wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 04:06 PM EDT

PDB ID	:	7M78 / pdb_00007m78
Title	:	Room Temperature XFEL Crystallography reveals asymmetry in the vicinity of the two phylloquinones in Photosystem I
Authors	:	Keable, S.M.; Simon, P.S.; Kolsch, A.; Kern, J.; Yachandra, V.K.; Zouni, A.; Yano, J.
Deposited on	:	2021-03-26
Resolution	:	3.00 Å(reported)

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

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

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

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

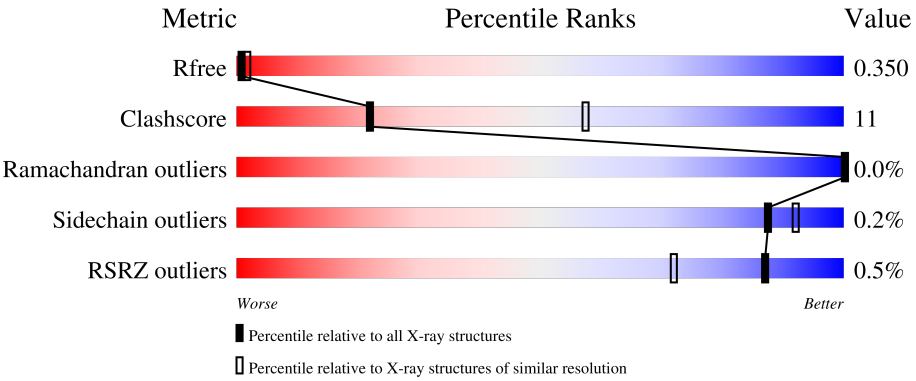
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

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



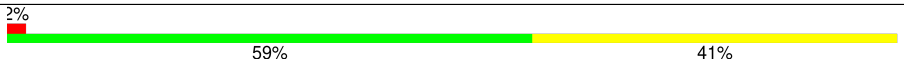
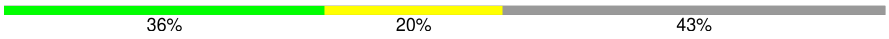
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	% 73% 25% .
2	B	740	75% 25%
3	C	80	75% 25%
4	D	138	78% 22%

Continued on next page...

Continued from previous page...

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	

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 48797 atoms, of which 24384 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
			Total	C	H	N	O	S			
1	A	740	11422	3794	5638	988	976	26	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	739	11507	3876	5618	987	1005	21	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	C	80	1174	367	576	103	117	11	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	D	138	2152	682	1077	186	204	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
5	E	69	1067	342	528	93	104	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
6	F	141	2141	680	1076	184	197	4	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
7	I	38	607	208	306	40	48	5	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
8	J	41	685	231	347	51	54	2	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
9	K	47	687	217	354	58	57	1	0	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
10	L	151	2244	735	1125	179	201	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

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

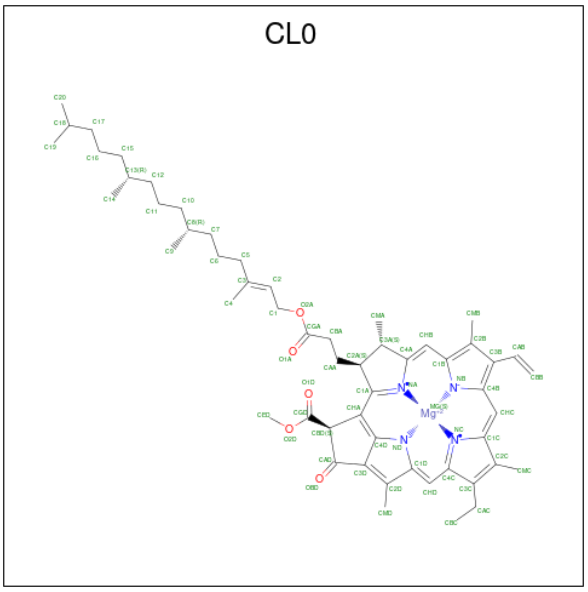
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
11	M	31	505	161	264	36	43	1	0	0	0

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

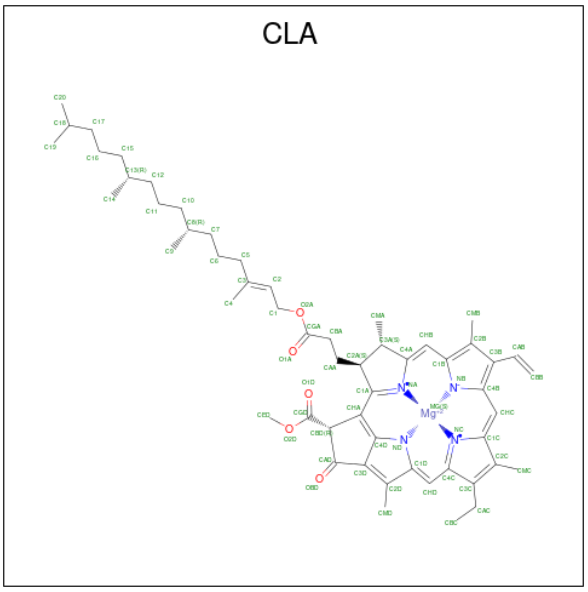
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
12	X	29	459	172	217	35	35	0	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
13	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			72	35	29	1	4	3		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	A	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			89	40	39	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			95	42	43	1	4	5		
14	A	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			117	49	58	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			104	45	49	1	4	5		

Continued on next page...

Continued from previous page...

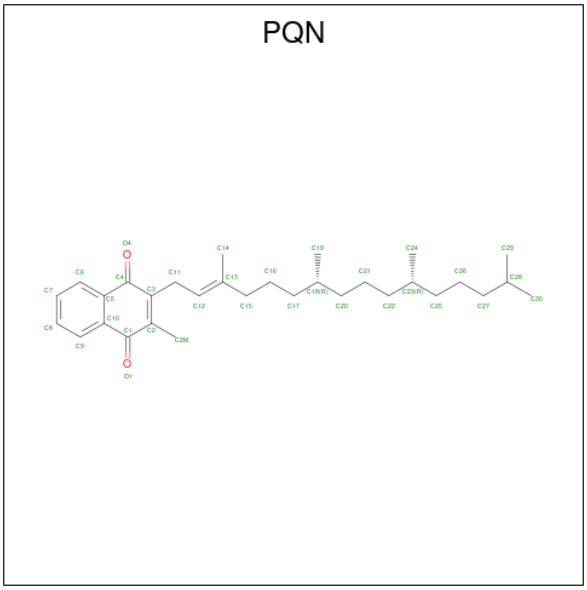
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			102	44	48	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			79	36	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			88	39	39	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			113	48	55	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			119	50	59	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			82	37	35	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	B	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			92	41	41	1	4	5		
14	F	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

Continued on next page...

Continued from previous page...

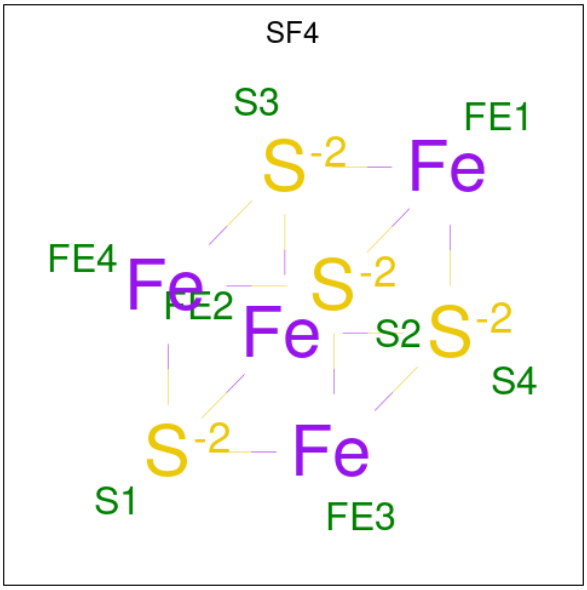
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	J	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	J	1	Total	C	H	Mg	N	O	0	0
			62	31	25	1	4	1		
14	K	1	Total	C	H	Mg	N	O	0	0
			70	33	29	1	4	3		
14	K	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	L	1	Total	C	H	Mg	N	O	0	0
			137	55	72	1	4	5		
14	M	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		
14	X	1	Total	C	H	Mg	N	O	0	0
			78	35	33	1	4	5		

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



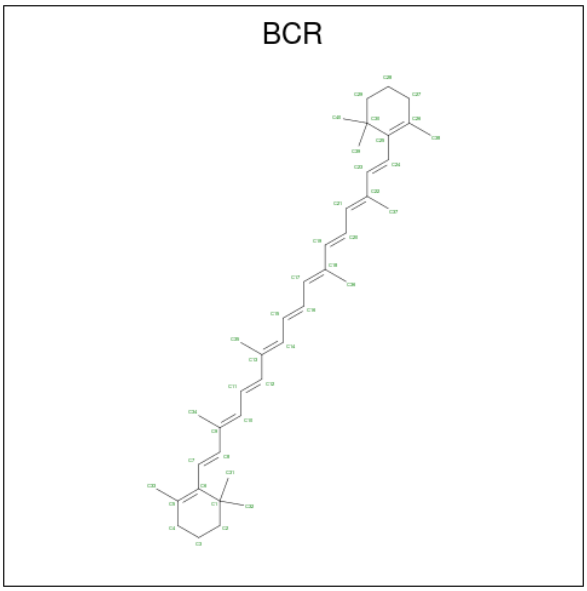
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			79	31	46	2		
15	B	1	Total	C	H	O	0	0
			79	31	46	2		

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



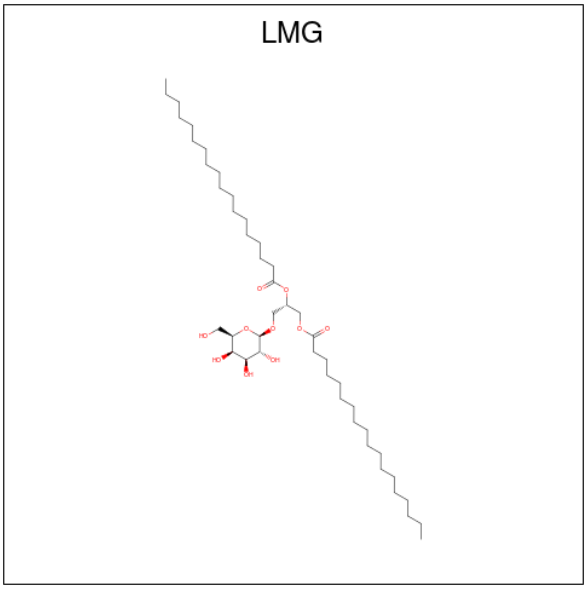
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total Fe S 8 4 4	0	0
16	C	1	Total Fe S 8 4 4	0	0
16	C	1	Total Fe S 8 4 4	0	0

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



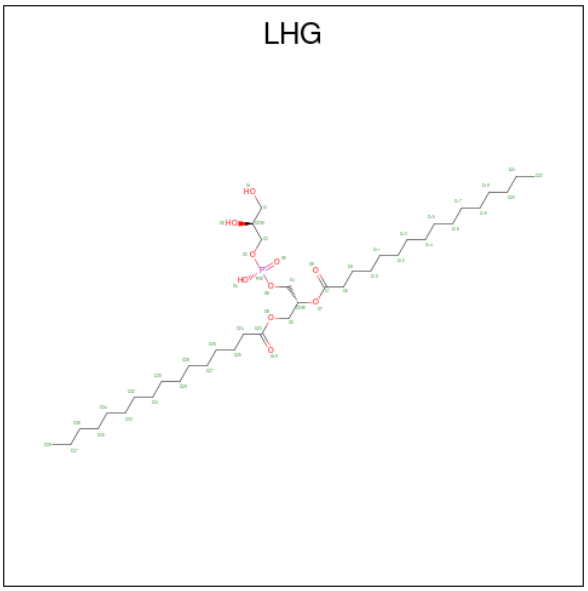
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	A	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	B	1	Total C H 96 40 56	0	0
17	F	1	Total C H 96 40 56	0	0
17	I	1	Total C H 96 40 56	0	0
17	I	1	Total C H 96 40 56	0	0
17	J	1	Total C H 96 40 56	0	0
17	J	1	Total C H 96 40 56	0	0
17	J	1	Total C H 96 40 56	0	0
17	L	1	Total C H 96 40 56	0	0
17	L	1	Total C H 96 40 56	0	0
17	M	1	Total C H 96 40 56	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	H	O	0	0
			118	38	70	10		
18	A	1	Total	C	H	O	0	0
			67	22	37	8		
18	B	1	Total	C	H	O	0	0
			141	45	86	10		
18	I	1	Total	C	H	O	0	0
			91	30	51	10		

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).

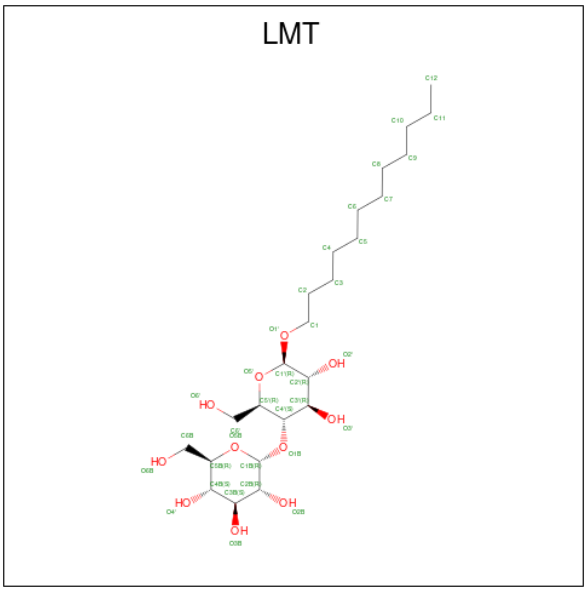


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	A	1	Total	C	H	O	P	0	0
			123	38	74	10	1		
19	A	1	Total	C	H	O	P	0	0
			53	16	26	10	1		
19	B	1	Total	C	H	O	P	0	0
			43	12	20	10	1		
19	M	1	Total	C	H	O	P	0	0
			123	38	74	10	1		

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

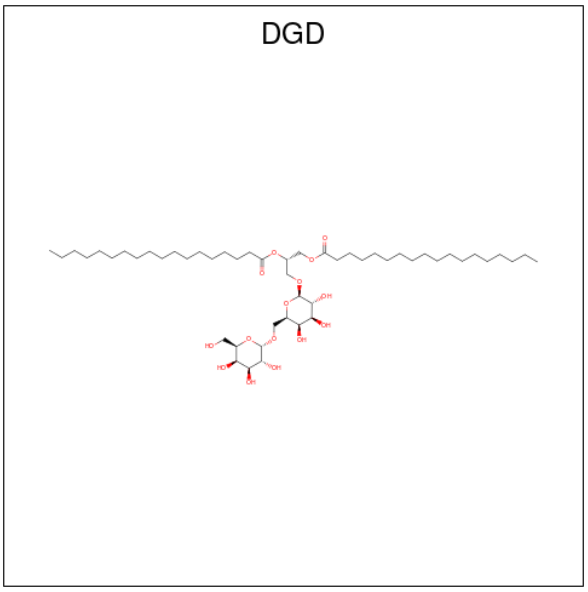
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	B	1	Total	Ca	0	0
			1	1		
20	L	1	Total	Ca	0	0
			1	1		

- Molecule 21 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	L	1	Total	C	H	O	0	0
			81	24	46	11		

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	L	1	Total	C	H	O	0	0
			162	51	96	15		

- Molecule 23 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	6	Total O 6 6	0	0
23	B	8	Total O 8 8	0	0
23	F	1	Total O 1 1	0	0
23	J	1	Total O 1 1	0	0
23	L	3	Total O 3 3	0	0
23	M	1	Total O 1 1	0	0

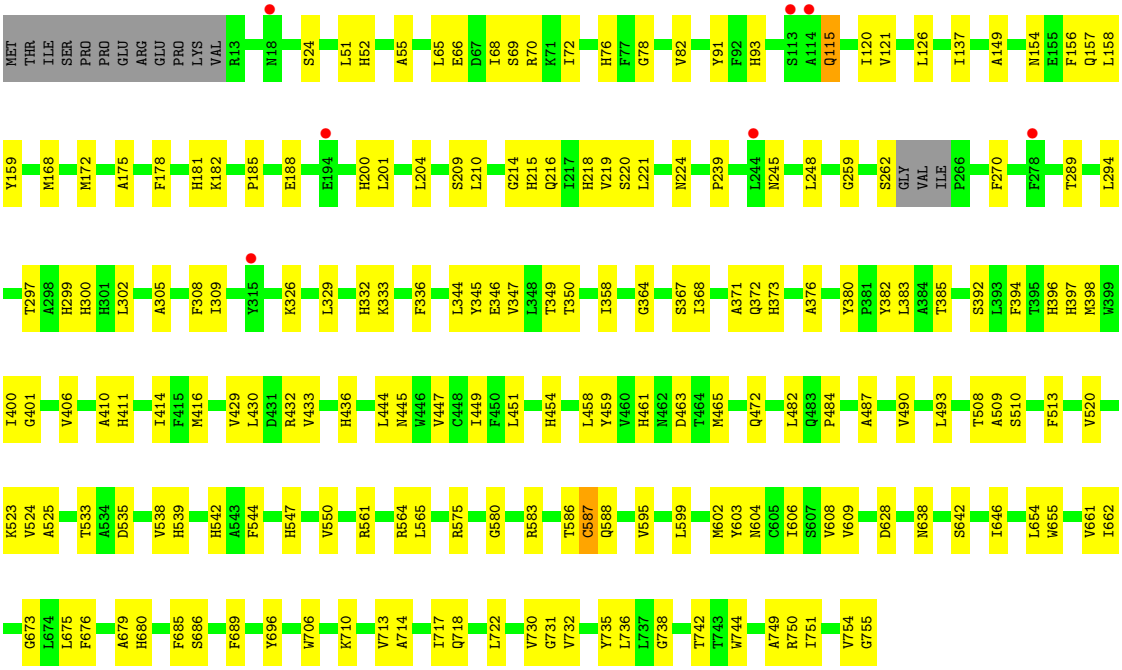
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain A:

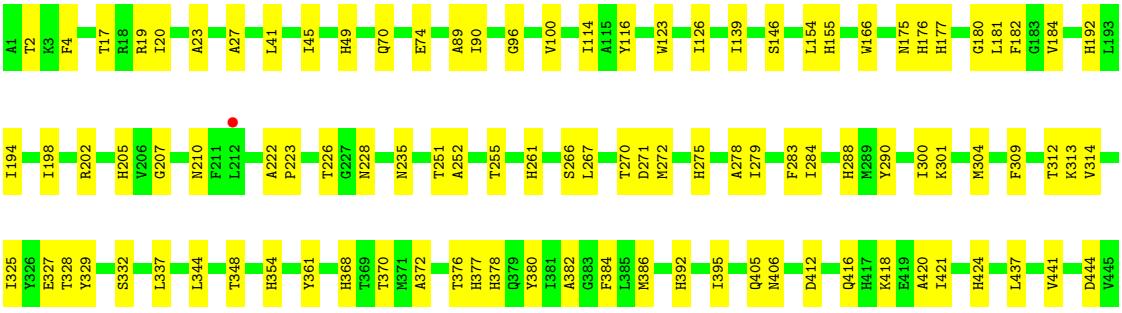


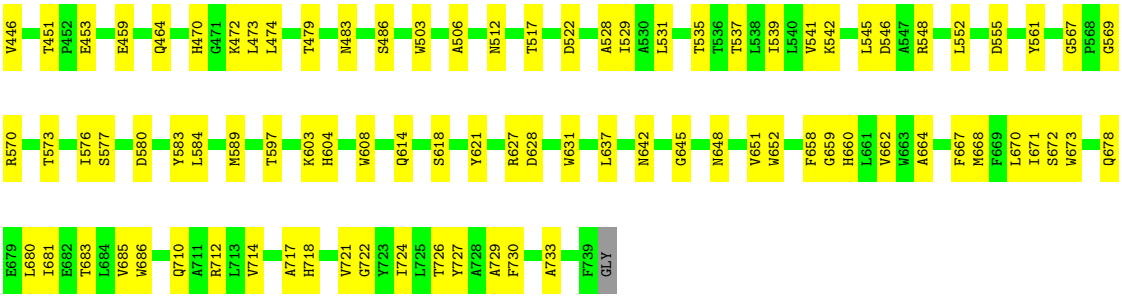


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

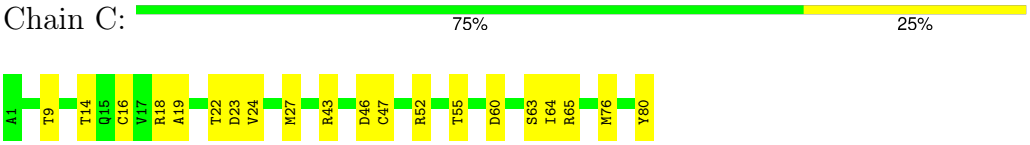
Chain B:



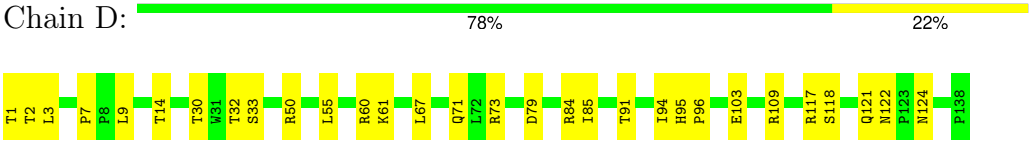




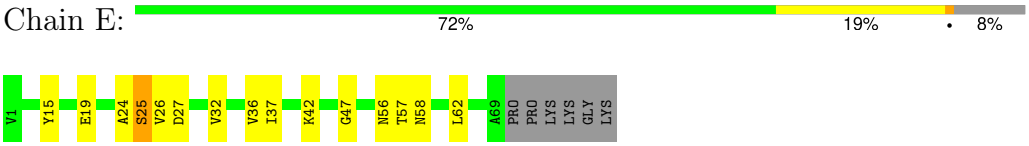
• Molecule 3: Photosystem I iron-sulfur center



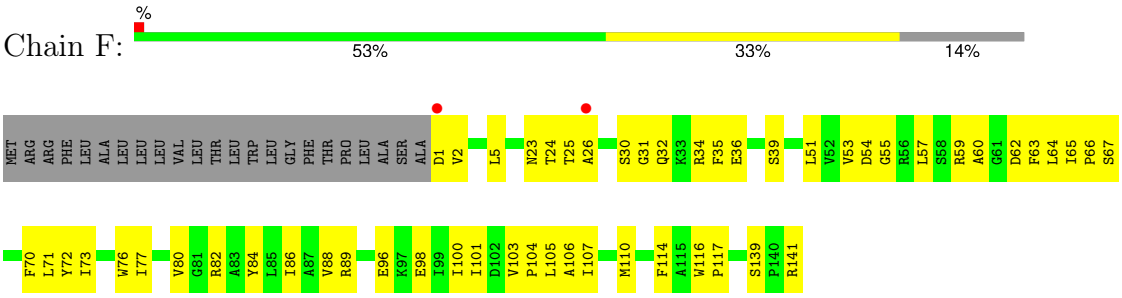
• Molecule 4: Photosystem I reaction center subunit II



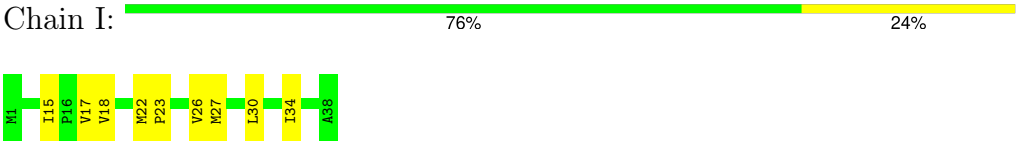
• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III

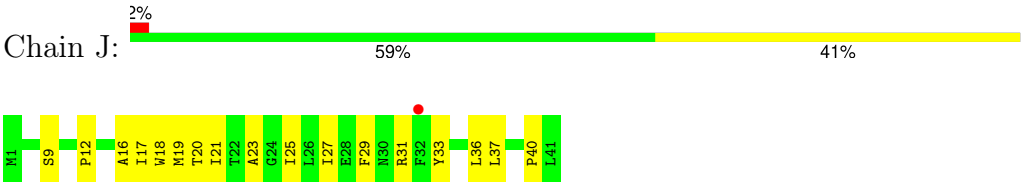


• Molecule 7: Photosystem I reaction center subunit VIII



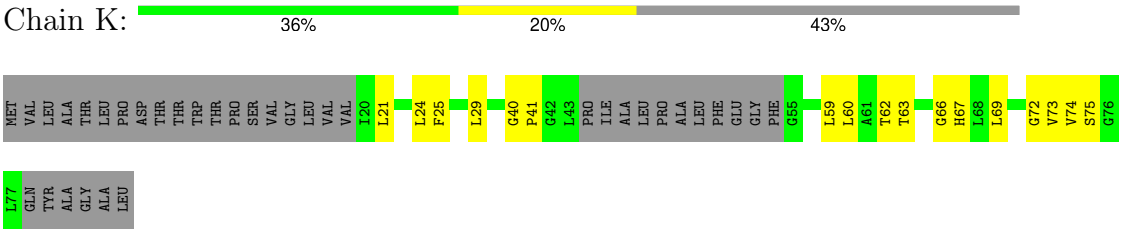
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



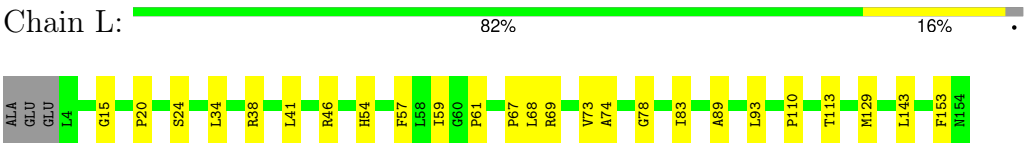
• Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:



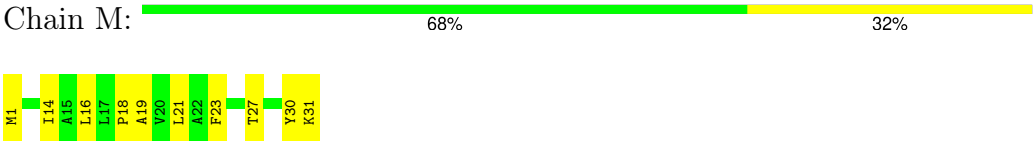
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



• 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	284.86Å 284.86Å 166.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.63 – 3.00 31.63 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.63-3.00) 94.3 (31.63-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.88 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.334 , 0.350 0.335 , 0.350	Depositor DCC
R_{free} test set	1995 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å^2)	32.5	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.13 , 0.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.146 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	48797	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: PQN, CA, LMG, SF4, CLA, DGD, CL0, BCR, LMT, LHG

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	0.14	0/5983	0.33	0/8158
2	B	0.14	0/6107	0.32	0/8345
3	C	0.12	0/608	0.30	0/824
4	D	0.13	0/1101	0.33	0/1492
5	E	0.12	0/551	0.34	0/750
6	F	0.14	0/1087	0.30	0/1476
7	I	0.17	0/312	0.44	0/425
8	J	0.17	0/350	0.30	0/477
9	K	0.13	0/337	0.35	0/454
10	L	0.15	0/1148	0.31	0/1558
11	M	0.19	0/244	0.36	0/332
12	X	0.14	0/251	0.29	0/342
All	All	0.14	0/18079	0.32	0/24633

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5784	5638	5639	157	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5889	5618	5649	150	0
3	C	598	576	580	16	0
4	D	1075	1077	1077	20	0
5	E	539	528	528	11	0
6	F	1065	1076	1077	41	0
7	I	301	306	306	8	0
8	J	338	347	347	23	0
9	K	333	354	354	16	0
10	L	1119	1125	1125	17	1
11	M	241	264	264	8	0
12	X	242	217	249	10	0
13	A	65	72	72	4	0
14	A	2577	2574	2574	77	0
14	B	2284	2232	2232	55	0
14	F	96	74	74	6	0
14	J	82	58	58	7	0
14	K	86	62	62	5	0
14	L	195	216	216	3	0
14	M	45	33	33	0	0
14	X	45	33	33	4	0
15	A	33	46	46	4	0
15	B	33	46	46	1	0
16	A	8	0	0	0	0
16	C	16	0	0	1	0
17	A	240	336	336	12	0
17	B	280	392	392	14	0
17	F	40	56	56	3	0
17	I	80	112	112	8	0
17	J	120	168	168	16	0
17	L	80	112	112	4	0
17	M	40	56	56	0	0
18	A	78	107	105	1	0
18	B	55	86	86	1	0
18	I	40	51	50	0	0
19	A	76	100	98	1	0
19	B	23	20	16	1	0
19	M	49	74	74	0	0
20	B	1	0	0	0	0
20	L	1	0	0	0	0
21	L	35	46	46	0	0
22	L	66	96	96	2	0
23	A	6	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	B	8	0	0	0	0
23	F	1	0	0	0	0
23	J	1	0	0	1	0
23	L	3	0	0	1	2
23	M	1	0	0	0	0
All	All	24413	24384	24444	524	2

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 11.

The worst 5 of 524 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)
10:L:153:PHE:O	23:L:302:HOH:O	1.68	1.10
2:B:583:TYR:OH	2:B:670:LEU:HD22	1.60	1.00
2:B:506:ALA:O	2:B:512:ASN:ND2	1.97	0.98
1:A:336:PHE:O	1:A:432:ARG:NH1	2.10	0.85
6:F:1:ASP:N	6:F:5:LEU:O	2.12	0.83

All (2) 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)
23:L:301:HOH:O	23:L:302:HOH:O[3_455]	1.08	1.12
10:L:67:PRO:O	23:L:302:HOH:O[3_455]	2.05	0.15

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%)	688 (94%)	48 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	737/740 (100%)	695 (94%)	42 (6%)	0	100 100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100 100
4	D	136/138 (99%)	124 (91%)	12 (9%)	0	100 100
5	E	67/75 (89%)	60 (90%)	6 (9%)	1 (2%)	8 35
6	F	139/164 (85%)	128 (92%)	11 (8%)	0	100 100
7	I	36/38 (95%)	30 (83%)	6 (17%)	0	100 100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100 100
9	K	43/83 (52%)	38 (88%)	5 (12%)	0	100 100
10	L	149/154 (97%)	146 (98%)	3 (2%)	0	100 100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100 100
12	X	27/35 (77%)	26 (96%)	1 (4%)	0	100 100
All	All	2216/2334 (95%)	2074 (94%)	141 (6%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	25	SER

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%)	587 (100%)	2 (0%)	86 91
2	B	597/597 (100%)	597 (100%)	0	100 100
3	C	67/67 (100%)	66 (98%)	1 (2%)	57 80
4	D	115/115 (100%)	115 (100%)	0	100 100
5	E	59/64 (92%)	59 (100%)	0	100 100
6	F	109/128 (85%)	109 (100%)	0	100 100
7	I	32/32 (100%)	32 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	J	36/36 (100%)	36 (100%)	0	100 100
9	K	33/61 (54%)	33 (100%)	0	100 100
10	L	117/119 (98%)	117 (100%)	0	100 100
11	M	26/26 (100%)	26 (100%)	0	100 100
12	X	23/27 (85%)	23 (100%)	0	100 100
All	All	1803/1875 (96%)	1800 (100%)	3 (0%)	87 92

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	587	CYS
3	C	16	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	604	HIS
11	M	7	GLN
4	D	6	GLN
10	L	16	HIS
3	C	37	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 135 ligands modelled in this entry, 2 are monoatomic - leaving 133 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	$\#\|Z\| > 2$
14	CLA	A	822	23	69,73,73	1.18	6 (8%)	82,113,113	1.22	5 (6%)
14	CLA	K	101	9	45,49,73	1.45	8 (17%)	54,83,113	1.32	4 (7%)
14	CLA	B	802	2	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
14	CLA	A	823	1	53,57,73	1.34	6 (11%)	61,93,113	1.38	5 (8%)
14	CLA	A	821	1	46,50,73	1.41	6 (13%)	54,84,113	1.47	4 (7%)
14	CLA	B	807	2	69,73,73	1.18	7 (10%)	82,113,113	1.20	4 (4%)
17	BCR	A	849	-	41,41,41	1.11	2 (4%)	56,56,56	1.20	6 (10%)
14	CLA	B	825	23	50,54,73	1.37	6 (12%)	59,90,113	1.35	4 (6%)
14	CLA	A	813	1	58,62,73	1.29	7 (12%)	68,99,113	1.31	5 (7%)
14	CLA	A	809	1	69,73,73	1.18	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	B	812	2	49,53,73	1.42	7 (14%)	58,89,113	1.38	5 (8%)
18	LMG	A	856	-	30,30,55	1.01	2 (6%)	37,37,63	1.30	5 (13%)
14	CLA	A	806	1	69,73,73	1.18	6 (8%)	82,113,113	1.29	6 (7%)
16	SF4	C	101	3	0,12,12	-	-	-		
18	LMG	A	853	-	48,48,55	0.77	1 (2%)	56,56,63	1.28	6 (10%)
14	CLA	M	102	23	49,53,73	1.42	8 (16%)	58,89,113	1.40	4 (6%)
22	DGD	L	207	-	67,67,67	0.93	2 (2%)	81,81,81	1.40	14 (17%)
17	BCR	L	201	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	8 (14%)
14	CLA	A	804	1	69,73,73	1.19	6 (8%)	82,113,113	1.20	5 (6%)
14	CLA	A	810	1	69,73,73	1.20	8 (11%)	82,113,113	1.26	6 (7%)
14	CLA	B	806	2	69,73,73	1.20	6 (8%)	82,113,113	1.22	4 (4%)
14	CLA	B	804	2	58,62,73	1.28	6 (10%)	68,99,113	1.33	7 (10%)
14	CLA	B	817	2	63,67,73	1.25	5 (7%)	74,105,113	1.25	6 (8%)
17	BCR	A	850	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	B	840	23	69,73,73	1.18	6 (8%)	82,113,113	1.23	6 (7%)
14	CLA	A	833	1	69,73,73	1.18	7 (10%)	82,113,113	1.18	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	SF4	A	846	1,2	0,12,12	-	-	-		
14	CLA	A	811	1	49,53,73	1.41	6 (12%)	58,89,113	1.39	6 (10%)
14	CLA	A	844	19	56,60,73	1.31	6 (10%)	65,97,113	1.38	6 (9%)
17	BCR	J	103	-	41,41,41	1.15	2 (4%)	56,56,56	1.28	7 (12%)
16	SF4	C	102	3	0,12,12	-	-	-		
17	BCR	A	847	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
14	CLA	B	834	2	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
14	CLA	X	1701	12	49,53,73	1.40	6 (12%)	58,89,113	1.34	5 (8%)
18	LMG	B	849	-	55,55,55	0.71	1 (1%)	63,63,63	1.37	8 (12%)
14	CLA	B	829	2	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
14	CLA	B	815	2	49,53,73	1.40	6 (12%)	58,89,113	1.35	4 (6%)
14	CLA	F	201	23	55,59,73	1.33	6 (10%)	64,96,113	1.35	6 (9%)
17	BCR	M	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
14	CLA	A	817	23	53,57,73	1.34	7 (13%)	61,93,113	1.31	5 (8%)
14	CLA	B	830	2	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
14	CLA	A	818	1	58,62,73	1.29	7 (12%)	68,99,113	1.33	5 (7%)
14	CLA	L	206	23	69,73,73	1.18	5 (7%)	82,113,113	1.35	8 (9%)
15	PQN	A	845	-	34,34,34	2.06	7 (20%)	43,45,45	1.23	5 (11%)
14	CLA	A	807	1	69,73,73	1.21	6 (8%)	82,113,113	1.19	4 (4%)
14	CLA	B	805	2	69,73,73	1.18	6 (8%)	82,113,113	1.21	4 (4%)
14	CLA	L	205	10	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
14	CLA	A	805	1,14	63,67,73	1.25	6 (9%)	74,105,113	1.24	6 (8%)
17	BCR	J	104	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	10 (17%)
14	CLA	B	837	2	64,68,73	1.24	6 (9%)	76,107,113	1.30	7 (9%)
14	CLA	A	830	1	69,73,73	1.19	6 (8%)	82,113,113	1.23	5 (6%)
14	CLA	F	202	23	49,53,73	1.41	6 (12%)	58,89,113	1.32	4 (6%)
14	CLA	B	813	2	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
14	CLA	A	812	1,14	69,73,73	1.18	6 (8%)	82,113,113	1.19	4 (4%)
14	CLA	B	822	23	59,63,73	1.27	6 (10%)	70,101,113	1.26	5 (7%)
14	CLA	A	834	1	69,73,73	1.19	5 (7%)	82,113,113	1.16	5 (6%)
14	CLA	J	101	8	49,53,73	1.40	6 (12%)	58,89,113	1.40	4 (6%)
14	CLA	B	811	2	49,53,73	1.40	6 (12%)	58,89,113	1.48	5 (8%)
14	CLA	B	816	2	59,63,73	1.28	6 (10%)	70,101,113	1.28	5 (7%)
17	BCR	B	851	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	7 (12%)
14	CLA	A	825	1	63,67,73	1.24	6 (9%)	74,105,113	1.26	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	824	2	58,62,73	1.29	7 (12%)	68,99,113	1.29	5 (7%)
17	BCR	J	105	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	9 (16%)
17	BCR	B	848	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)
14	CLA	B	839	2	51,55,73	1.36	8 (15%)	60,91,113	1.33	6 (10%)
14	CLA	B	831	2	53,57,73	1.35	7 (13%)	61,93,113	1.35	6 (9%)
14	CLA	A	816	1	49,53,73	1.40	7 (14%)	58,89,113	1.38	4 (6%)
14	CLA	B	809	2	69,73,73	1.20	8 (11%)	82,113,113	1.32	8 (9%)
14	CLA	B	814	2	69,73,73	1.19	6 (8%)	82,113,113	1.22	5 (6%)
14	CLA	L	204	10	69,73,73	1.17	8 (11%)	82,113,113	1.32	6 (7%)
14	CLA	A	831	1	69,73,73	1.18	7 (10%)	82,113,113	1.22	6 (7%)
14	CLA	A	857	23	69,73,73	1.17	6 (8%)	82,113,113	1.21	5 (6%)
14	CLA	B	810	2	69,73,73	1.18	7 (10%)	82,113,113	1.31	6 (7%)
15	PQN	B	842	-	34,34,34	2.05	7 (20%)	43,45,45	1.17	4 (9%)
14	CLA	A	828	1	69,73,73	1.20	6 (8%)	82,113,113	1.20	5 (6%)
14	CLA	A	815	1	49,53,73	1.42	7 (14%)	58,89,113	1.32	4 (6%)
14	CLA	B	833	2	62,66,73	1.24	6 (9%)	73,104,113	1.27	5 (6%)
17	BCR	A	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.36	8 (14%)
17	BCR	A	851	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	B	818	2	64,68,73	1.22	6 (9%)	76,107,113	1.25	4 (5%)
14	CLA	B	823	2	49,53,73	1.42	7 (14%)	58,89,113	1.40	4 (6%)
19	LHG	A	854	-	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
14	CLA	A	803	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
17	BCR	A	852	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	9 (16%)
21	LMT	L	202	-	36,36,36	1.13	3 (8%)	47,47,47	1.04	2 (4%)
17	BCR	B	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
14	CLA	B	835	23	49,53,73	1.42	7 (14%)	58,89,113	1.37	5 (8%)
14	CLA	A	838	1	55,59,73	1.34	7 (12%)	64,96,113	1.35	5 (7%)
17	BCR	B	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.23	6 (10%)
14	CLA	B	836	23	49,53,73	1.44	7 (14%)	58,89,113	1.36	4 (6%)
14	CLA	A	829	1	69,73,73	1.19	6 (8%)	82,113,113	1.15	4 (4%)
14	CLA	J	102	8	41,45,73	1.49	7 (17%)	50,78,113	1.34	3 (6%)
17	BCR	B	844	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	9 (16%)
14	CLA	A	808	1	55,59,73	1.35	7 (12%)	64,96,113	1.38	7 (10%)
14	CLA	A	840	1	51,55,73	1.36	7 (13%)	60,91,113	1.36	5 (8%)
14	CLA	B	826	2	69,73,73	1.19	6 (8%)	82,113,113	1.23	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
14	CLA	B	808	2	69,73,73	1.19	7 (10%)	82,113,113	1.21	6 (7%)
17	BCR	I	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	6 (10%)
14	CLA	B	828	2	69,73,73	1.18	6 (8%)	82,113,113	1.17	5 (6%)
14	CLA	K	102	-	49,53,73	1.40	6 (12%)	58,89,113	1.41	5 (8%)
19	LHG	B	850	-	22,22,48	0.92	2 (9%)	25,28,54	1.23	1 (4%)
14	CLA	A	826	23	69,73,73	1.19	7 (10%)	82,113,113	1.25	4 (4%)
14	CLA	B	841	2	69,73,73	1.19	7 (10%)	82,113,113	1.25	5 (6%)
14	CLA	A	802	23	69,73,73	1.18	6 (8%)	82,113,113	1.18	3 (3%)
13	CL0	A	801	1	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
19	LHG	A	855	14	26,26,48	0.85	2 (7%)	29,32,54	1.32	3 (10%)
14	CLA	A	843	23	69,73,73	1.20	6 (8%)	82,113,113	1.25	4 (4%)
14	CLA	B	821	2	49,53,73	1.40	7 (14%)	58,89,113	1.39	4 (6%)
14	CLA	B	827	2	69,73,73	1.19	7 (10%)	82,113,113	1.14	5 (6%)
18	LMG	I	102	-	40,40,55	0.89	1 (2%)	48,48,63	1.26	6 (12%)
14	CLA	B	803	-	69,73,73	1.19	6 (8%)	82,113,113	1.21	4 (4%)
14	CLA	B	819	23	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
17	BCR	F	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.23	7 (12%)
14	CLA	A	832	1	54,58,73	1.33	7 (12%)	64,95,113	1.34	5 (7%)
17	BCR	B	846	-	41,41,41	1.06	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	A	820	1	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
17	BCR	I	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	A	841	1	69,73,73	1.17	7 (10%)	82,113,113	1.21	4 (4%)
14	CLA	A	836	1	58,62,73	1.31	6 (10%)	68,99,113	1.25	5 (7%)
14	CLA	A	842	1	69,73,73	1.18	7 (10%)	82,113,113	1.29	4 (4%)
14	CLA	A	824	1	55,59,73	1.32	6 (10%)	64,96,113	1.29	6 (9%)
14	CLA	A	837	1	49,53,73	1.41	5 (10%)	58,89,113	1.35	4 (6%)
14	CLA	A	839	1	69,73,73	1.17	7 (10%)	82,113,113	1.24	6 (7%)
14	CLA	B	820	2	51,55,73	1.36	6 (11%)	60,91,113	1.33	4 (6%)
14	CLA	B	838	2	69,73,73	1.20	6 (8%)	82,113,113	1.25	5 (6%)
14	CLA	A	827	23	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
19	LHG	M	101	-	48,48,48	0.63	0	51,54,54	1.22	6 (11%)
14	CLA	A	814	1	64,68,73	1.23	6 (9%)	76,107,113	1.27	6 (7%)
14	CLA	A	819	1	58,62,73	1.31	8 (13%)	68,99,113	1.30	6 (8%)
17	BCR	B	843	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	9 (16%)
14	CLA	B	832	2	69,73,73	1.18	6 (8%)	82,113,113	1.19	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
17	BCR	L	208	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
14	CLA	A	835	1	69,73,73	1.20	6 (8%)	82,113,113	1.20	5 (6%)

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
14	CLA	A	822	23	-	13/39/115/115	-
14	CLA	K	101	9	-	1/9/81/115	-
14	CLA	B	802	2	-	13/39/115/115	-
14	CLA	A	823	1	-	10/20/96/115	-
14	CLA	A	821	1	-	2/10/86/115	-
14	CLA	B	807	2	-	7/39/115/115	-
17	BCR	A	849	-	-	12/29/63/63	0/2/2/2
14	CLA	B	825	23	-	4/17/93/115	-
14	CLA	A	813	1	-	8/26/102/115	-
14	CLA	A	809	1	-	12/39/115/115	-
14	CLA	B	812	2	-	6/15/91/115	-
18	LMG	A	856	-	-	12/23/43/70	0/1/1/1
14	CLA	A	806	1	-	14/39/115/115	-
16	SF4	C	101	3	-	-	0/6/5/5
18	LMG	A	853	-	-	25/43/63/70	0/1/1/1
14	CLA	M	102	23	-	5/15/91/115	-
22	DGD	L	207	-	-	23/55/95/95	0/2/2/2
17	BCR	L	201	-	-	11/29/63/63	0/2/2/2
14	CLA	A	804	1	-	10/39/115/115	-
14	CLA	A	810	1	-	10/39/115/115	-
14	CLA	B	806	2	-	9/39/115/115	-
14	CLA	B	804	2	-	7/26/102/115	-
14	CLA	B	817	2	-	7/32/108/115	-
17	BCR	A	850	-	-	12/29/63/63	0/2/2/2
14	CLA	B	840	23	-	8/39/115/115	-
14	CLA	A	833	1	-	10/39/115/115	-
16	SF4	A	846	1,2	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	811	1	-	8/15/91/115	-
14	CLA	A	844	19	-	6/24/100/115	-
17	BCR	J	103	-	-	18/29/63/63	0/2/2/2
16	SF4	C	102	3	-	-	0/6/5/5
17	BCR	A	847	-	-	11/29/63/63	0/2/2/2
14	CLA	B	834	2	-	6/15/91/115	-
14	CLA	X	1701	12	-	6/15/91/115	-
18	LMG	B	849	-	-	18/50/70/70	0/1/1/1
14	CLA	B	829	2	-	8/39/115/115	-
14	CLA	B	815	2	-	4/15/91/115	-
14	CLA	F	201	23	-	6/23/99/115	-
17	BCR	M	103	-	-	18/29/63/63	0/2/2/2
14	CLA	A	817	23	-	6/20/96/115	-
14	CLA	B	830	2	-	9/15/91/115	-
14	CLA	A	818	1	-	3/26/102/115	-
14	CLA	L	206	23	-	7/39/115/115	-
15	PQN	A	845	-	-	11/23/43/43	0/2/2/2
14	CLA	A	807	1	-	14/39/115/115	-
14	CLA	B	805	2	-	11/39/115/115	-
14	CLA	L	205	10	-	11/39/115/115	-
14	CLA	A	805	1,14	-	6/32/108/115	-
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
14	CLA	B	837	2	-	5/33/109/115	-
14	CLA	A	830	1	-	14/39/115/115	-
14	CLA	F	202	23	-	4/15/91/115	-
14	CLA	B	813	2	-	18/39/115/115	-
14	CLA	A	812	1,14	-	5/39/115/115	-
14	CLA	B	822	23	-	7/27/103/115	-
14	CLA	A	834	1	-	9/39/115/115	-
14	CLA	J	101	8	-	3/15/91/115	-
14	CLA	B	811	2	-	2/15/91/115	-
14	CLA	B	816	2	-	6/27/103/115	-
17	BCR	B	851	-	-	8/29/63/63	0/2/2/2
14	CLA	A	825	1	-	10/32/108/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	824	2	-	7/26/102/115	-
17	BCR	J	105	-	-	10/29/63/63	0/2/2/2
17	BCR	B	848	-	-	6/29/63/63	0/2/2/2
14	CLA	B	839	2	-	4/18/94/115	-
14	CLA	B	831	2	-	7/20/96/115	-
14	CLA	A	816	1	-	5/15/91/115	-
14	CLA	B	809	2	-	14/39/115/115	-
14	CLA	B	814	2	-	13/39/115/115	-
14	CLA	L	204	10	-	13/39/115/115	-
14	CLA	A	831	1	-	10/39/115/115	-
14	CLA	A	857	23	-	17/39/115/115	-
14	CLA	B	810	2	-	16/39/115/115	-
15	PQN	B	842	-	-	8/23/43/43	0/2/2/2
14	CLA	A	828	1	-	11/39/115/115	-
14	CLA	A	815	1	-	3/15/91/115	-
14	CLA	B	833	2	-	4/31/107/115	-
17	BCR	A	848	-	-	17/29/63/63	0/2/2/2
17	BCR	A	851	-	-	7/29/63/63	0/2/2/2
14	CLA	B	818	2	-	10/33/109/115	-
14	CLA	B	823	2	-	6/15/91/115	-
19	LHG	A	854	-	-	21/53/53/53	-
14	CLA	A	803	-	-	6/39/115/115	-
17	BCR	A	852	-	-	19/29/63/63	0/2/2/2
21	LMT	L	202	-	-	12/21/61/61	0/2/2/2
17	BCR	B	847	-	-	13/29/63/63	0/2/2/2
14	CLA	B	835	23	-	7/15/91/115	-
14	CLA	A	838	1	-	5/23/99/115	-
17	BCR	B	845	-	-	9/29/63/63	0/2/2/2
14	CLA	B	836	23	-	4/15/91/115	-
14	CLA	A	829	1	-	11/39/115/115	-
14	CLA	J	102	8	-	1/4/76/115	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	A	808	1	-	9/23/99/115	-
14	CLA	A	840	1	-	2/18/94/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	826	2	-	16/39/115/115	-
14	CLA	B	808	2	-	7/39/115/115	-
17	BCR	I	101	-	-	15/29/63/63	0/2/2/2
14	CLA	B	828	2	-	19/39/115/115	-
14	CLA	K	102	-	-	6/15/91/115	-
19	LHG	B	850	-	-	13/26/26/53	-
14	CLA	A	826	23	-	14/39/115/115	-
14	CLA	B	841	2	-	8/39/115/115	-
14	CLA	A	802	23	-	11/39/115/115	-
13	CL0	A	801	1	-	15/39/115/115	-
19	LHG	A	855	14	-	10/31/31/53	-
14	CLA	A	843	23	-	8/39/115/115	-
14	CLA	B	821	2	-	6/15/91/115	-
14	CLA	B	827	2	-	13/39/115/115	-
18	LMG	I	102	-	-	9/35/55/70	0/1/1/1
14	CLA	B	803	-	-	11/39/115/115	-
14	CLA	B	819	23	-	12/39/115/115	-
17	BCR	F	203	-	-	9/29/63/63	0/2/2/2
14	CLA	A	832	1	-	6/21/97/115	-
17	BCR	B	846	-	-	13/29/63/63	0/2/2/2
14	CLA	A	820	1	-	16/39/115/115	-
17	BCR	I	103	-	-	14/29/63/63	0/2/2/2
14	CLA	A	841	1	-	6/39/115/115	-
14	CLA	A	836	1	-	3/26/102/115	-
14	CLA	A	842	1	-	9/39/115/115	-
14	CLA	A	824	1	-	3/23/99/115	-
14	CLA	A	837	1	-	6/15/91/115	-
14	CLA	A	839	1	-	13/39/115/115	-
14	CLA	B	820	2	-	6/18/94/115	-
14	CLA	B	838	2	-	10/39/115/115	-
14	CLA	A	827	23	-	5/39/115/115	-
19	LHG	M	101	-	-	26/53/53/53	-
14	CLA	A	814	1	-	7/33/109/115	-
14	CLA	A	819	1	-	9/26/102/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	B	843	-	-	7/29/63/63	0/2/2/2
14	CLA	B	832	2	-	11/39/115/115	-
17	BCR	L	208	-	-	11/29/63/63	0/2/2/2
14	CLA	A	835	1	-	11/39/115/115	-

The worst 5 of 703 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	845	PQN	O1-C1	6.00	1.35	1.23
15	B	842	PQN	O4-C4	5.96	1.35	1.23
15	B	842	PQN	O1-C1	5.96	1.35	1.23
15	A	845	PQN	O4-C4	5.95	1.35	1.23
15	A	845	PQN	C10-C1	-4.75	1.38	1.48

The worst 5 of 715 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	842	CLA	C4A-NA-C1A	7.29	110.00	106.68
14	B	802	CLA	C4A-NA-C1A	7.21	109.97	106.68
14	B	810	CLA	C4A-NA-C1A	7.10	109.92	106.68
14	B	811	CLA	C4A-NA-C1A	6.92	109.83	106.68
14	L	204	CLA	C4A-NA-C1A	6.83	109.79	106.68

There are no chirality outliers.

5 of 1251 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	801	CL0	CBD-CGD-O2D-CED
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CHA-CBD-CGD-O1D
14	A	805	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

103 monomers are involved in 198 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	822	CLA	2	0
14	K	101	CLA	4	0
14	B	802	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	849	BCR	1	0
14	B	825	CLA	3	0
14	A	813	CLA	1	0
14	A	809	CLA	1	0
14	B	812	CLA	2	0
18	A	856	LMG	1	0
14	A	806	CLA	3	0
22	L	207	DGD	2	0
17	L	201	BCR	3	0
14	A	804	CLA	2	0
14	A	810	CLA	5	0
14	B	804	CLA	1	0
14	B	817	CLA	3	0
17	A	850	BCR	1	0
14	B	840	CLA	2	0
14	A	833	CLA	1	0
14	A	811	CLA	3	0
14	A	844	CLA	2	0
17	J	103	BCR	2	0
16	C	102	SF4	1	0
17	A	847	BCR	1	0
14	B	834	CLA	1	0
14	X	1701	CLA	4	0
18	B	849	LMG	1	0
14	B	829	CLA	2	0
14	F	201	CLA	1	0
14	A	817	CLA	1	0
14	B	830	CLA	1	0
14	A	818	CLA	1	0
14	L	206	CLA	2	0
15	A	845	PQN	4	0
14	A	807	CLA	1	0
14	B	805	CLA	2	0
14	A	805	CLA	6	0
17	J	104	BCR	6	0
14	B	837	CLA	1	0
14	A	830	CLA	1	0
14	F	202	CLA	5	0
14	B	813	CLA	2	0
14	A	812	CLA	2	0
14	J	101	CLA	7	0
14	B	811	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	816	CLA	1	0
17	B	851	BCR	1	0
14	A	825	CLA	2	0
14	B	824	CLA	1	0
17	J	105	BCR	8	0
17	B	848	BCR	1	0
14	B	839	CLA	1	0
14	B	831	CLA	3	0
14	B	809	CLA	4	0
14	B	814	CLA	2	0
14	L	204	CLA	1	0
14	A	831	CLA	3	0
14	A	857	CLA	4	0
15	B	842	PQN	1	0
14	A	828	CLA	2	0
14	A	815	CLA	3	0
14	B	833	CLA	3	0
17	A	848	BCR	4	0
17	A	851	BCR	1	0
14	B	818	CLA	1	0
19	A	854	LHG	1	0
14	A	803	CLA	3	0
17	A	852	BCR	5	0
17	B	847	BCR	5	0
14	A	838	CLA	1	0
17	B	845	BCR	2	0
14	B	836	CLA	1	0
14	A	829	CLA	6	0
14	A	808	CLA	2	0
14	A	840	CLA	2	0
14	B	826	CLA	3	0
14	B	808	CLA	1	0
17	I	101	BCR	4	0
14	B	828	CLA	1	0
14	K	102	CLA	1	0
19	B	850	LHG	1	0
14	B	841	CLA	1	0
14	A	802	CLA	2	0
13	A	801	CL0	4	0
14	A	843	CLA	2	0
14	B	827	CLA	2	0
14	B	803	CLA	5	0

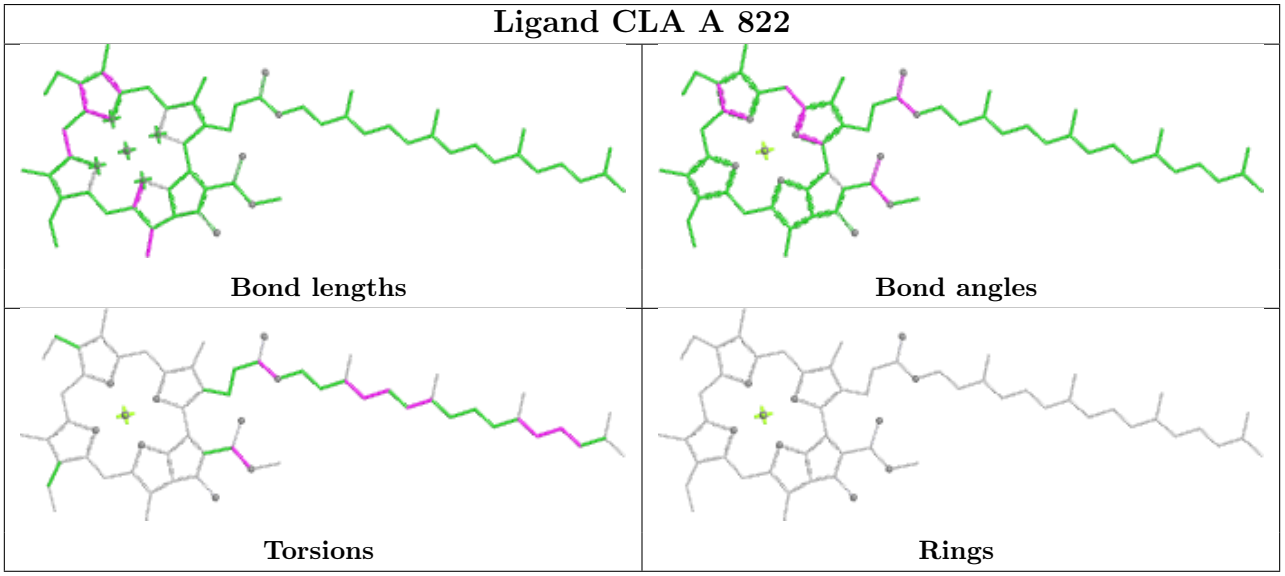
Continued on next page...

Continued from previous page...

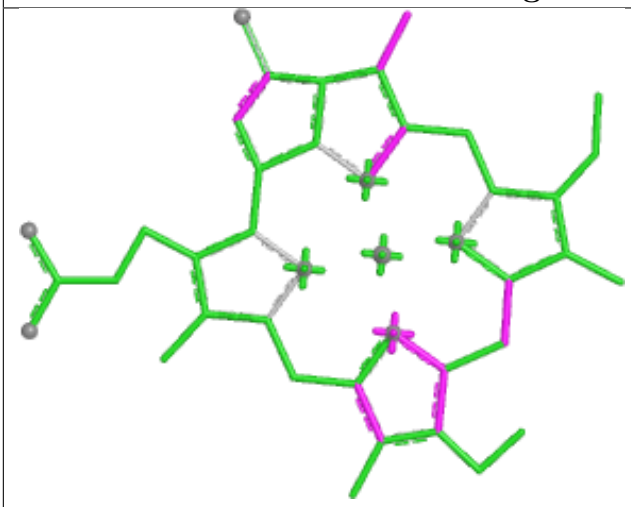
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	F	203	BCR	3	0
17	B	846	BCR	3	0
14	A	820	CLA	3	0
17	I	103	BCR	4	0
14	A	841	CLA	3	0
14	A	842	CLA	3	0
14	A	824	CLA	1	0
14	A	839	CLA	1	0
14	B	820	CLA	2	0
14	A	827	CLA	3	0
14	A	814	CLA	1	0
14	A	819	CLA	2	0
17	B	843	BCR	2	0
14	B	832	CLA	1	0
17	L	208	BCR	1	0
14	A	835	CLA	1	0

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

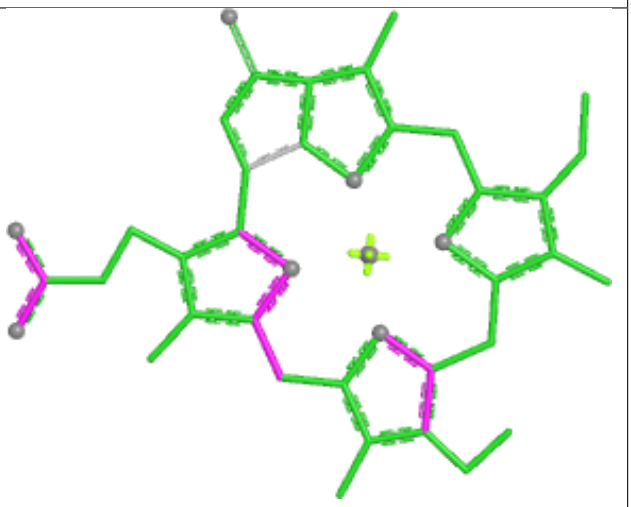
Ligand CLA A 822



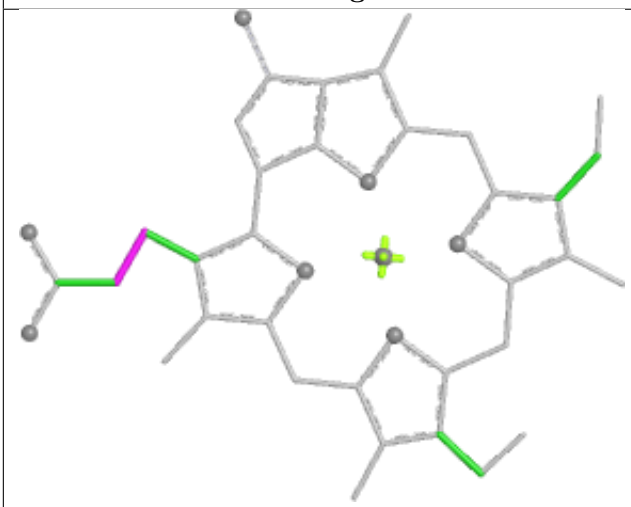
Ligand CLA K 101



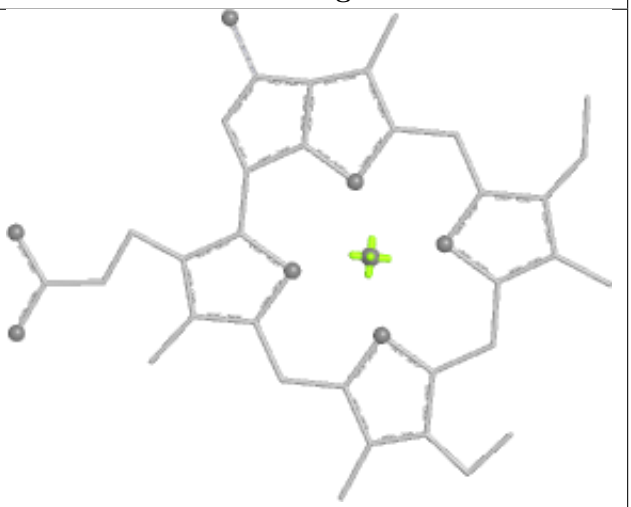
Bond lengths



Bond angles

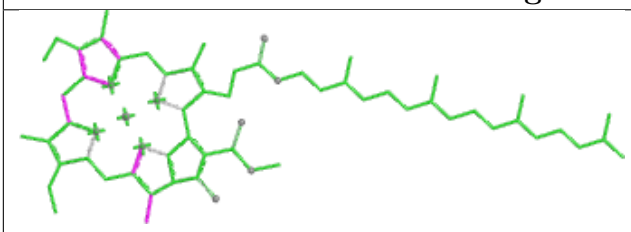


Torsions

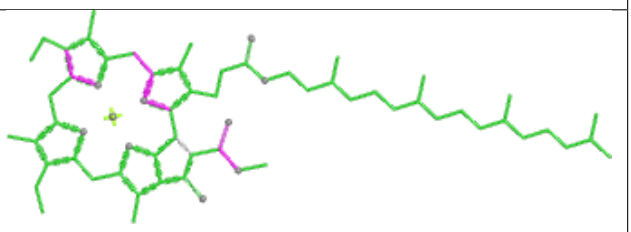


Rings

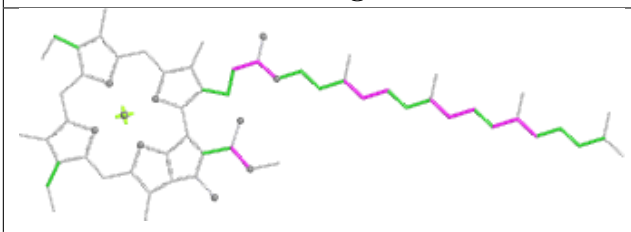
Ligand CLA B 802



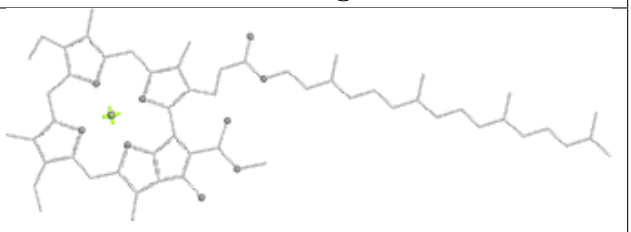
Bond lengths



Bond angles

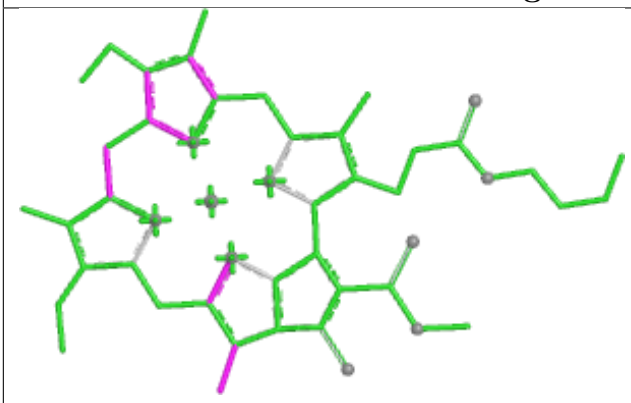


Torsions

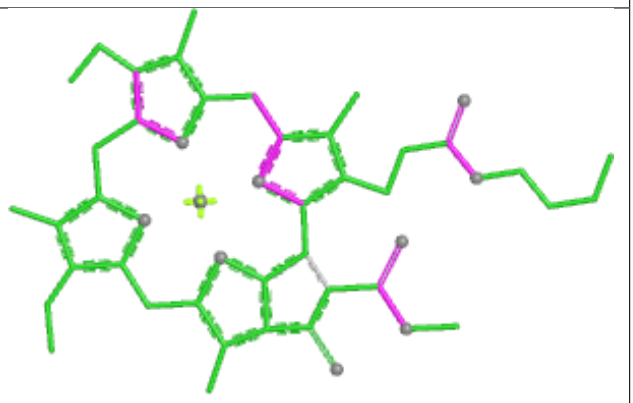


Rings

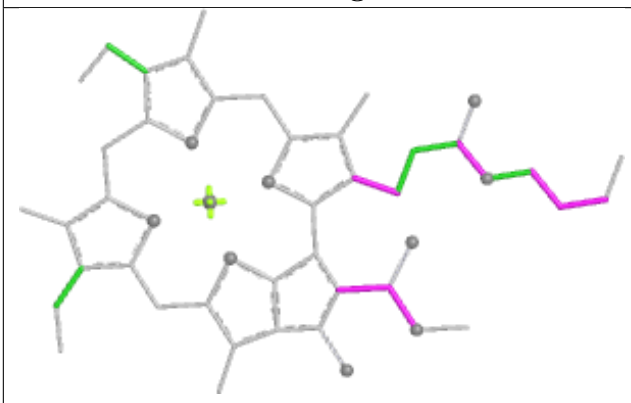
Ligand CLA A 823



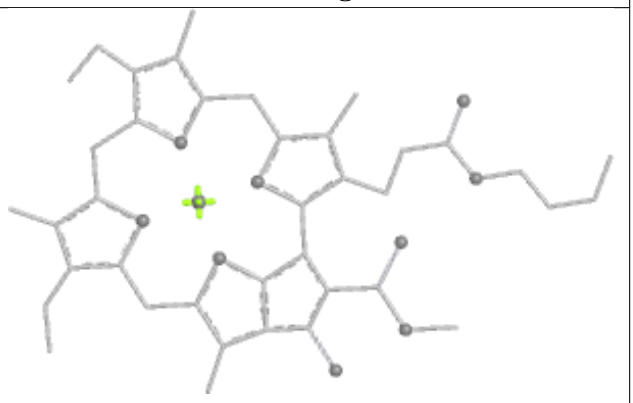
Bond lengths



Bond angles

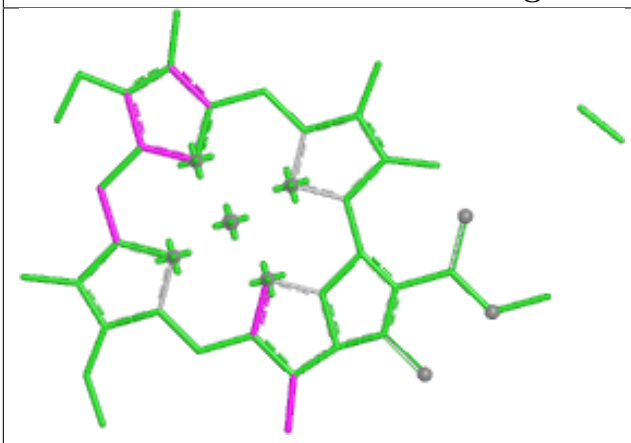


Torsions

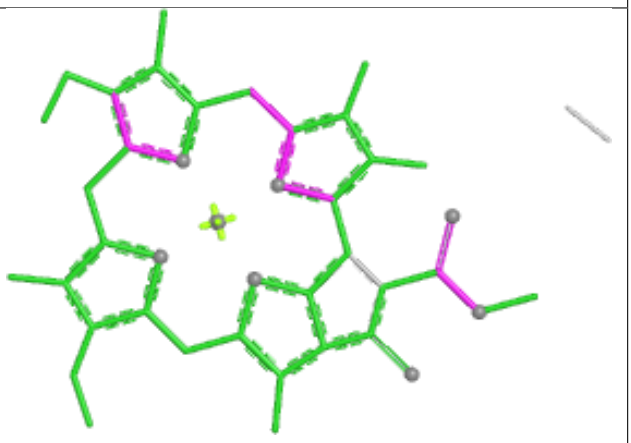


Rings

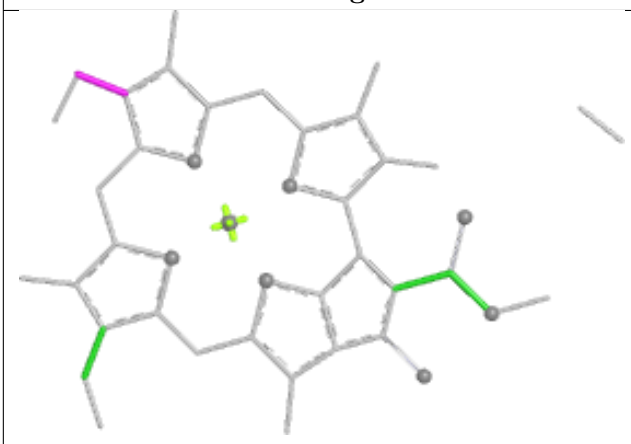
Ligand CLA A 821



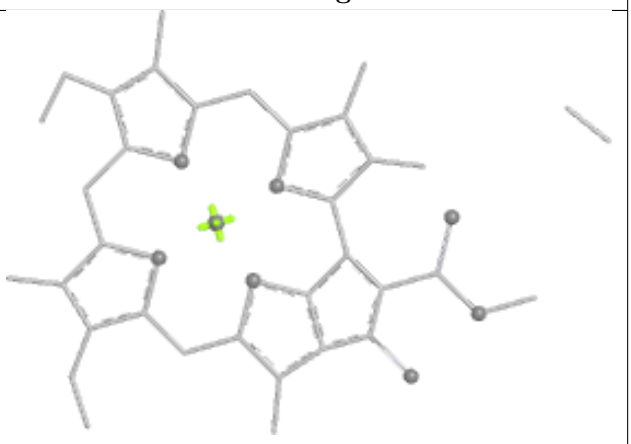
Bond lengths



Bond angles

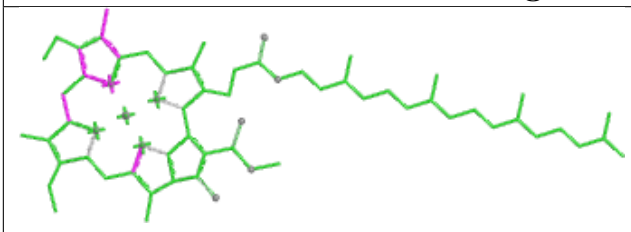


Torsions

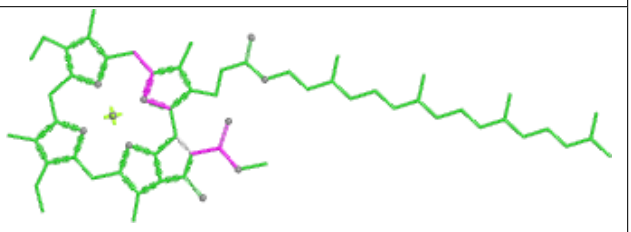


Rings

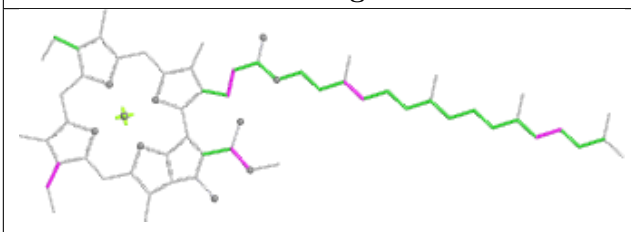
Ligand CLA B 807



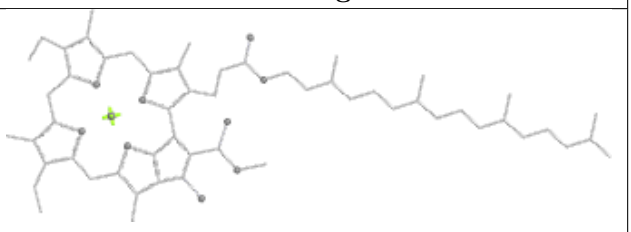
Bond lengths



Bond angles

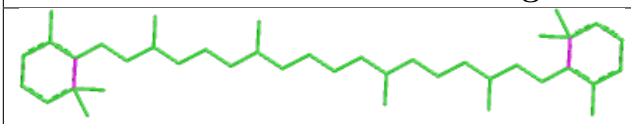


Torsions

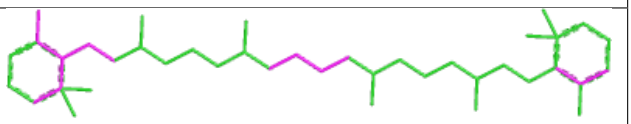


Rings

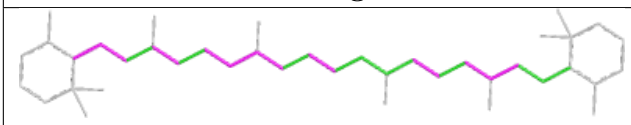
Ligand BCR A 849



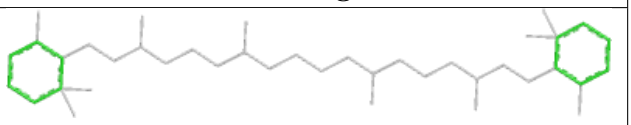
Bond lengths



Bond angles

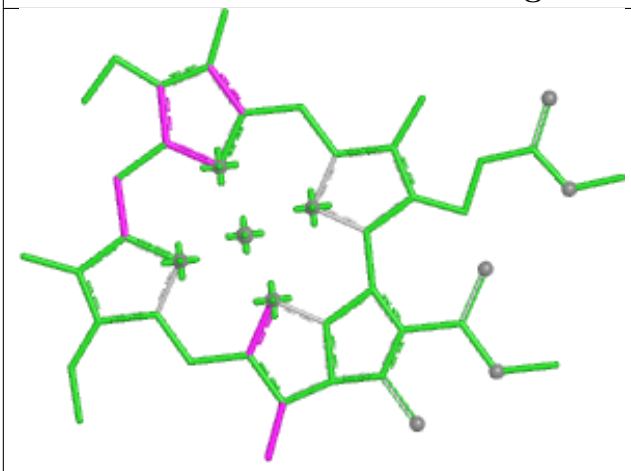


Torsions

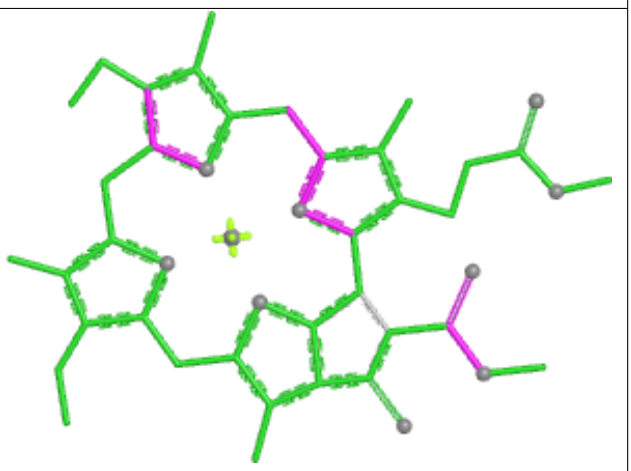


Rings

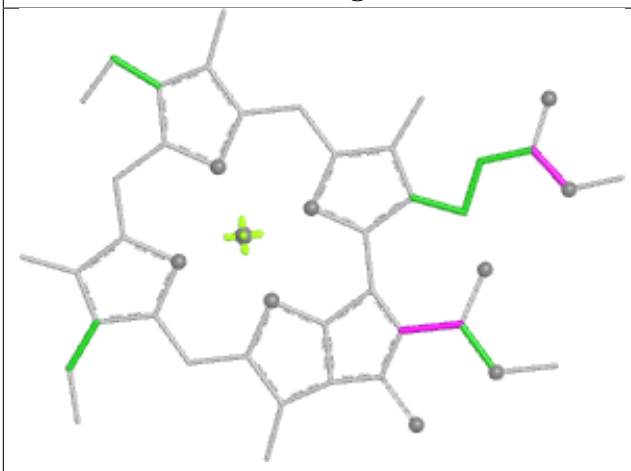
Ligand CLA B 825



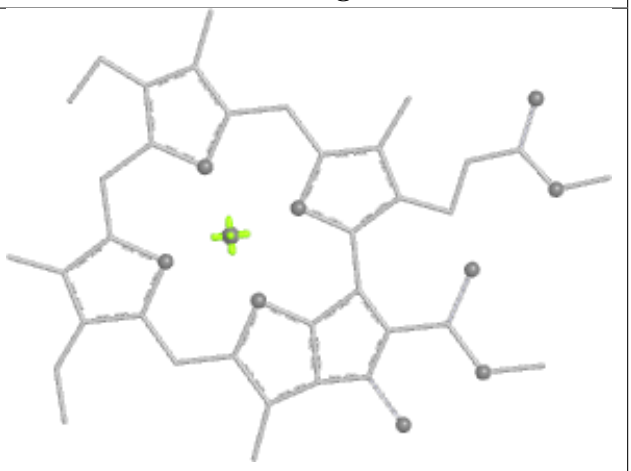
Bond lengths



Bond angles

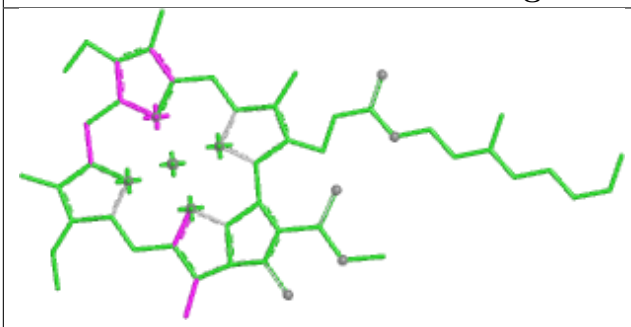


Torsions

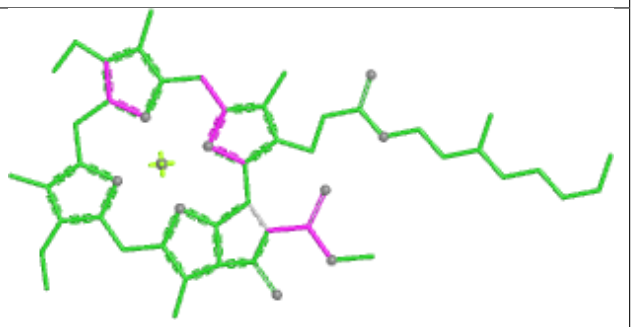


Rings

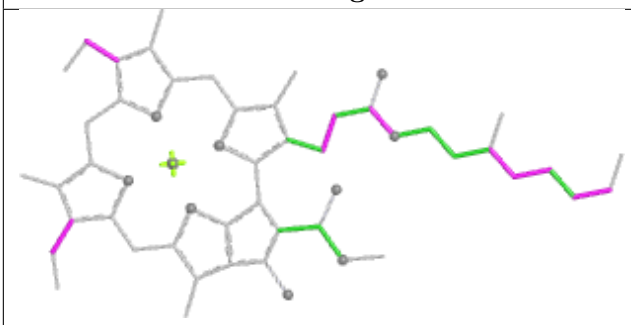
Ligand CLA A 813



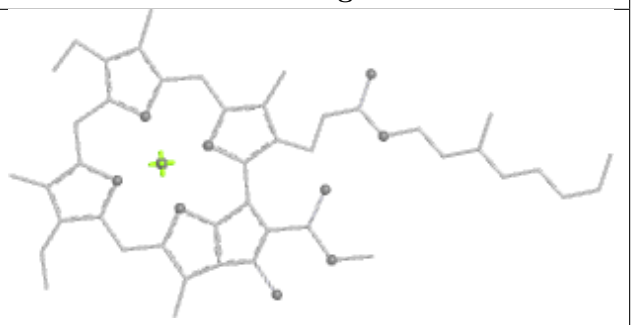
Bond lengths



Bond angles

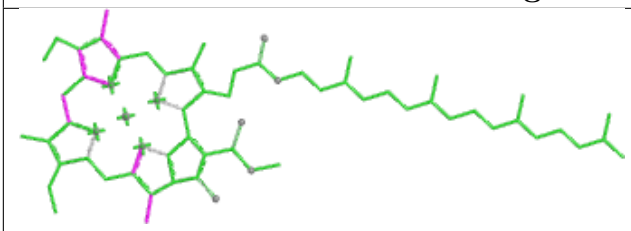


Torsions

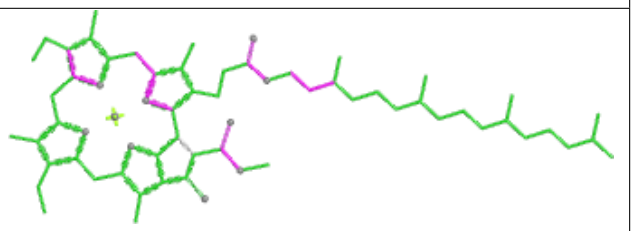


Rings

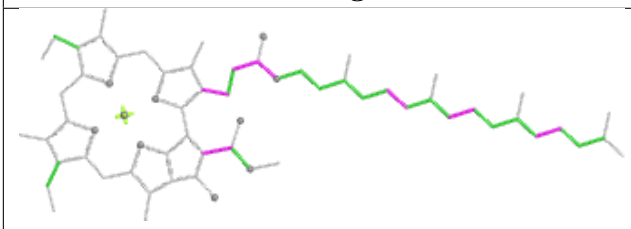
Ligand CLA A 809



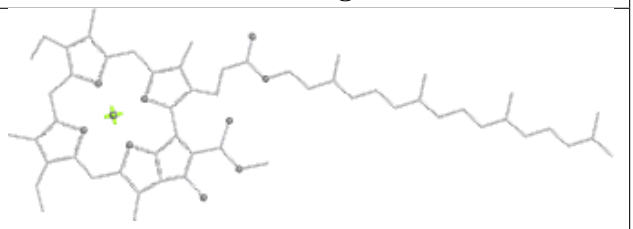
Bond lengths



Bond angles

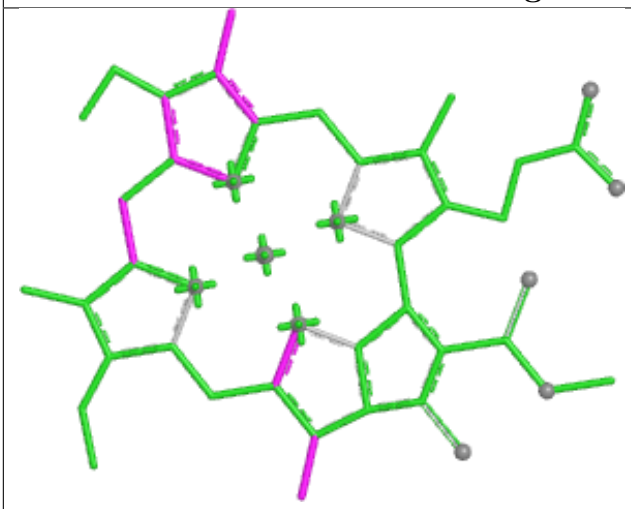


Torsions

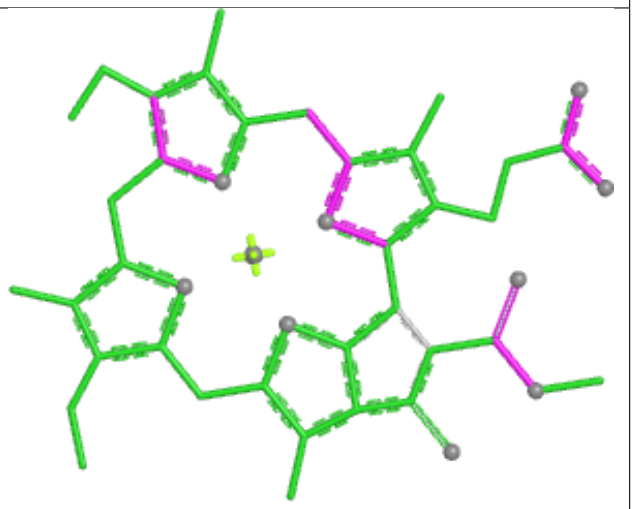


Rings

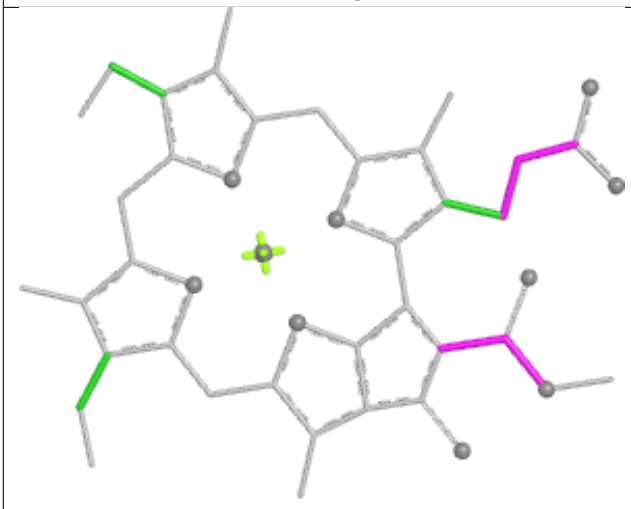
Ligand CLA B 812



Bond lengths



Bond angles

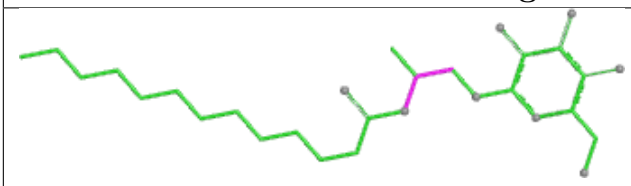


Torsions

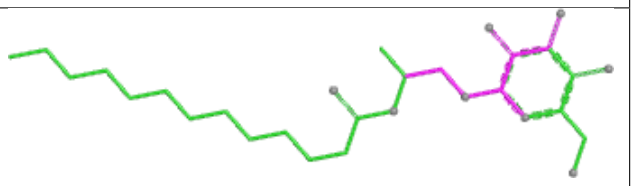


Rings

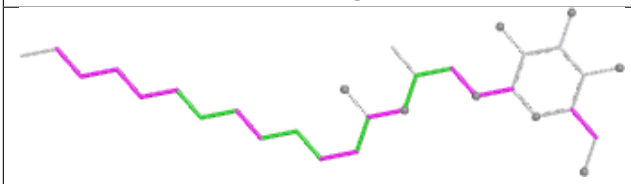
Ligand LMG A 856



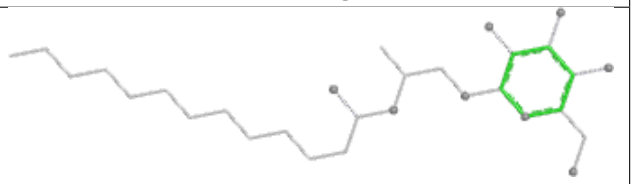
Bond lengths



Bond angles

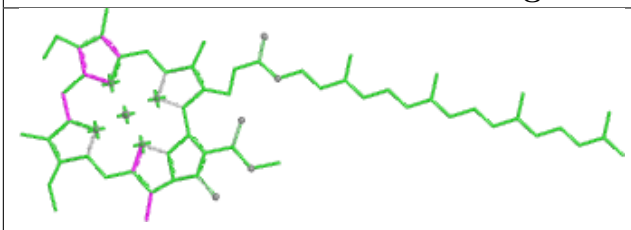


Torsions

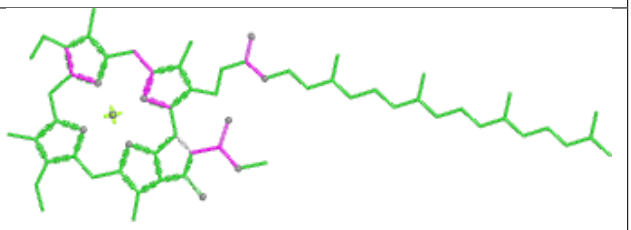


Rings

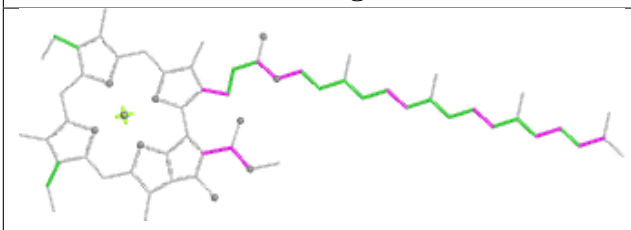
Ligand CLA A 806



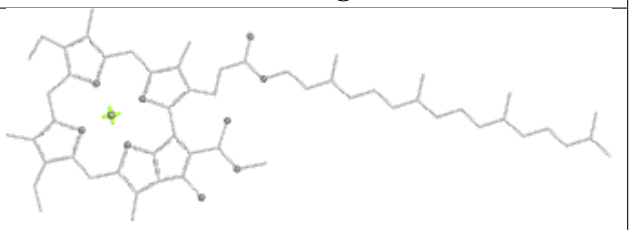
Bond lengths



Bond angles

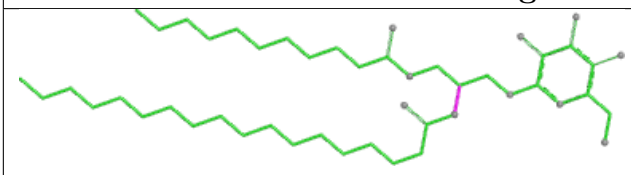


Torsions

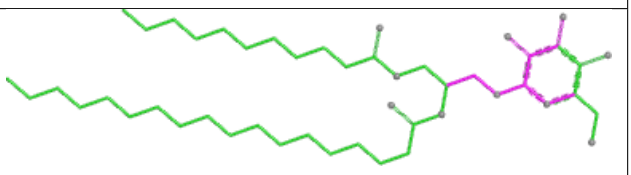


Rings

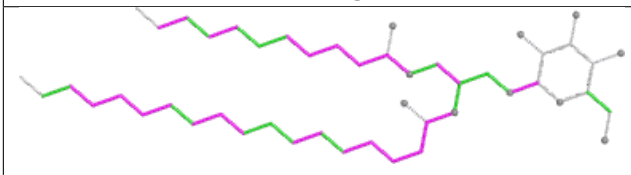
Ligand LMG A 853



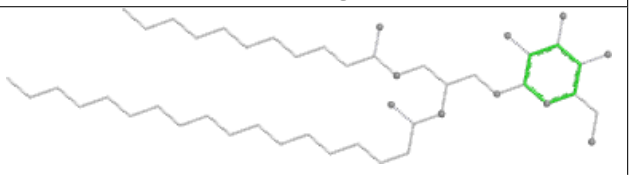
Bond lengths



Bond angles

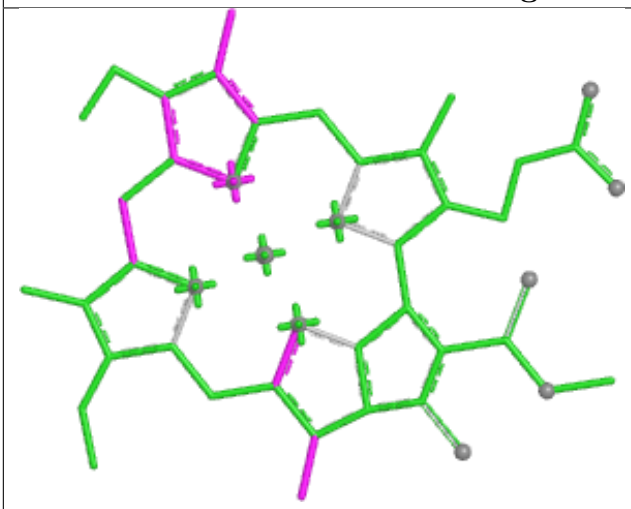


Torsions

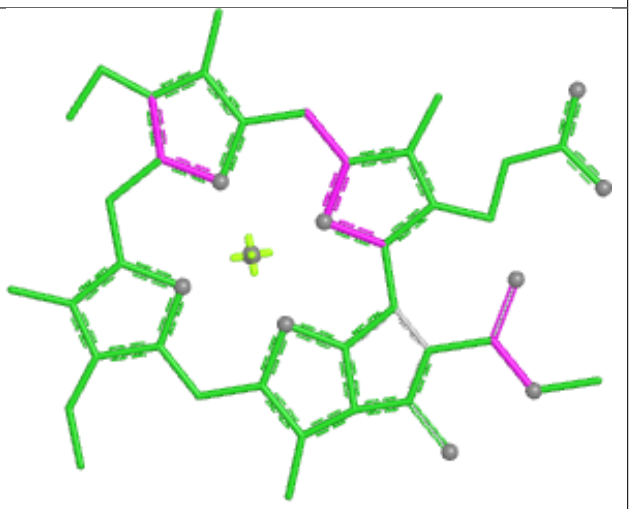


Rings

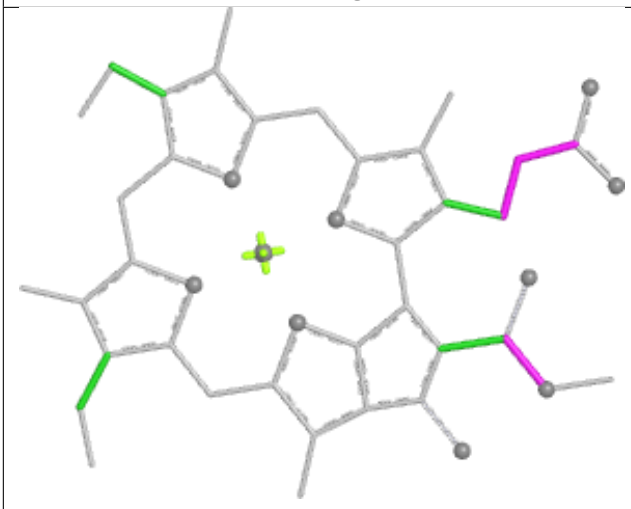
Ligand CLA M 102



Bond lengths



Bond angles

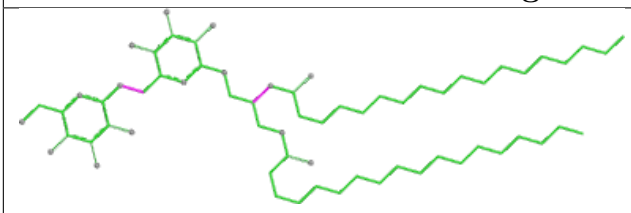


Torsions

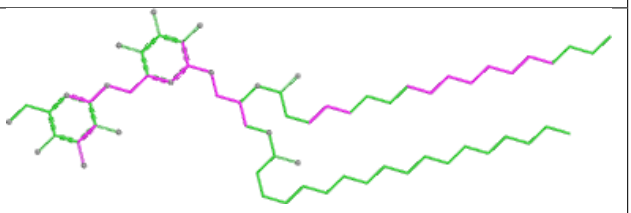


Rings

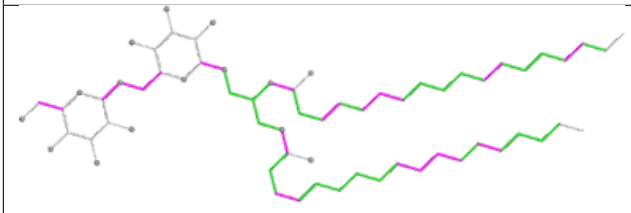
Ligand DGD L 207



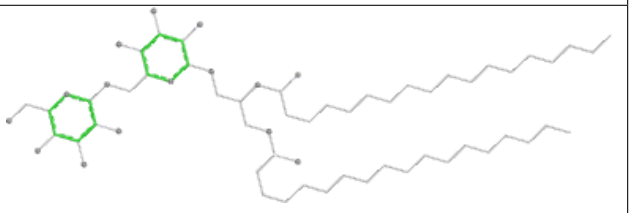
Bond lengths



Bond angles

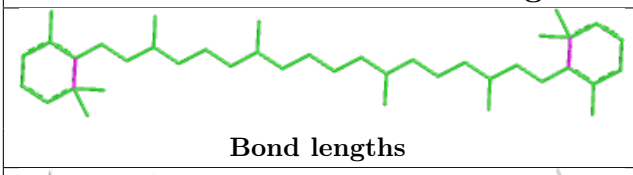


Torsions

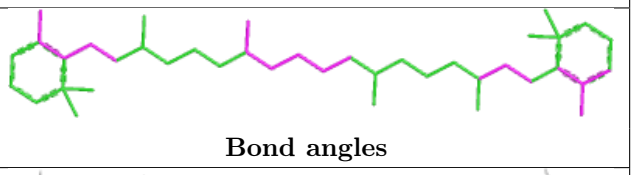


Rings

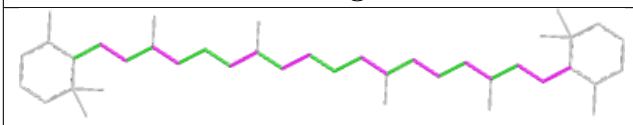
Ligand BCR L 201



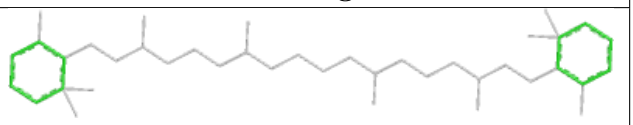
Bond lengths



Bond angles

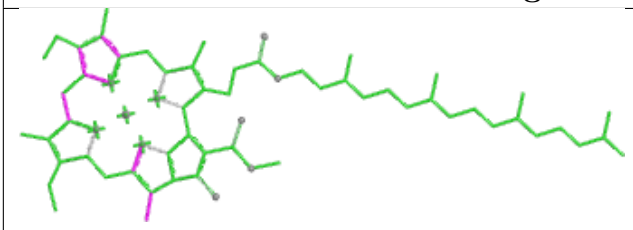


Torsions

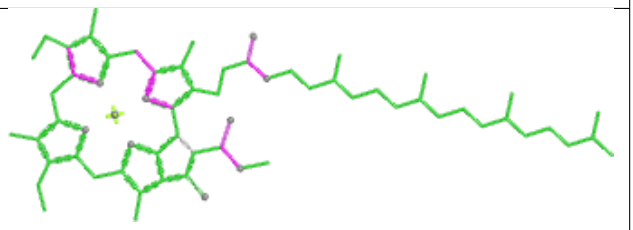


Rings

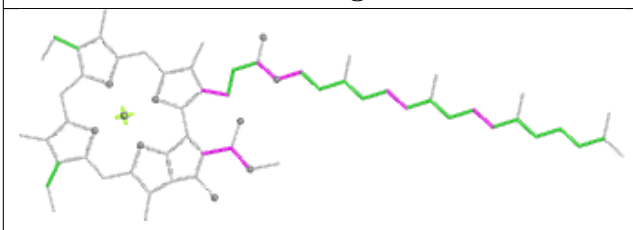
Ligand CLA A 804



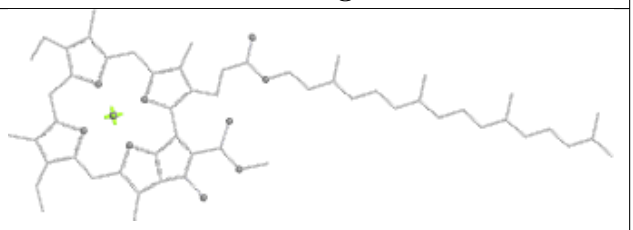
Bond lengths



Bond angles

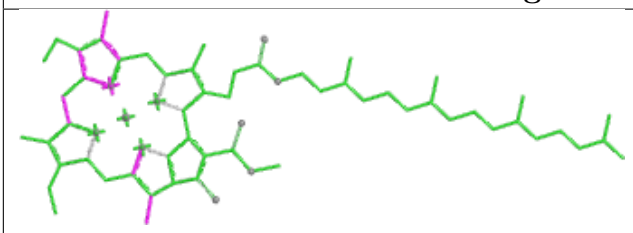


Torsions

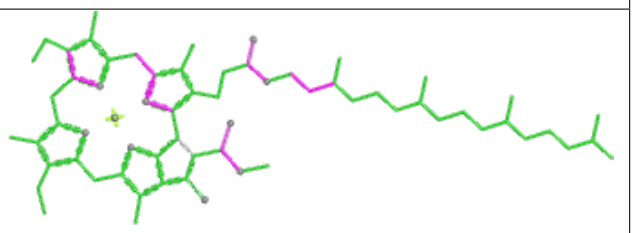


Rings

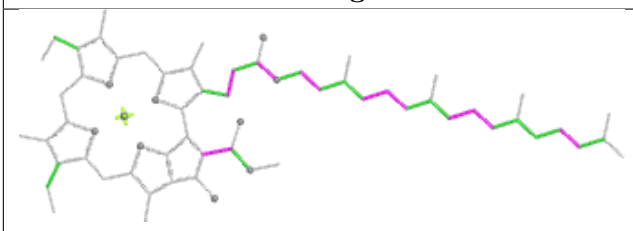
Ligand CLA A 810



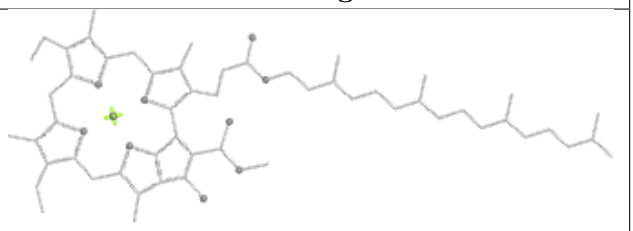
Bond lengths



Bond angles

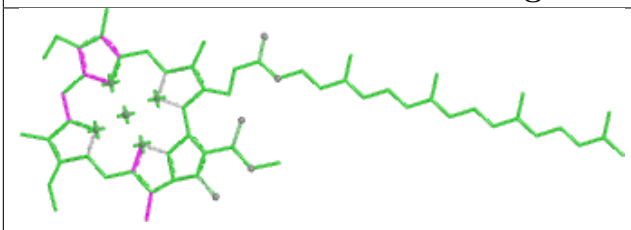


Torsions

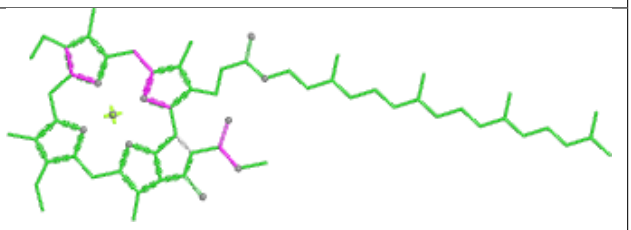


Rings

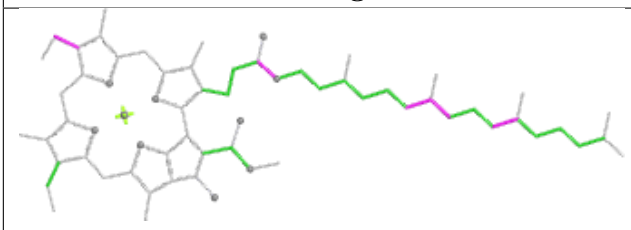
Ligand CLA B 806



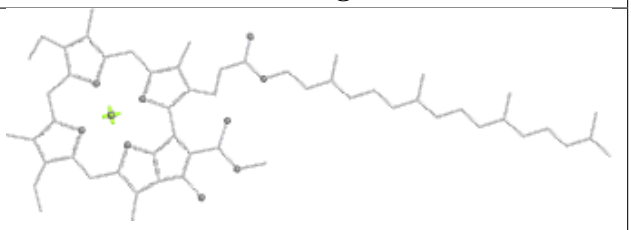
Bond lengths



Bond angles

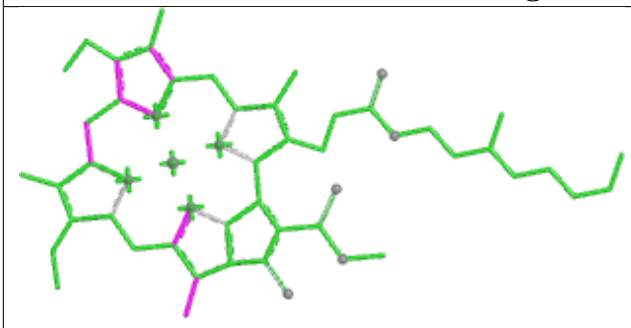


Torsions

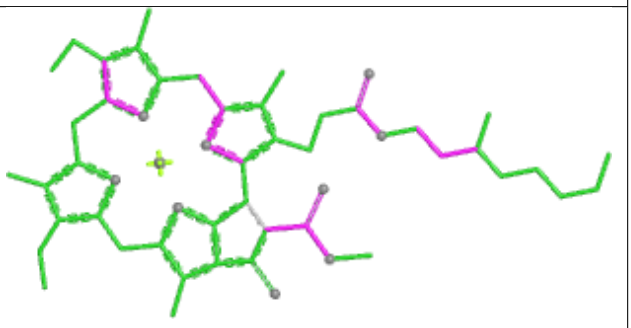


Rings

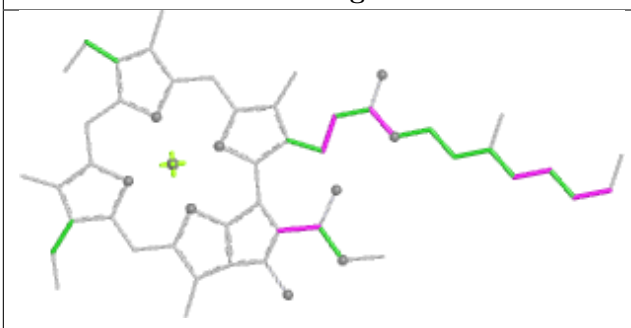
Ligand CLA B 804



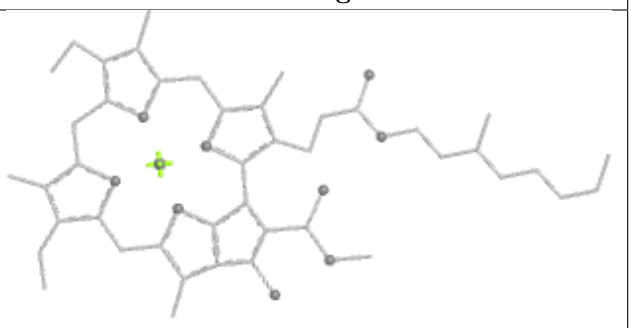
Bond lengths



Bond angles

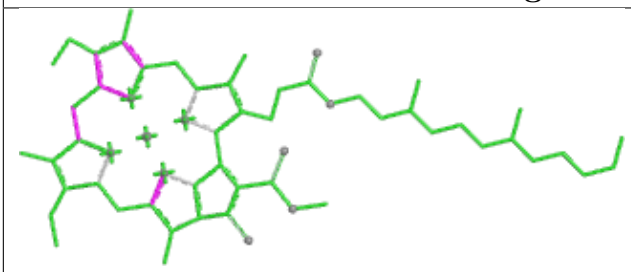


Torsions

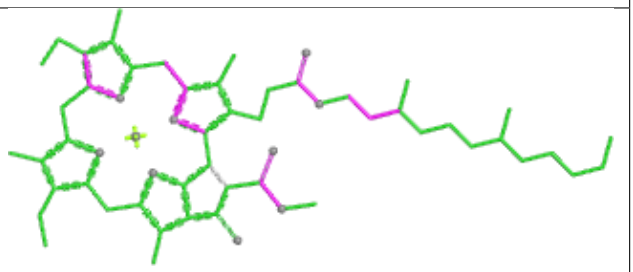


Rings

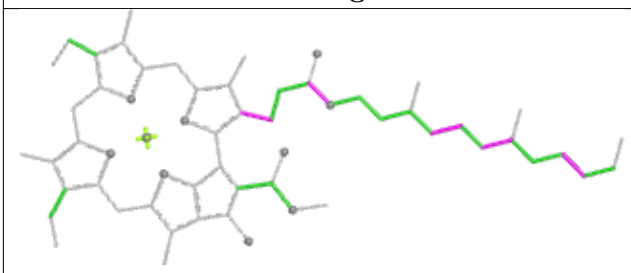
Ligand CLA B 817



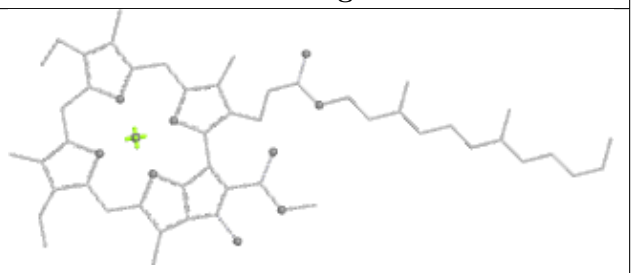
Bond lengths



Bond angles

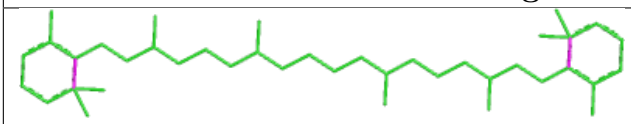


Torsions

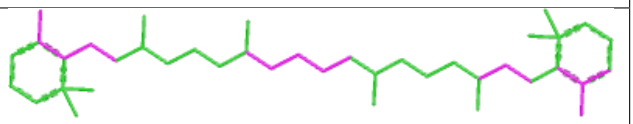


Rings

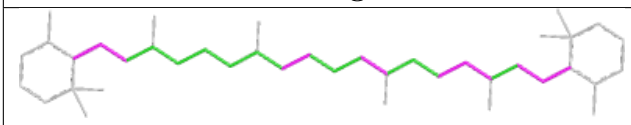
Ligand BCR A 850



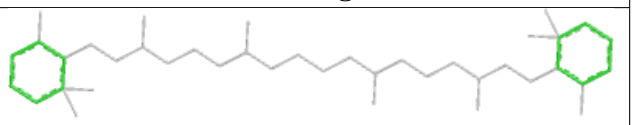
Bond lengths



Bond angles

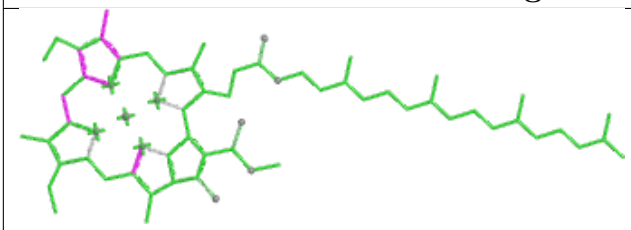


Torsions

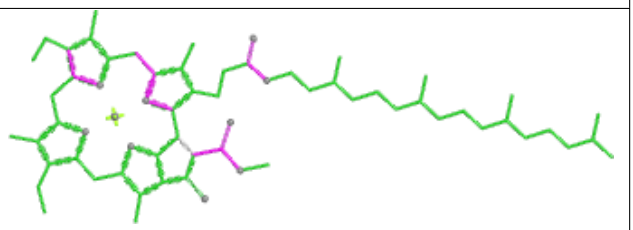


Rings

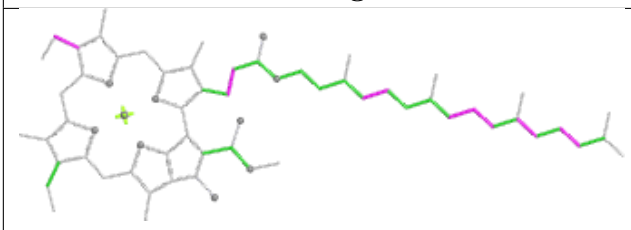
Ligand CLA B 840



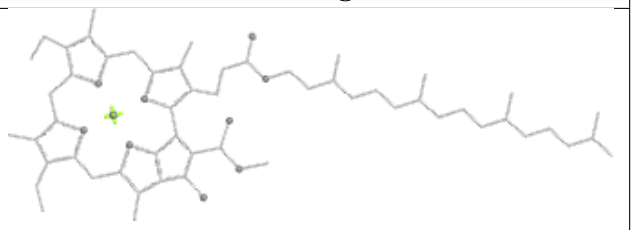
Bond lengths



Bond angles

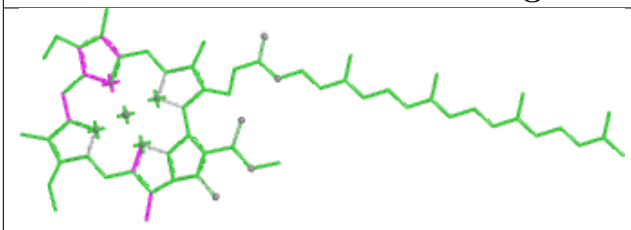


Torsions

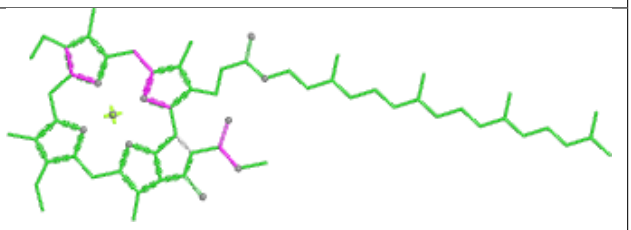


Rings

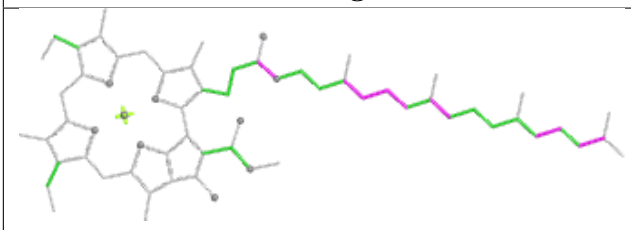
Ligand CLA A 833



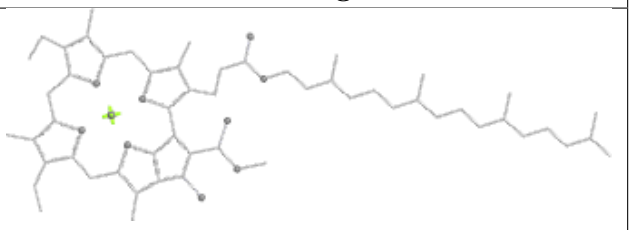
Bond lengths



Bond angles

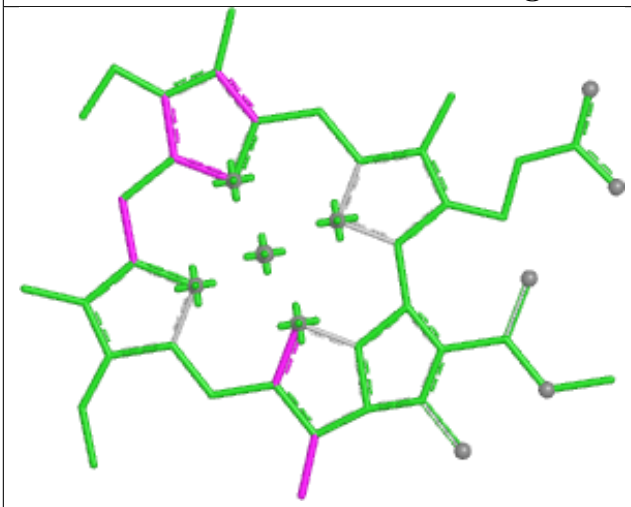


Torsions

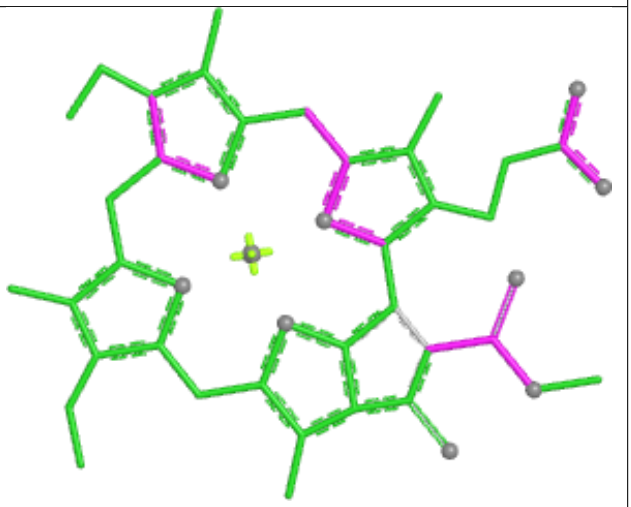


Rings

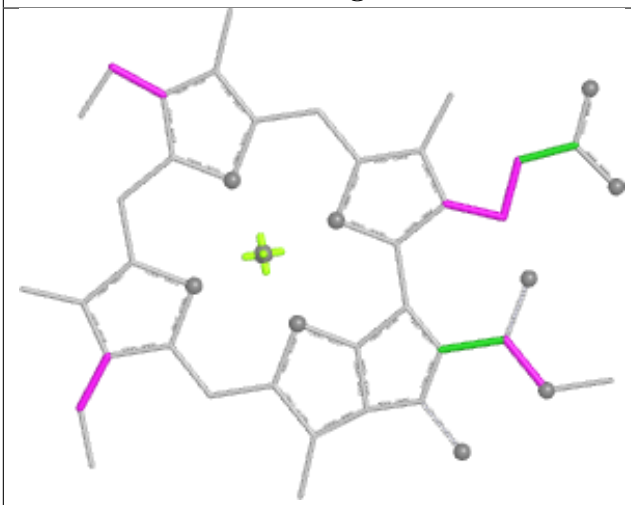
Ligand CLA A 811



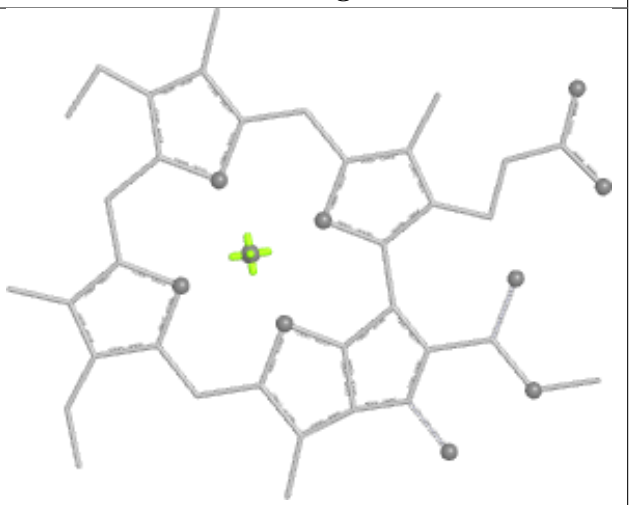
Bond lengths



Bond angles

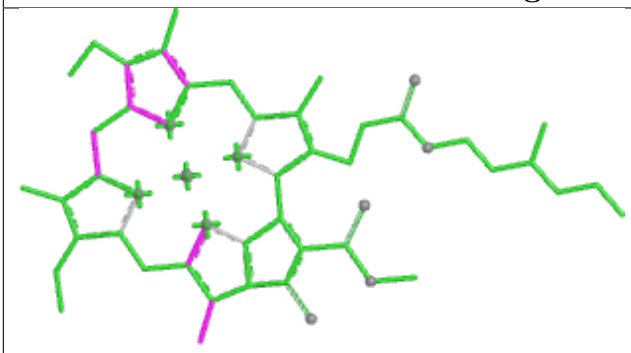


Torsions

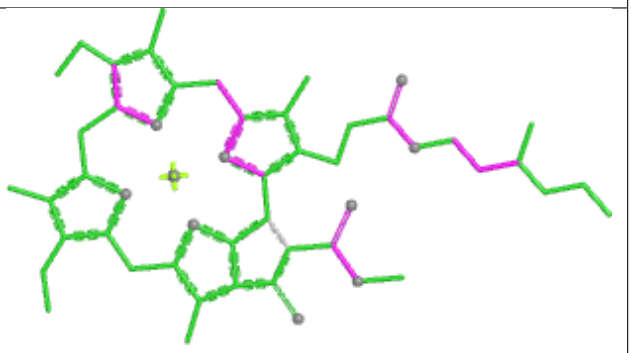


Rings

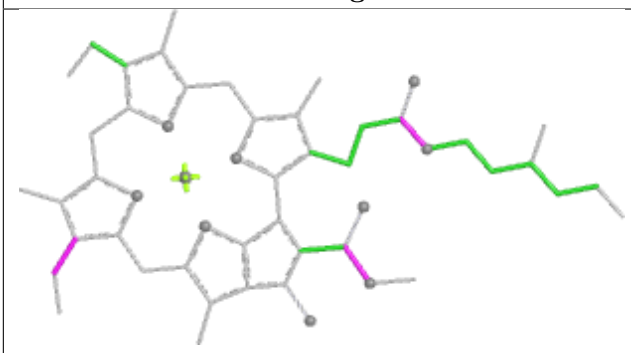
Ligand CLA A 844



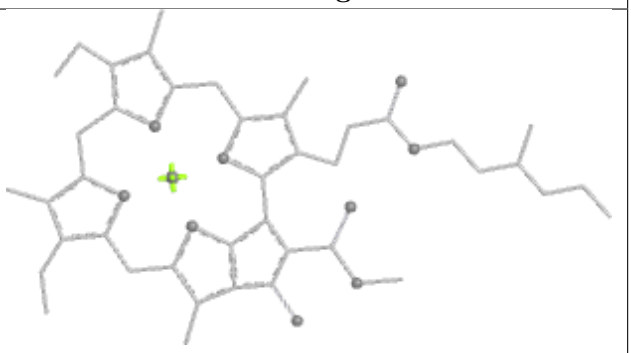
Bond lengths



Bond angles

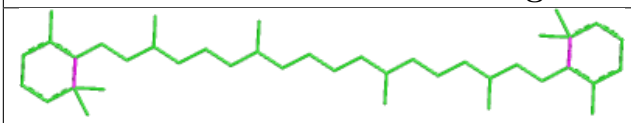


Torsions

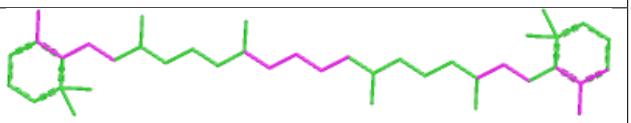


Rings

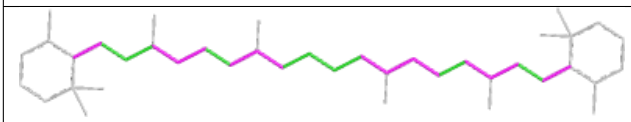
Ligand BCR J 103



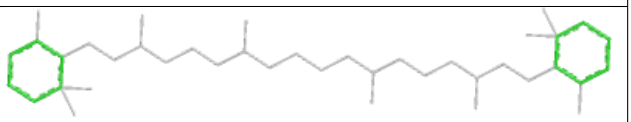
Bond lengths



Bond angles



Torsions

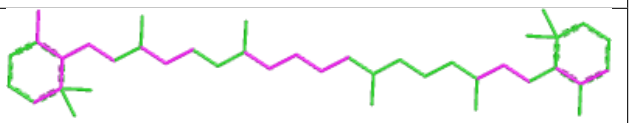


Rings

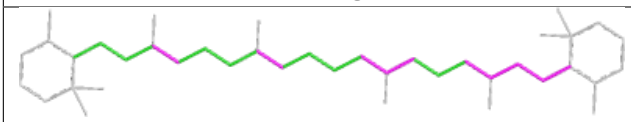
Ligand BCR A 847



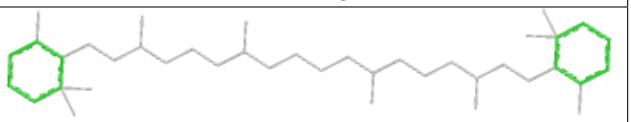
Bond lengths



Bond angles

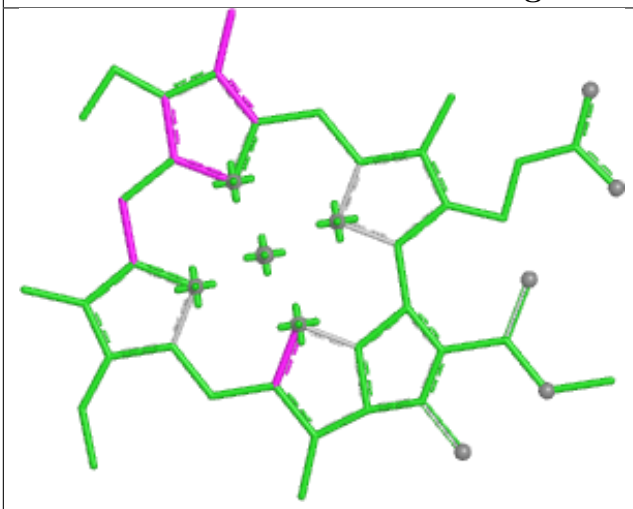


Torsions

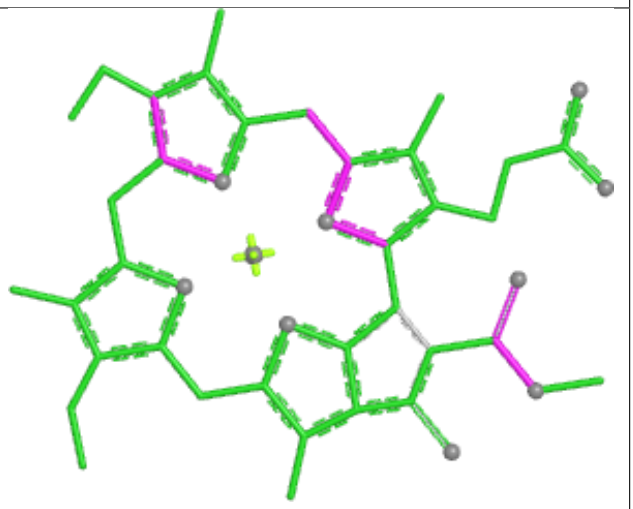


Rings

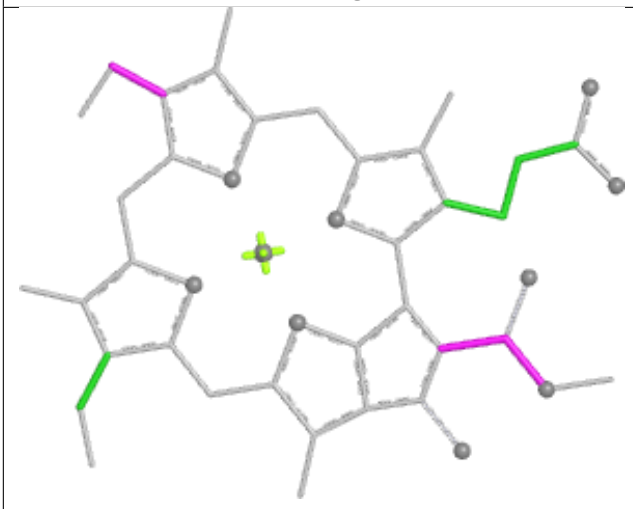
Ligand CLA B 834



Bond lengths



Bond angles

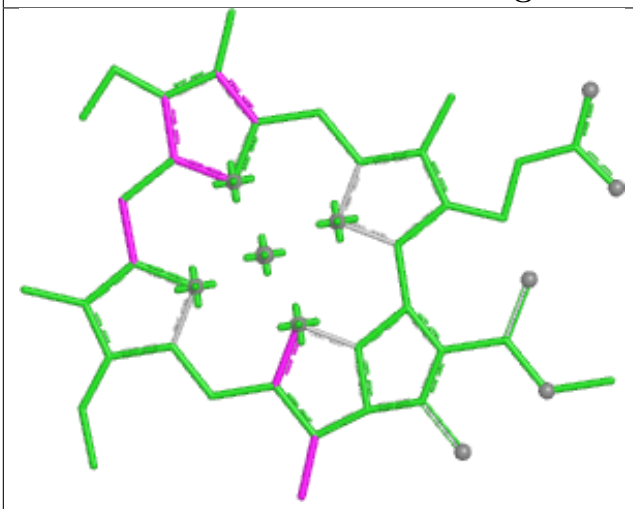


Torsions

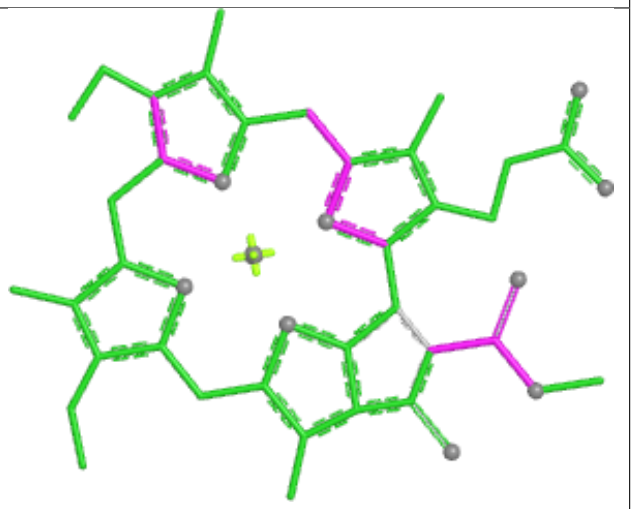


Rings

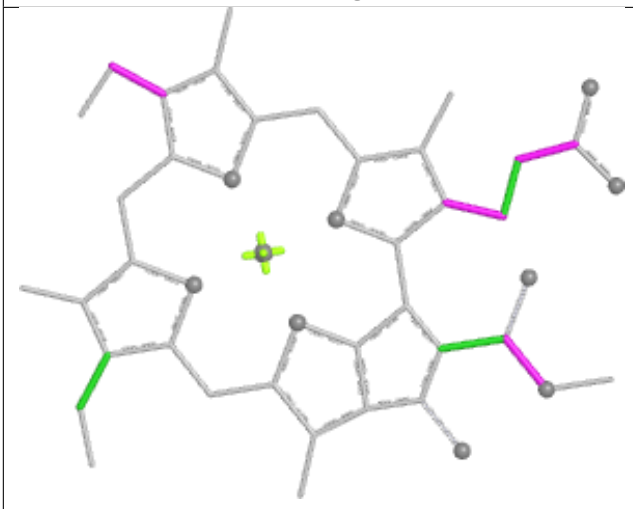
Ligand CLA X 1701



Bond lengths



Bond angles

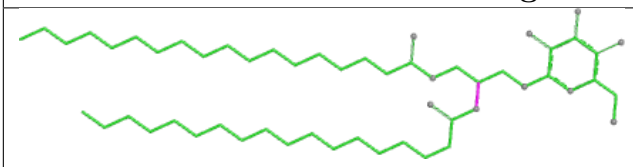


Torsions

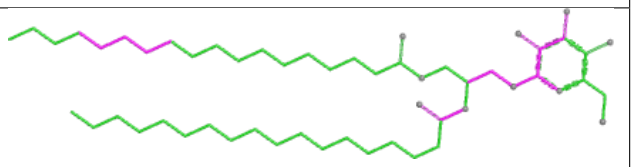


Rings

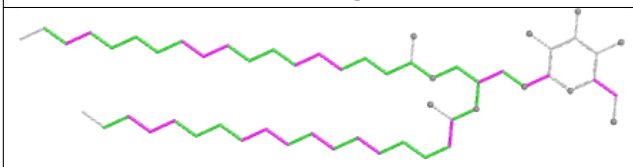
Ligand LMG B 849



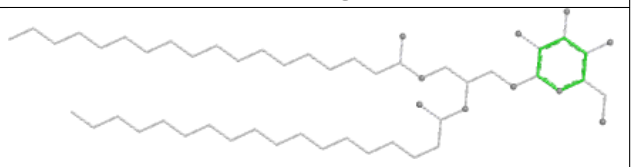
Bond lengths



Bond angles

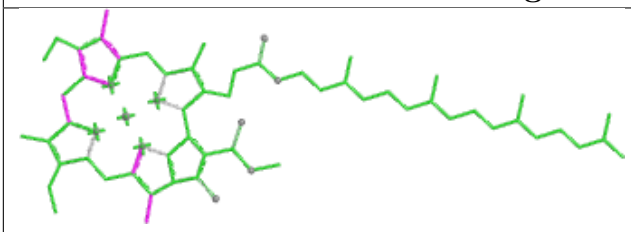


Torsions

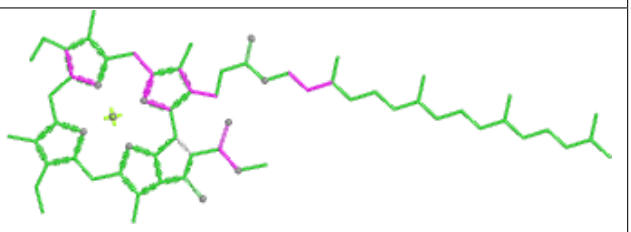


Rings

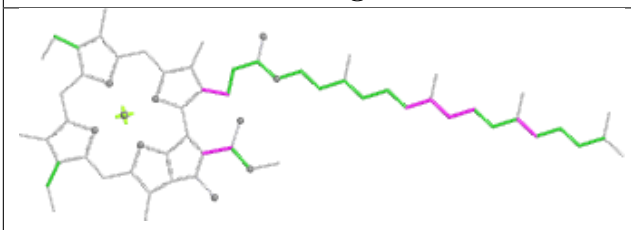
Ligand CLA B 829



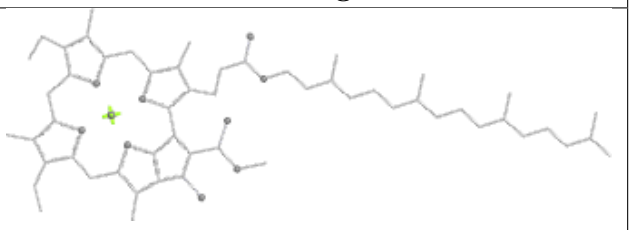
Bond lengths



Bond angles

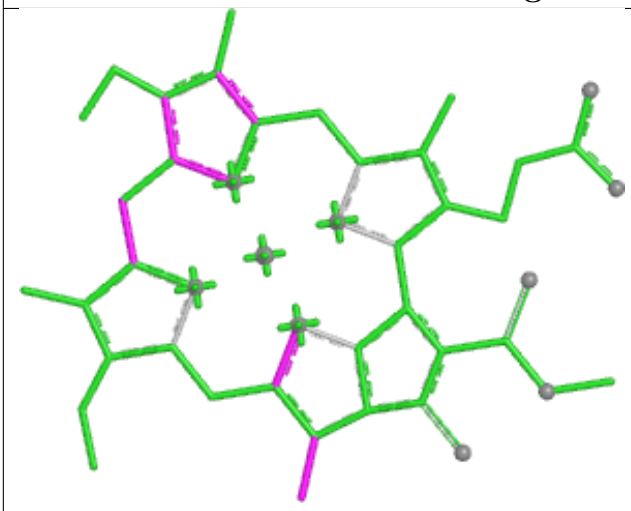


Torsions

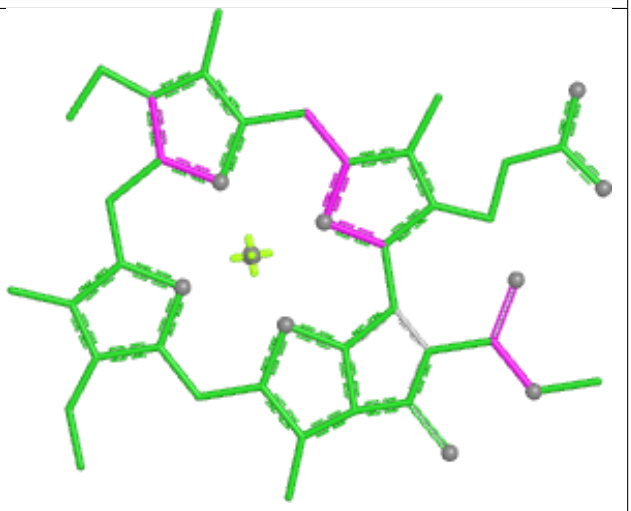


Rings

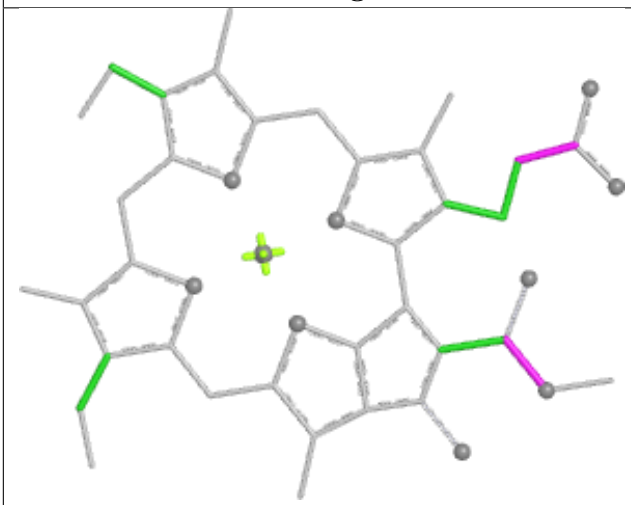
Ligand CLA B 815



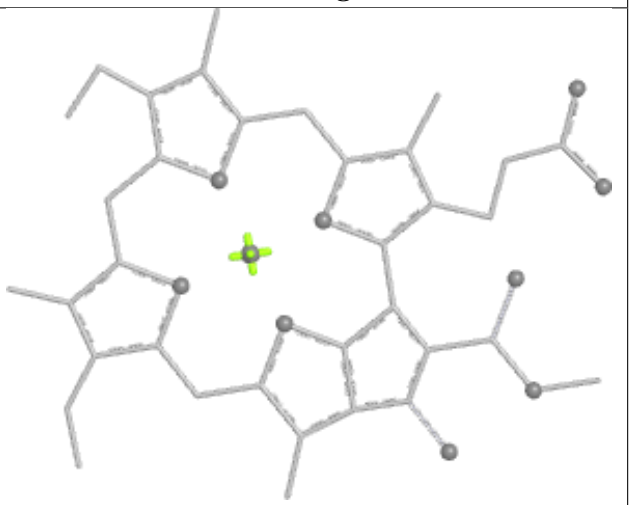
Bond lengths



Bond angles

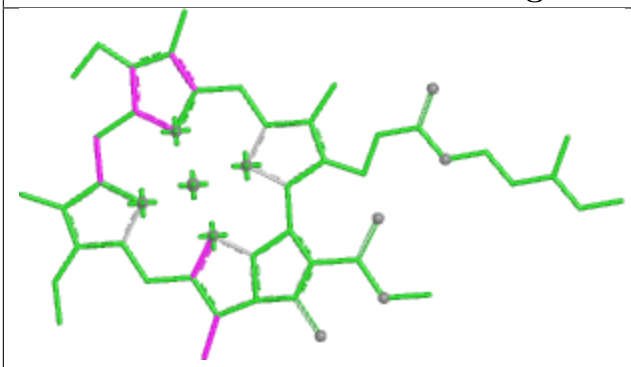


Torsions

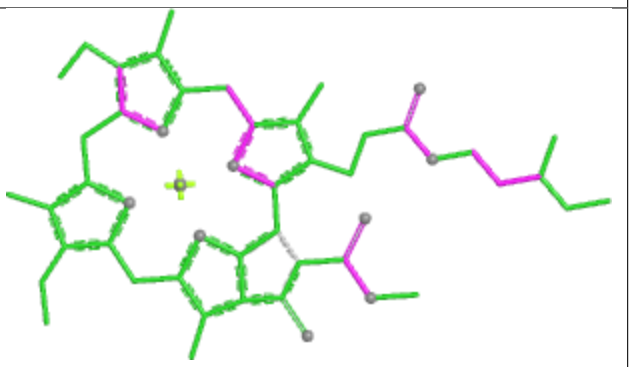


Rings

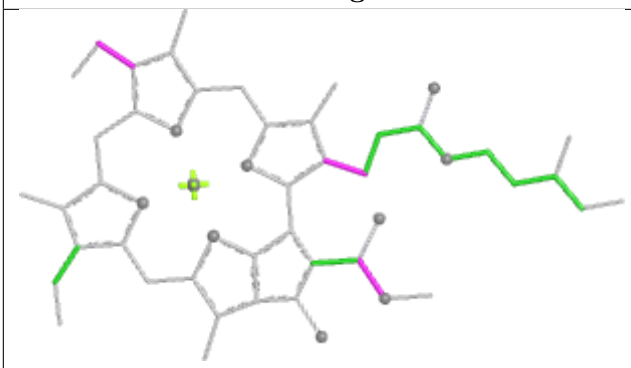
Ligand CLA F 201



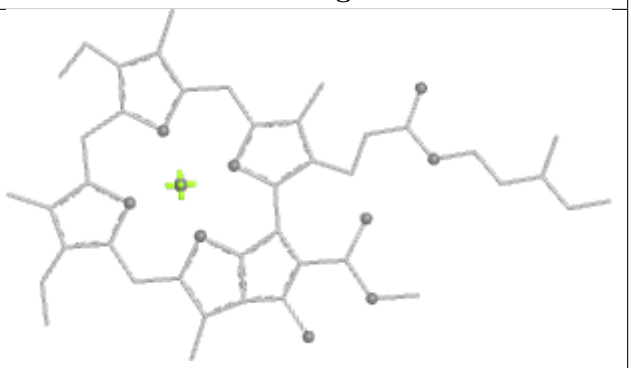
Bond lengths



Bond angles

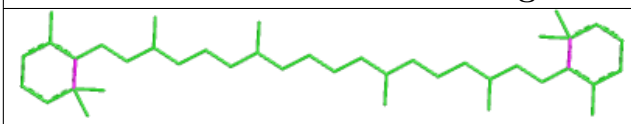


Torsions

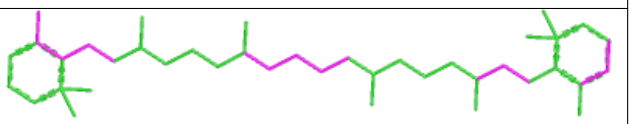


Rings

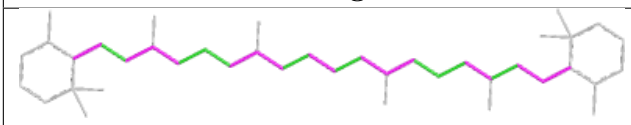
Ligand BCR M 103



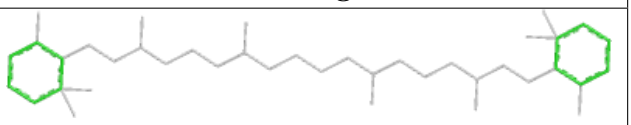
Bond lengths



Bond angles

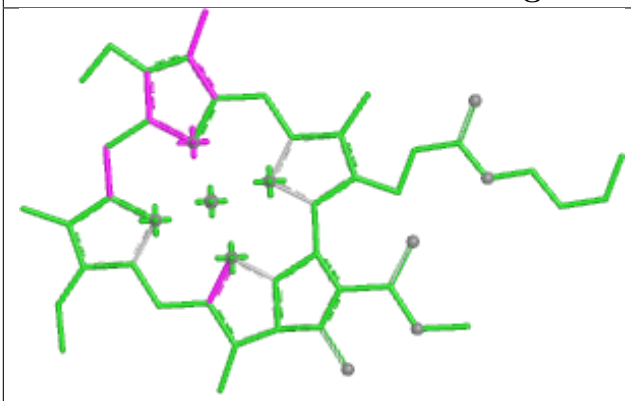


Torsions

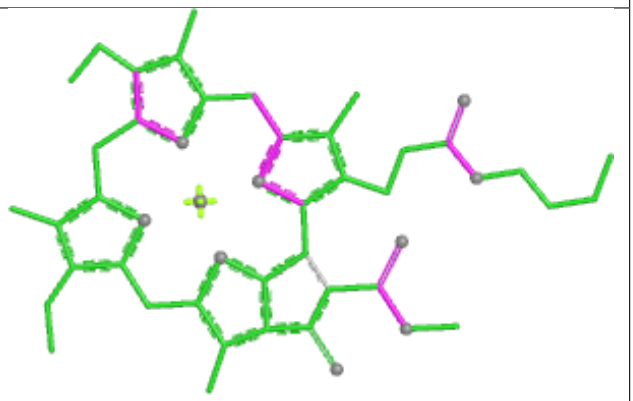


Rings

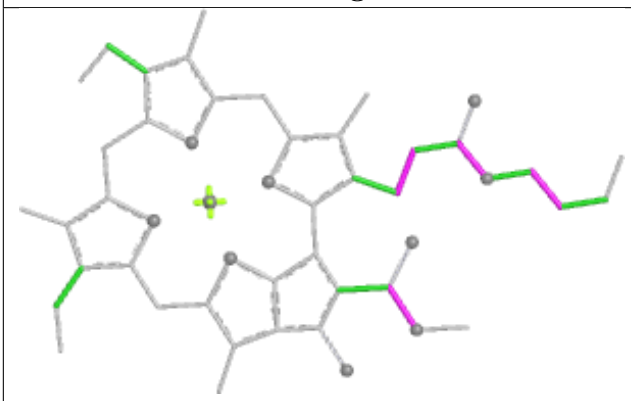
Ligand CLA A 817



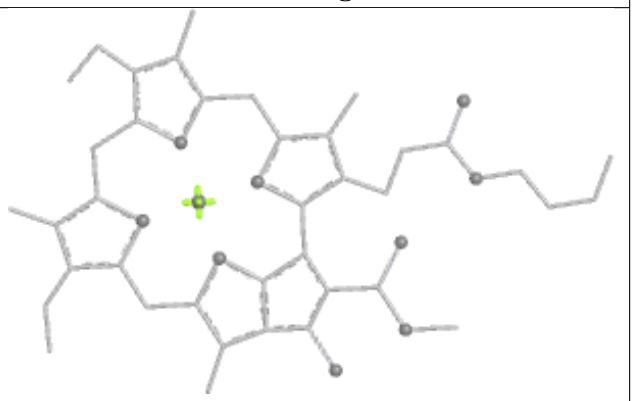
Bond lengths



Bond angles

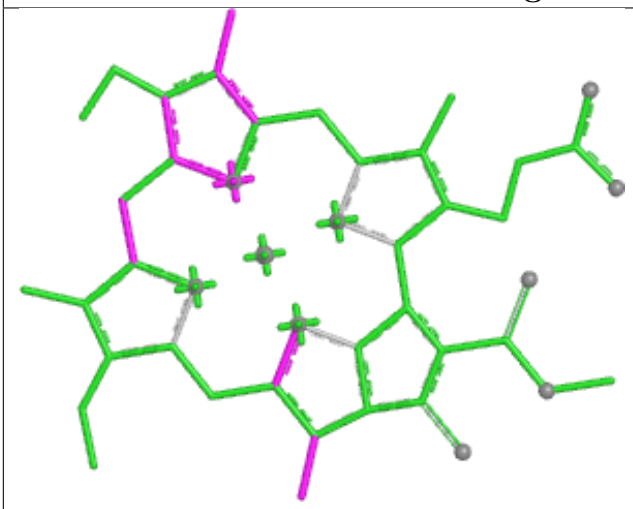


Torsions

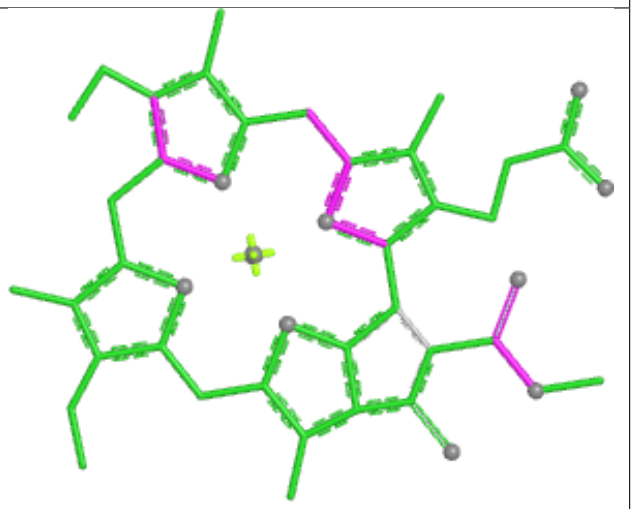


Rings

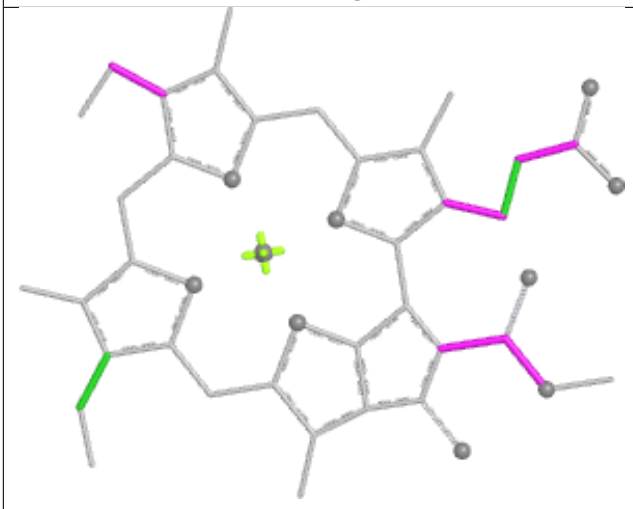
Ligand CLA B 830



Bond lengths



Bond angles

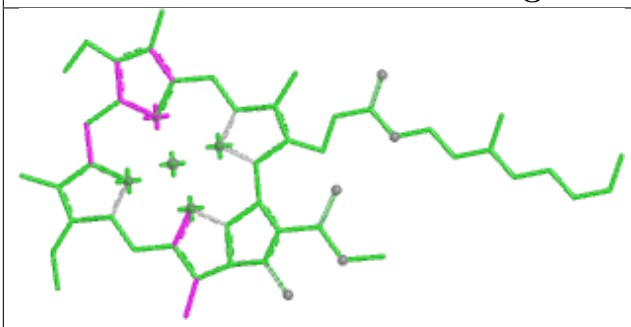


Torsions

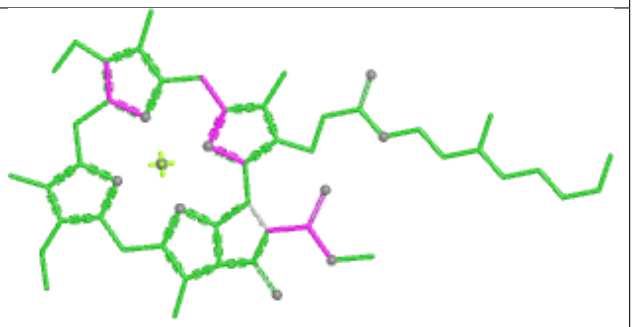


Rings

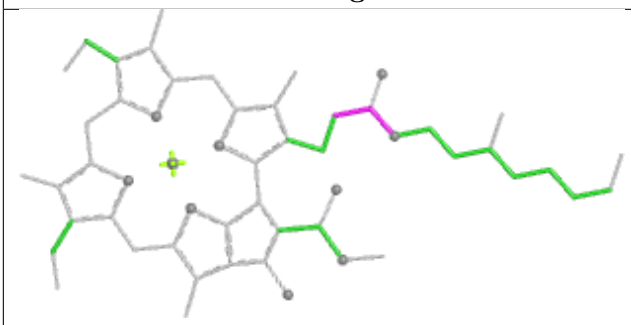
Ligand CLA A 818



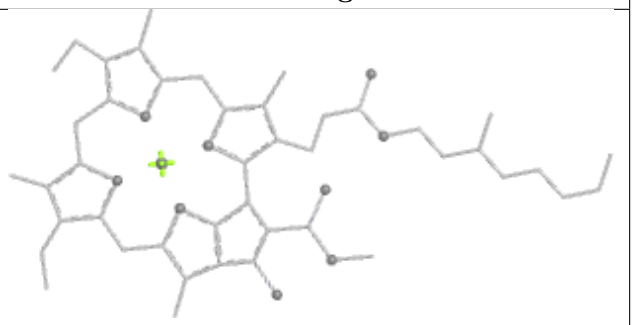
Bond lengths



Bond angles

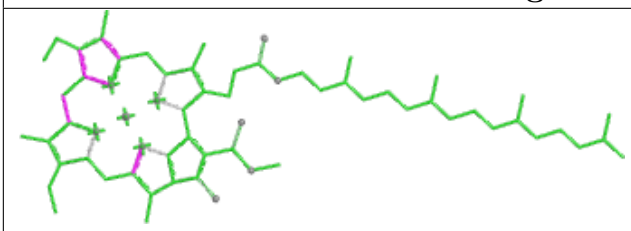


Torsions

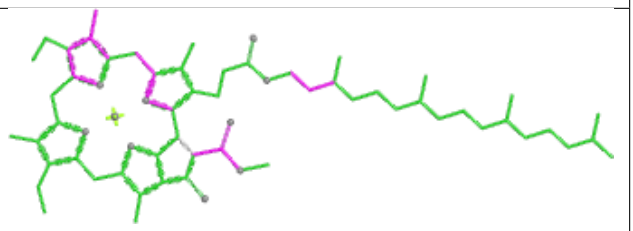


Rings

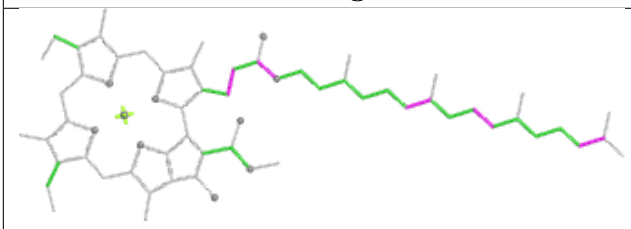
Ligand CLA L 206



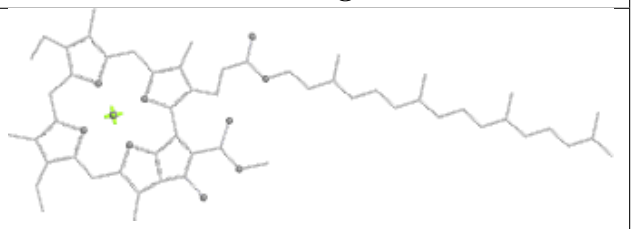
Bond lengths



Bond angles

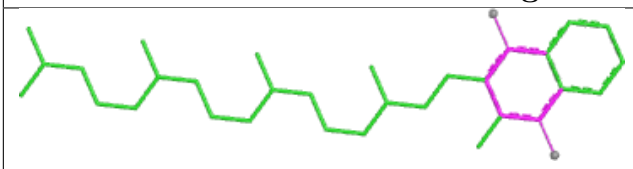


Torsions

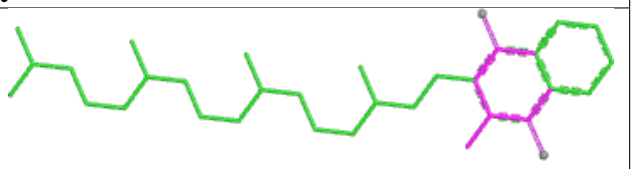


Rings

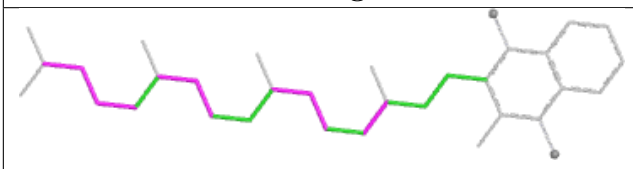
Ligand PQN A 845



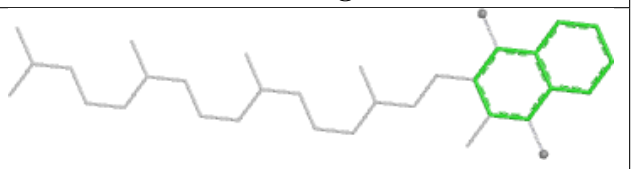
Bond lengths



Bond angles

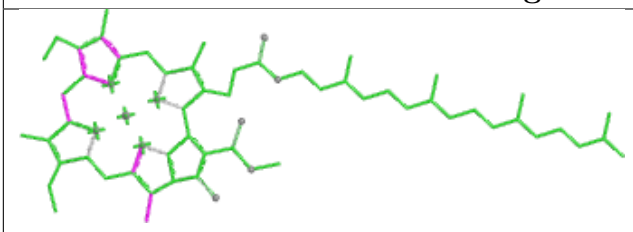


Torsions

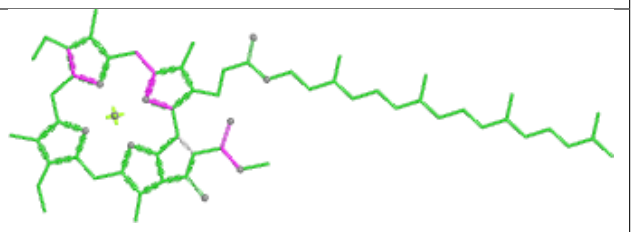


Rings

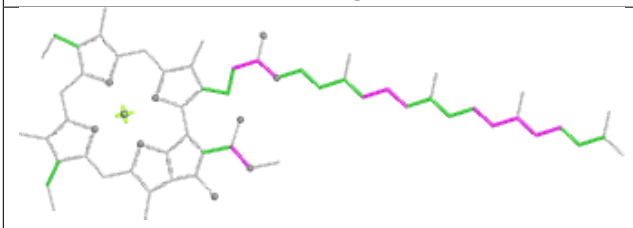
Ligand CLA A 807



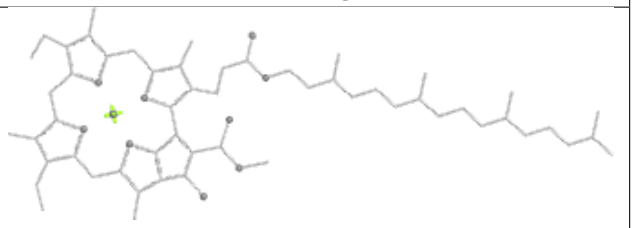
Bond lengths



Bond angles

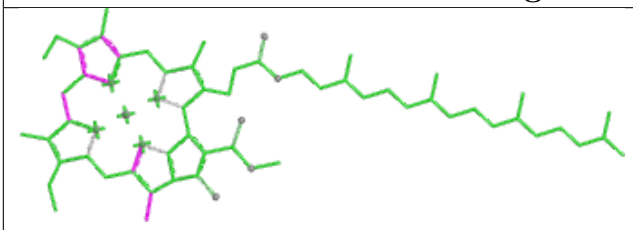


Torsions

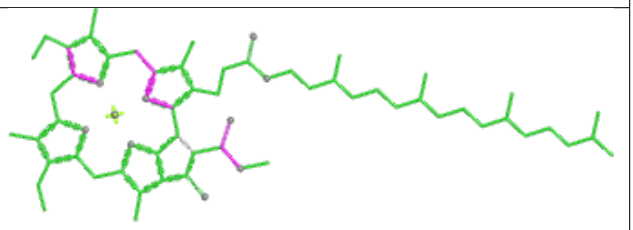


Rings

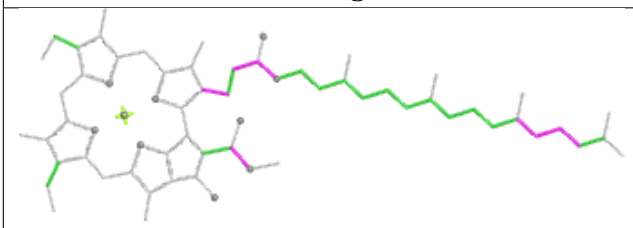
Ligand CLA B 805



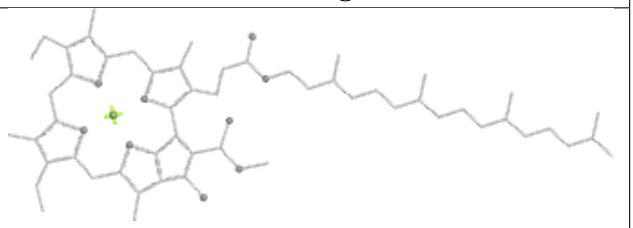
Bond lengths



Bond angles

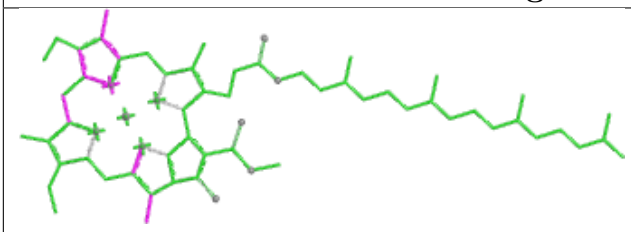


Torsions

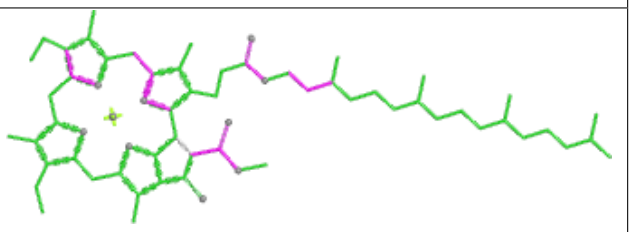


Rings

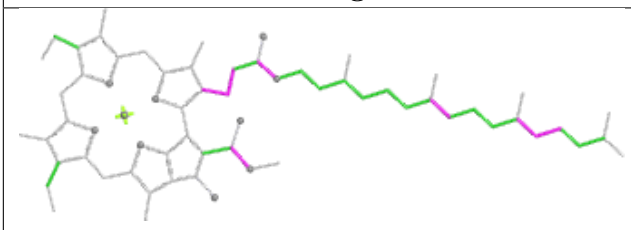
Ligand CLA L 205



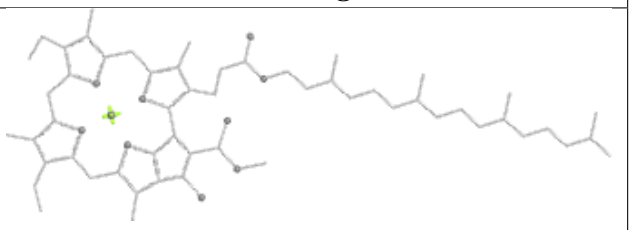
Bond lengths



Bond angles

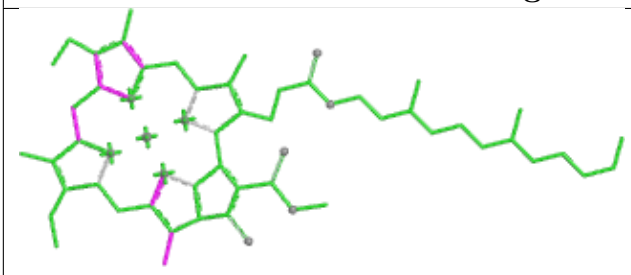


Torsions

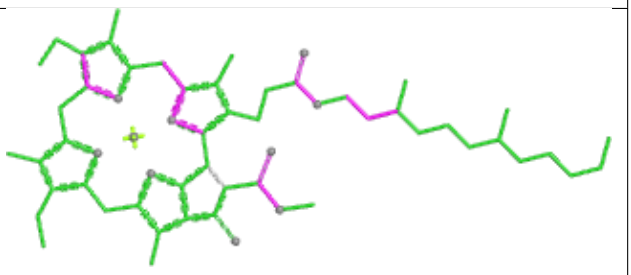


Rings

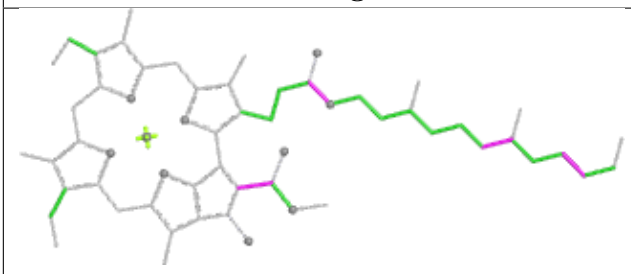
Ligand CLA A 805



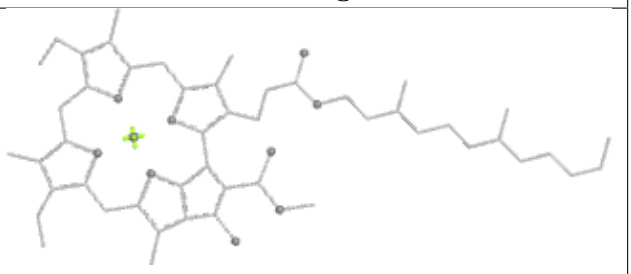
Bond lengths



Bond angles



Torsions

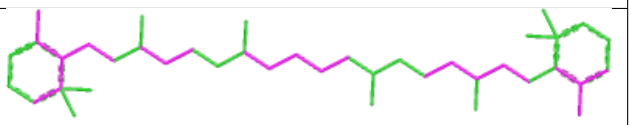


Rings

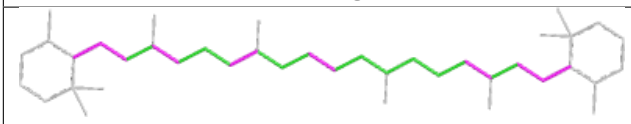
Ligand BCR J 104



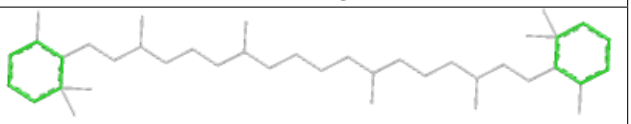
Bond lengths



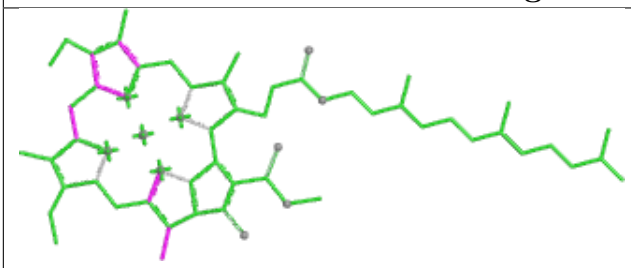
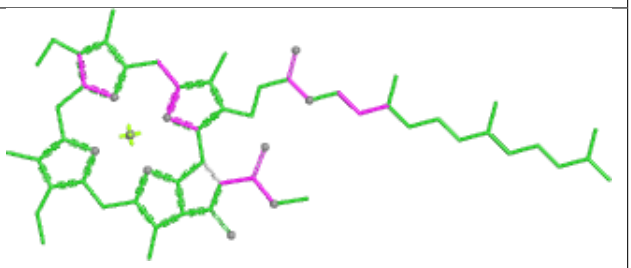
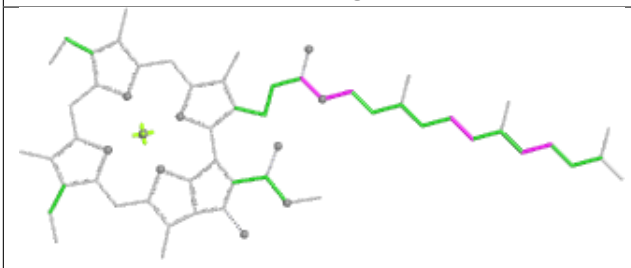
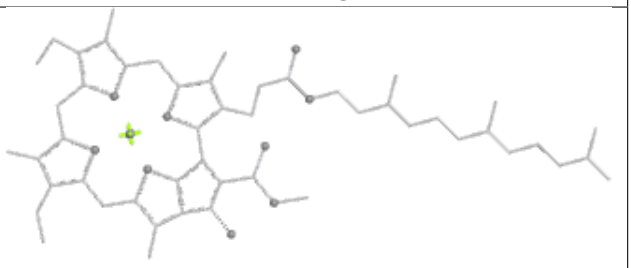
Bond angles

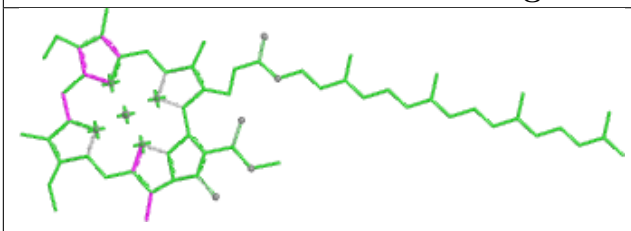
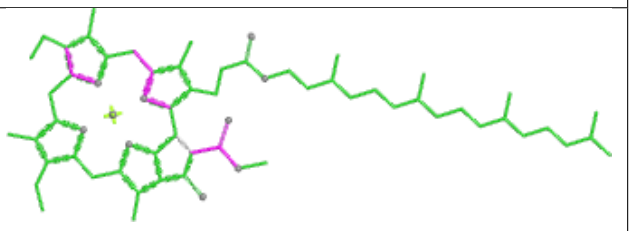
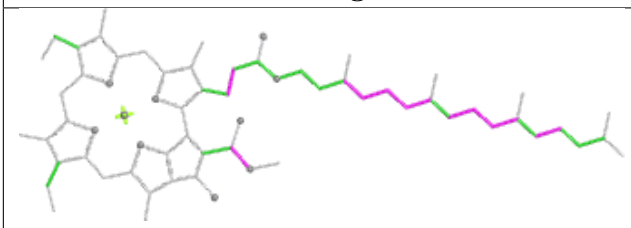
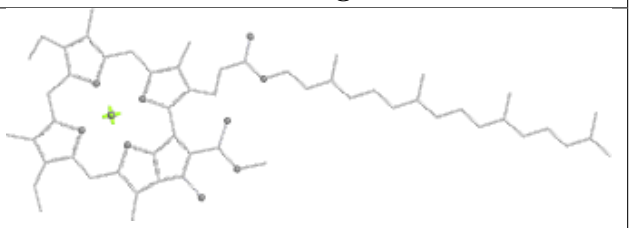


Torsions

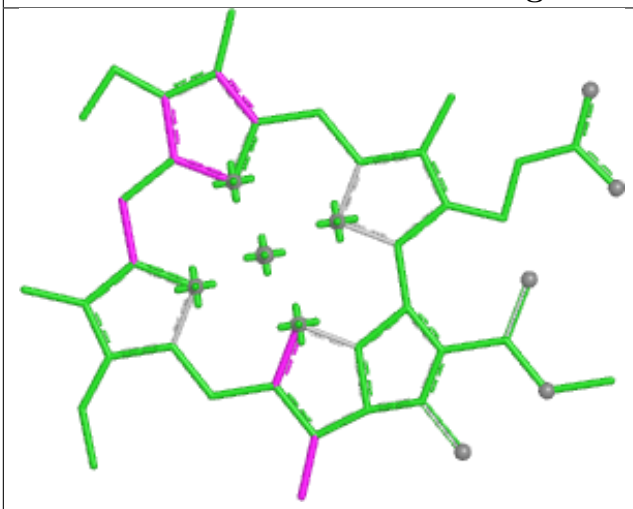


Rings

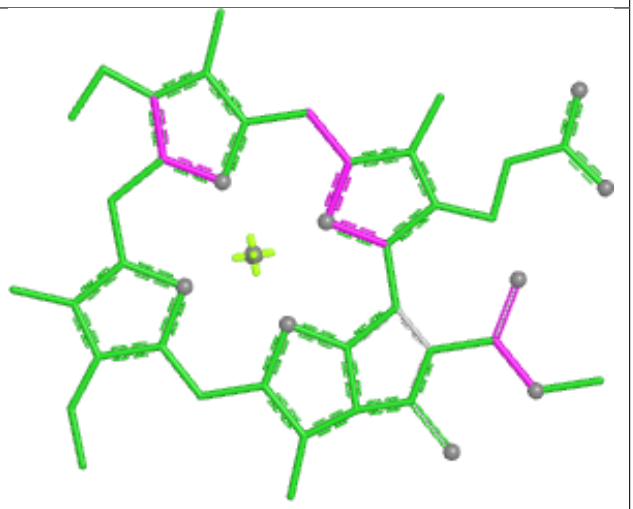
Ligand CLA B 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

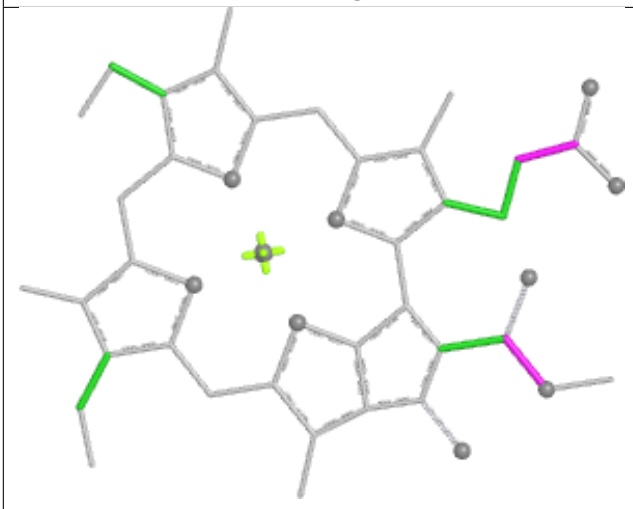
Ligand CLA F 202



Bond lengths



Bond angles

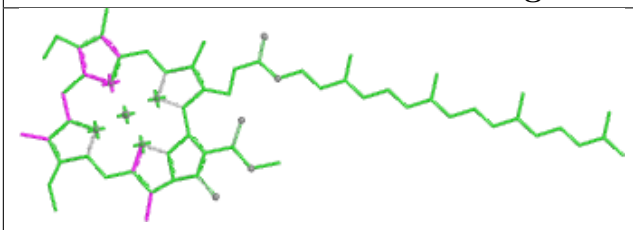


Torsions

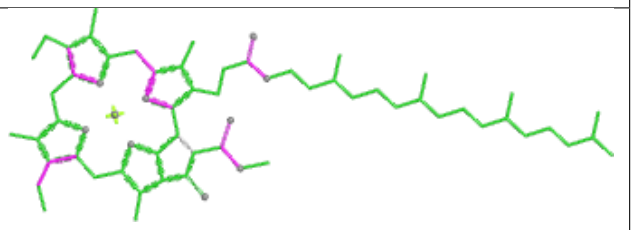


Rings

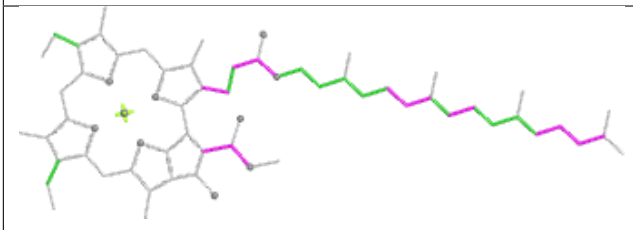
Ligand CLA B 813



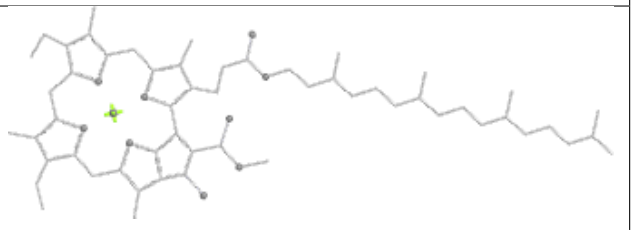
Bond lengths



Bond angles

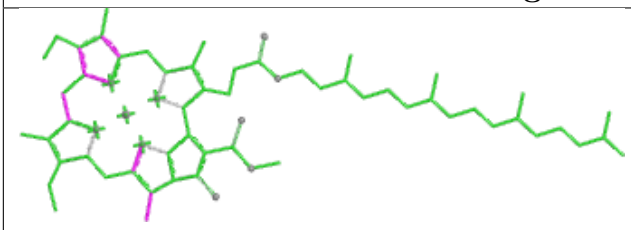


Torsions

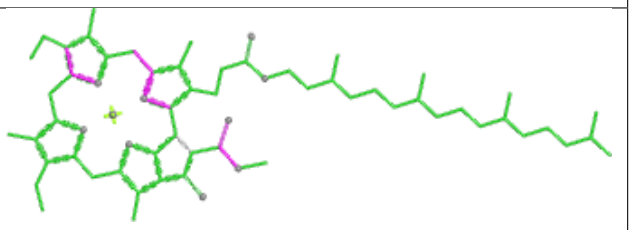


Rings

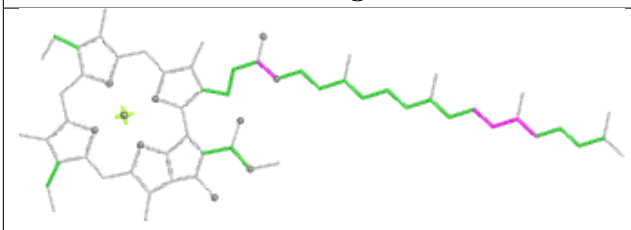
Ligand CLA A 812



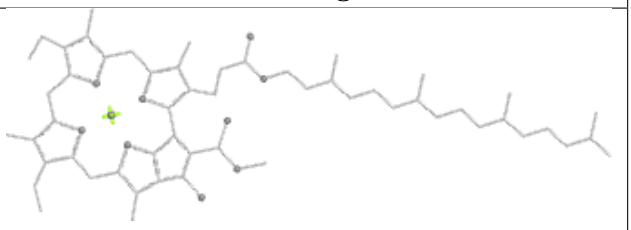
Bond lengths



Bond angles

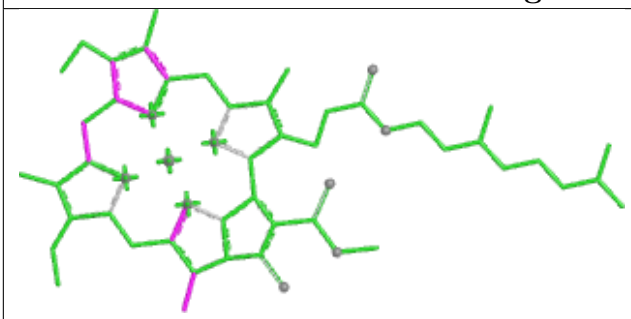


Torsions

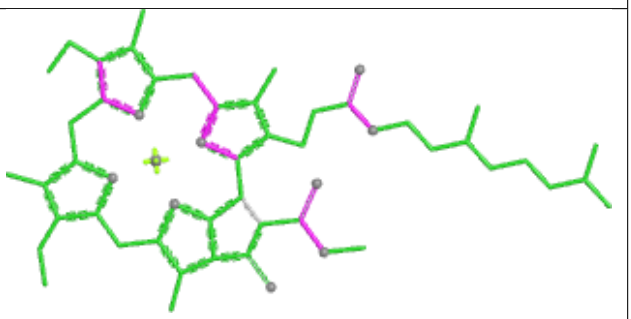


Rings

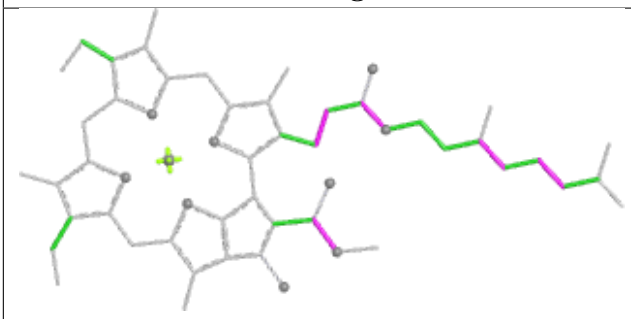
Ligand CLA B 822



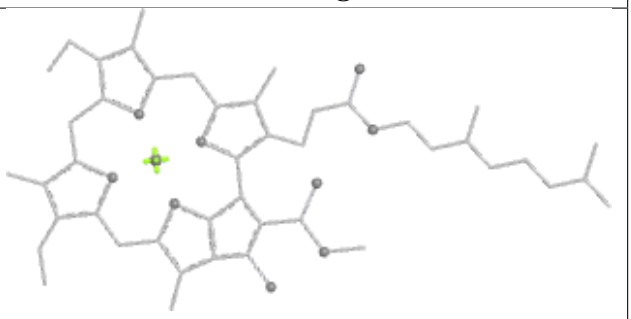
Bond lengths



Bond angles

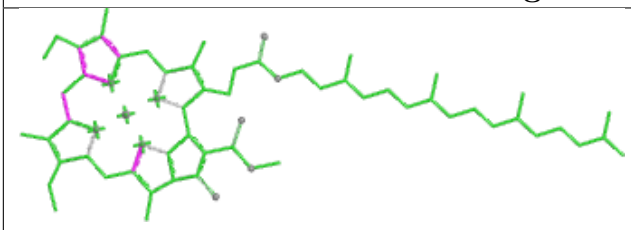


Torsions

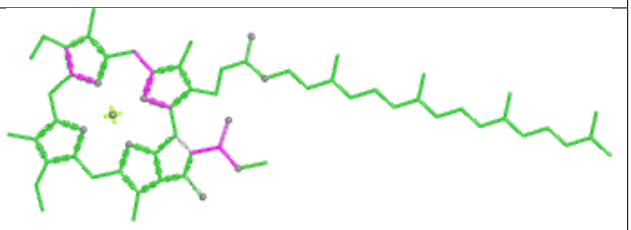


Rings

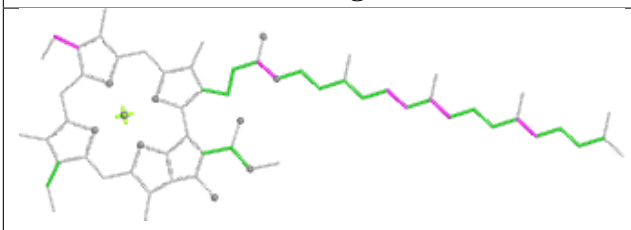
Ligand CLA A 834



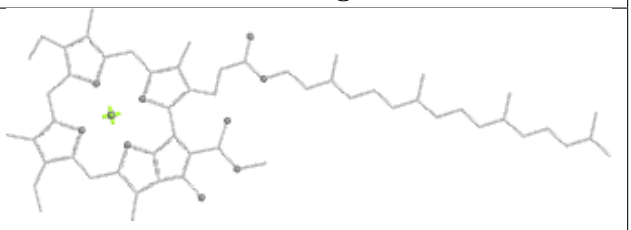
Bond lengths



Bond angles

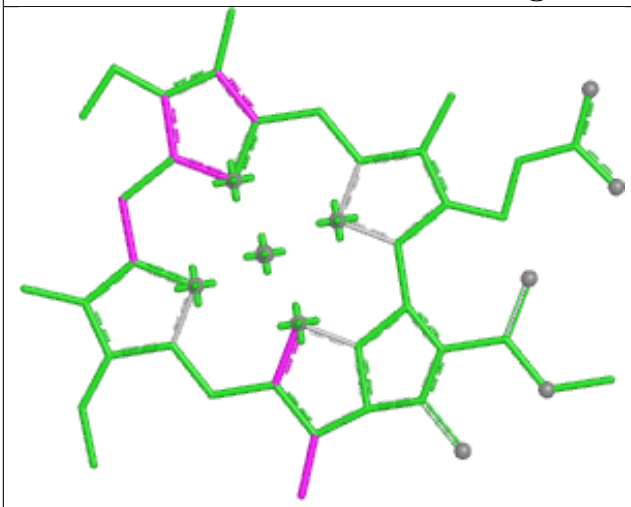


Torsions

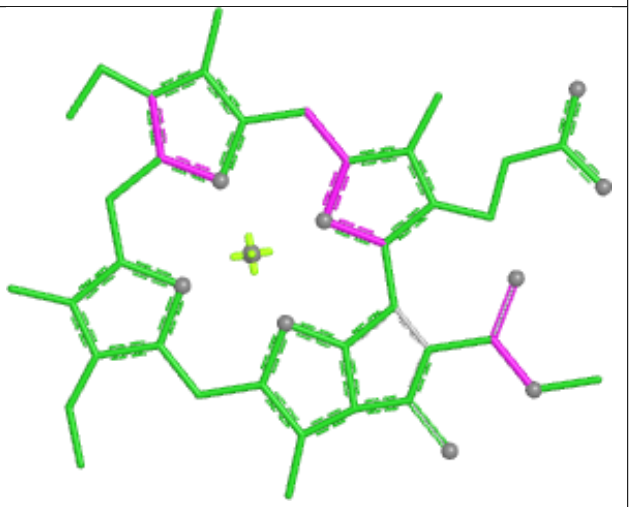


Rings

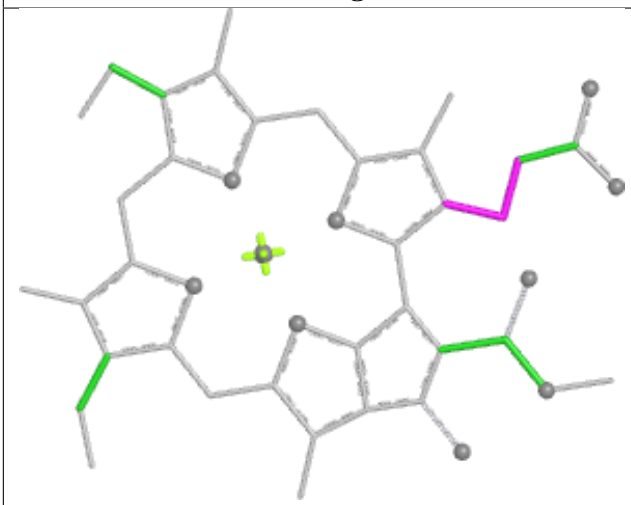
Ligand CLA J 101



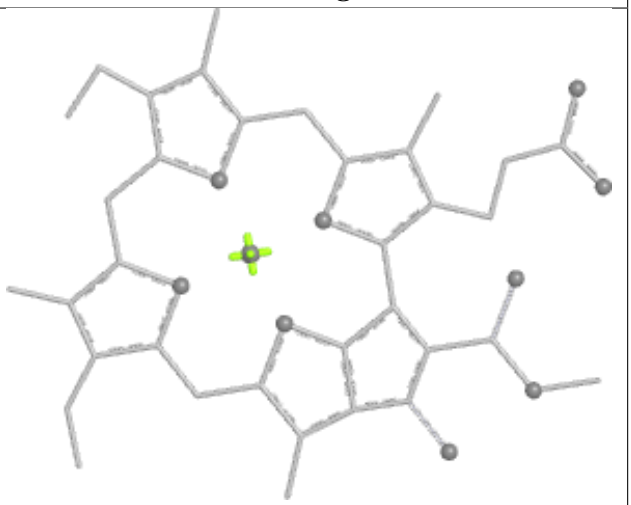
Bond lengths



Bond angles

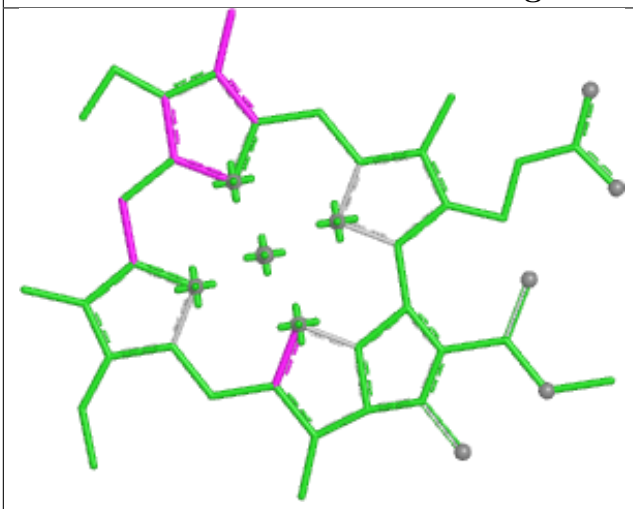


Torsions

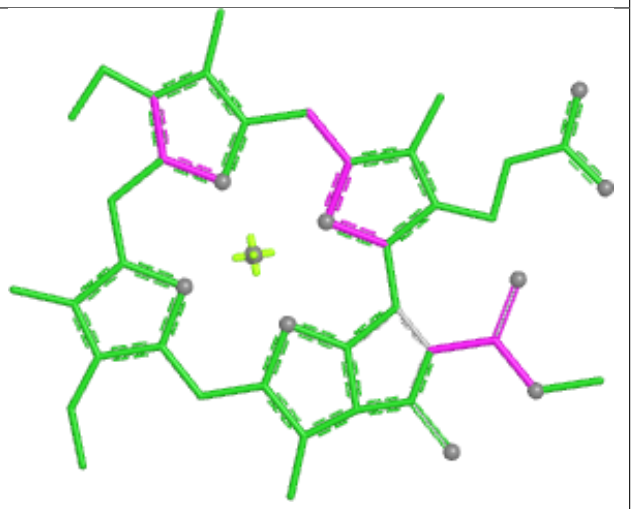


Rings

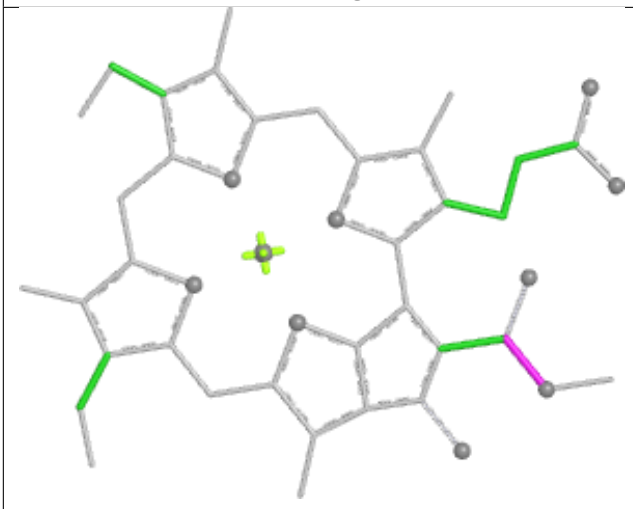
Ligand CLA B 811



Bond lengths



Bond angles

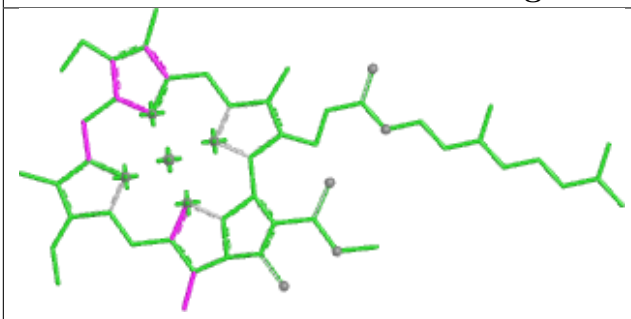


Torsions

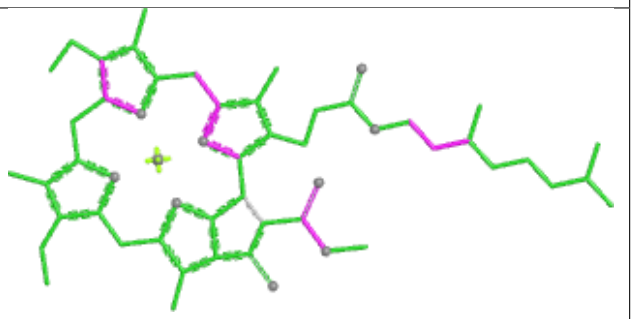


Rings

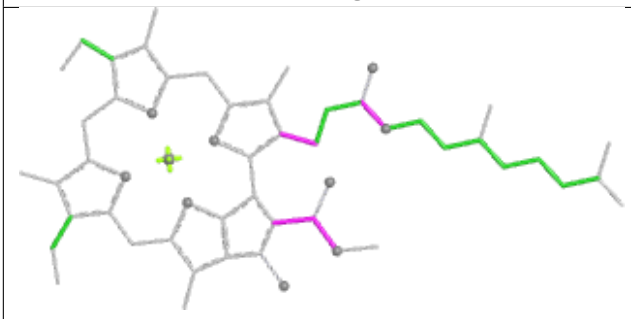
Ligand CLA B 816



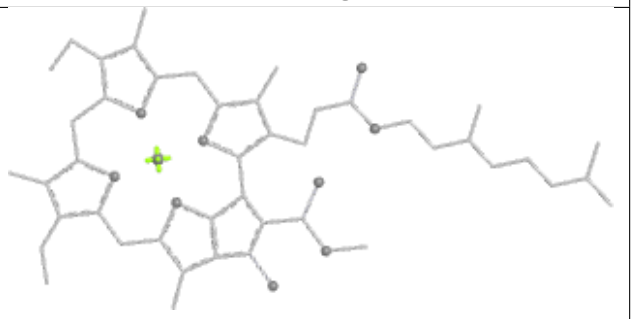
Bond lengths



Bond angles

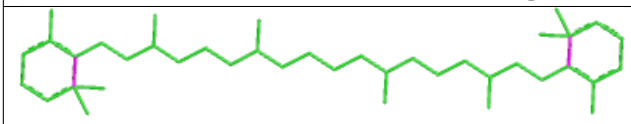


Torsions

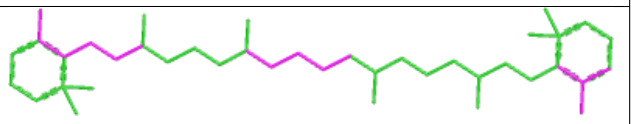


Rings

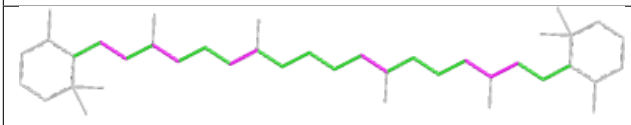
Ligand BCR B 851



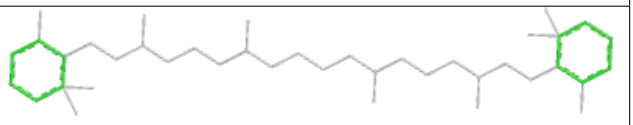
Bond lengths



Bond angles

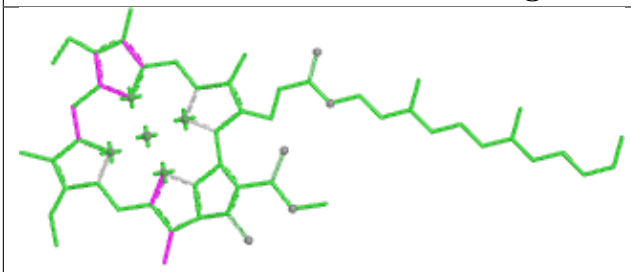


Torsions

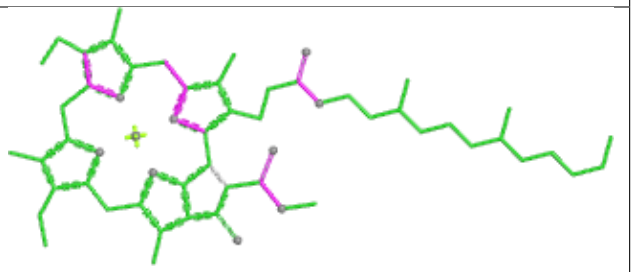


Rings

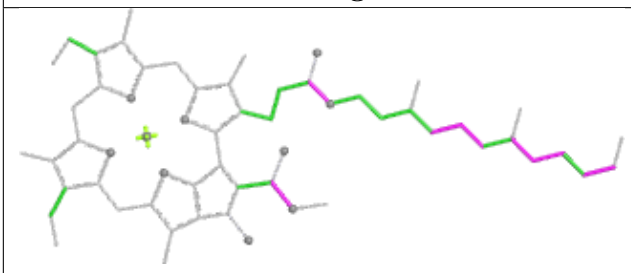
Ligand CLA A 825



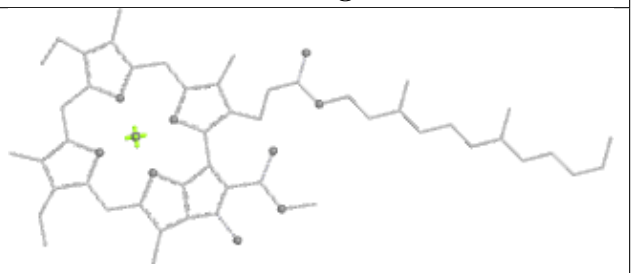
Bond lengths



Bond angles

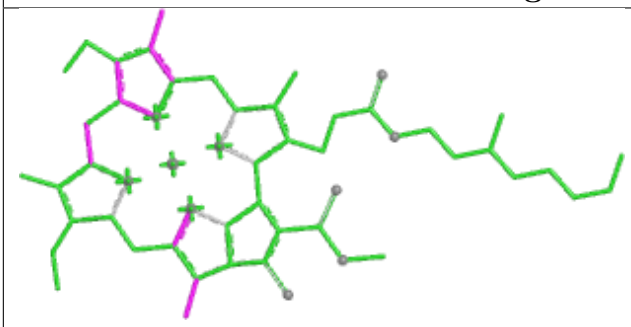


Torsions

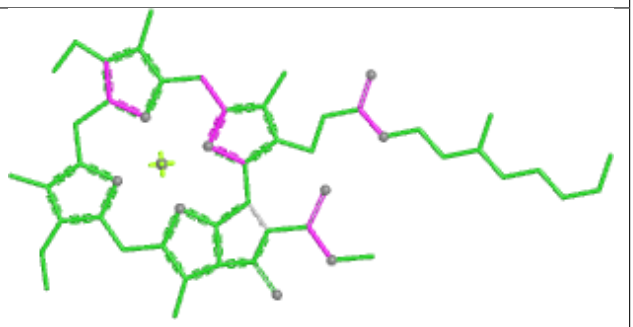


Rings

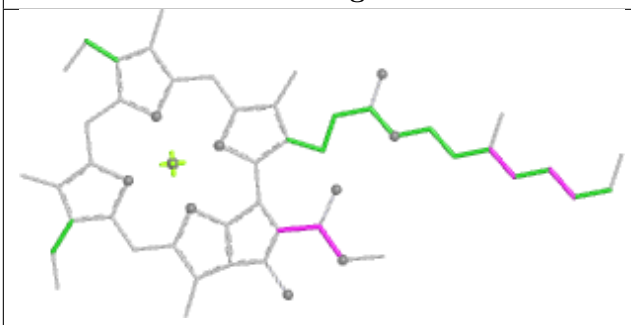
Ligand CLA B 824



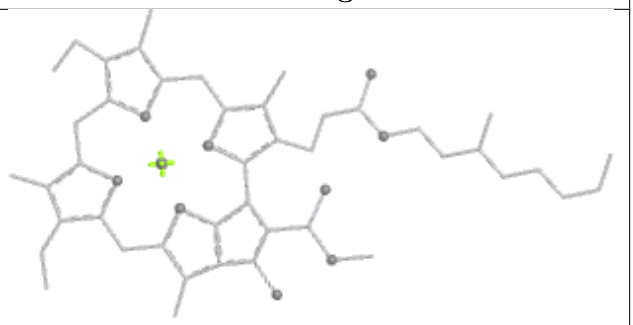
Bond lengths



Bond angles



Torsions

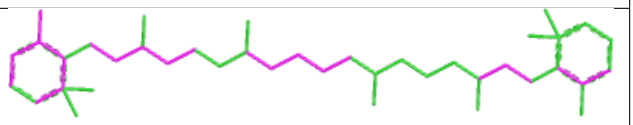


Rings

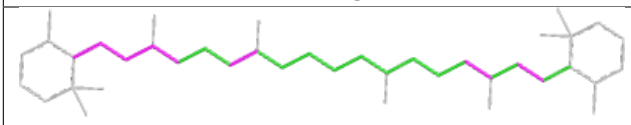
Ligand BCR J 105



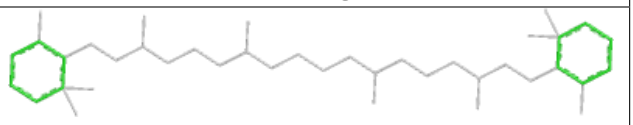
Bond lengths



Bond angles

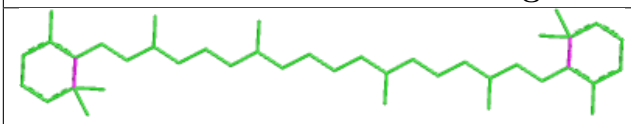


Torsions

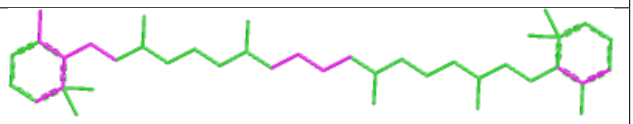


Rings

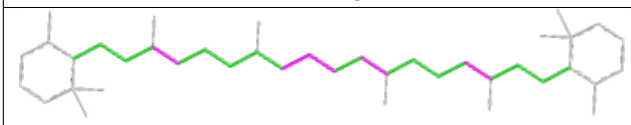
Ligand BCR B 848



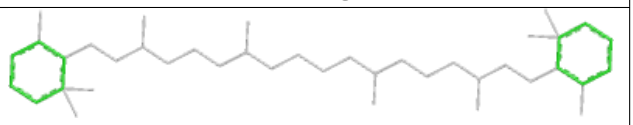
Bond lengths



Bond angles

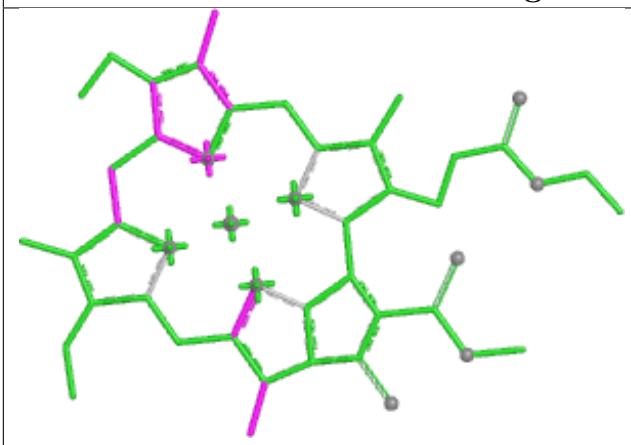


Torsions

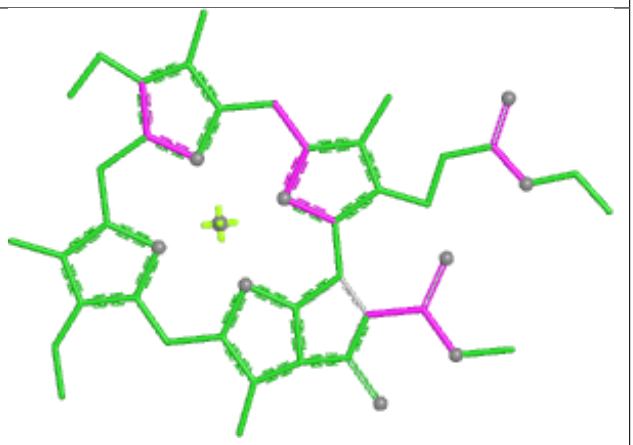


Rings

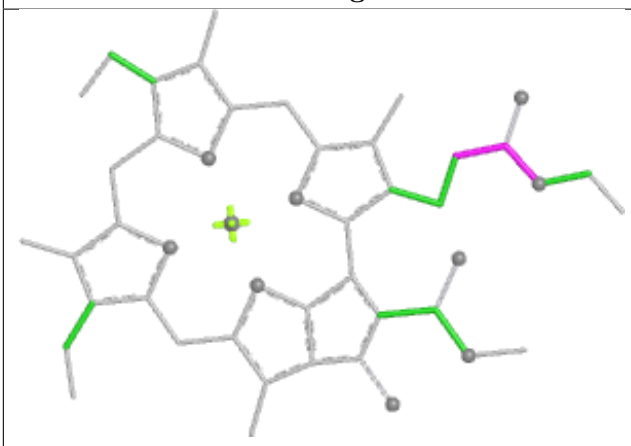
Ligand CLA B 839



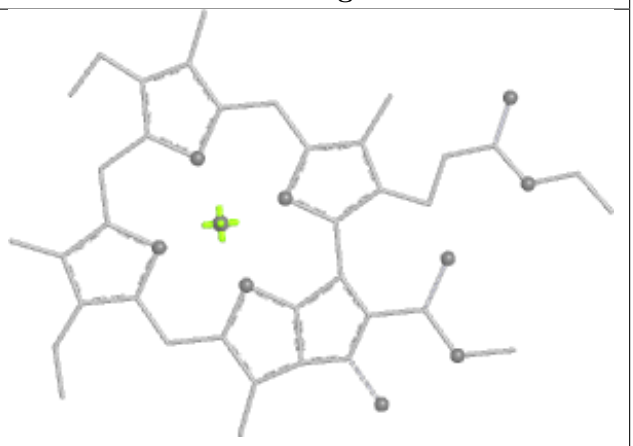
Bond lengths



Bond angles

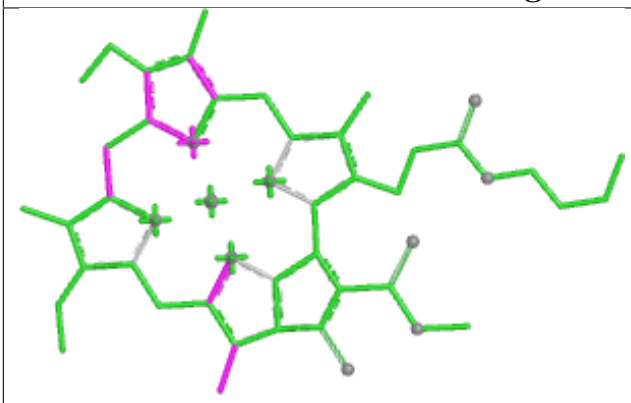


Torsions

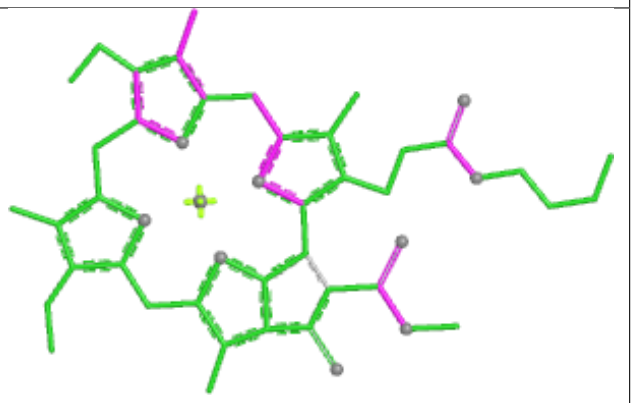


Rings

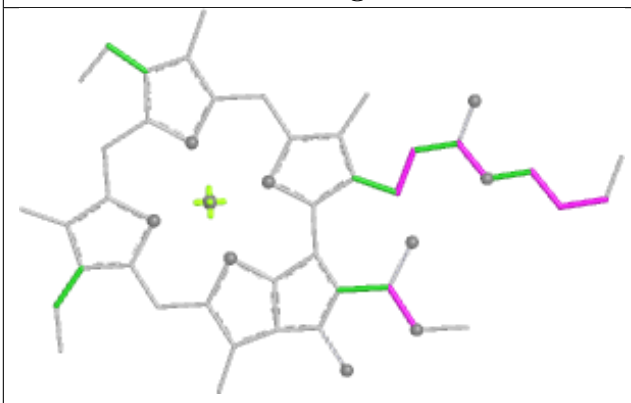
Ligand CLA B 831



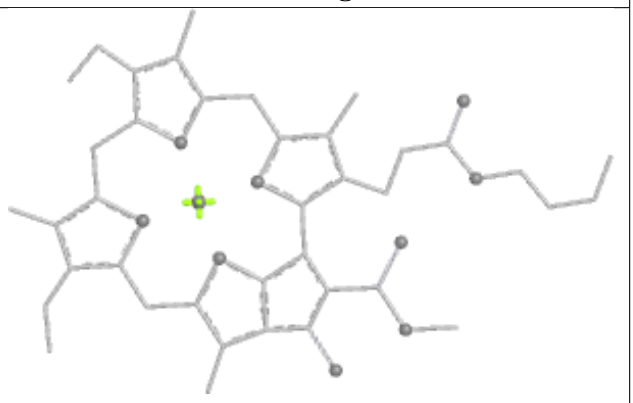
Bond lengths



Bond angles

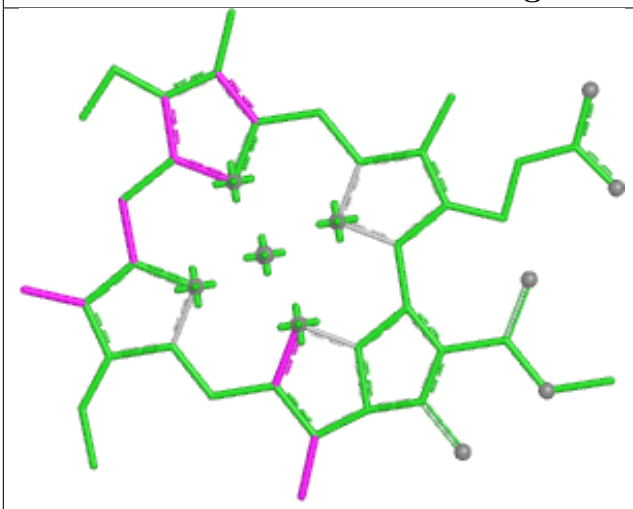


Torsions

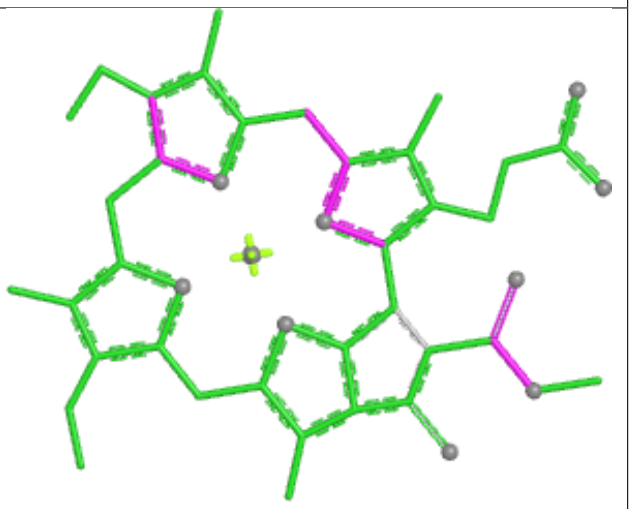


Rings

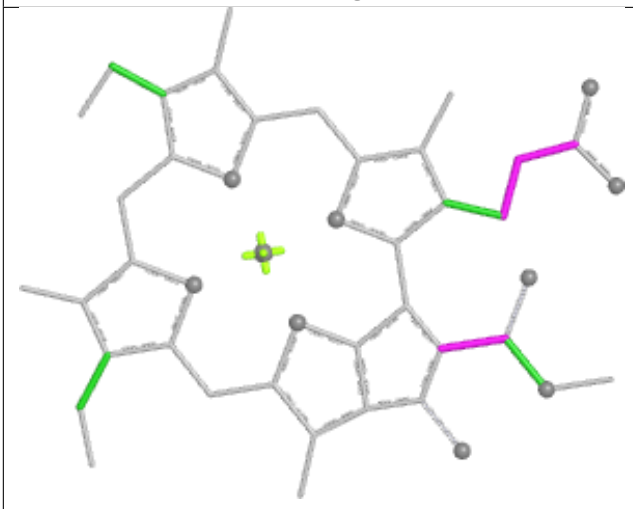
Ligand CLA A 816



Bond lengths



Bond angles

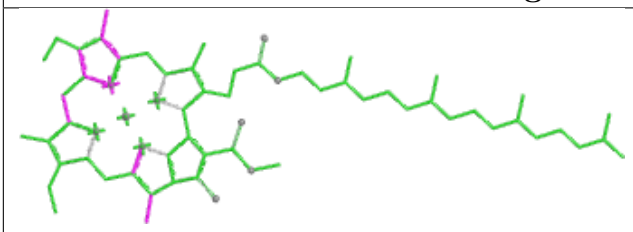


Torsions

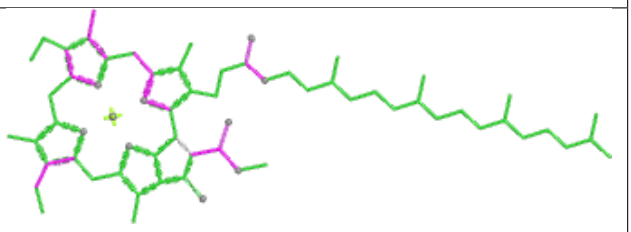


Rings

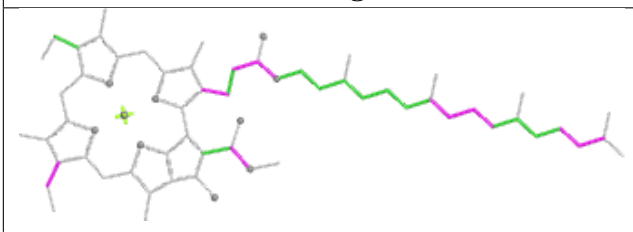
Ligand CLA B 809



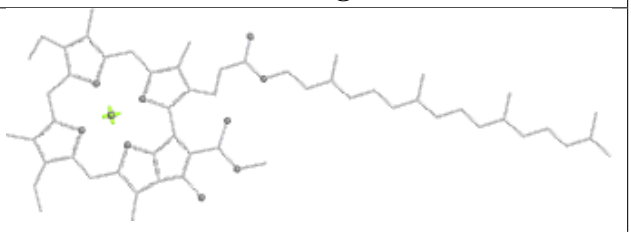
Bond lengths



Bond angles

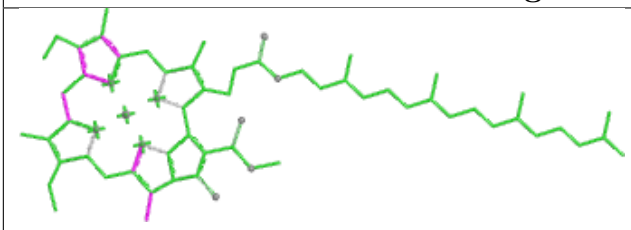


Torsions

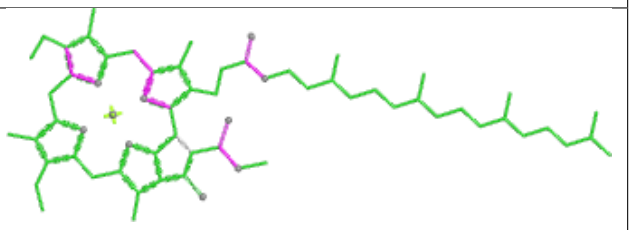


Rings

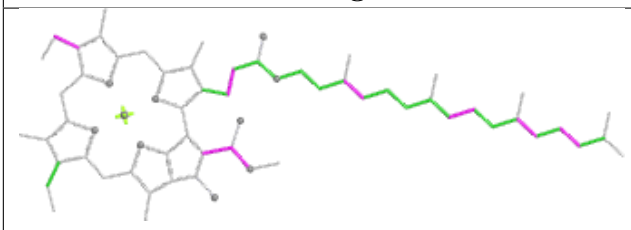
Ligand CLA B 814



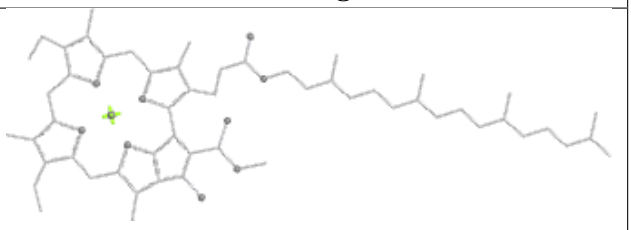
Bond lengths



Bond angles

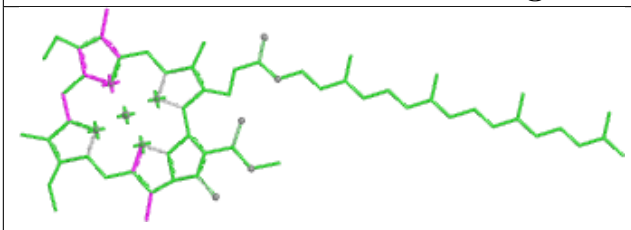


Torsions

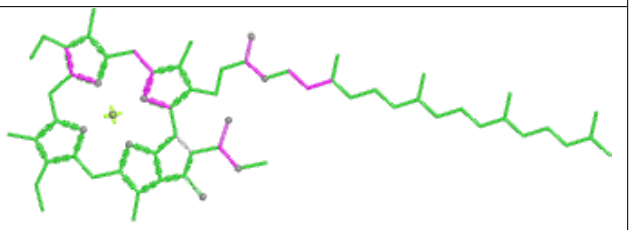


Rings

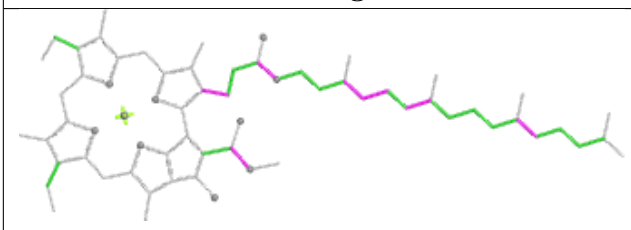
Ligand CLA L 204



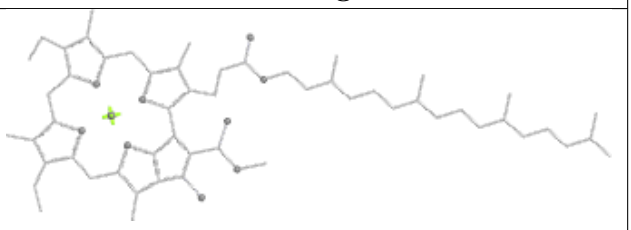
Bond lengths



Bond angles

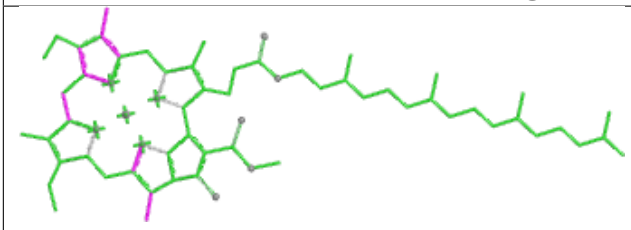


Torsions

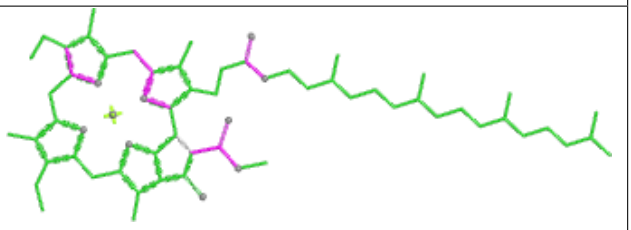


Rings

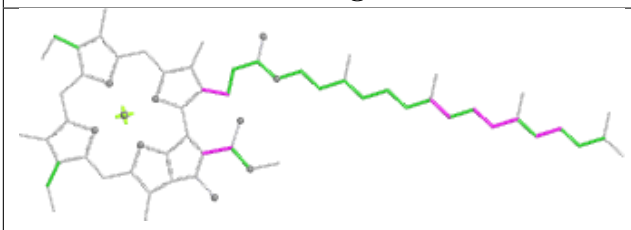
Ligand CLA A 831



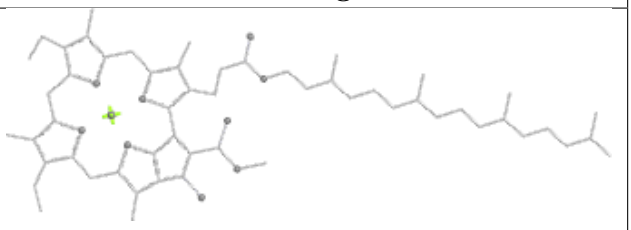
Bond lengths



Bond angles

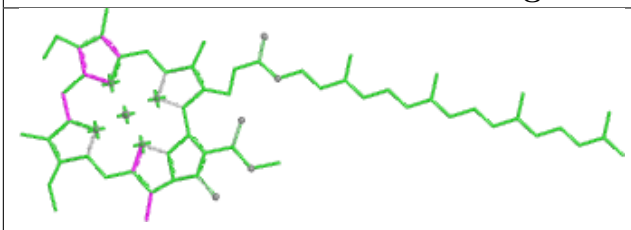


Torsions

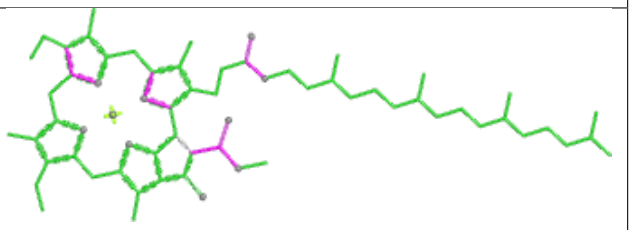


Rings

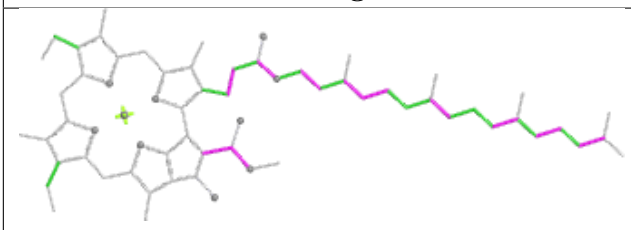
Ligand CLA A 857



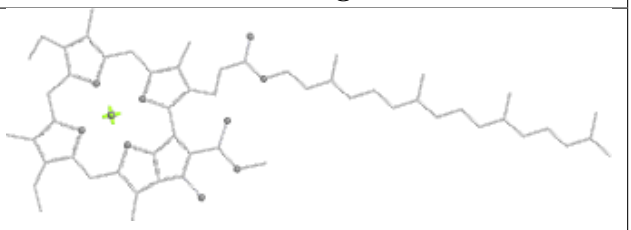
Bond lengths



Bond angles

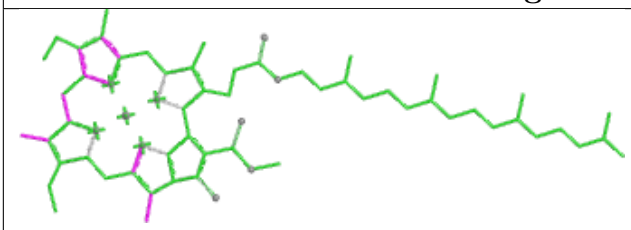


Torsions

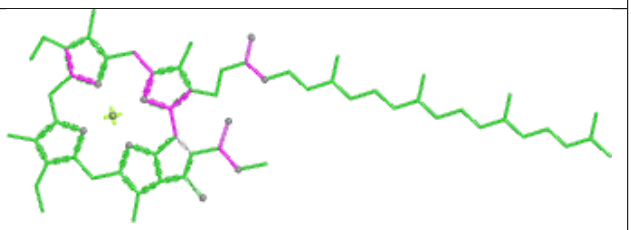


Rings

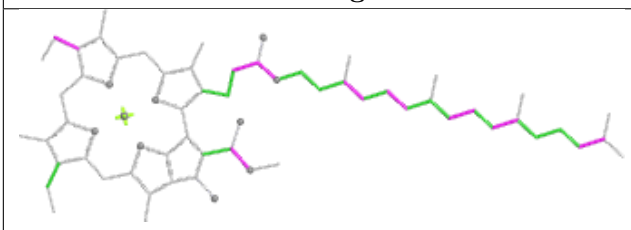
Ligand CLA B 810



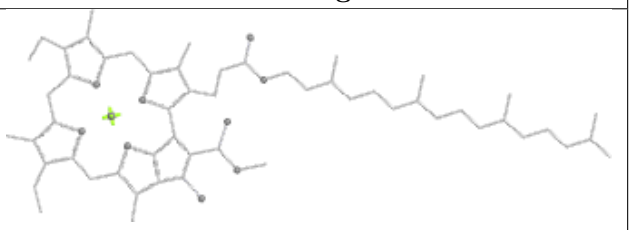
Bond lengths



Bond angles

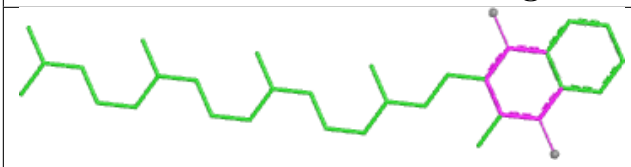


Torsions

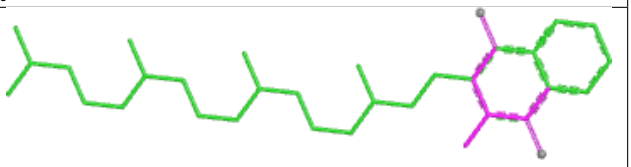


Rings

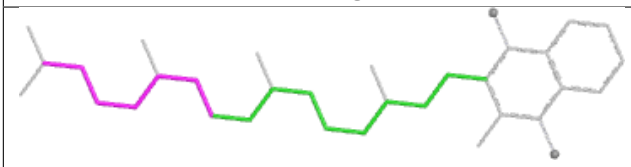
Ligand PQN B 842



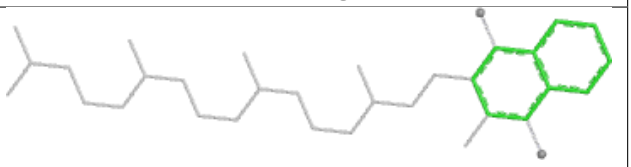
Bond lengths



Bond angles

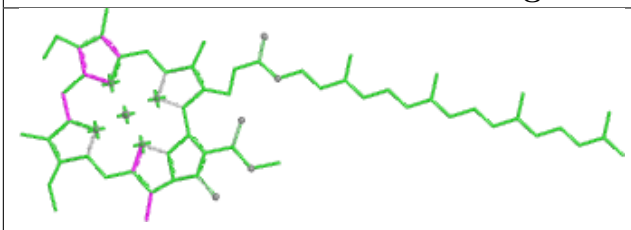


Torsions

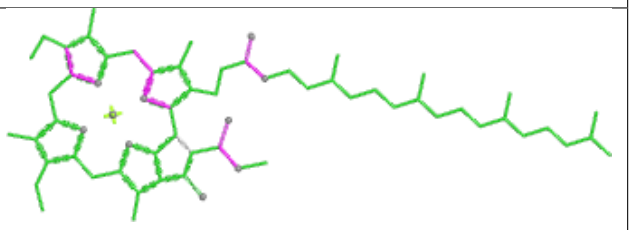


Rings

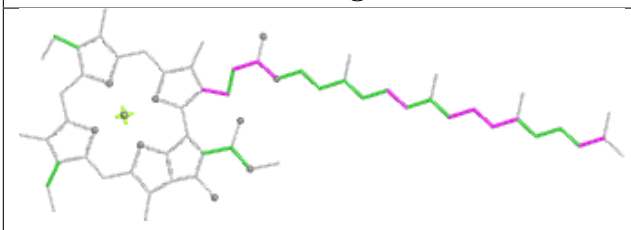
Ligand CLA A 828



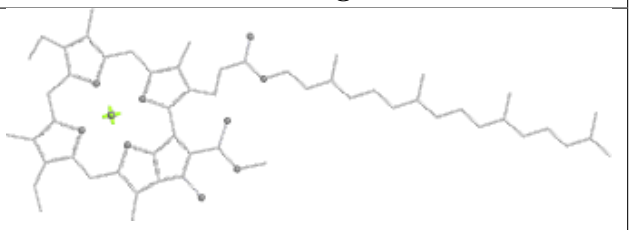
Bond lengths



Bond angles

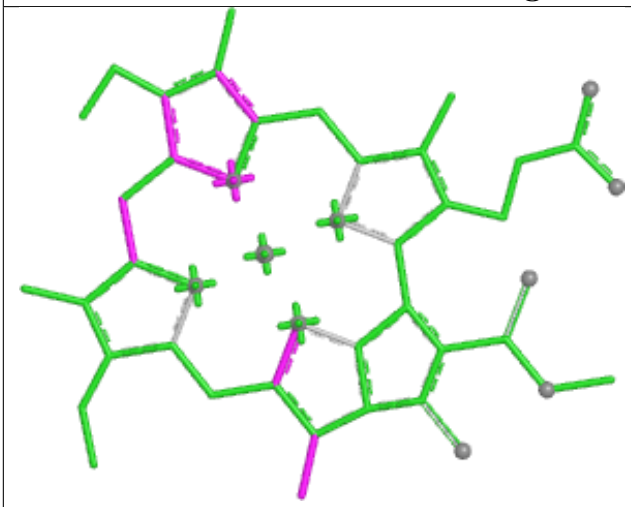


Torsions

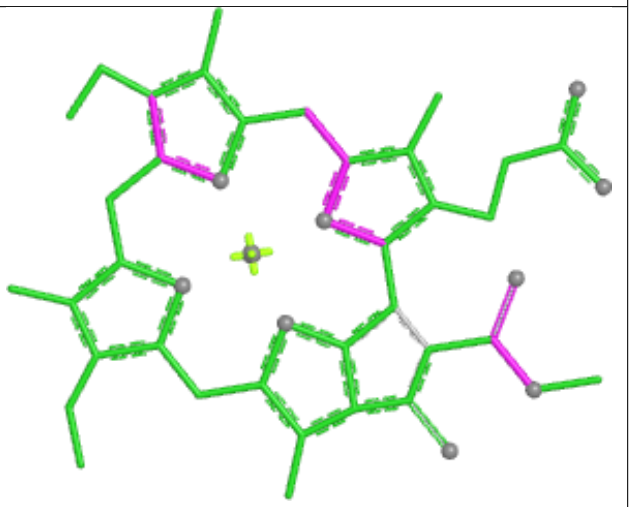


Rings

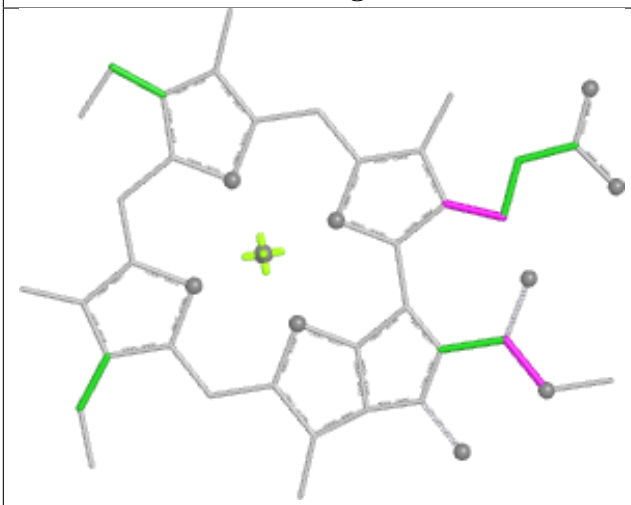
Ligand CLA A 815



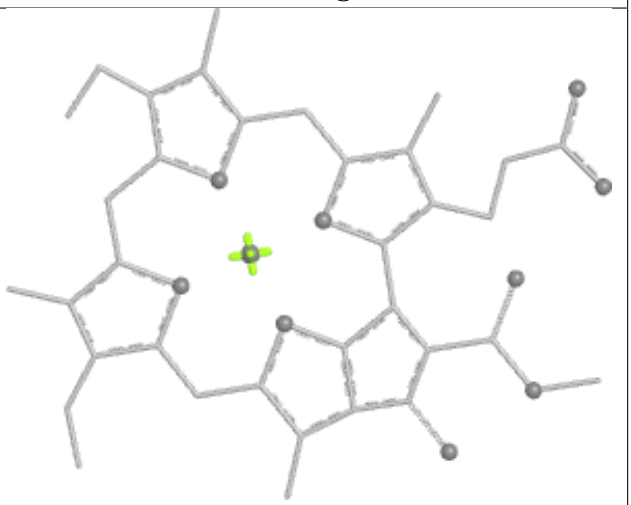
Bond lengths



Bond angles

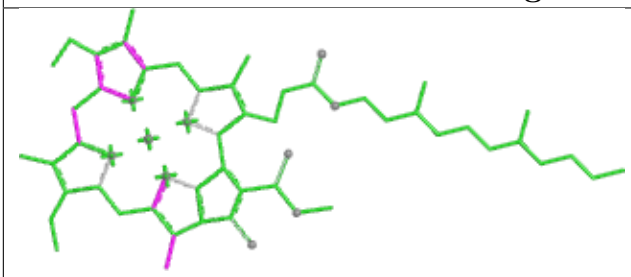


Torsions

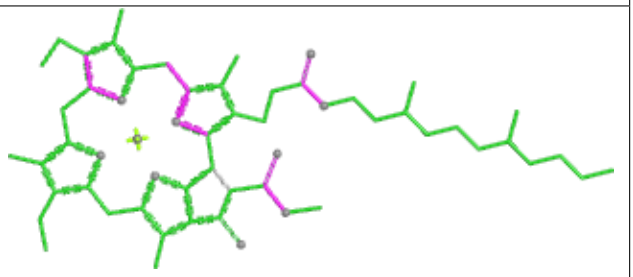


Rings

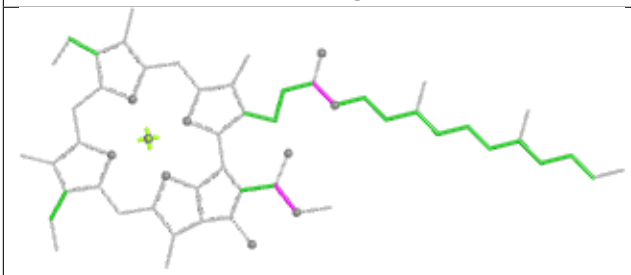
Ligand CLA B 833



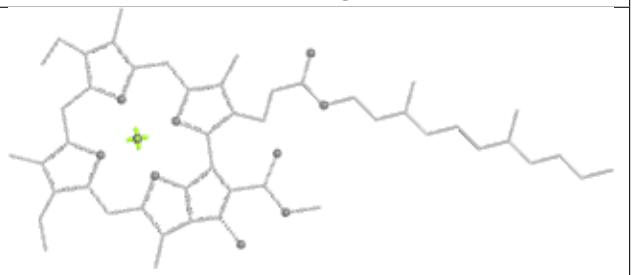
Bond lengths



Bond angles



Torsions

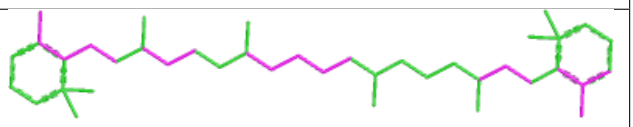


Rings

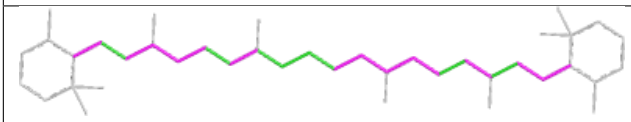
Ligand BCR A 848



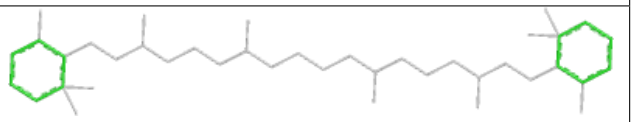
Bond lengths



Bond angles

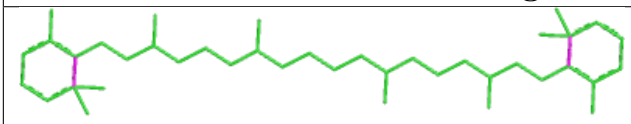


Torsions

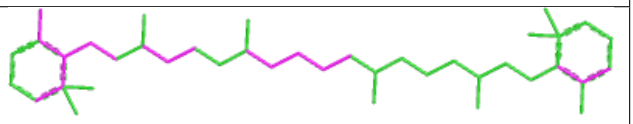


Rings

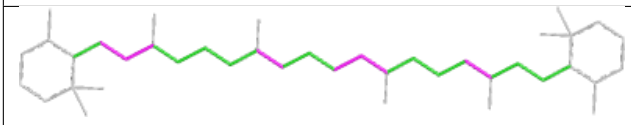
Ligand BCR A 851



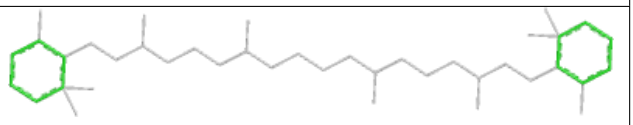
Bond lengths



Bond angles

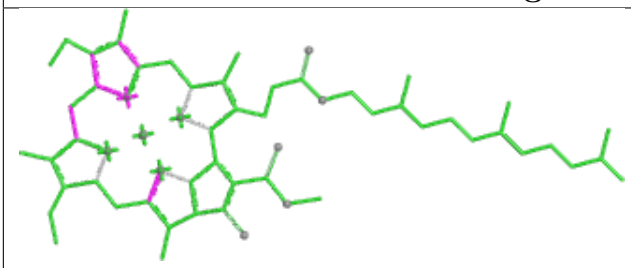


Torsions

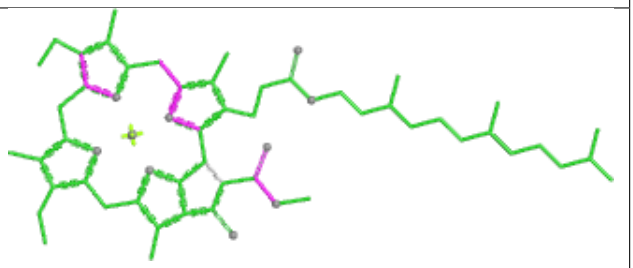


Rings

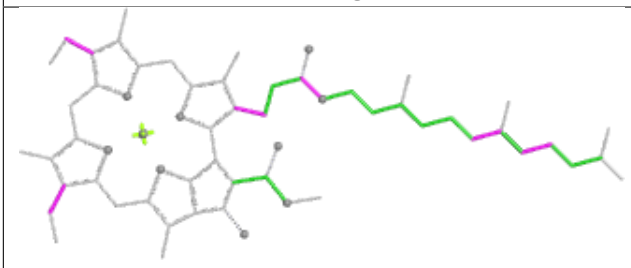
Ligand CLA B 818



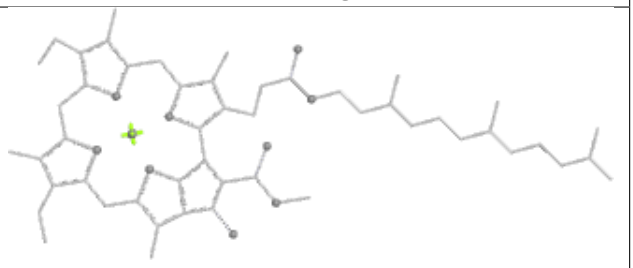
Bond lengths



Bond angles

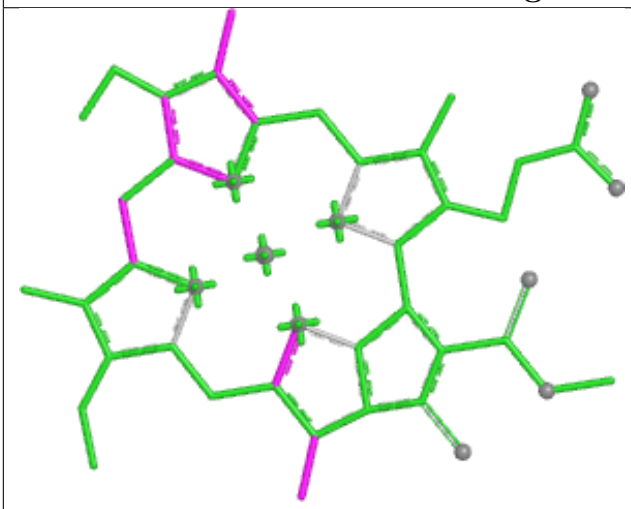


Torsions

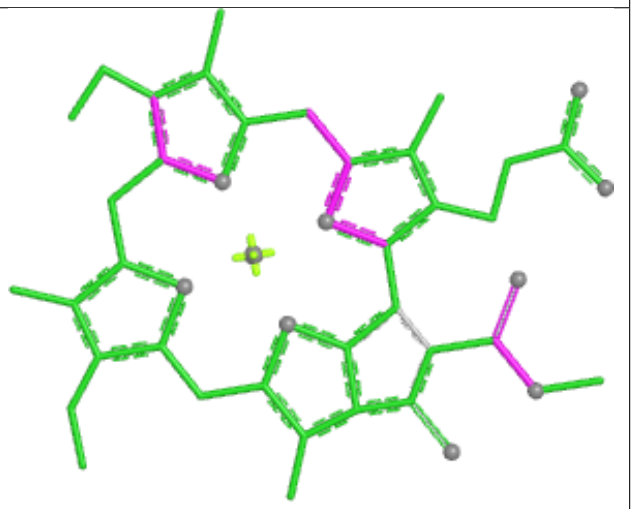


Rings

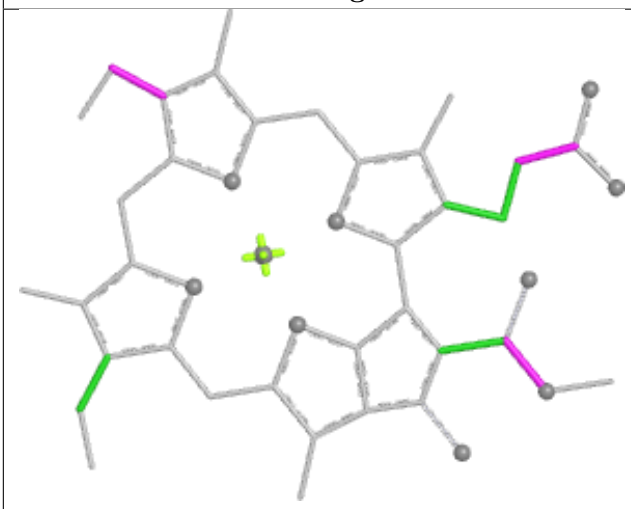
Ligand CLA B 823



Bond lengths



Bond angles

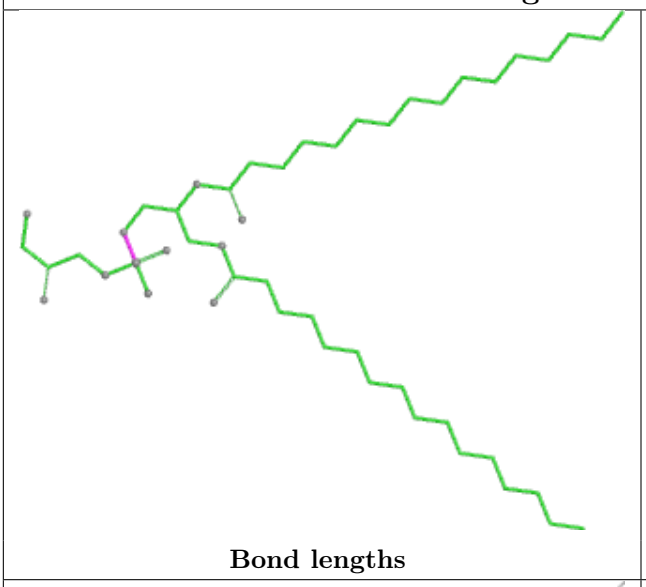


Torsions

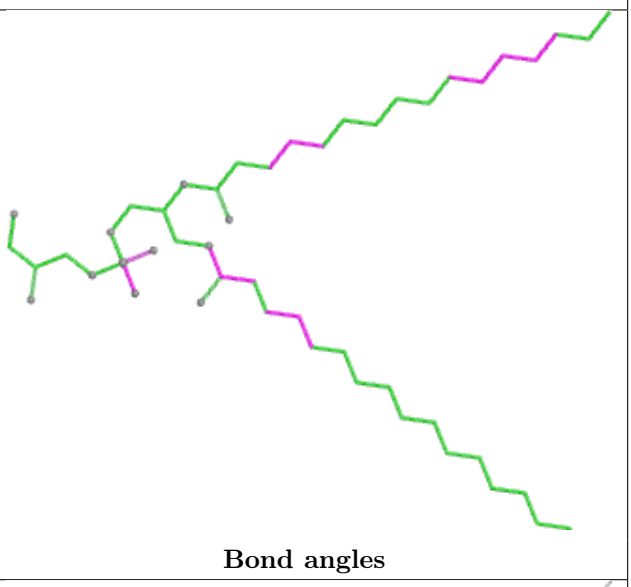


Rings

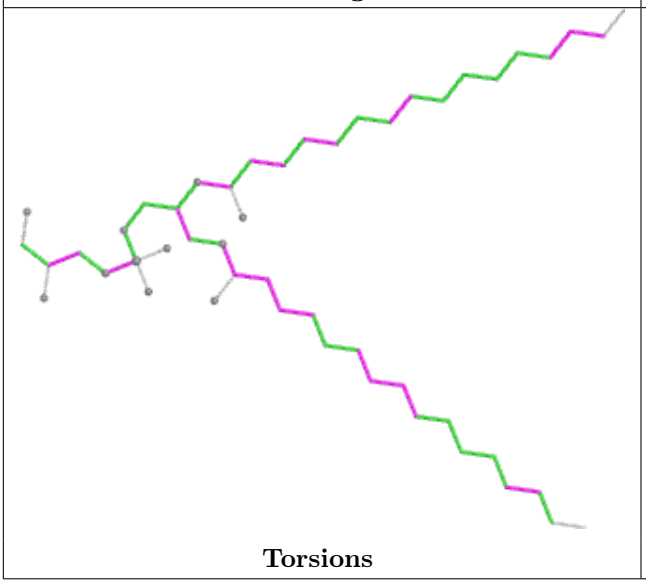
Ligand LHG A 854



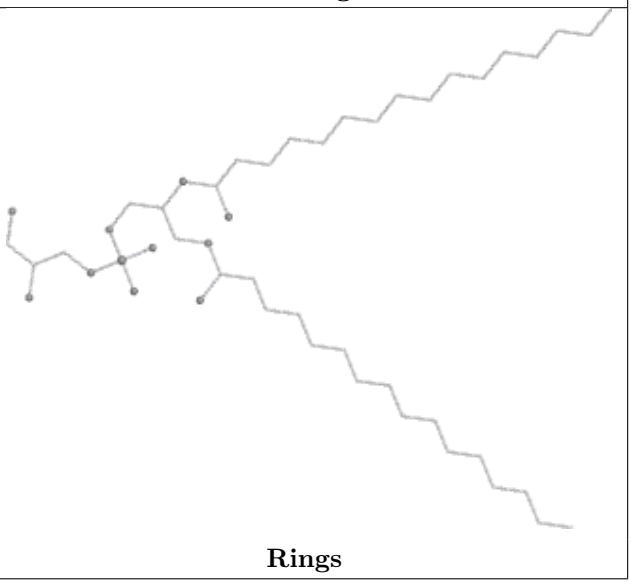
Bond lengths



Bond angles

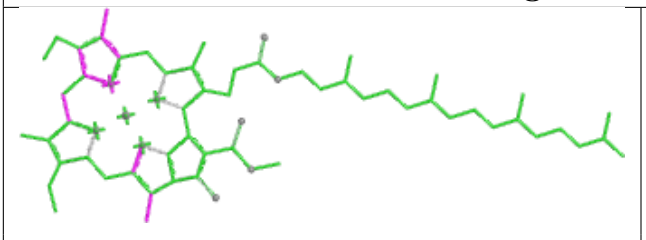


Torsions

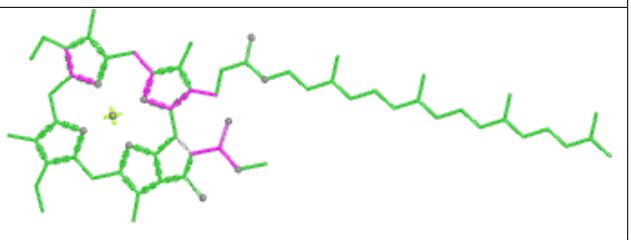


Rings

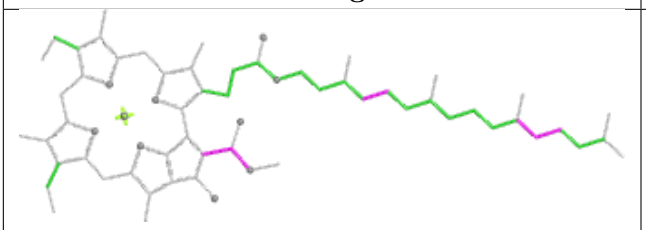
Ligand CLA A 803



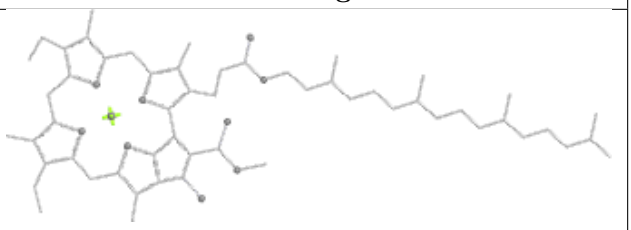
Bond lengths



Bond angles

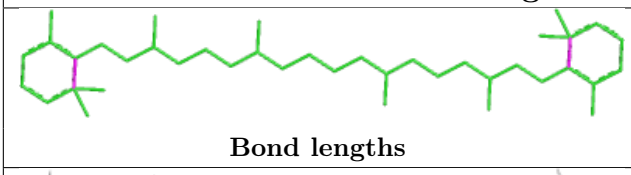


Torsions

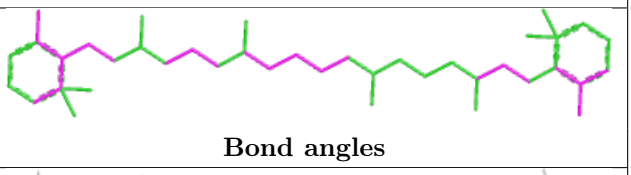


Rings

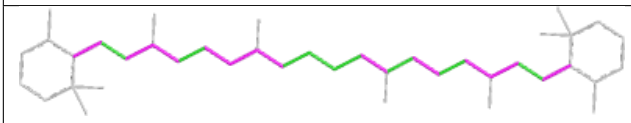
Ligand BCR A 852



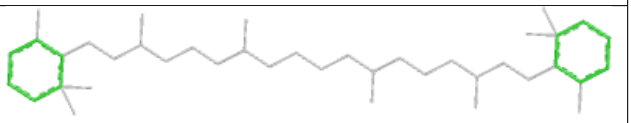
Bond lengths



Bond angles

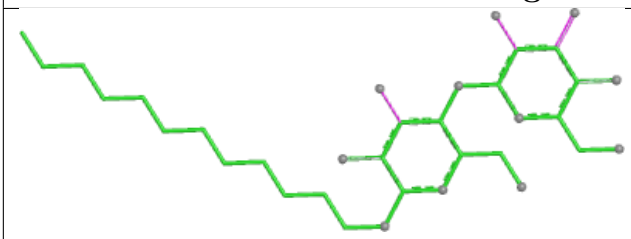


Torsions

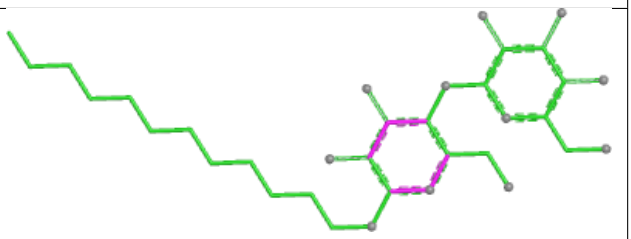


Rings

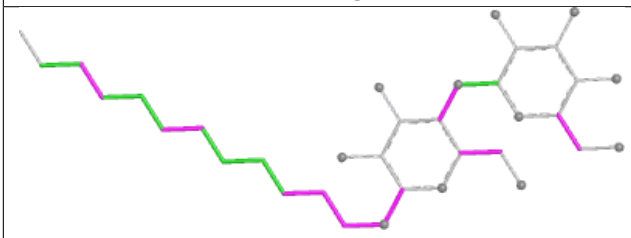
Ligand LMT L 202



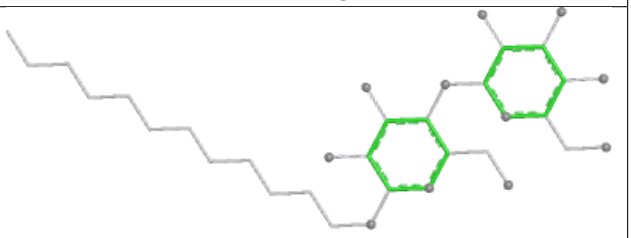
Bond lengths



Bond angles

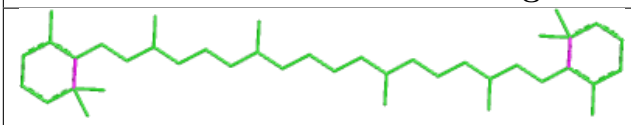


Torsions

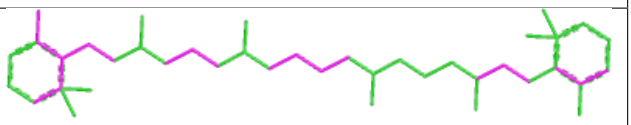


Rings

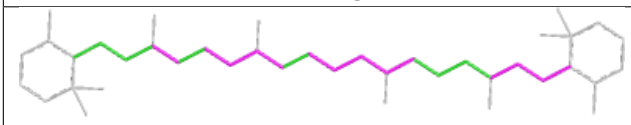
Ligand BCR B 847



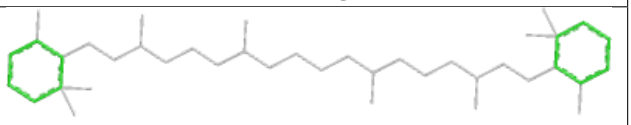
Bond lengths



Bond angles

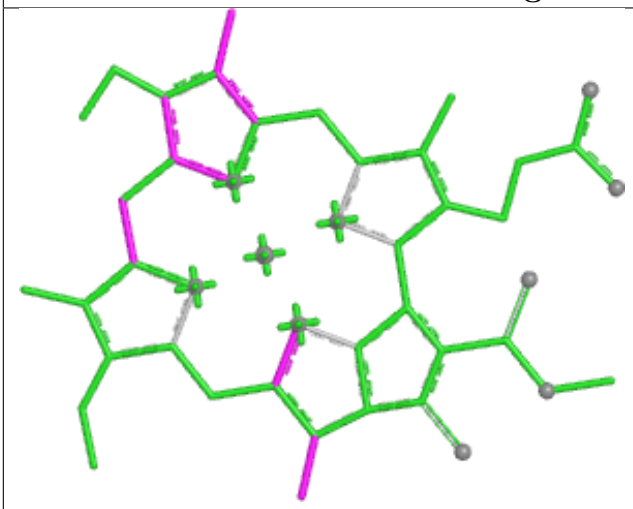


Torsions

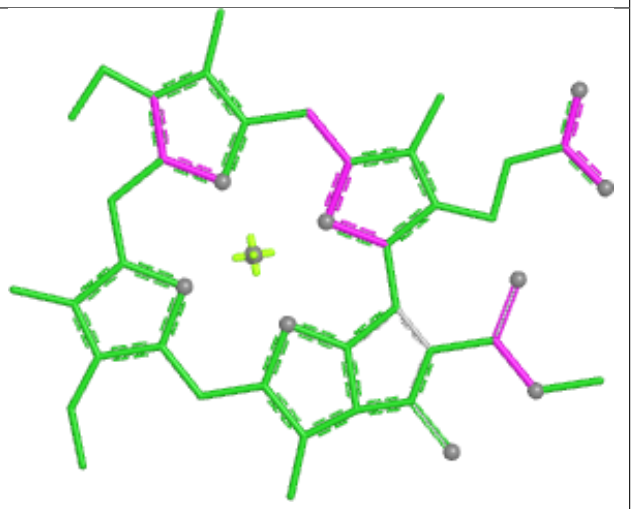


Rings

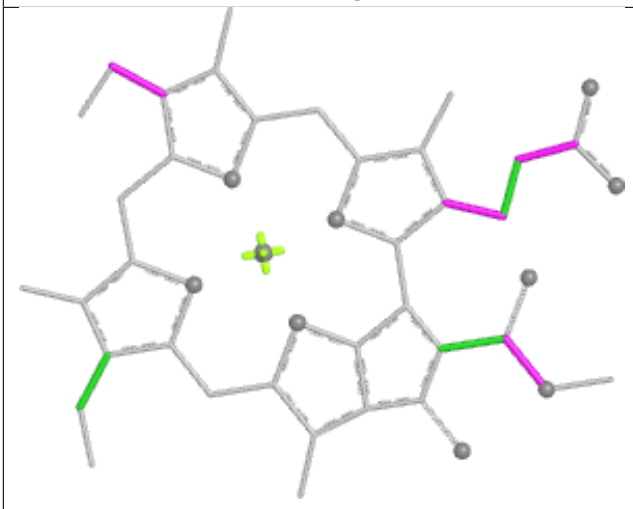
Ligand CLA B 835



Bond lengths



Bond angles

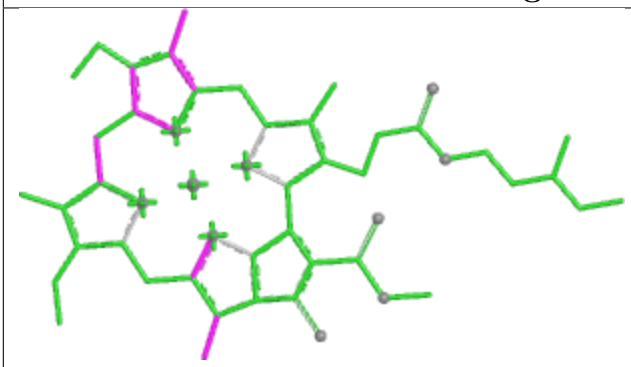


Torsions

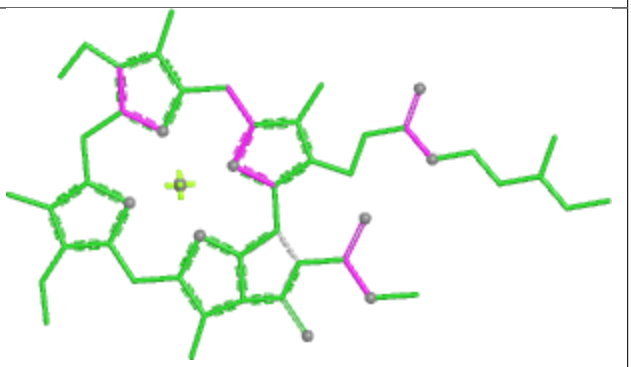


Rings

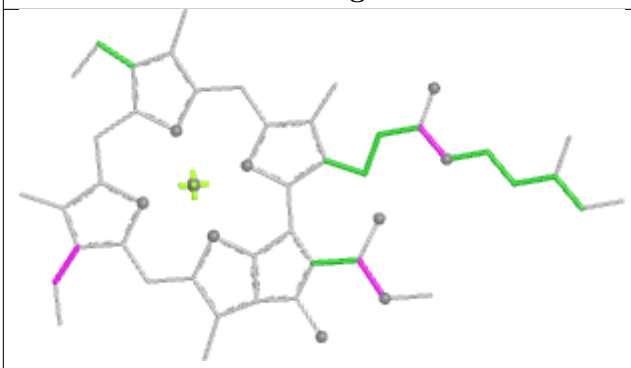
Ligand CLA A 838



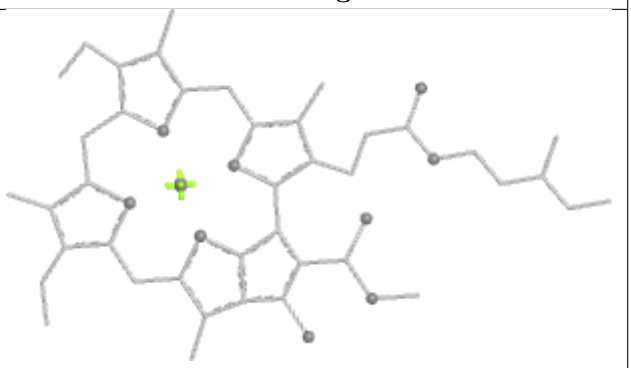
Bond lengths



Bond angles

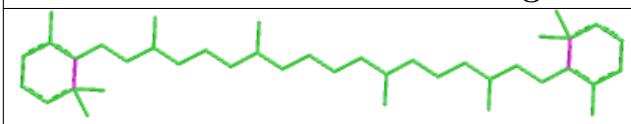


Torsions

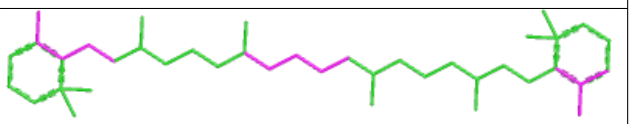


Rings

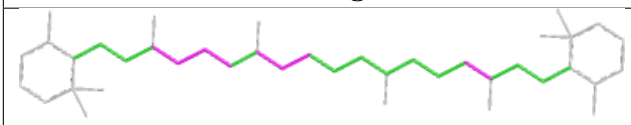
Ligand BCR B 845



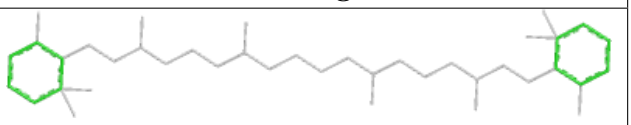
Bond lengths



Bond angles

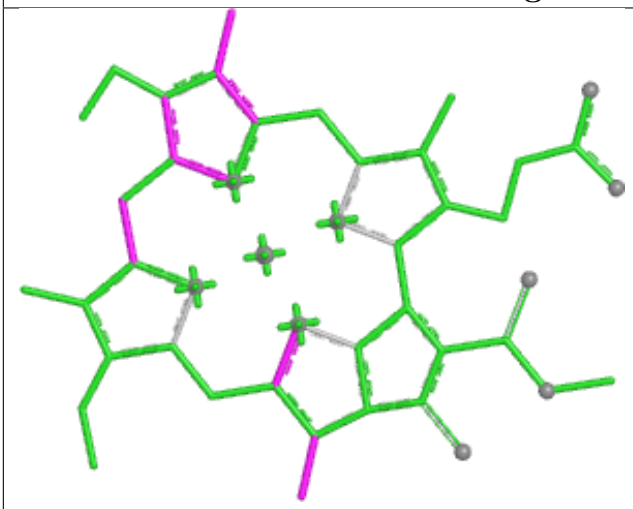


Torsions

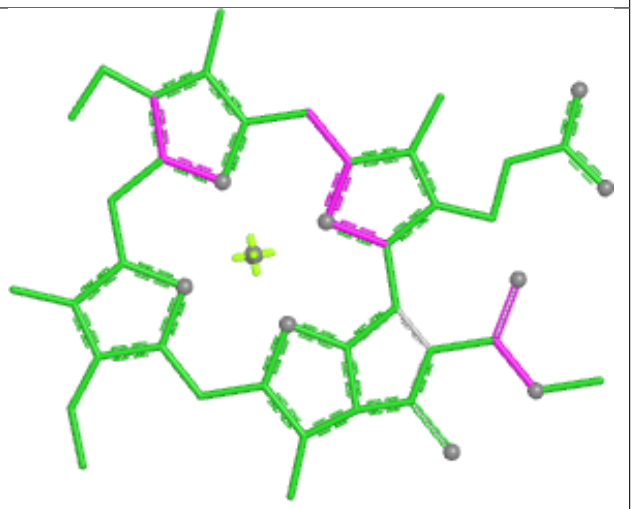


Rings

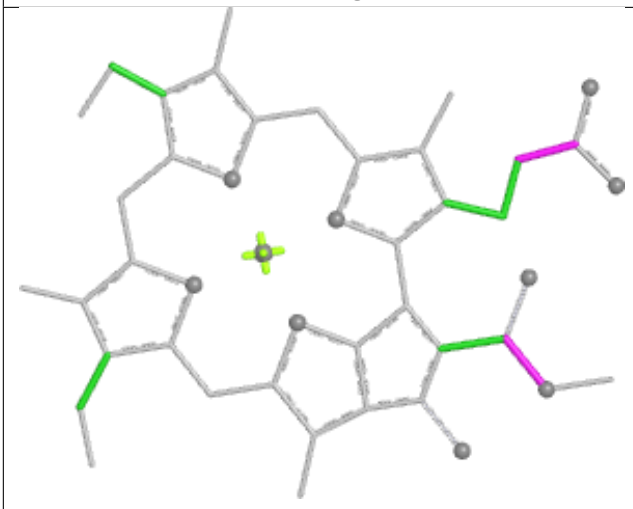
Ligand CLA B 836



Bond lengths



Bond angles

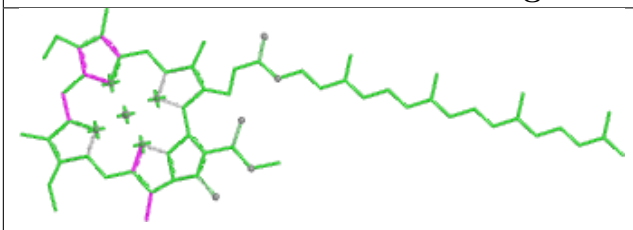


Torsions

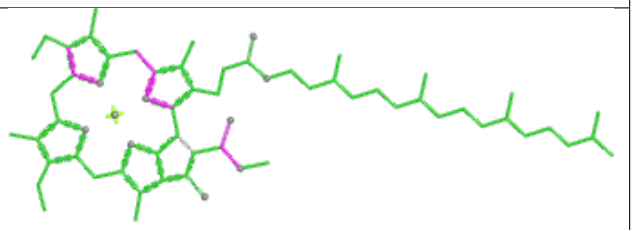


Rings

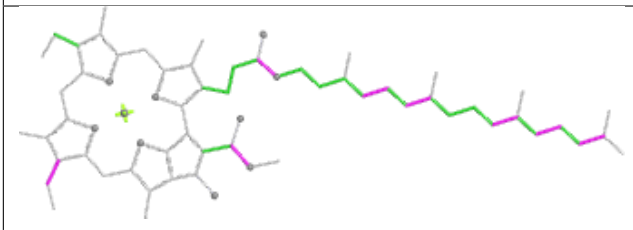
Ligand CLA A 829



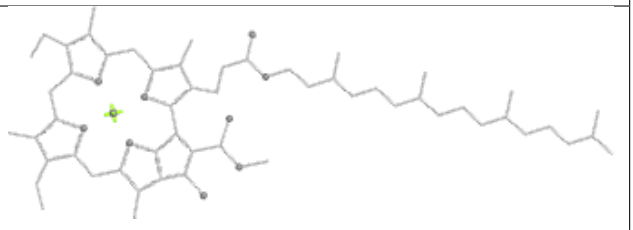
Bond lengths



Bond angles

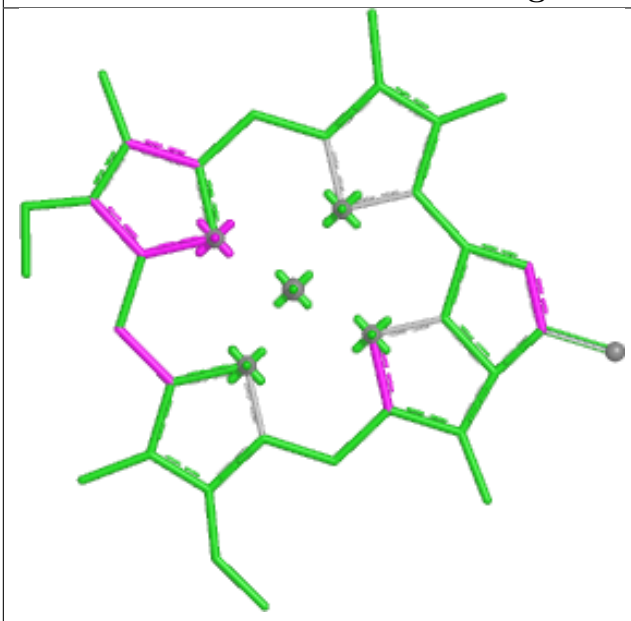


Torsions

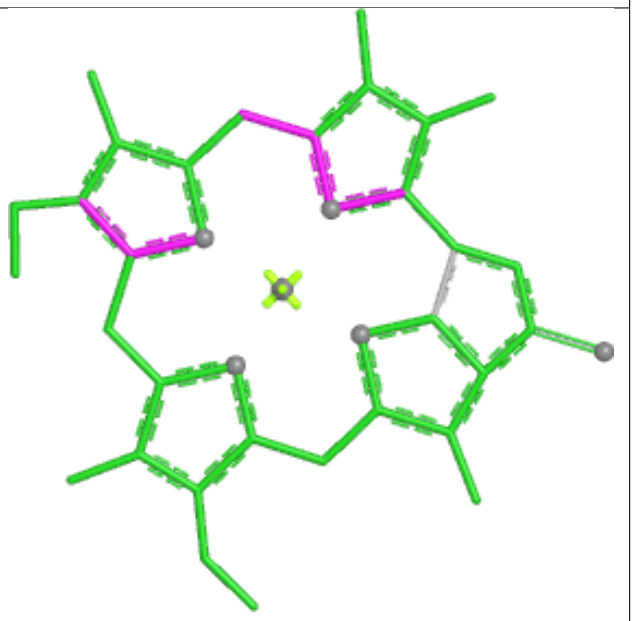


Rings

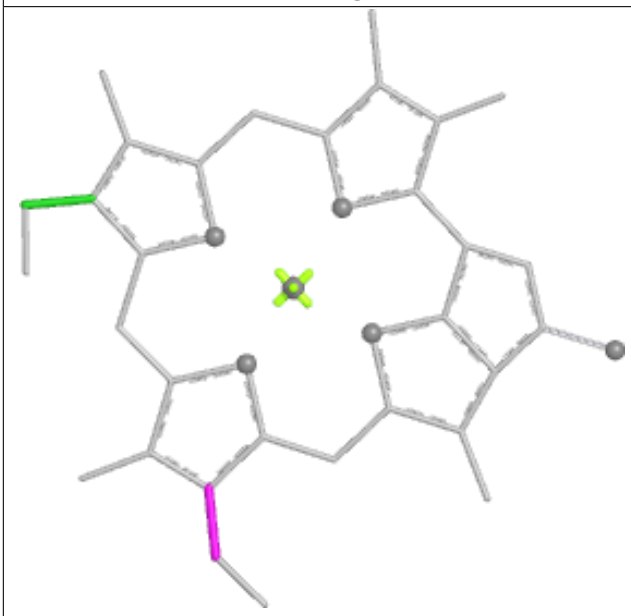
Ligand CLA J 102



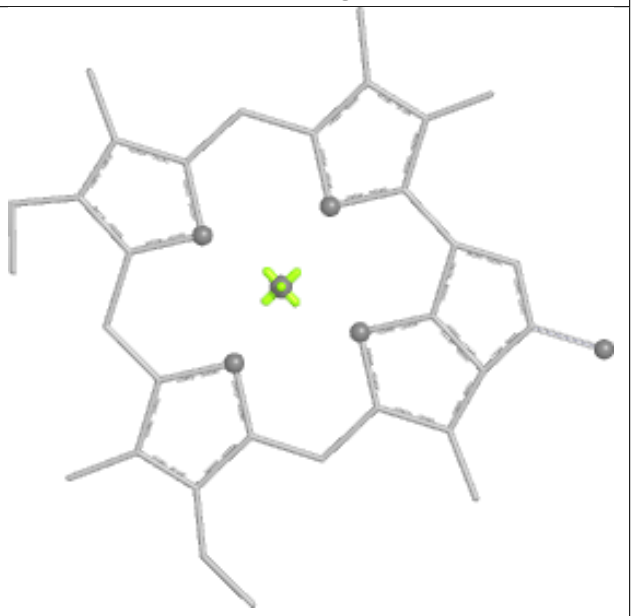
Bond lengths



Bond angles

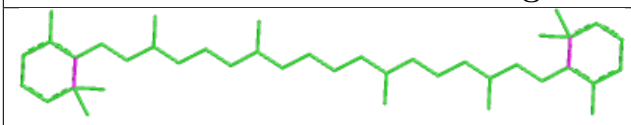


Torsions

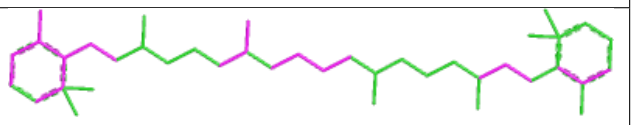


Rings

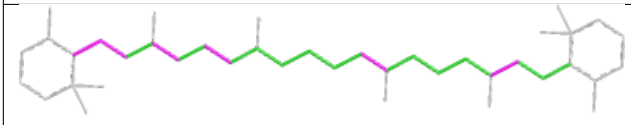
Ligand BCR B 844



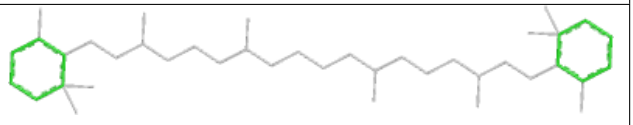
Bond lengths



Bond angles

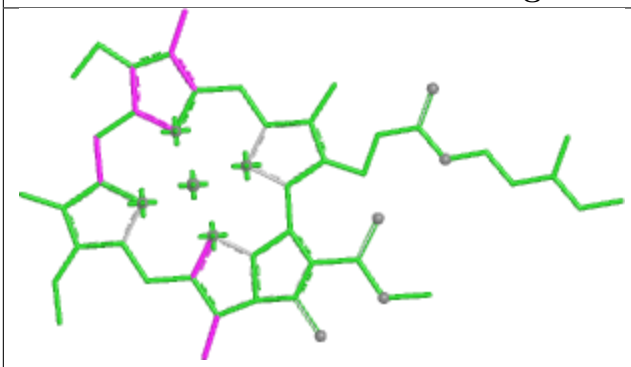


Torsions

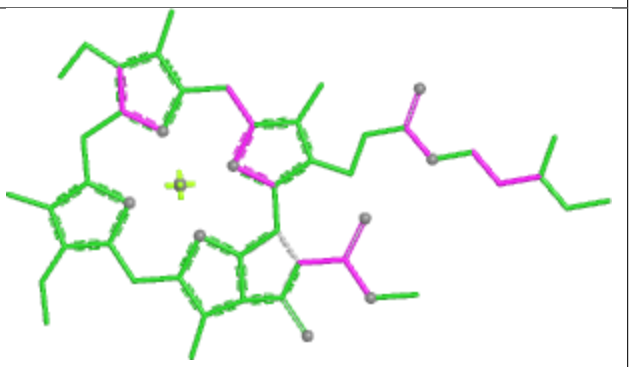


Rings

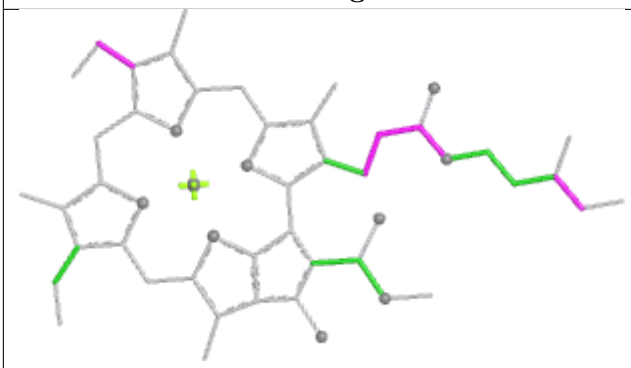
Ligand CLA A 808



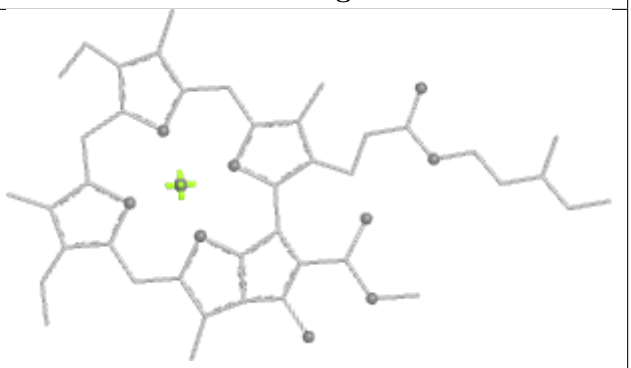
Bond lengths



Bond angles

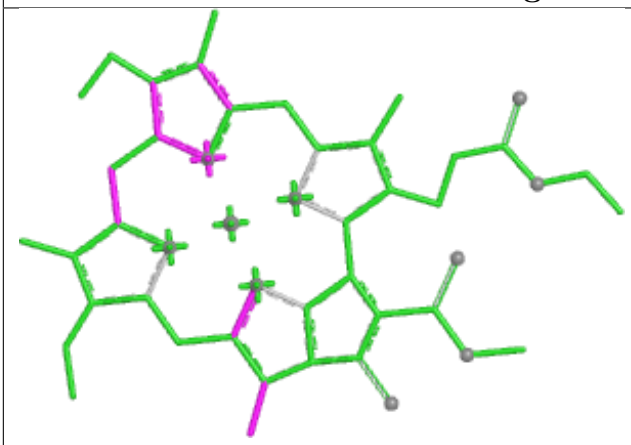


Torsions

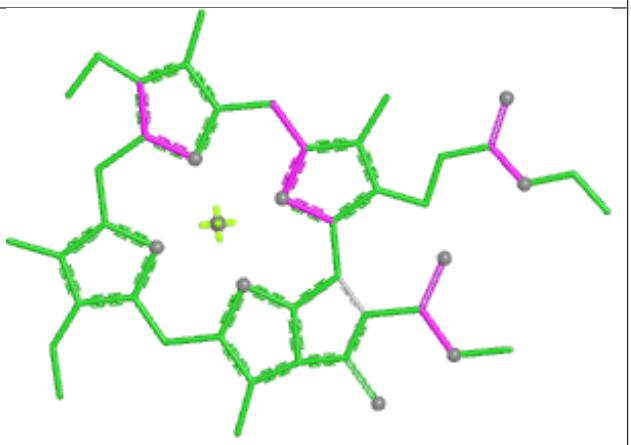


Rings

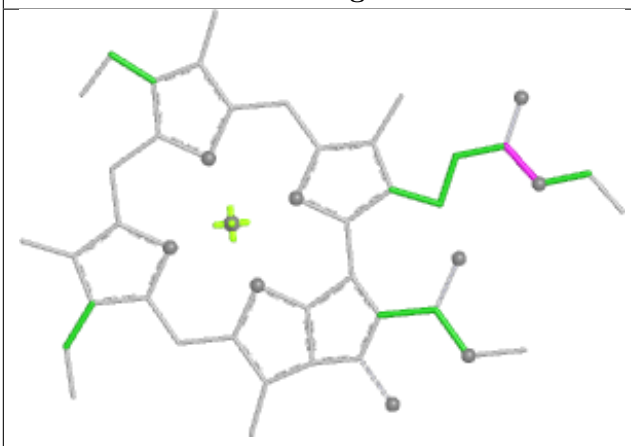
Ligand CLA A 840



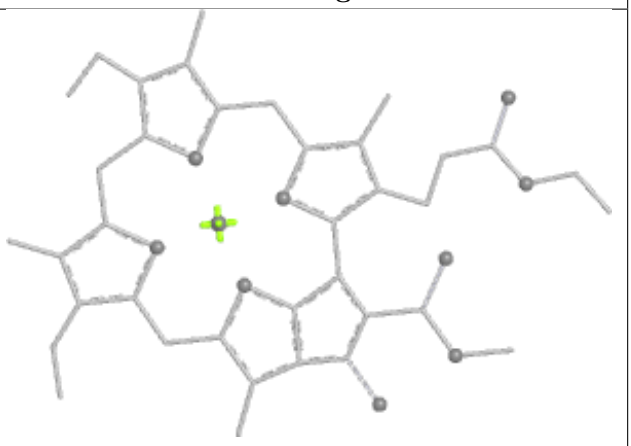
Bond lengths



Bond angles

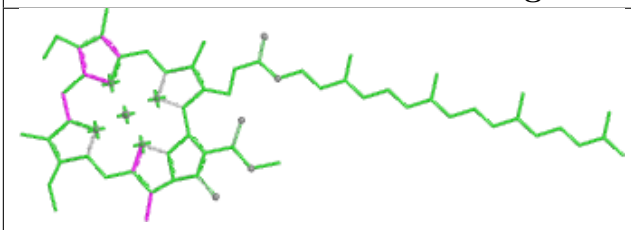


Torsions

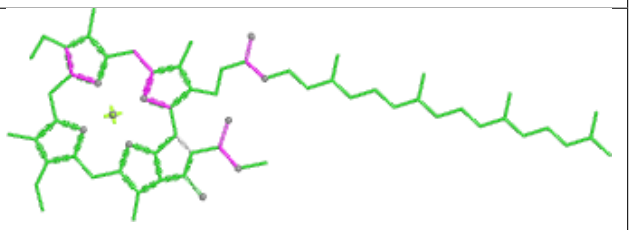


Rings

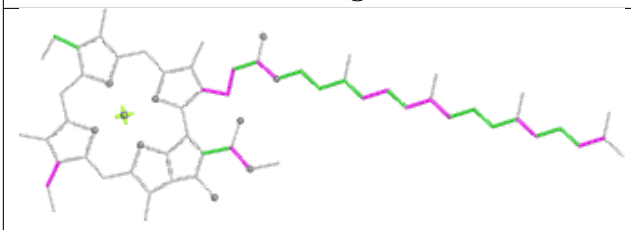
Ligand CLA B 826



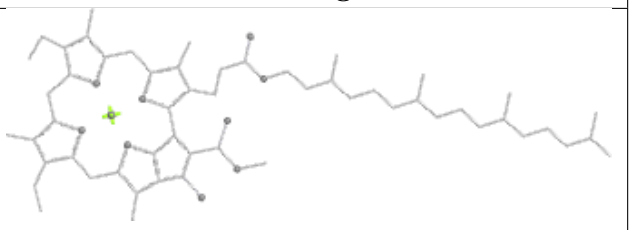
Bond lengths



Bond angles

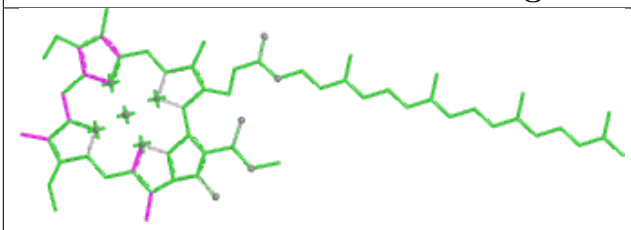


Torsions

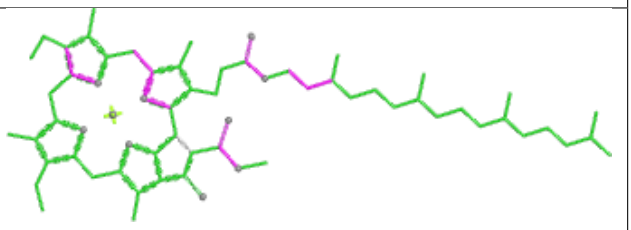


Rings

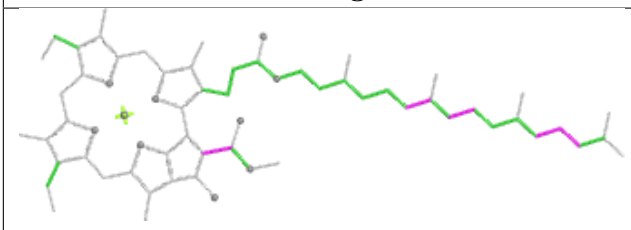
Ligand CLA B 808



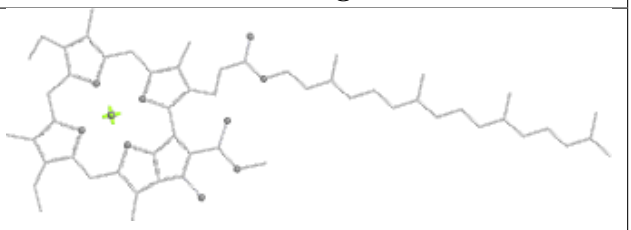
Bond lengths



Bond angles

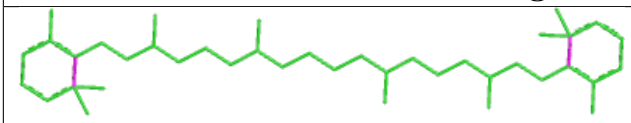


Torsions

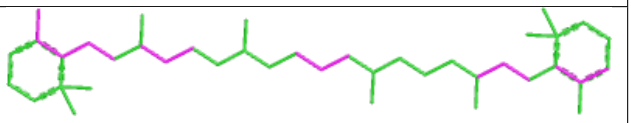


Rings

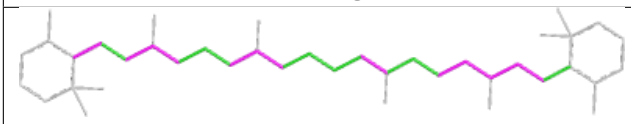
Ligand BCR I 101



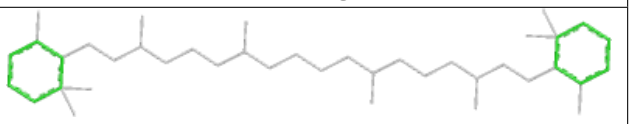
Bond lengths



Bond angles

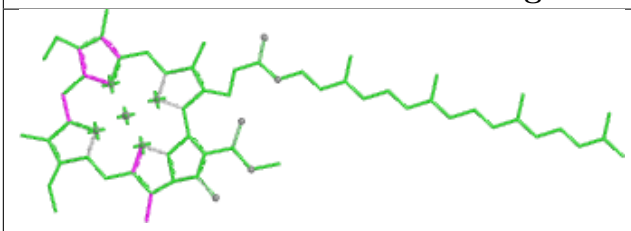


Torsions

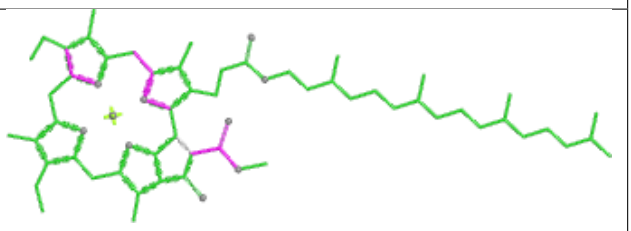


Rings

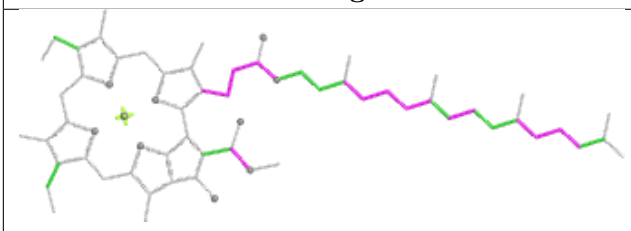
Ligand CLA B 828



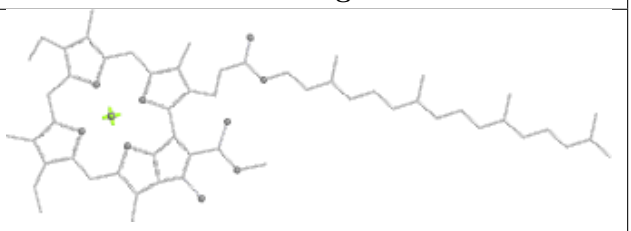
Bond lengths



Bond angles

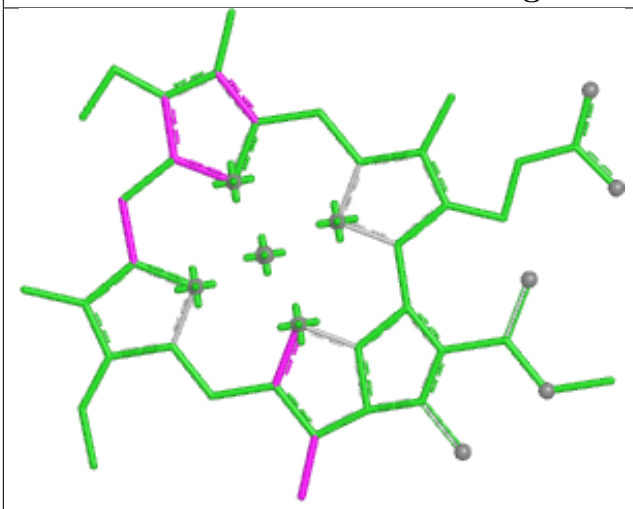


Torsions

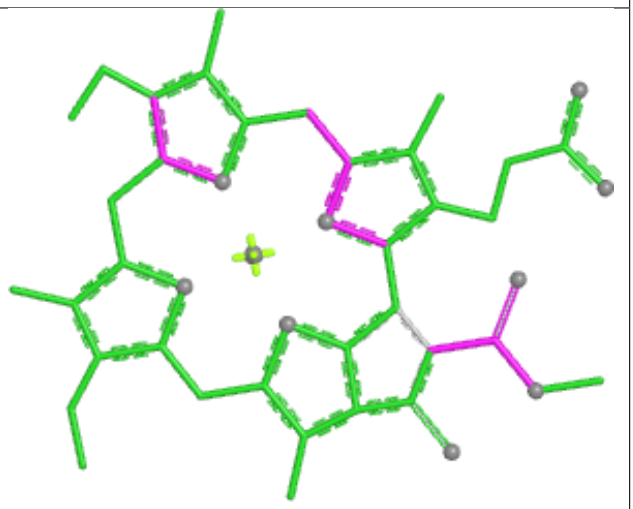


Rings

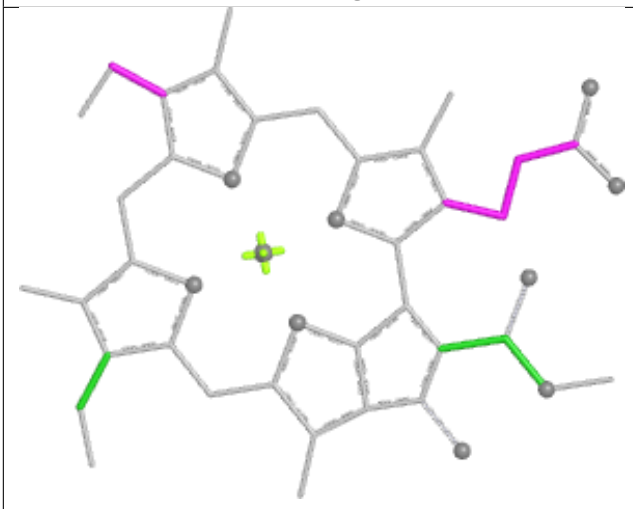
Ligand CLA K 102



Bond lengths



Bond angles

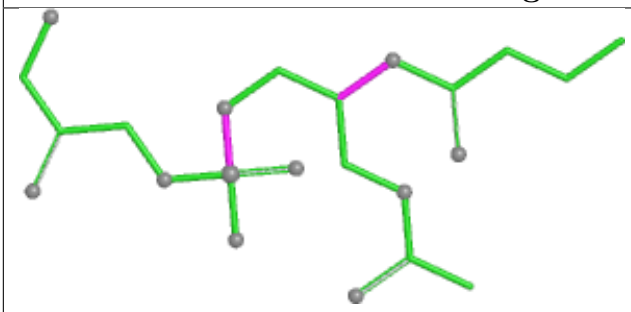


Torsions

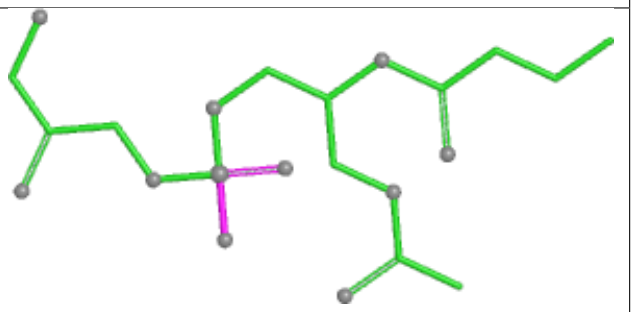


Rings

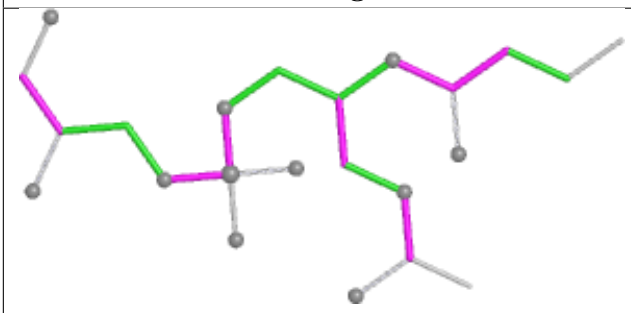
Ligand LHG B 850



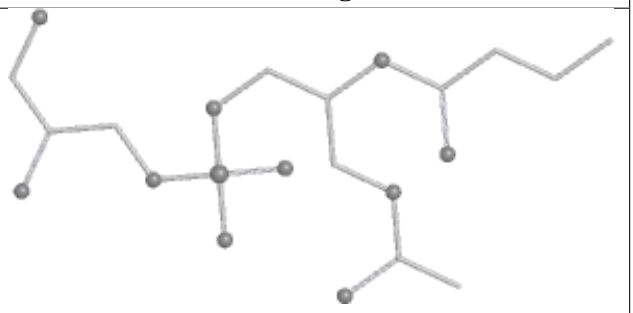
Bond lengths



Bond angles

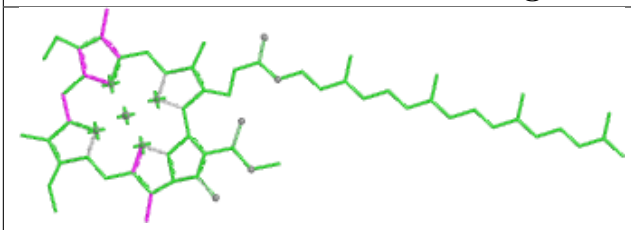


Torsions

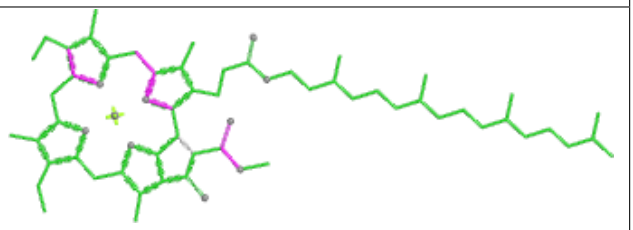


Rings

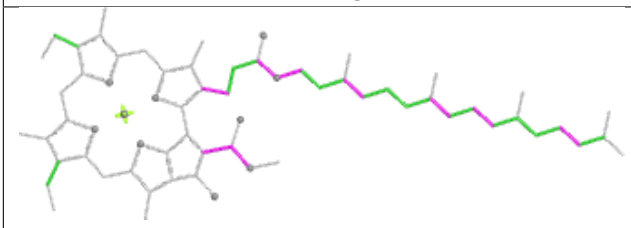
Ligand CLA A 826



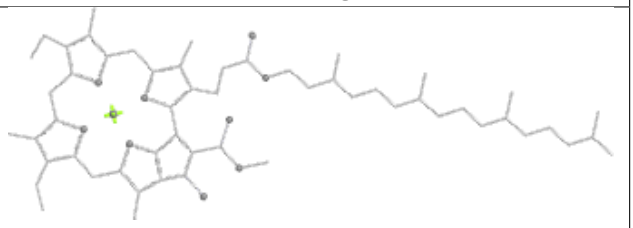
Bond lengths



Bond angles

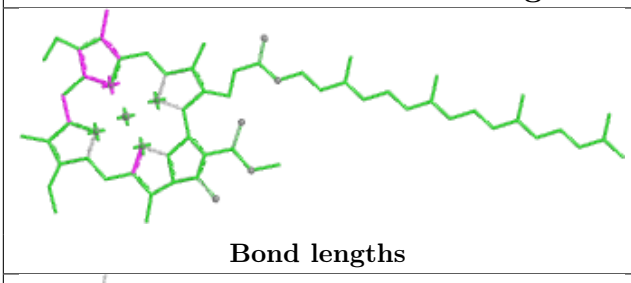


Torsions

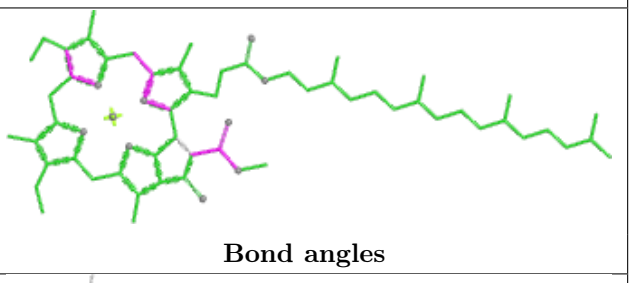


Rings

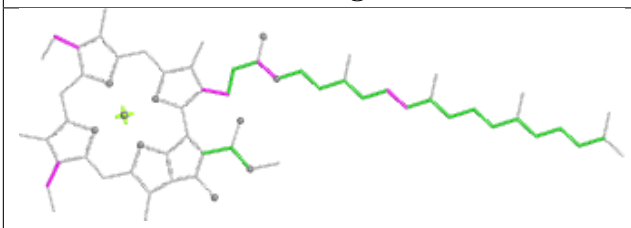
Ligand CLA B 841



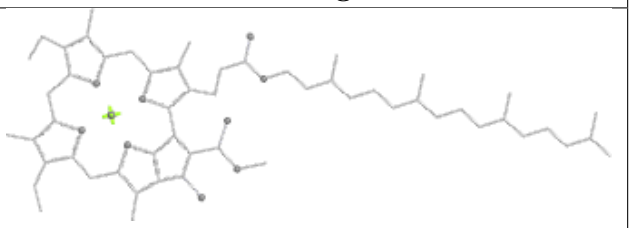
Bond lengths



Bond angles

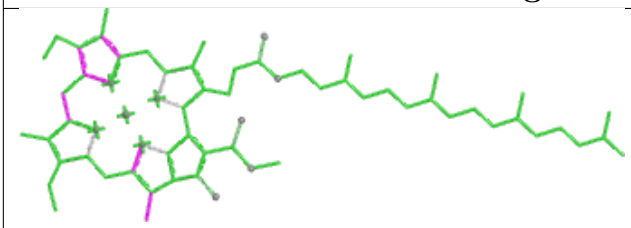


Torsions

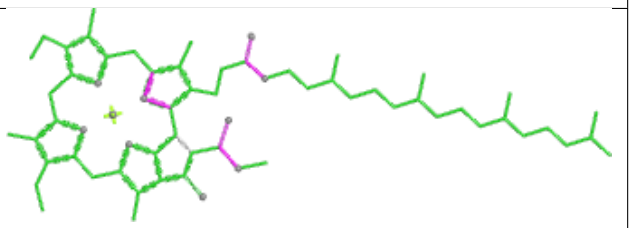


Rings

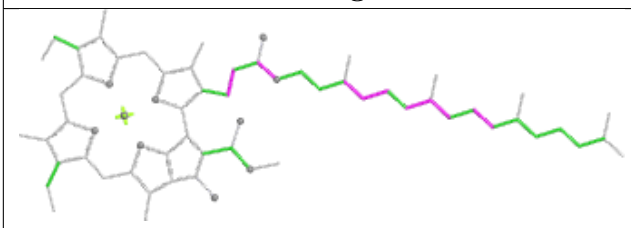
Ligand CLA A 802



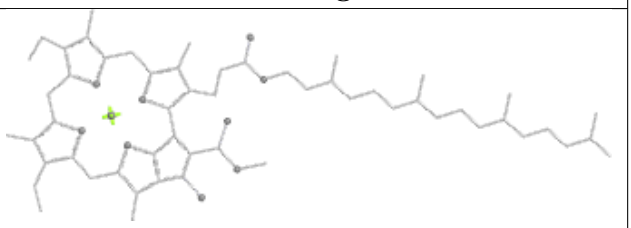
Bond lengths



Bond angles

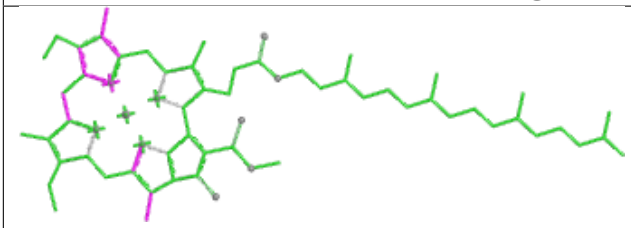


Torsions

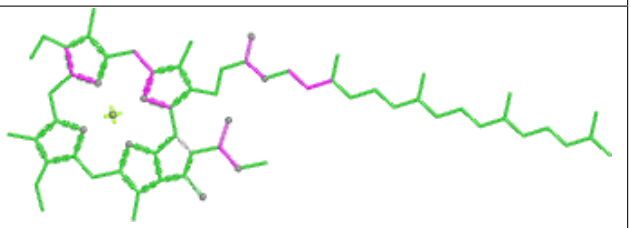


Rings

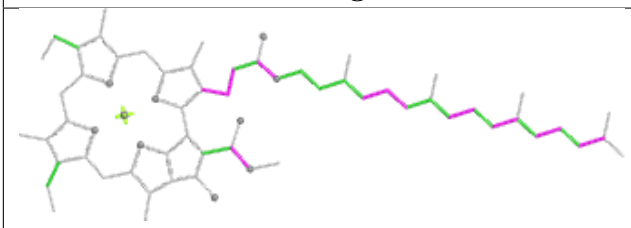
Ligand CL0 A 801



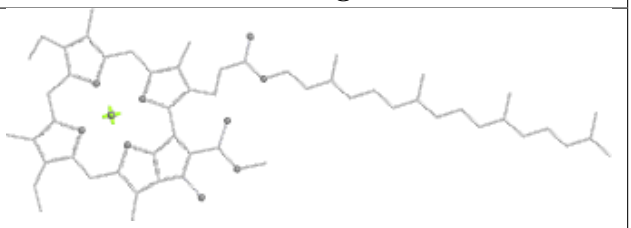
Bond lengths



Bond angles

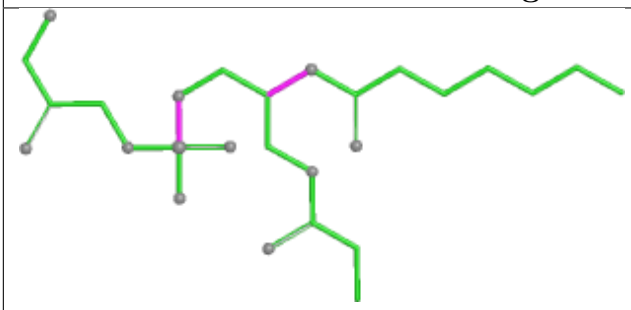


Torsions

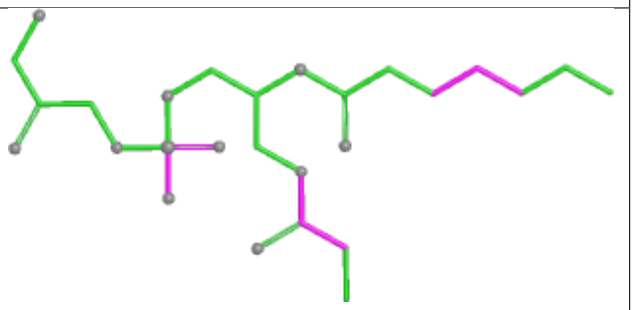


Rings

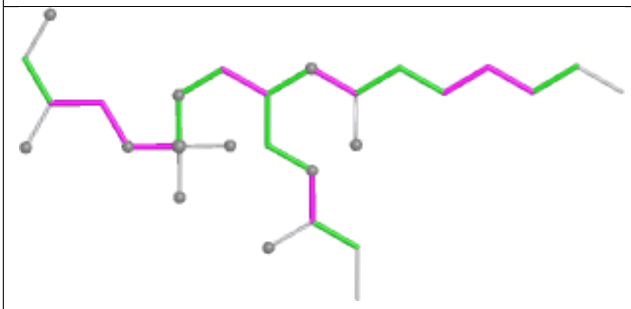
Ligand LHG A 855



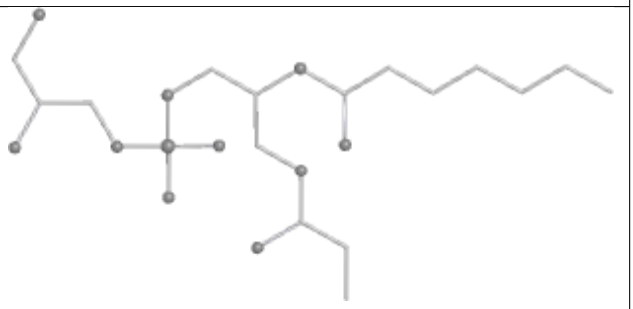
Bond lengths



Bond angles

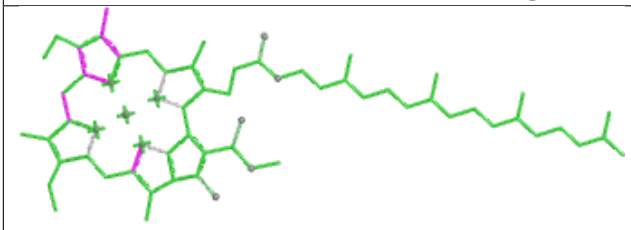


Torsions

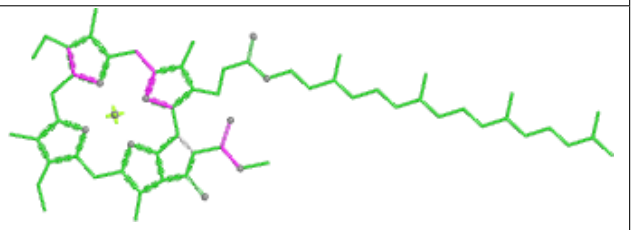


Rings

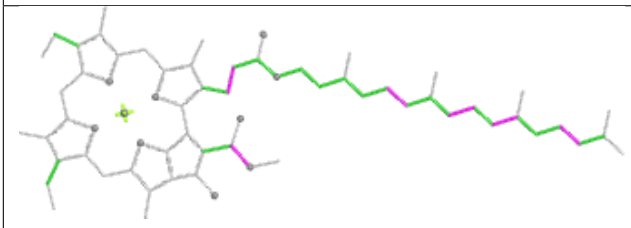
Ligand CLA A 843



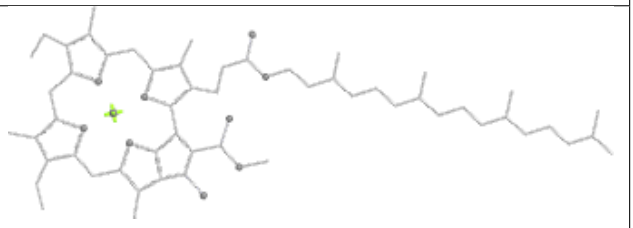
Bond lengths



Bond angles

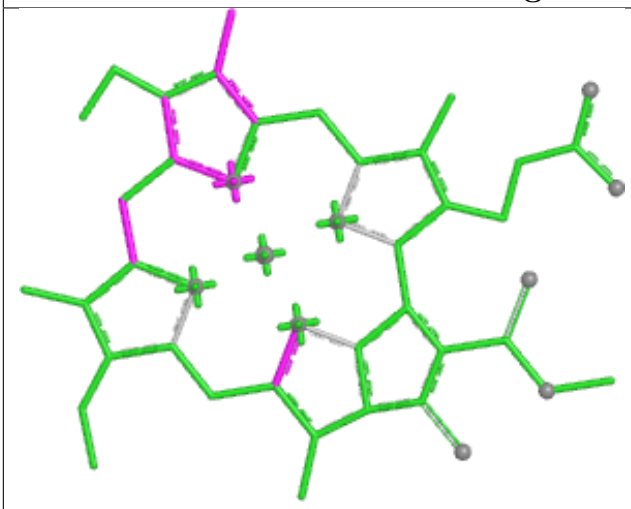


Torsions

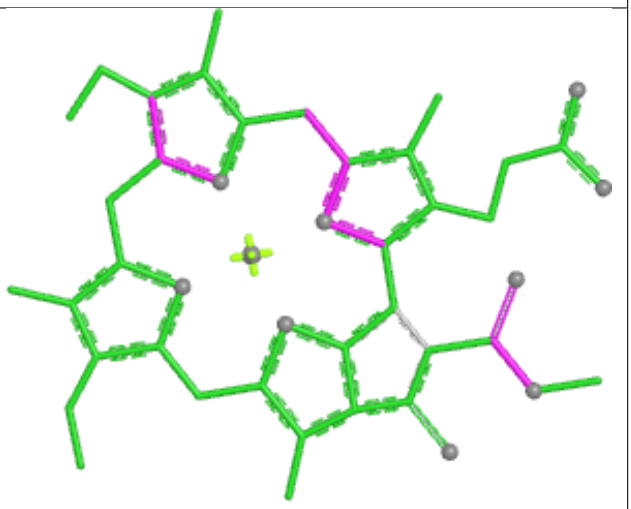


Rings

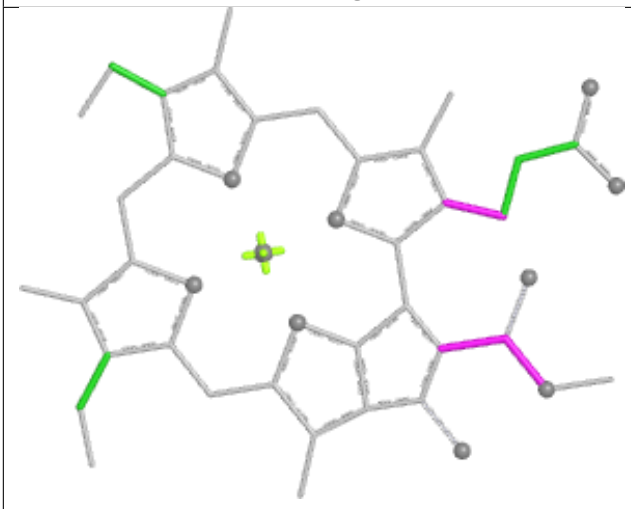
Ligand CLA B 821



Bond lengths



Bond angles

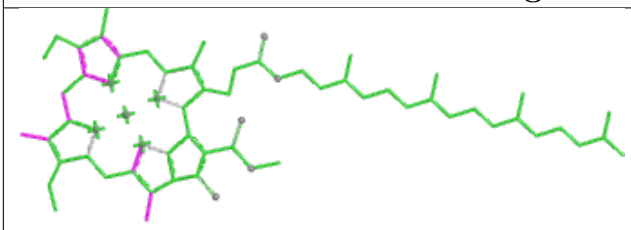


Torsions

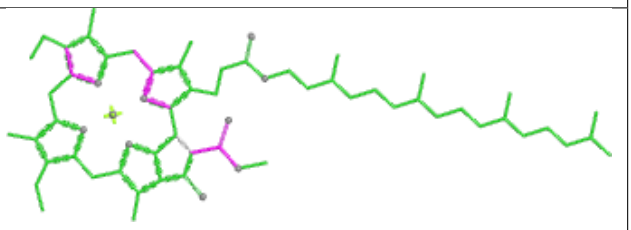


Rings

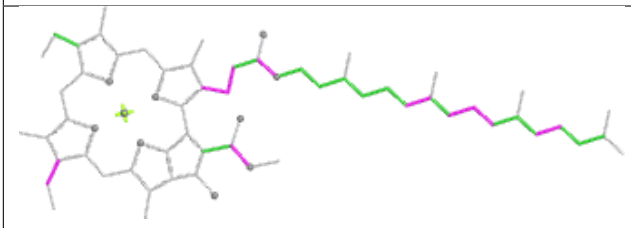
Ligand CLA B 827



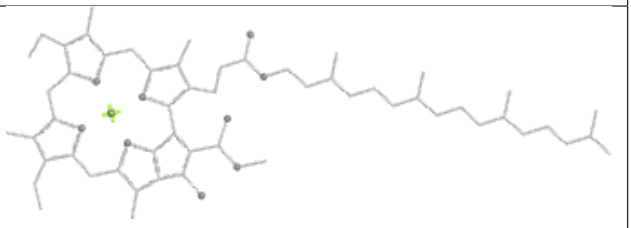
Bond lengths



Bond angles

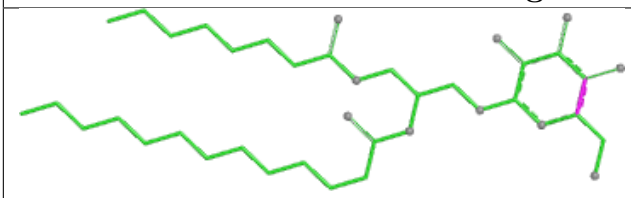


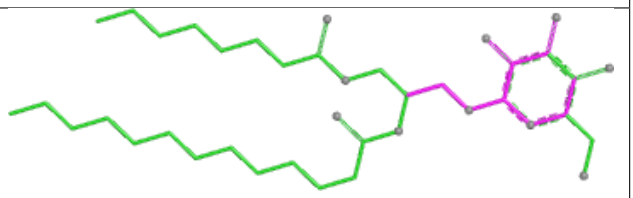
Torsions

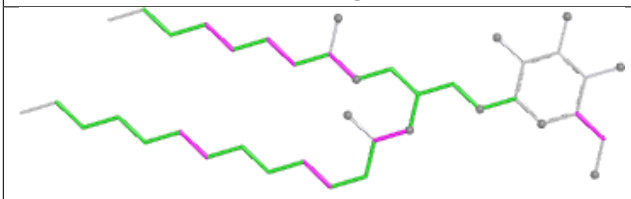


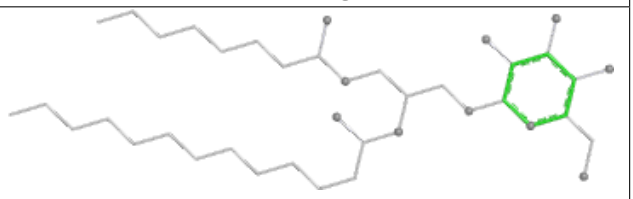
Rings

Ligand LMG I 102

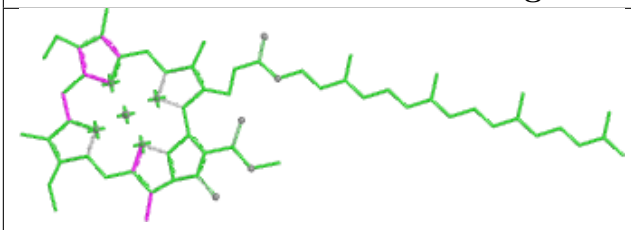

Bond lengths

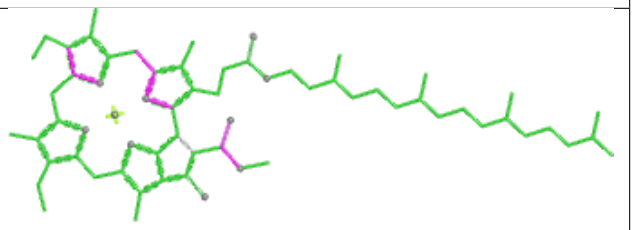

Bond angles

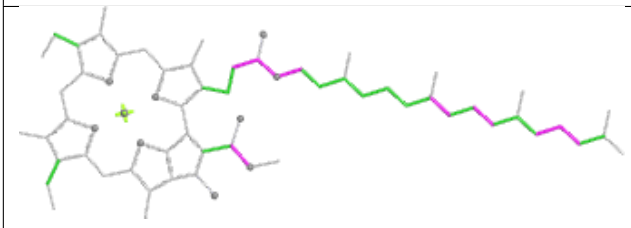

Torsions

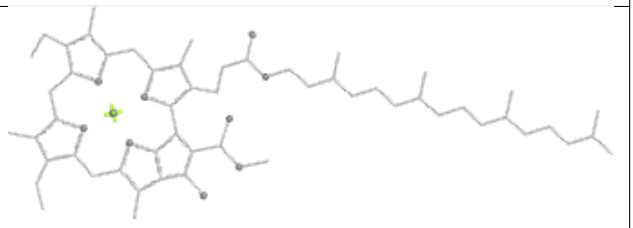

Rings

Ligand CLA B 803

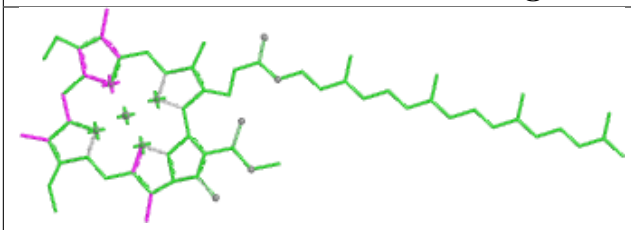

Bond lengths

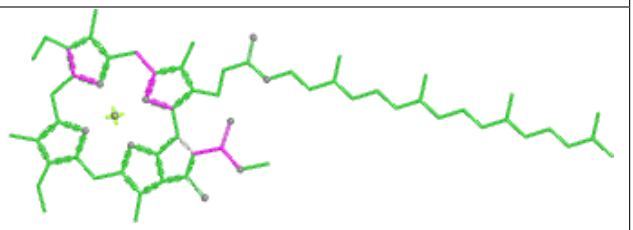

Bond angles

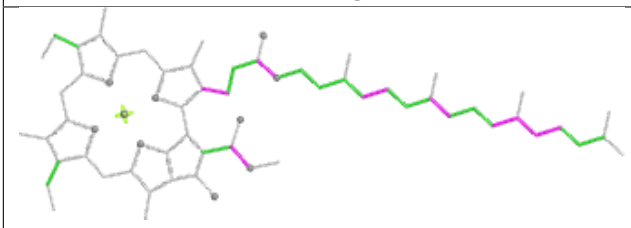

Torsions

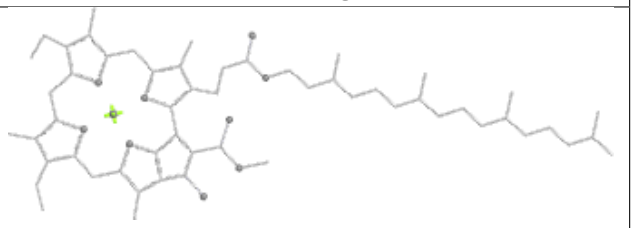

Rings

Ligand CLA B 819

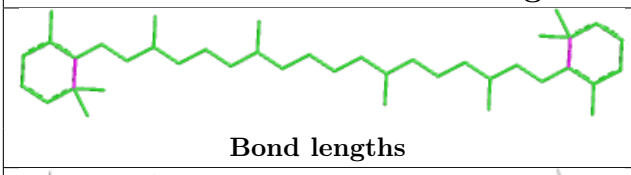

Bond lengths


Bond angles

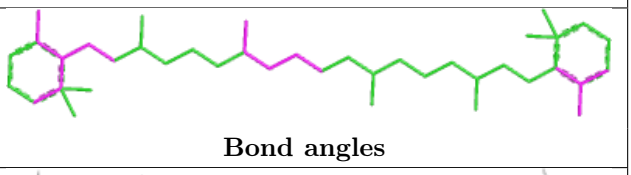

Torsions


Rings

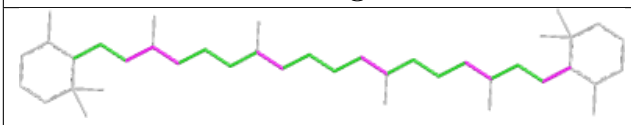
Ligand BCR F 203



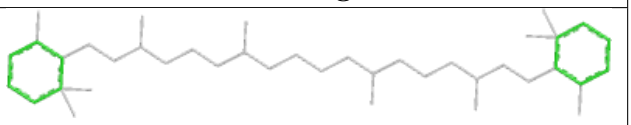
Bond lengths



Bond angles

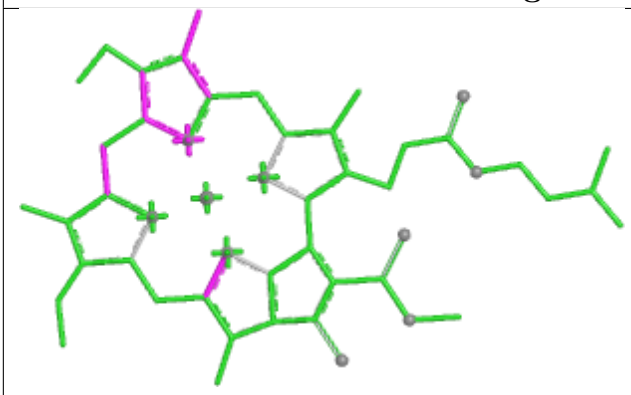


Torsions

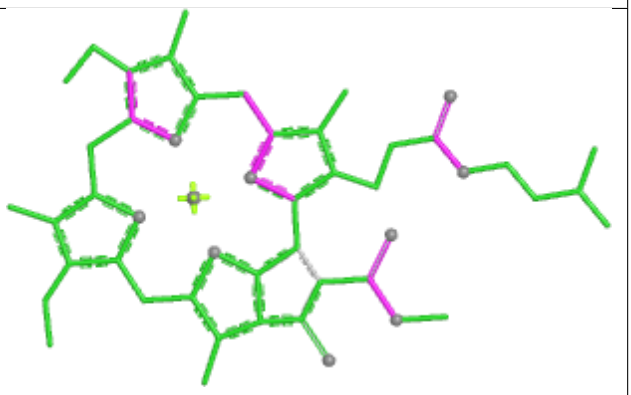


Rings

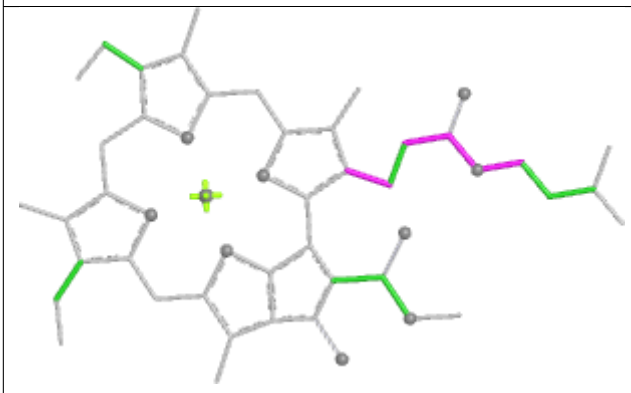
Ligand CLA A 832



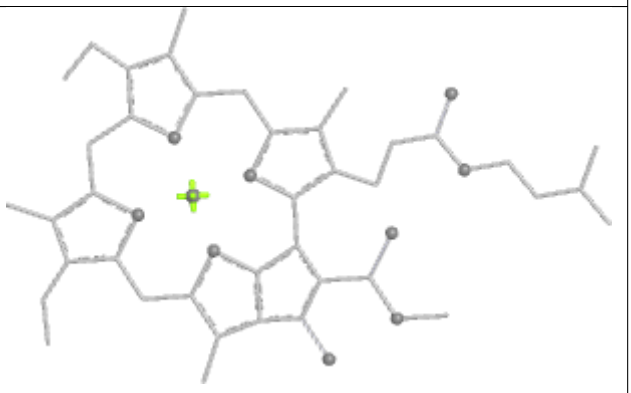
Bond lengths



Bond angles

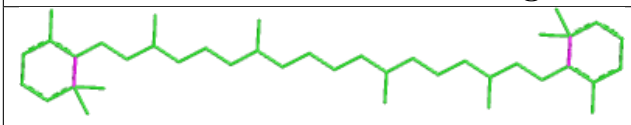


Torsions

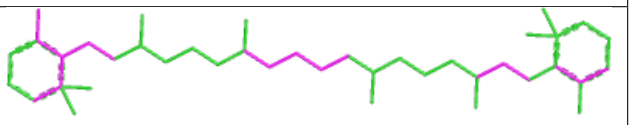


Rings

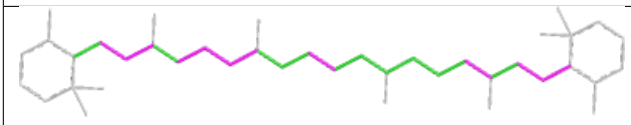
Ligand BCR B 846



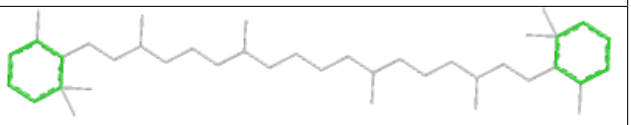
Bond lengths



Bond angles

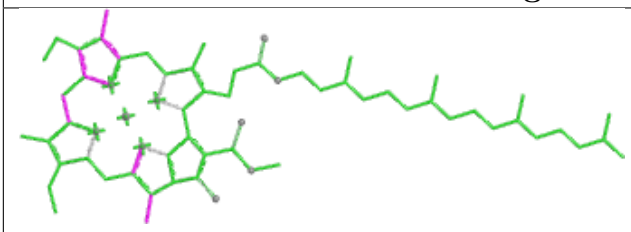


Torsions

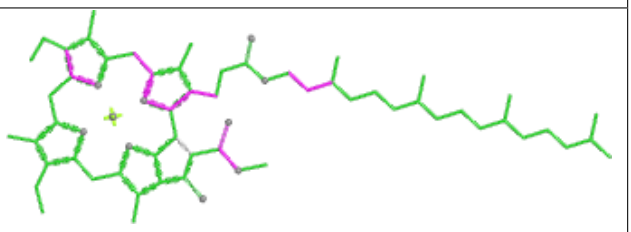


Rings

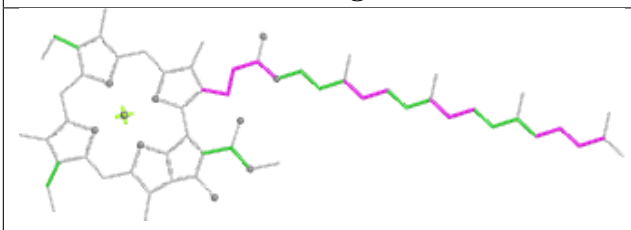
Ligand CLA A 820



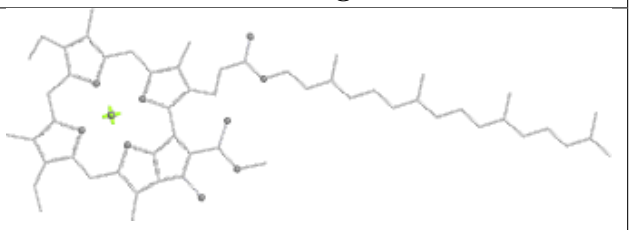
Bond lengths



Bond angles



Torsions

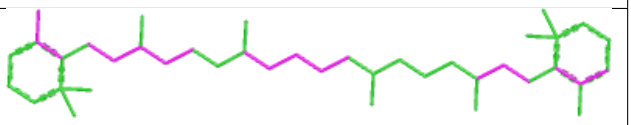


Rings

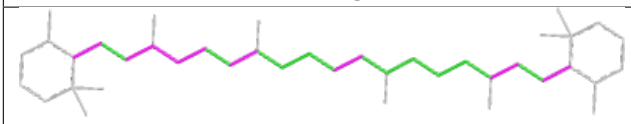
Ligand BCR I 103



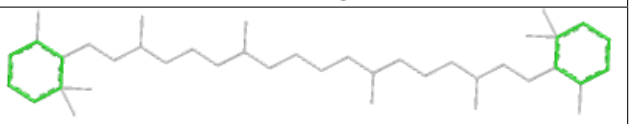
Bond lengths



Bond angles

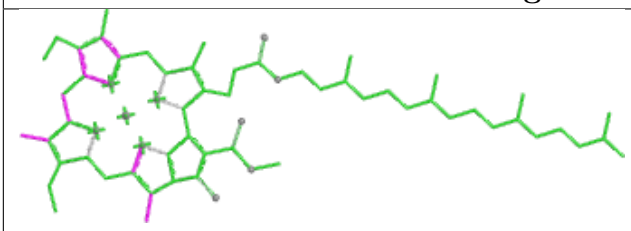


Torsions

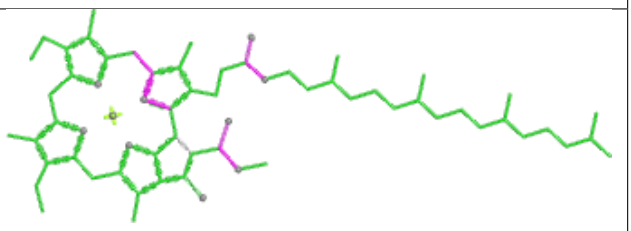


Rings

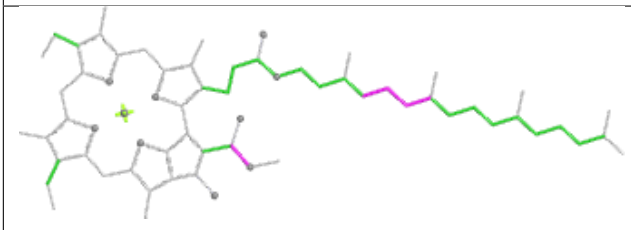
Ligand CLA A 841



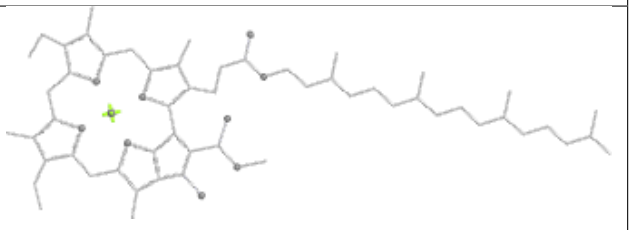
Bond lengths



Bond angles

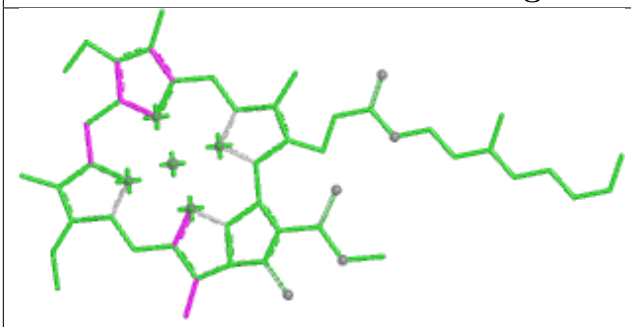


Torsions

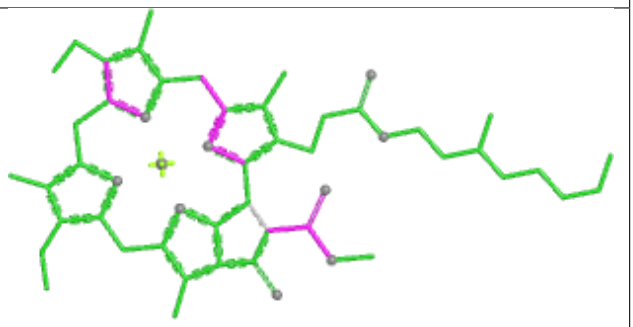


Rings

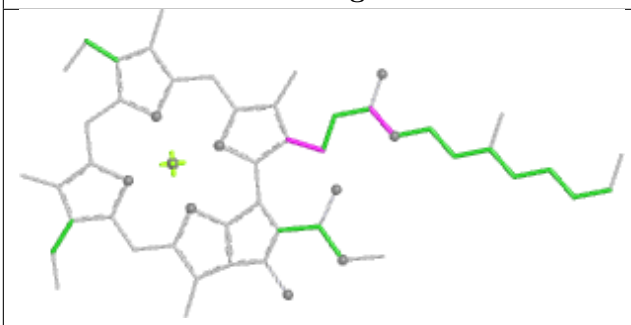
Ligand CLA A 836



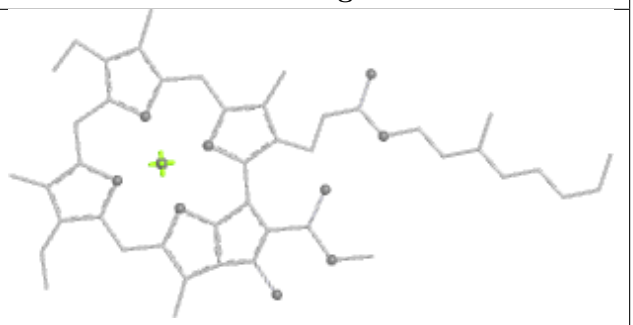
Bond lengths



Bond angles

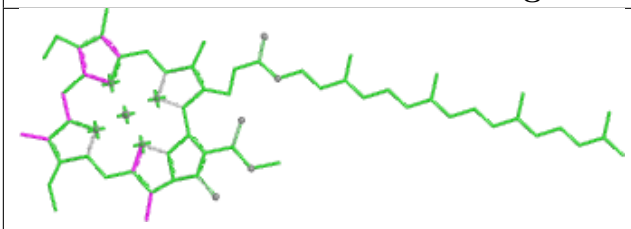


Torsions

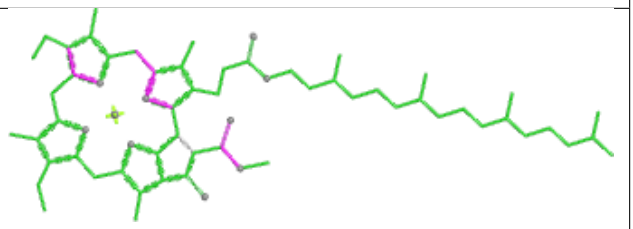


Rings

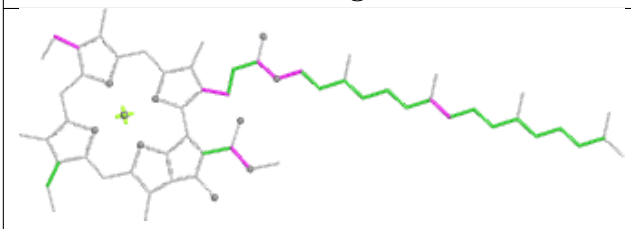
Ligand CLA A 842



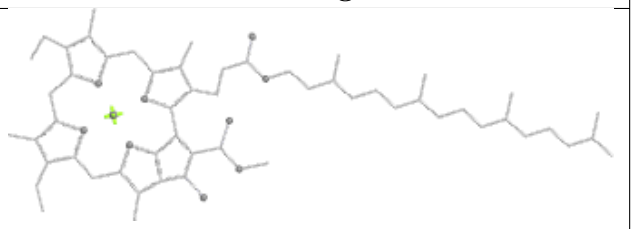
Bond lengths



Bond angles

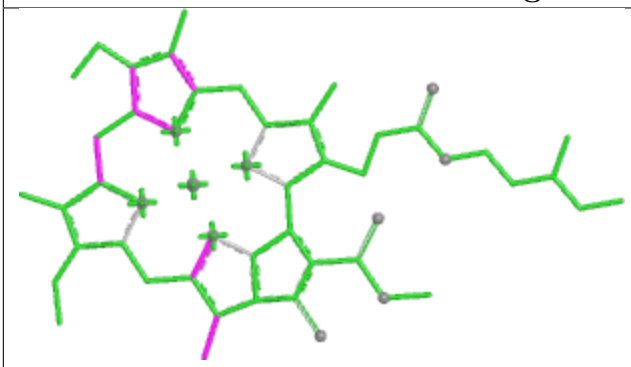


Torsions

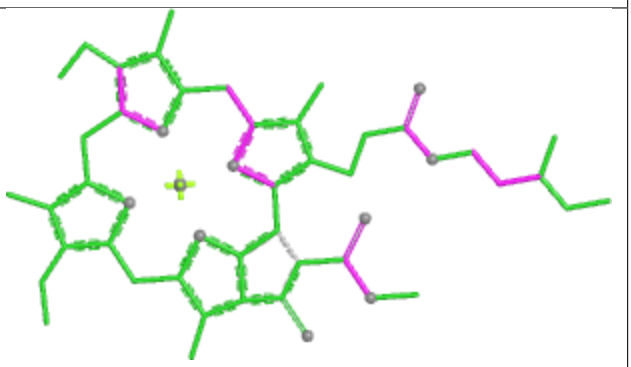


Rings

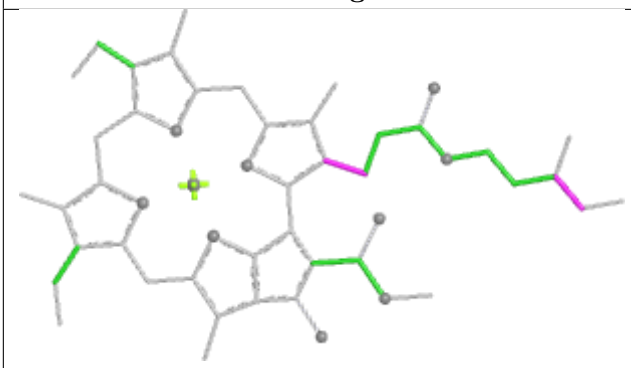
Ligand CLA A 824



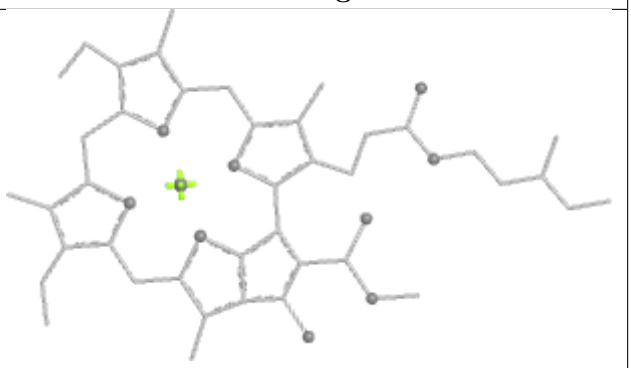
Bond lengths



Bond angles

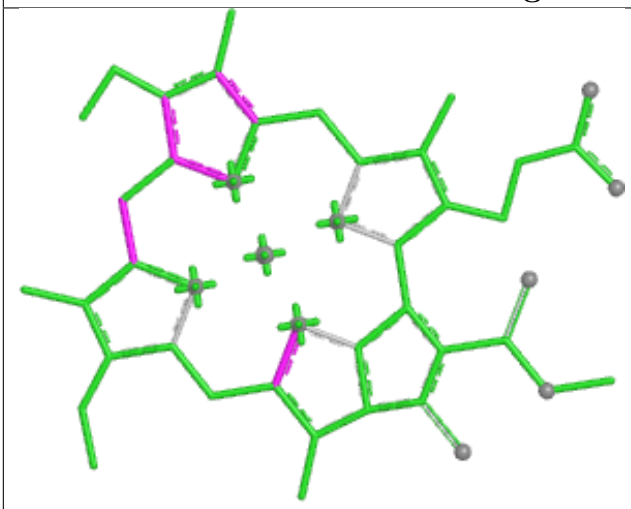


Torsions

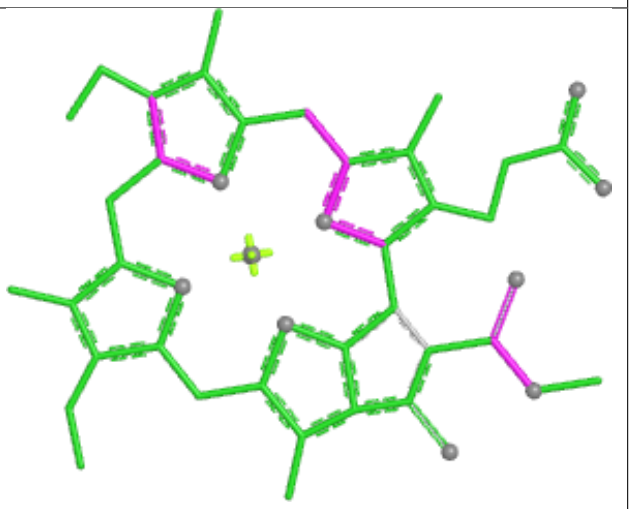


Rings

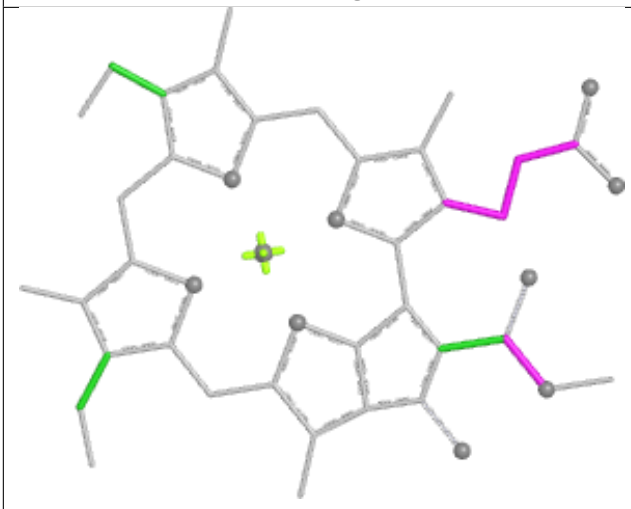
Ligand CLA A 837



Bond lengths



Bond angles

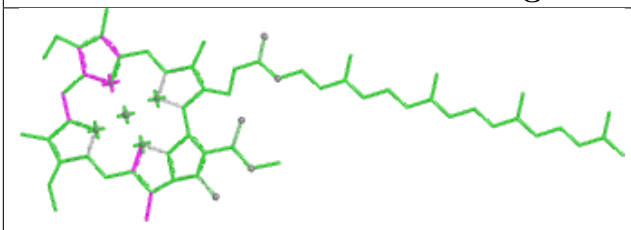


Torsions

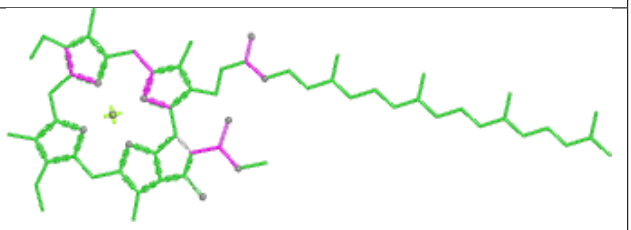


Rings

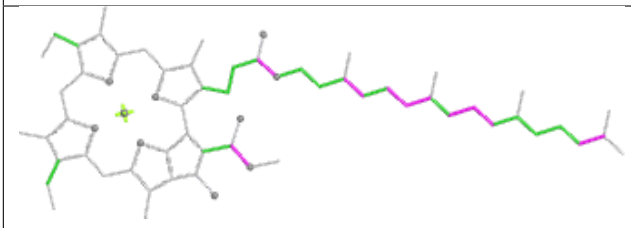
Ligand CLA A 839



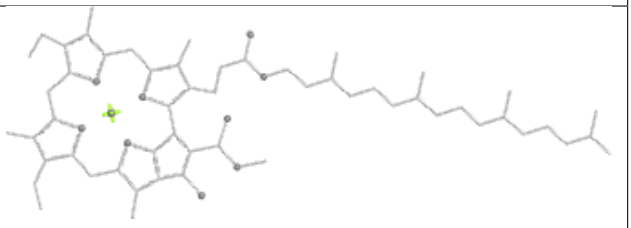
Bond lengths



Bond angles

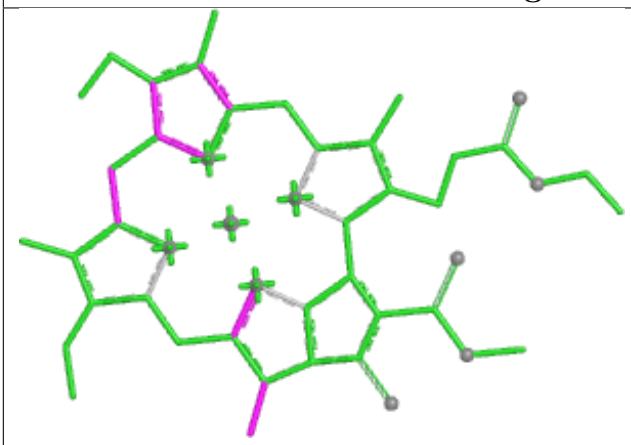


Torsions

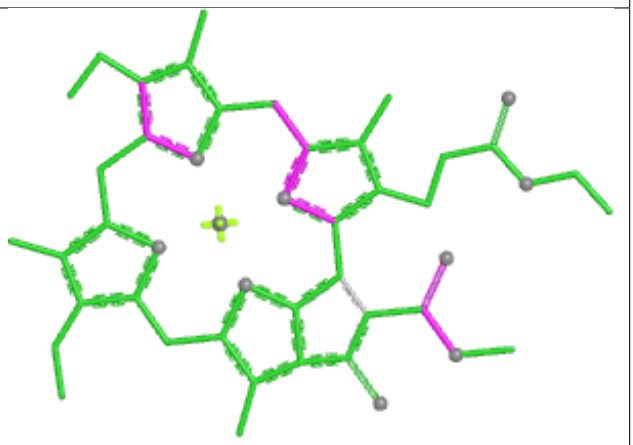


Rings

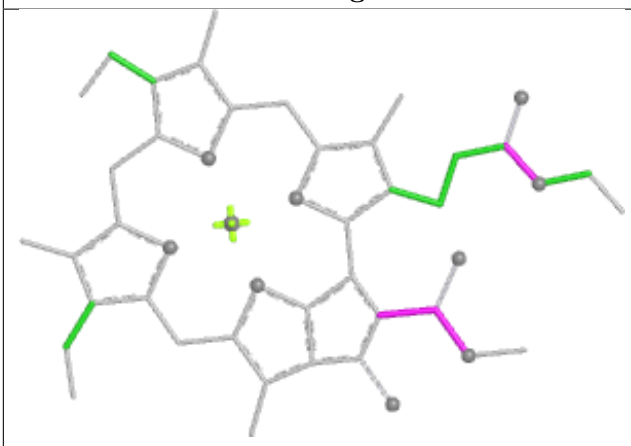
Ligand CLA B 820



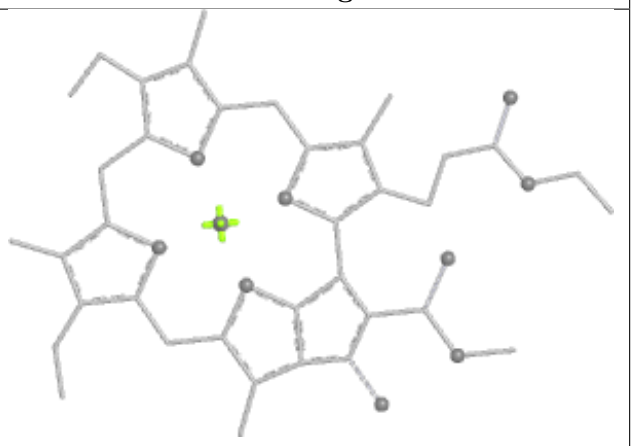
Bond lengths



Bond angles

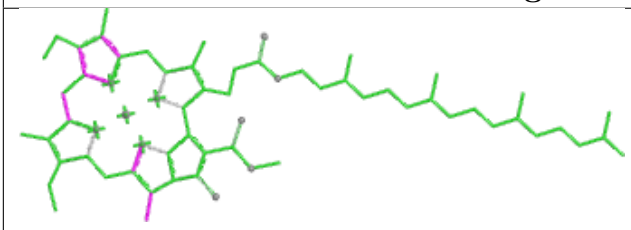


Torsions

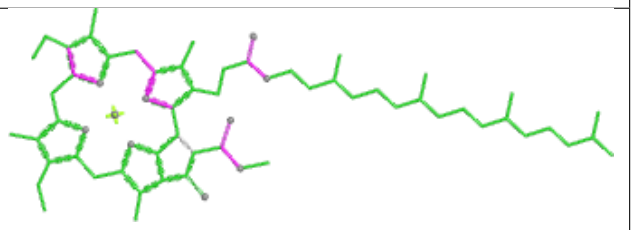


Rings

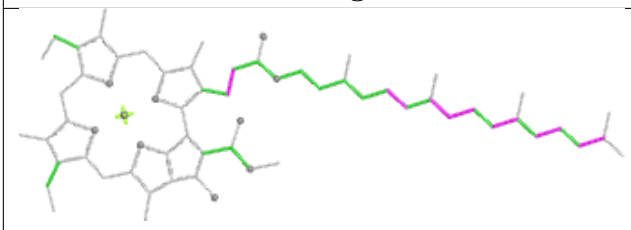
Ligand CLA B 838



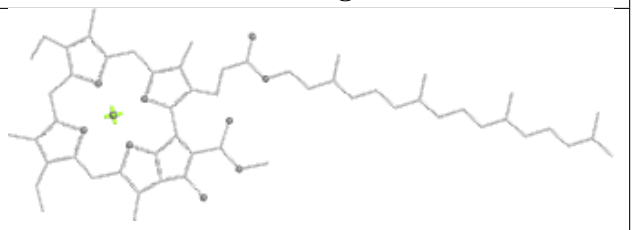
Bond lengths



Bond angles

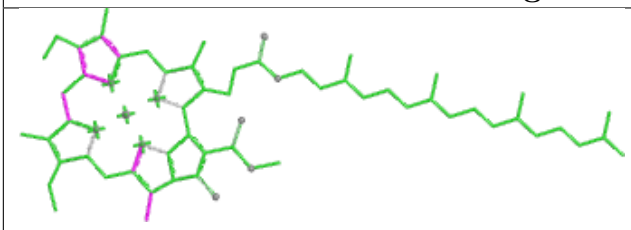


Torsions

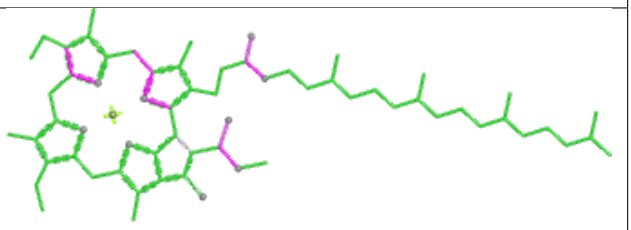


Rings

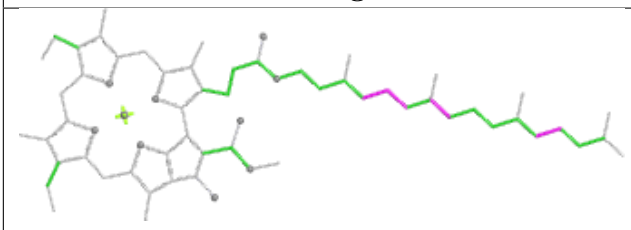
Ligand CLA A 827



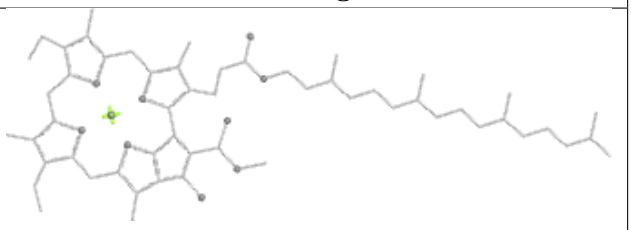
Bond lengths



Bond angles

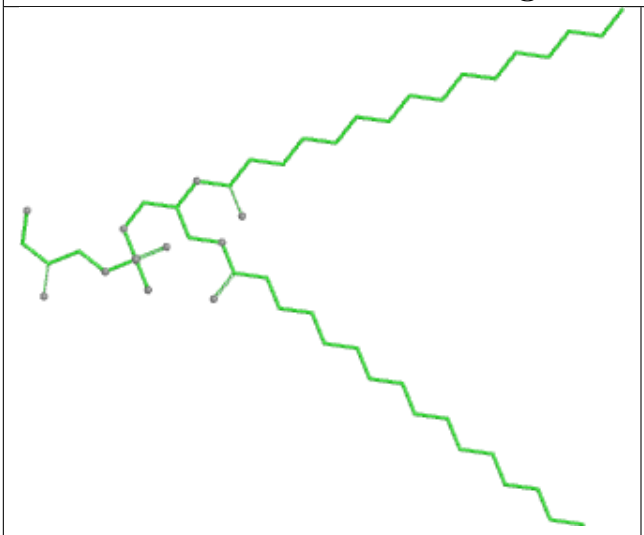


Torsions

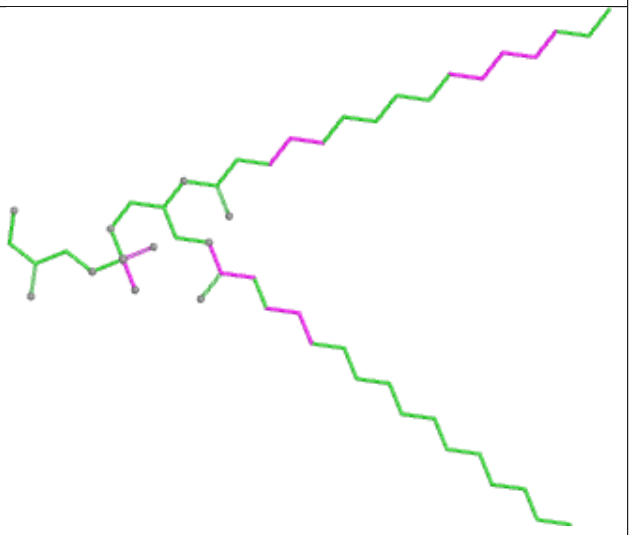


Rings

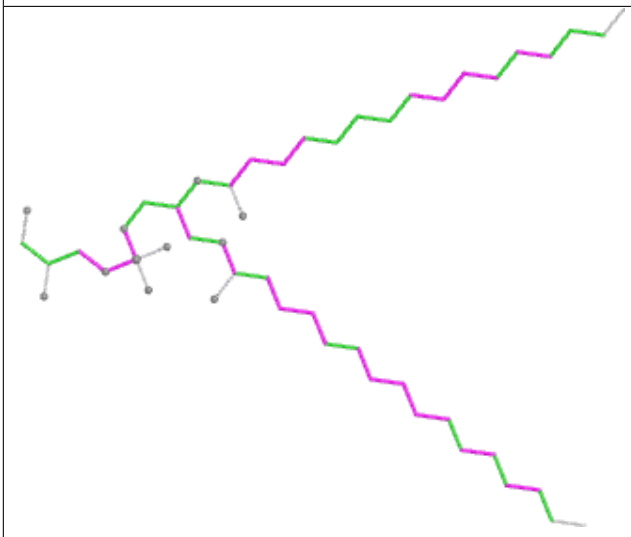
Ligand LHG M 101



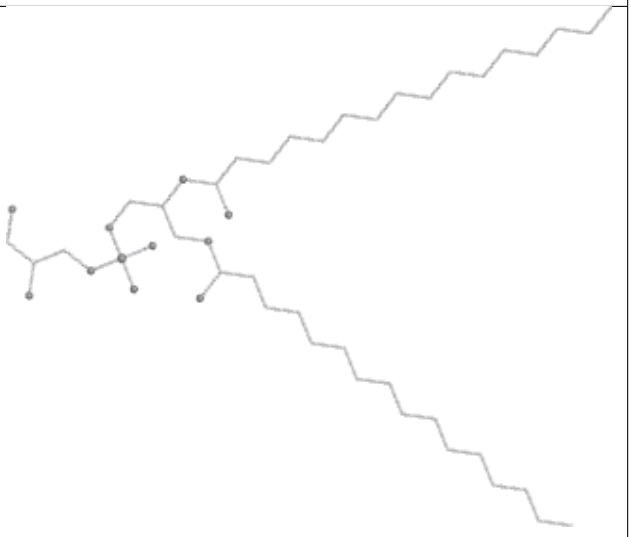
Bond lengths



Bond angles

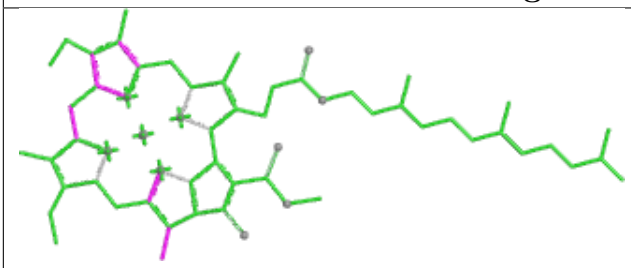


Torsions

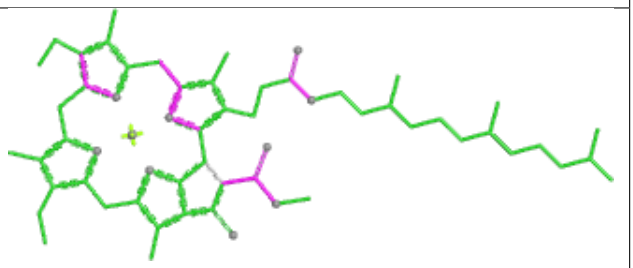


Rings

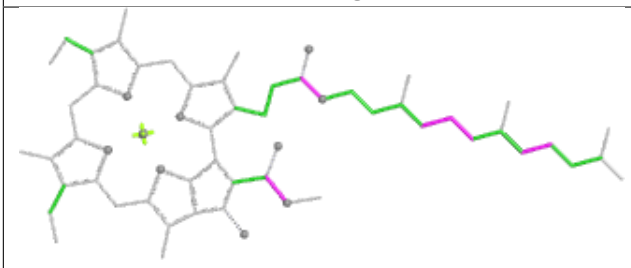
Ligand CLA A 814



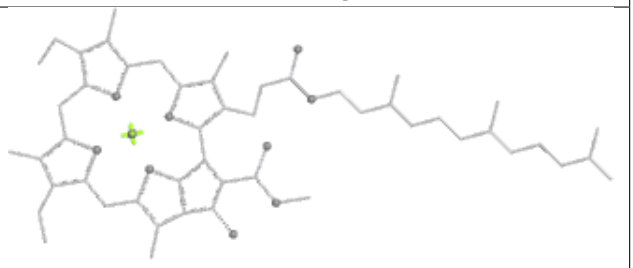
Bond lengths



Bond angles

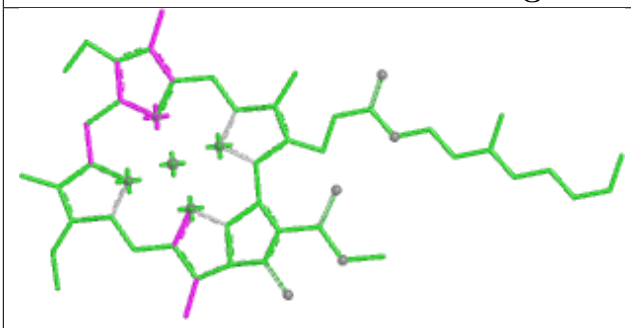


Torsions

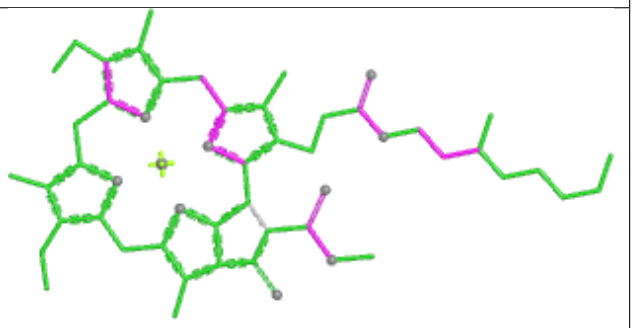


Rings

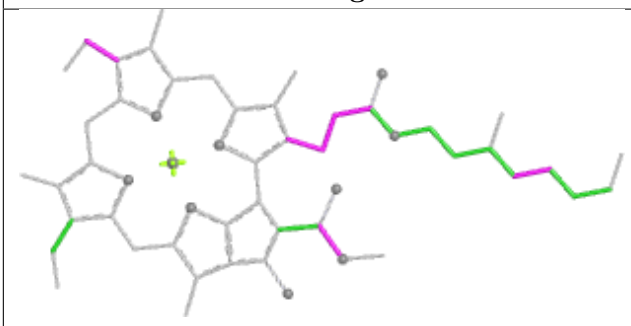
Ligand CLA A 819



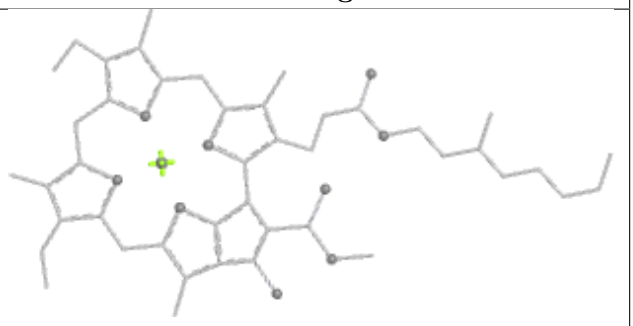
Bond lengths



Bond angles



Torsions

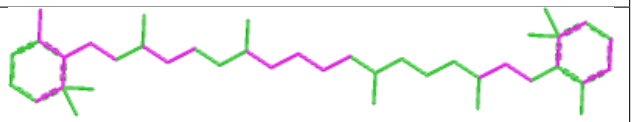


Rings

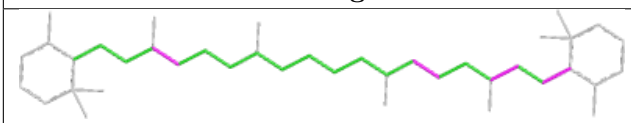
Ligand BCR B 843



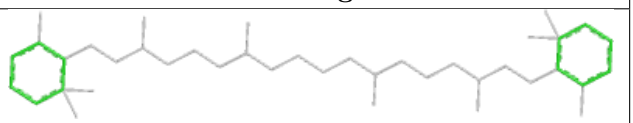
Bond lengths



Bond angles

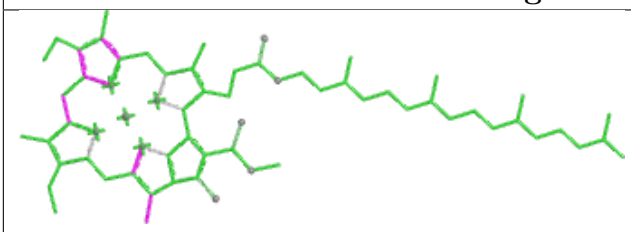


Torsions

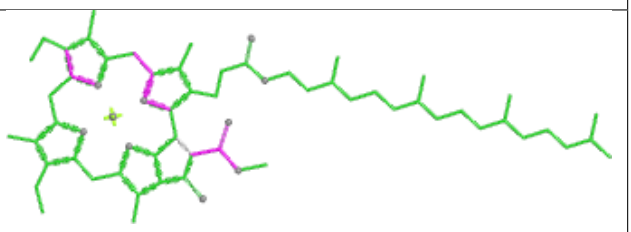


Rings

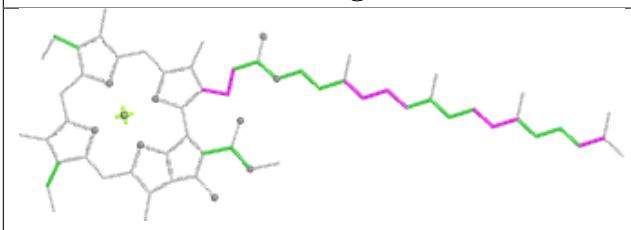
Ligand CLA B 832



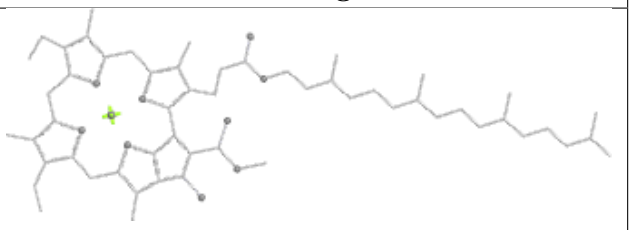
Bond lengths



Bond angles

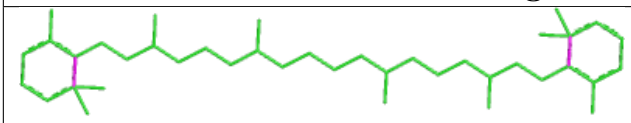


Torsions

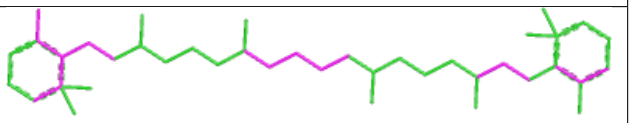


Rings

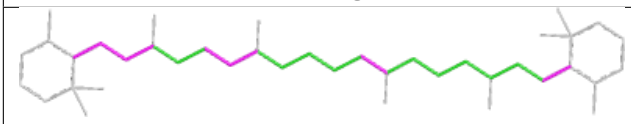
Ligand BCR L 208



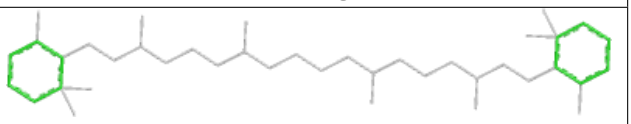
Bond lengths



Bond angles

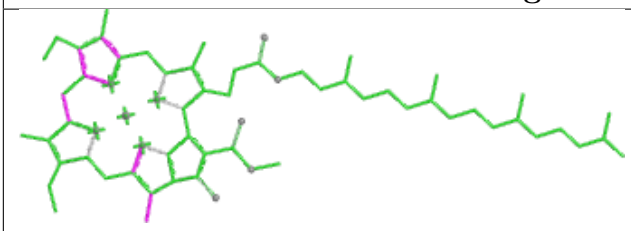


Torsions

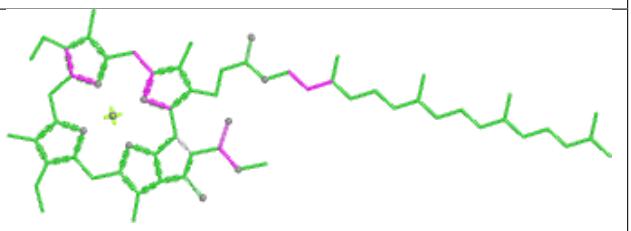


Rings

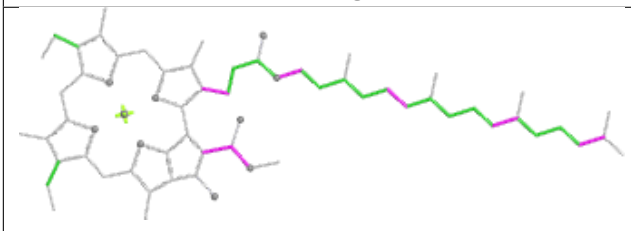
Ligand CLA A 835



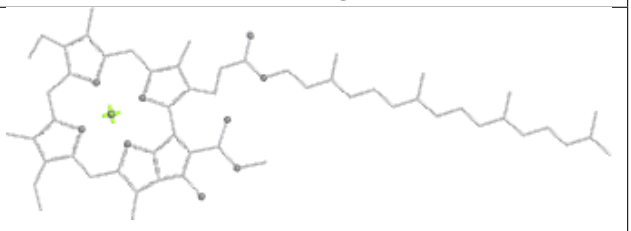
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	740/755 (98%)	-0.72	7 (0%) 81 61	3, 61, 113, 158	0
2	B	739/740 (99%)	-1.01	1 (0%) 92 86	2, 34, 80, 114	0
3	C	80/80 (100%)	-1.10	0 100 100	2, 27, 54, 65	0
4	D	138/138 (100%)	-1.10	0 100 100	7, 39, 66, 120	0
5	E	69/75 (92%)	-0.88	0 100 100	27, 56, 78, 94	0
6	F	141/164 (85%)	-0.76	2 (1%) 73 51	27, 80, 99, 107	0
7	I	38/38 (100%)	-1.17	0 100 100	2, 10, 36, 70	0
8	J	41/41 (100%)	-0.81	1 (2%) 59 36	70, 90, 104, 123	0
9	K	47/83 (56%)	-0.61	0 100 100	106, 140, 157, 174	0
10	L	151/154 (98%)	-1.22	0 100 100	2, 10, 46, 94	0
11	M	31/31 (100%)	-1.21	0 100 100	5, 27, 51, 76	0
12	X	29/35 (82%)	-0.97	0 100 100	51, 61, 90, 103	0
All	All	2244/2334 (96%)	-0.91	11 (0%) 87 72	2, 44, 106, 174	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	F	26	ALA	5.2
1	A	315	TYR	4.4
1	A	114	ALA	3.8
1	A	18	ASN	3.0
1	A	113	SER	3.0

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 oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CLA	A	816	45/65	0.96	0.10	79,117,143,153	0
14	CLA	A	817	49/65	0.96	0.07	37,101,133,134	0
14	CLA	A	823	49/65	0.96	0.09	52,90,119,131	0
14	CLA	A	824	51/65	0.96	0.08	41,74,106,112	0
14	CLA	A	828	65/65	0.96	0.11	33,66,102,109	0
14	CLA	B	820	47/65	0.96	0.07	43,72,103,108	0
14	CLA	J	101	45/65	0.96	0.09	91,111,145,149	0
14	CLA	J	102	37/65	0.96	0.09	76,99,123,137	0
17	BCR	B	843	40/40	0.96	0.13	49,84,117,135	0
18	LMG	A	856	30/55	0.96	0.10	6,57,119,135	0
18	LMG	I	102	40/55	0.96	0.11	23,59,94,118	0
14	CLA	B	811	45/65	0.97	0.07	18,41,61,84	0
14	CLA	B	816	55/65	0.97	0.08	35,70,107,140	0
14	CLA	B	817	59/65	0.97	0.09	21,55,83,91	0
14	CLA	B	819	65/65	0.97	0.09	22,65,95,106	0
14	CLA	A	818	54/65	0.97	0.08	69,98,125,135	0
14	CLA	B	833	58/65	0.97	0.09	36,72,110,115	0
14	CLA	B	837	60/65	0.97	0.09	15,55,86,96	0
14	CLA	A	814	60/65	0.97	0.10	47,88,113,115	0
14	CLA	A	811	45/65	0.97	0.06	66,99,125,133	0
14	CLA	K	101	41/65	0.97	0.07	86,123,158,168	0
14	CLA	K	102	45/65	0.97	0.08	75,105,138,139	0
14	CLA	M	102	45/65	0.97	0.12	57,105,140,154	0
17	BCR	A	847	40/40	0.97	0.11	81,120,140,149	0
17	BCR	A	848	40/40	0.97	0.10	70,105,135,149	0
17	BCR	A	850	40/40	0.97	0.09	35,65,129,131	0
14	CLA	A	813	54/65	0.97	0.07	47,74,102,110	0
17	BCR	B	844	40/40	0.97	0.07	22,48,88,97	0
17	BCR	B	847	40/40	0.97	0.10	19,65,98,106	0
17	BCR	B	851	40/40	0.97	0.09	20,58,101,108	0
17	BCR	J	105	40/40	0.97	0.13	41,87,128,135	0
18	LMG	A	853	48/55	0.97	0.09	30,87,126,134	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CLA	A	836	54/65	0.97	0.07	20,61,102,109	0
14	CLA	A	844	52/65	0.97	0.07	18,57,85,93	0
19	LHG	M	101	49/49	0.97	0.08	21,63,138,155	0
22	DGD	L	207	66/66	0.97	0.08	19,73,129,142	0
14	CLA	B	812	45/65	0.98	0.05	31,63,89,93	0
14	CLA	B	813	65/65	0.98	0.08	15,46,72,76	0
14	CLA	B	815	45/65	0.98	0.06	35,56,89,92	0
14	CLA	A	815	45/65	0.98	0.07	59,88,123,130	0
14	CLA	A	806	65/65	0.98	0.09	40,74,110,115	0
14	CLA	B	818	60/65	0.98	0.08	23,44,74,81	0
14	CLA	A	807	65/65	0.98	0.08	30,58,84,90	0
14	CLA	A	808	51/65	0.98	0.06	55,76,104,107	0
14	CLA	B	821	45/65	0.98	0.05	40,67,93,94	0
14	CLA	B	822	55/65	0.98	0.06	42,68,95,96	0
14	CLA	B	823	45/65	0.98	0.07	4,35,68,80	0
14	CLA	B	825	46/65	0.98	0.07	10,38,62,64	0
14	CLA	B	826	65/65	0.98	0.06	11,39,65,70	0
14	CLA	B	828	65/65	0.98	0.07	2,35,53,71	0
14	CLA	B	830	45/65	0.98	0.06	19,47,69,87	0
14	CLA	B	832	65/65	0.98	0.08	29,60,86,95	0
14	CLA	A	820	65/65	0.98	0.08	39,74,99,107	0
14	CLA	B	834	45/65	0.98	0.07	28,47,69,71	0
14	CLA	B	836	45/65	0.98	0.05	37,62,94,95	0
14	CLA	A	822	65/65	0.98	0.07	25,61,95,101	0
14	CLA	B	838	65/65	0.98	0.07	16,62,101,117	0
14	CLA	F	201	51/65	0.98	0.07	10,49,98,117	0
14	CLA	F	202	45/65	0.98	0.08	60,89,119,125	0
14	CLA	A	809	65/65	0.98	0.08	12,58,97,102	0
14	CLA	A	810	65/65	0.98	0.07	18,73,122,135	0
14	CLA	A	825	59/65	0.98	0.07	23,57,97,109	0
14	CLA	A	826	65/65	0.98	0.08	45,74,105,108	0
14	CLA	L	204	65/65	0.98	0.06	2,15,46,67	0
14	CLA	L	205	65/65	0.98	0.06	2,19,91,104	0
14	CLA	L	206	65/65	0.98	0.06	2,20,49,59	0
14	CLA	A	827	65/65	0.98	0.06	3,42,119,141	0
14	CLA	X	1701	45/65	0.98	0.07	49,78,108,114	0
15	PQN	A	845	33/33	0.98	0.09	61,89,118,121	0
14	CLA	A	803	65/65	0.98	0.07	16,41,61,82	0
14	CLA	A	829	65/65	0.98	0.08	33,59,84,91	0
17	BCR	A	849	40/40	0.98	0.11	51,93,145,150	0
14	CLA	A	830	65/65	0.98	0.08	29,62,92,95	0
17	BCR	A	851	40/40	0.98	0.06	15,47,82,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CLA	A	831	65/65	0.98	0.08	29,61,84,92	0
14	CLA	A	832	50/65	0.98	0.07	6,35,65,91	0
17	BCR	B	845	40/40	0.98	0.07	16,50,105,117	0
17	BCR	B	846	40/40	0.98	0.07	27,53,73,79	0
14	CLA	A	834	65/65	0.98	0.06	2,11,39,45	0
14	CLA	A	812	65/65	0.98	0.10	55,87,118,120	0
17	BCR	F	203	40/40	0.98	0.10	17,68,100,121	0
17	BCR	I	101	40/40	0.98	0.06	2,2,24,41	0
17	BCR	J	103	40/40	0.98	0.07	34,76,98,103	0
17	BCR	J	104	40/40	0.98	0.07	52,90,119,124	0
14	CLA	A	837	45/65	0.98	0.06	54,78,101,111	0
17	BCR	M	103	40/40	0.98	0.06	2,22,50,56	0
14	CLA	A	838	51/65	0.98	0.07	10,33,53,76	0
14	CLA	A	804	65/65	0.98	0.07	33,72,99,106	0
14	CLA	A	857	65/65	0.98	0.07	12,39,65,76	0
19	LHG	A	854	49/49	0.98	0.09	12,58,82,92	0
19	LHG	B	850	23/49	0.98	0.07	46,85,113,119	0
14	CLA	B	804	54/65	0.98	0.07	2,22,41,48	0
21	LMT	L	202	35/35	0.98	0.07	48,116,152,165	0
14	CLA	A	805	59/65	0.98	0.08	48,72,99,115	0
14	CLA	B	803	65/65	0.99	0.05	2,7,27,38	0
14	CLA	B	824	54/65	0.99	0.05	21,38,60,61	0
14	CLA	A	835	65/65	0.99	0.05	2,6,35,63	0
15	PQN	B	842	33/33	0.99	0.07	27,47,66,70	0
14	CLA	B	805	65/65	0.99	0.06	2,30,63,75	0
14	CLA	B	827	65/65	0.99	0.06	2,22,74,76	0
14	CLA	B	806	65/65	0.99	0.05	2,24,51,64	0
14	CLA	B	829	65/65	0.99	0.05	2,21,53,72	0
14	CLA	B	807	65/65	0.99	0.06	2,9,40,63	0
17	BCR	A	852	40/40	0.99	0.06	2,37,64,66	0
14	CLA	B	831	49/65	0.99	0.05	8,43,70,96	0
14	CLA	B	808	65/65	0.99	0.05	2,13,45,50	0
14	CLA	B	809	65/65	0.99	0.06	2,12,40,63	0
14	CLA	B	810	65/65	0.99	0.05	2,2,33,43	0
14	CLA	B	835	45/65	0.99	0.06	18,53,81,85	0
17	BCR	B	848	40/40	0.99	0.05	2,8,34,35	0
14	CLA	A	802	65/65	0.99	0.05	2,12,28,48	0
14	CLA	A	819	54/65	0.99	0.06	35,68,90,106	0
13	CL0	A	801	65/65	0.99	0.05	2,20,45,48	0
17	BCR	I	103	40/40	0.99	0.04	2,2,21,39	0
14	CLA	B	839	47/65	0.99	0.06	23,48,67,79	0
14	CLA	B	840	65/65	0.99	0.04	2,2,26,31	0

Continued on next page...

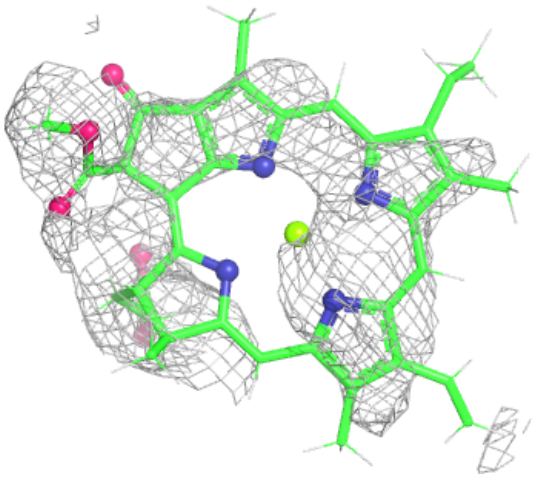
Continued from previous page...

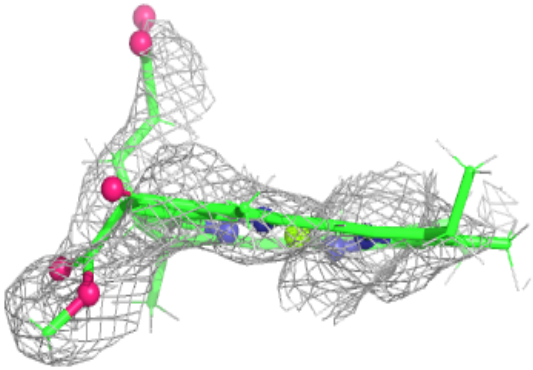
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	CLA	B	841	65/65	0.99	0.04	2,3,26,29	0
17	BCR	L	201	40/40	0.99	0.04	2,8,33,35	0
17	BCR	L	208	40/40	0.99	0.05	2,12,60,72	0
14	CLA	B	814	65/65	0.99	0.06	19,51,86,91	0
14	CLA	A	839	65/65	0.99	0.05	2,32,71,94	0
14	CLA	A	840	47/65	0.99	0.04	2,28,49,67	0
18	LMG	B	849	55/55	0.99	0.06	2,31,57,61	0
14	CLA	A	841	65/65	0.99	0.07	6,42,97,106	0
14	CLA	A	842	65/65	0.99	0.06	11,47,91,109	0
19	LHG	A	855	27/49	0.99	0.06	20,53,90,91	0
14	CLA	A	843	65/65	0.99	0.05	2,2,24,33	0
14	CLA	A	833	65/65	0.99	0.05	2,37,109,114	0
20	CA	B	801	1/1	0.99	0.07	43,43,43,43	0
14	CLA	A	821	43/65	0.99	0.07	46,104,144,150	0
14	CLA	B	802	65/65	0.99	0.06	2,23,44,50	0
16	SF4	A	846	8/8	1.00	0.02	3,20,62,92	0
20	CA	L	203	1/1	1.00	0.03	2,2,2,2	0
16	SF4	C	101	8/8	1.00	0.02	2,25,32,45	0
16	SF4	C	102	8/8	1.00	0.02	12,19,36,38	0

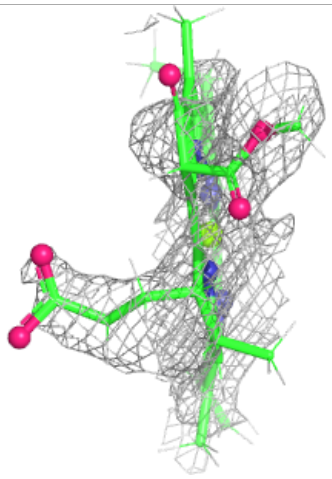
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA A 816:

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

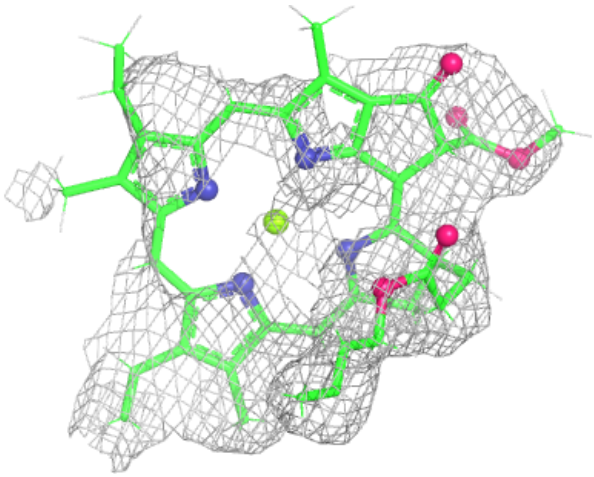


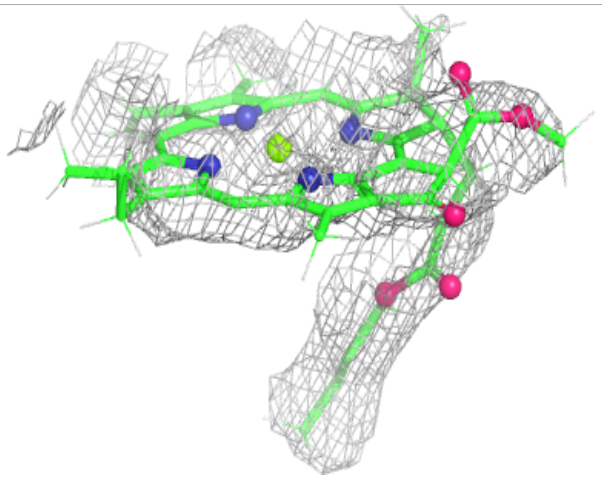


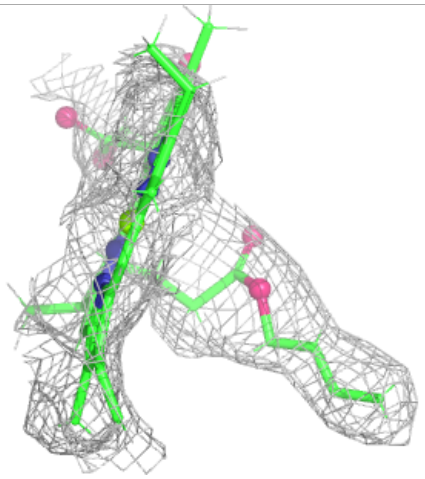


Electron density around CLA A 817:

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

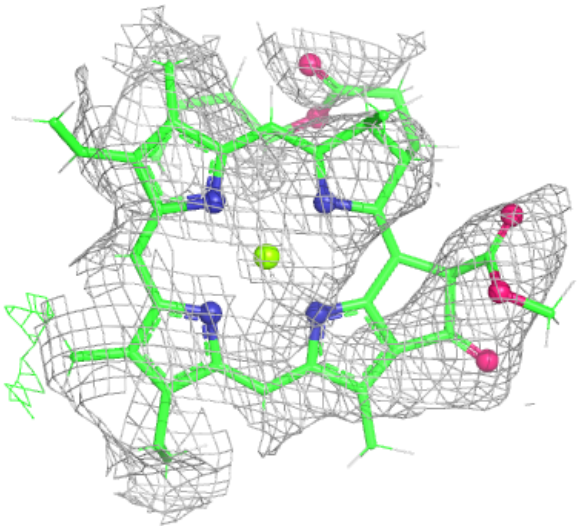


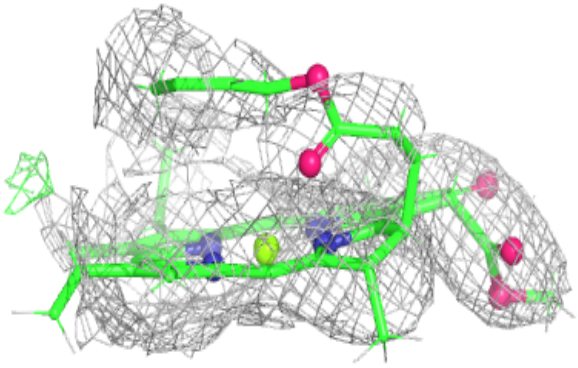


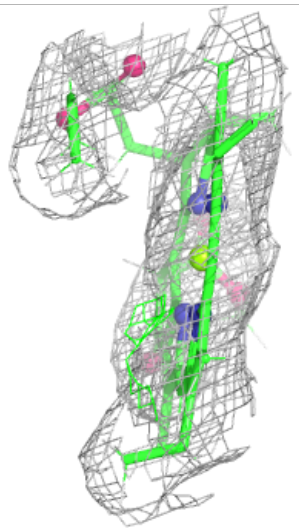


Electron density around CLA A 823:

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

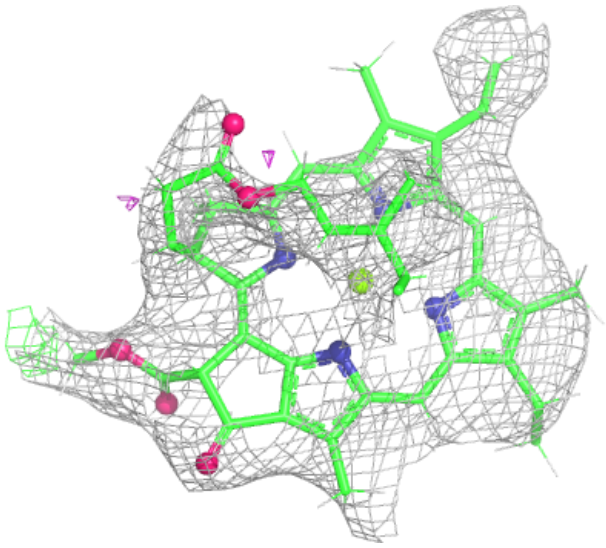


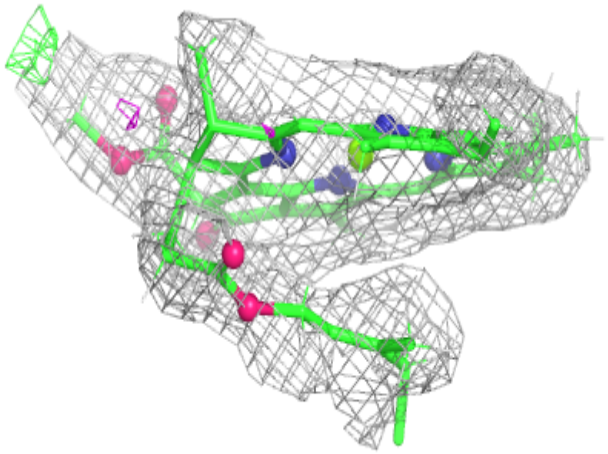


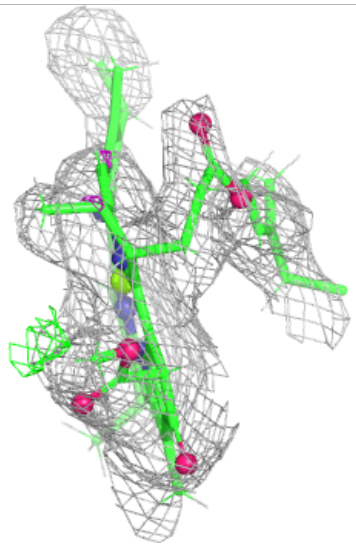


Electron density around CLA A 824:

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

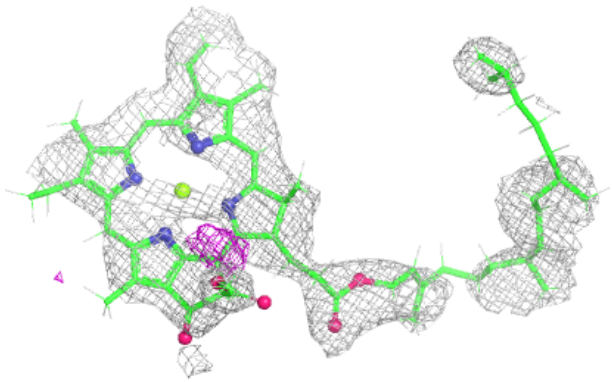


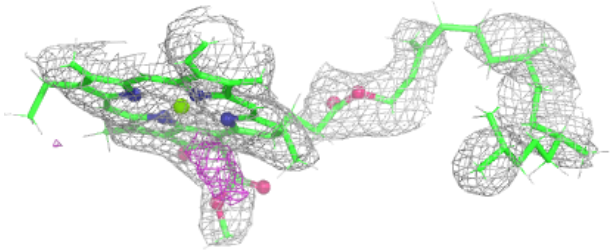


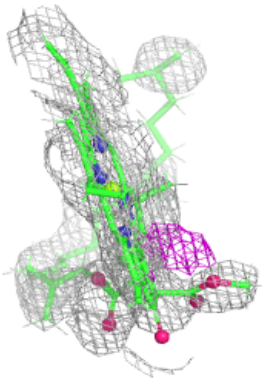


Electron density around CLA A 828:

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

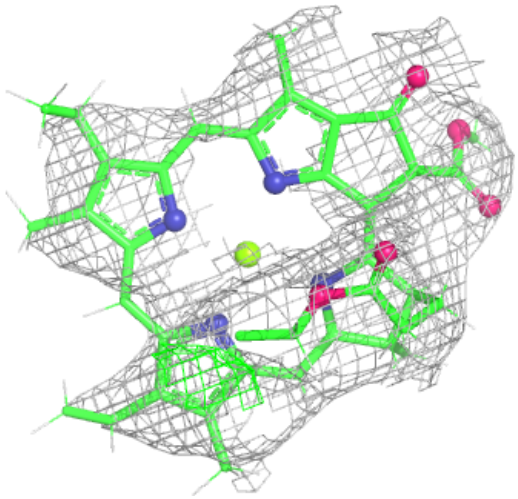


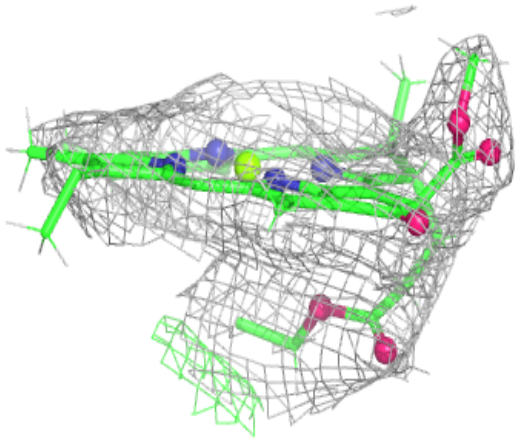


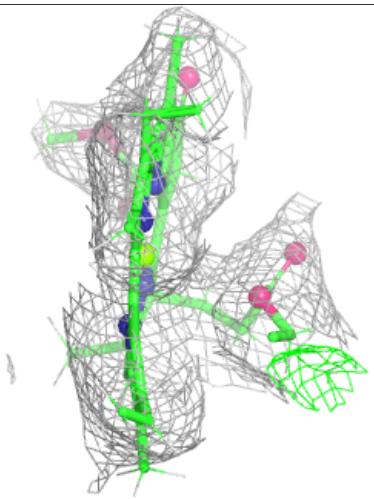


Electron density around CLA B 820:

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

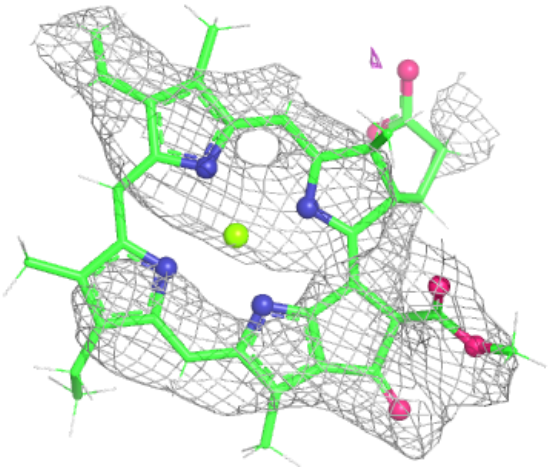


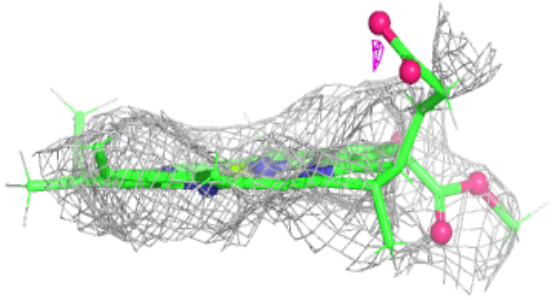


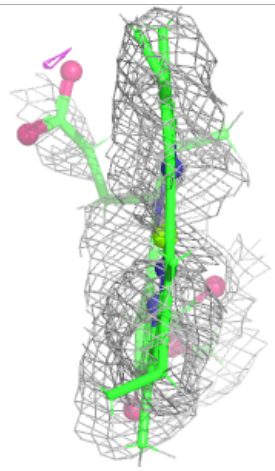


Electron density around CLA J 101:

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

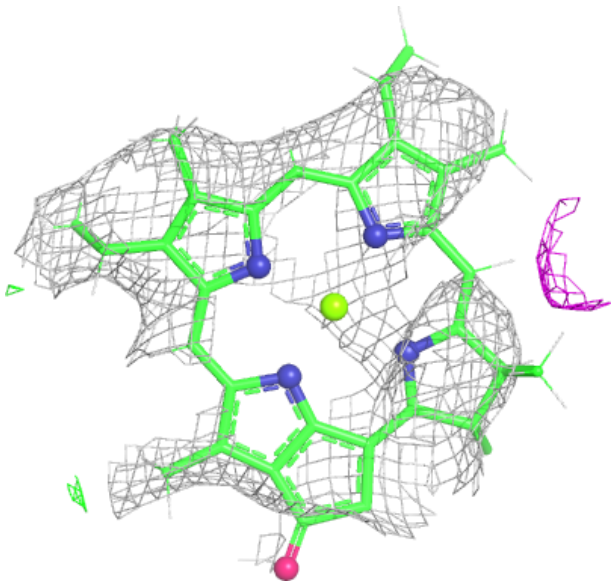


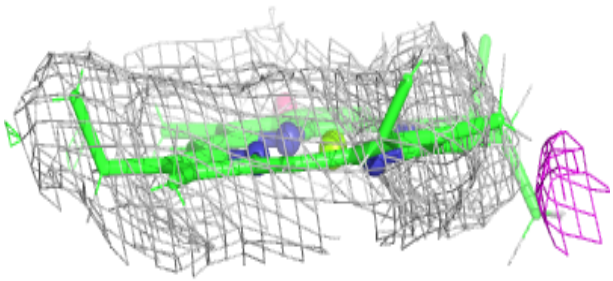


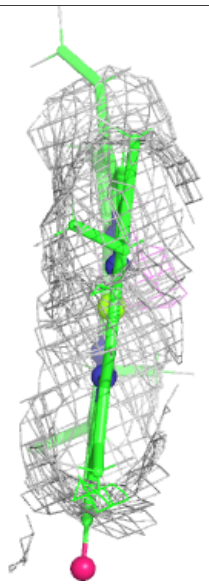


Electron density around CLA J 102:

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

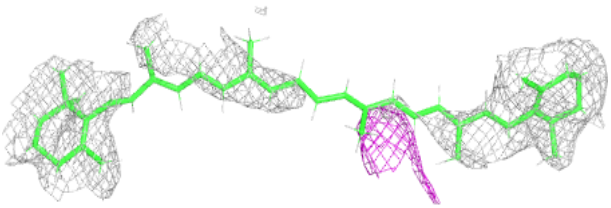


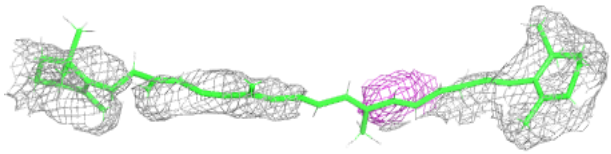


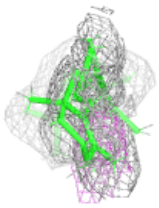


Electron density around BCR B 843:

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

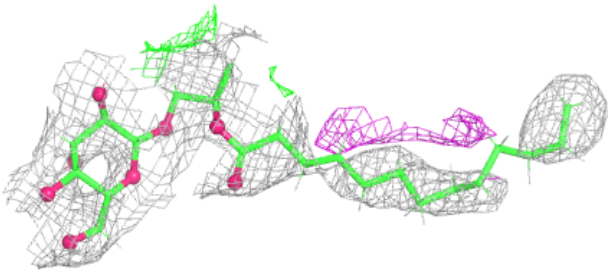


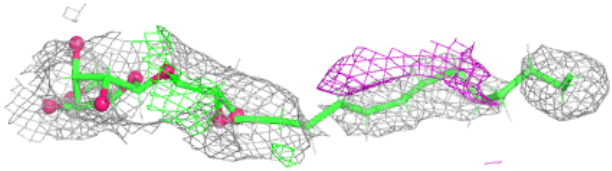


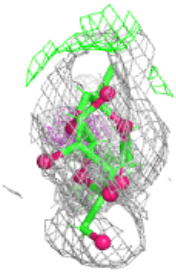


Electron density around LMG A 856:

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

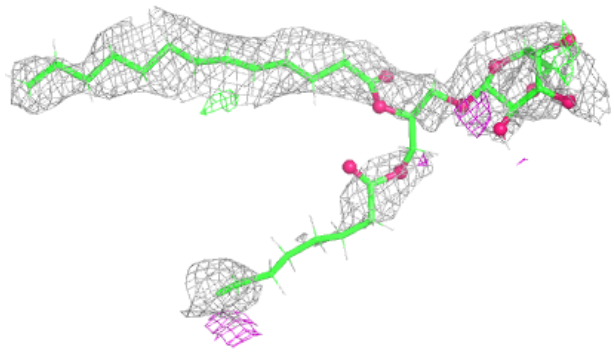


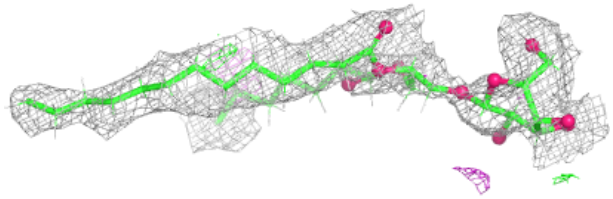


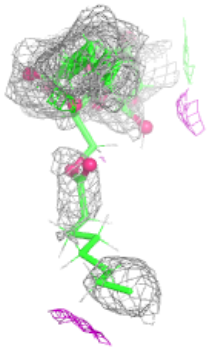


Electron density around LMG I 102:

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

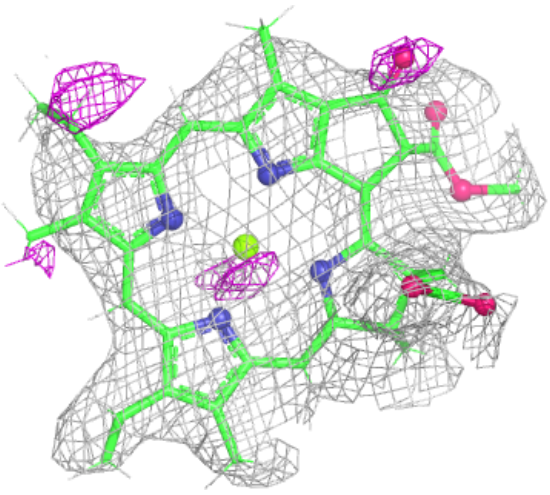


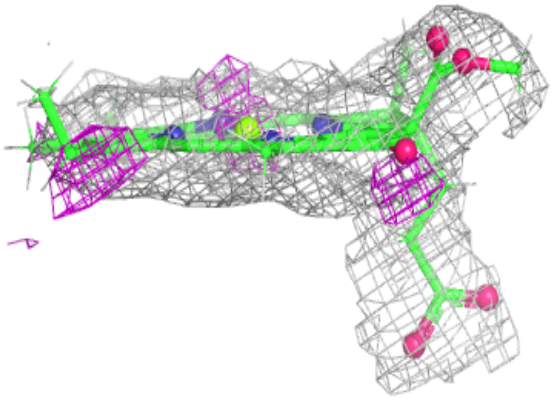




Electron density around CLA B 811:

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

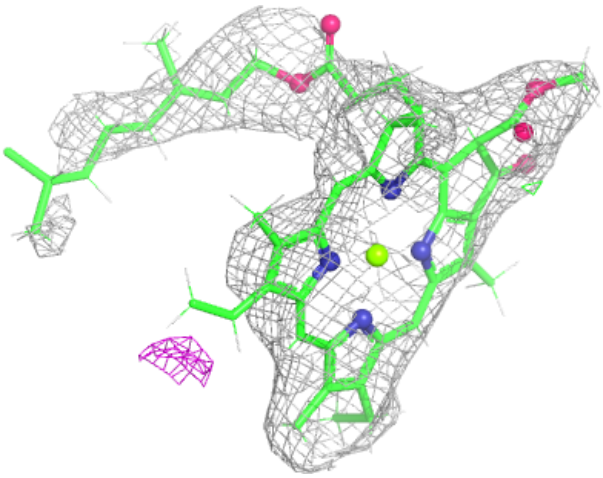


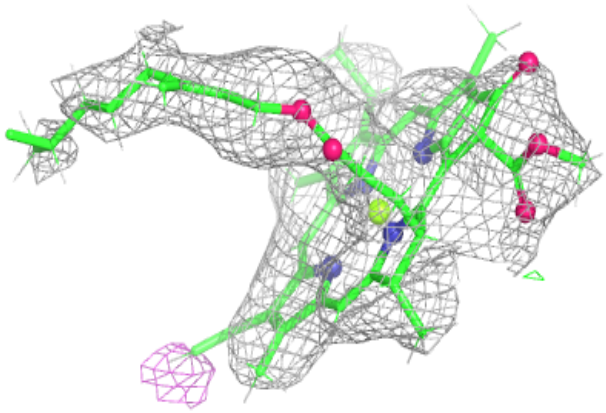


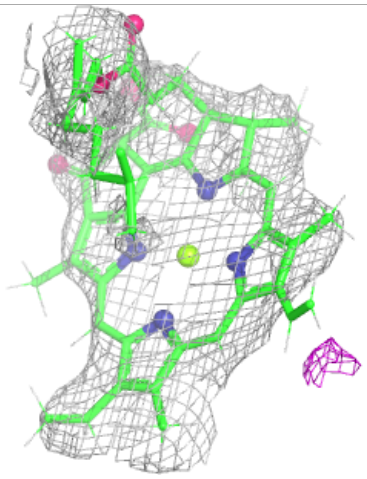


Electron density around CLA B 816:

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

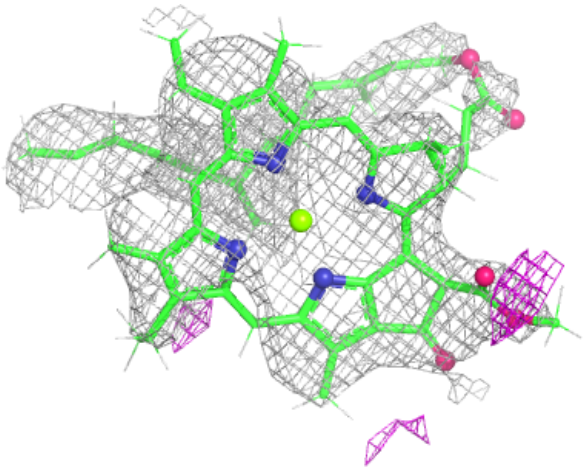


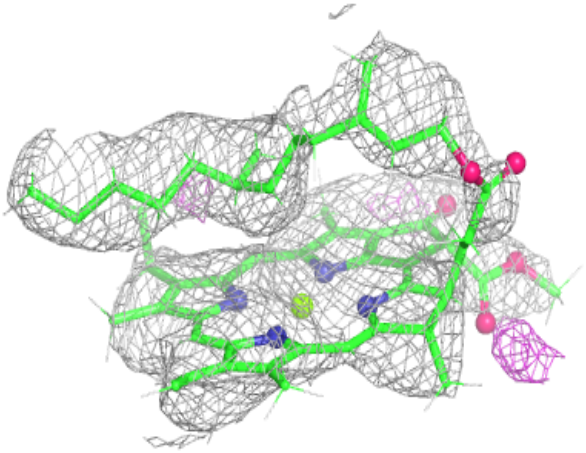


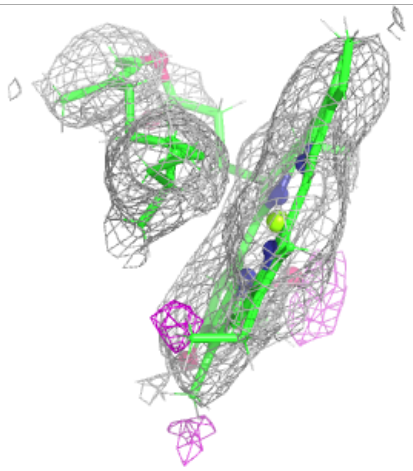


Electron density around CLA B 817:

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

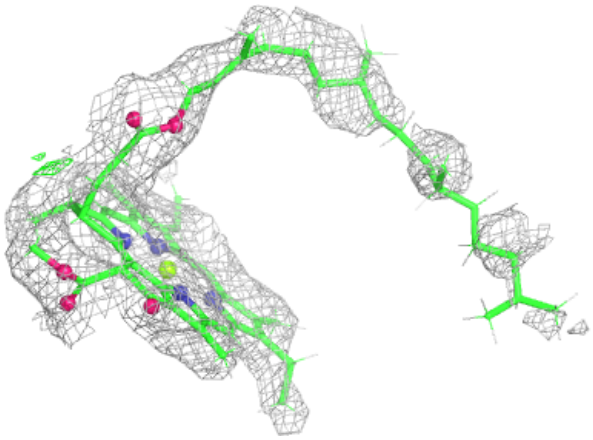


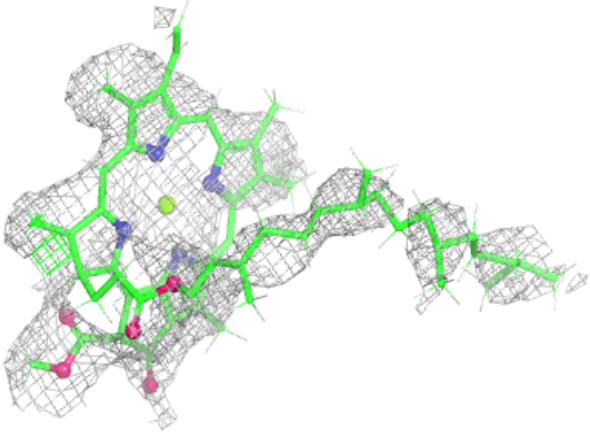


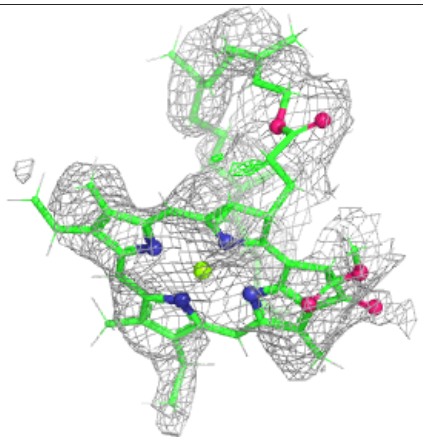


Electron density around CLA B 819:

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

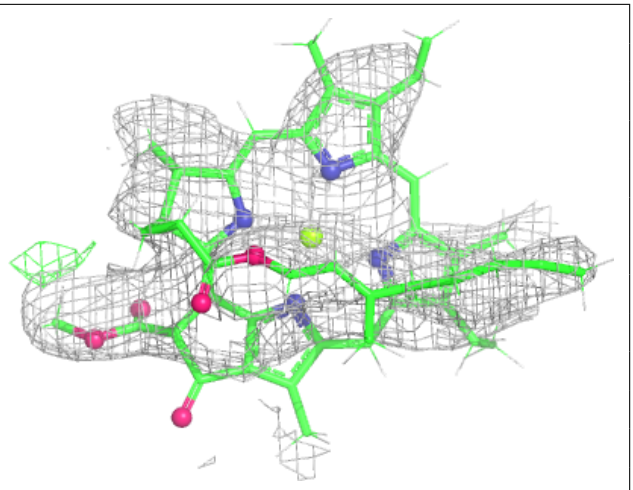




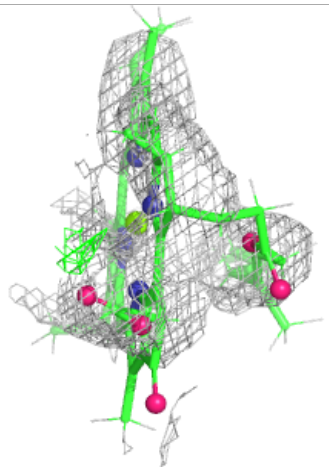


Electron density around CLA A 818:

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

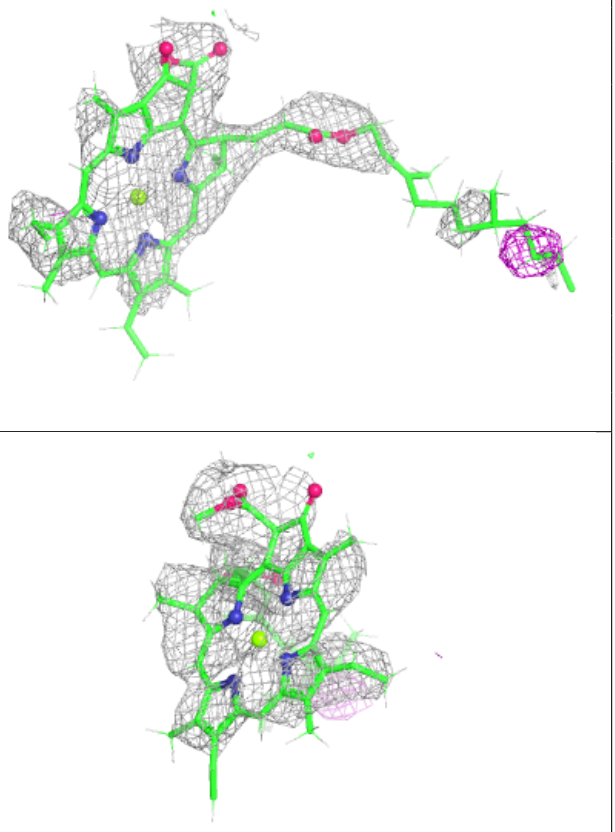






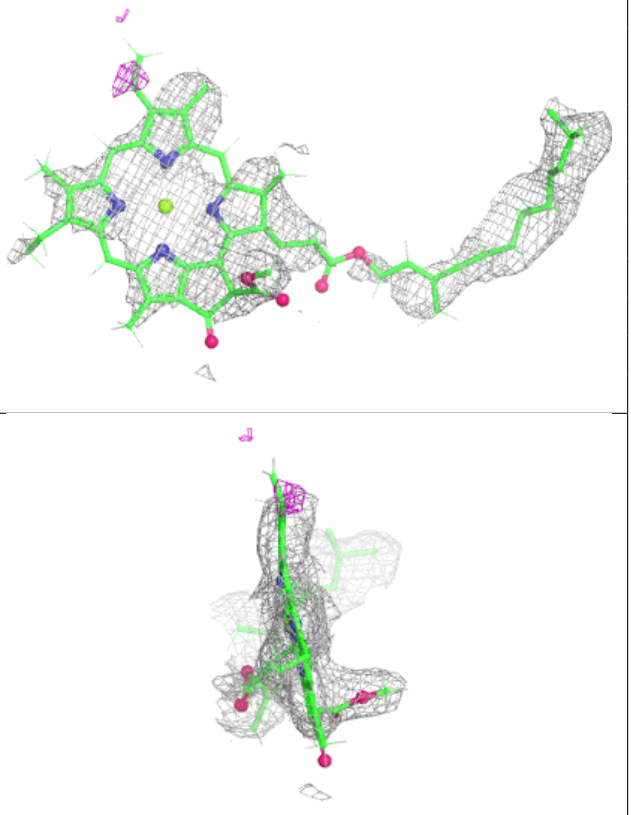
Electron density around CLA B 833:

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



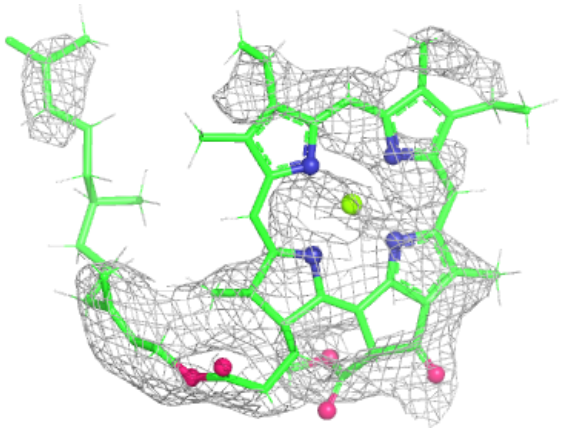
Electron density around CLA B 837:

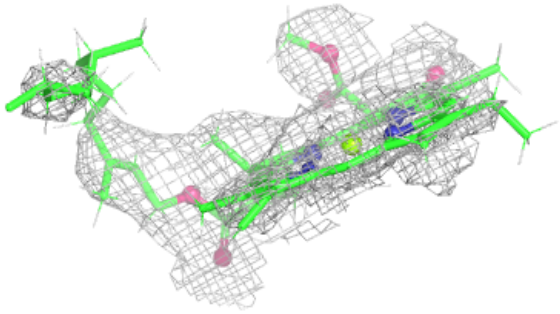
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

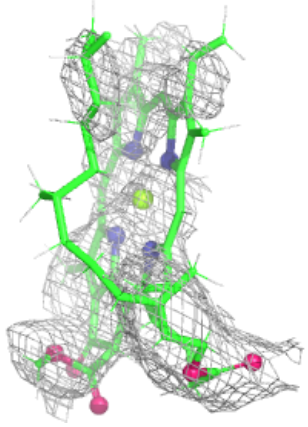


Electron density around CLA A 814:

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

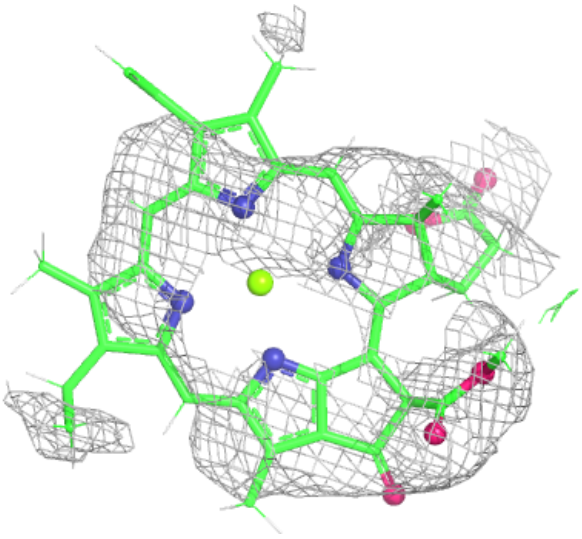


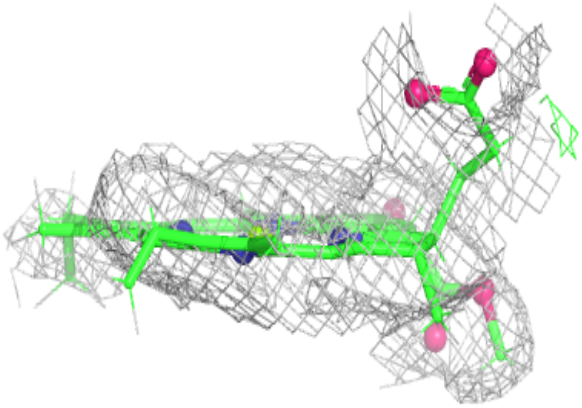


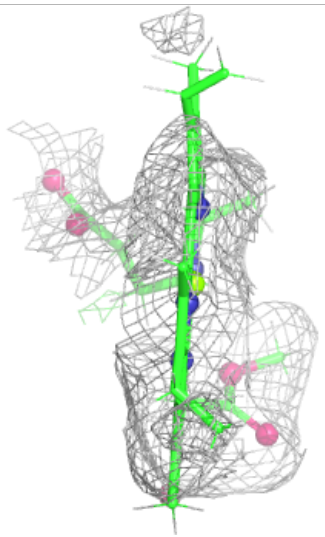


Electron density around CLA A 811:

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

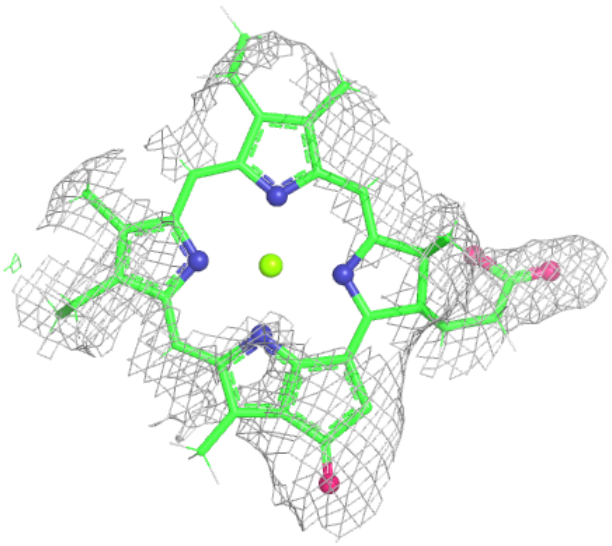


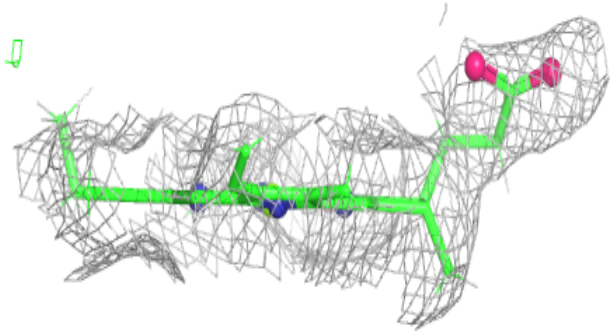


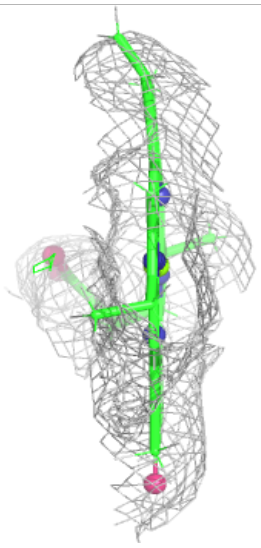


Electron density around CLA K 101:

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

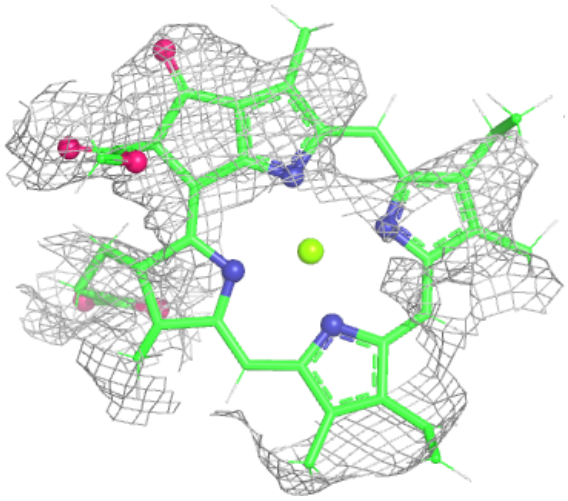


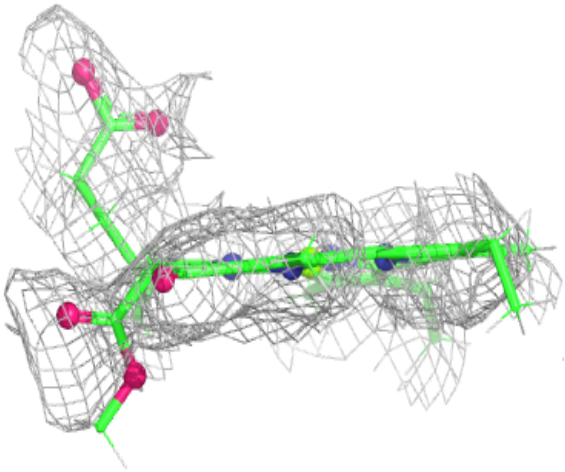


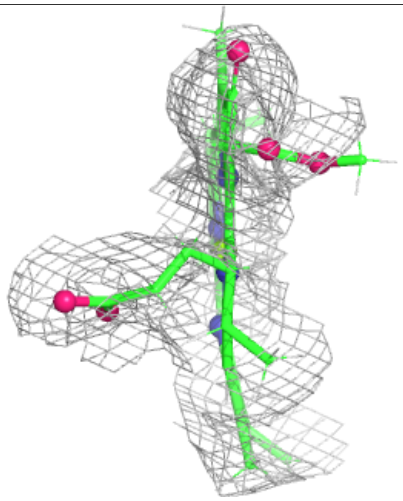


Electron density around CLA K 102:

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

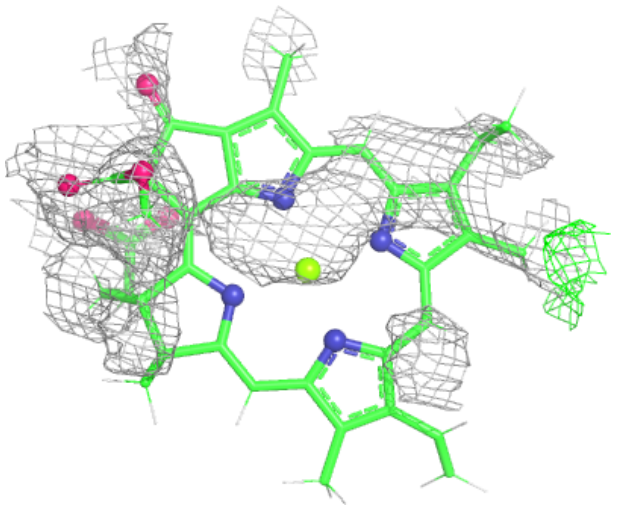


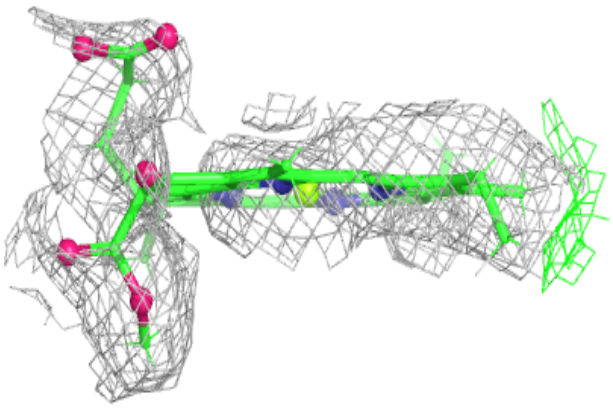


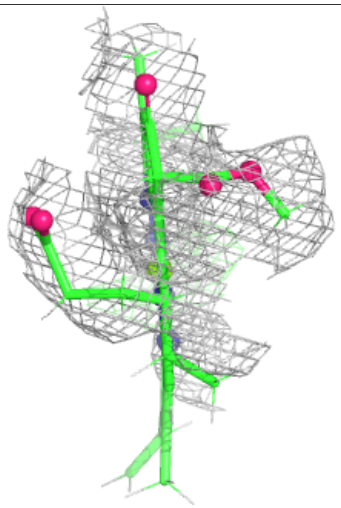


Electron density around CLA M 102:

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

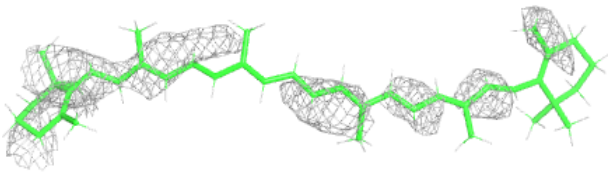


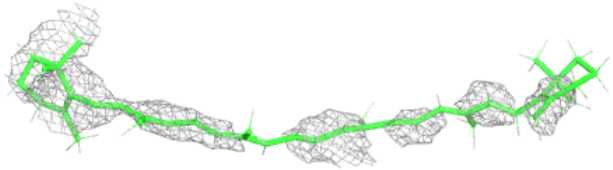


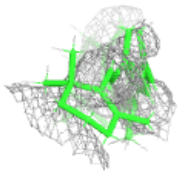


Electron density around BCR A 847:

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

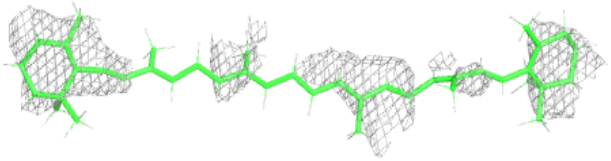


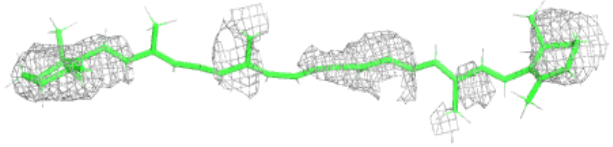


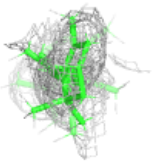


Electron density around BCR A 848:

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

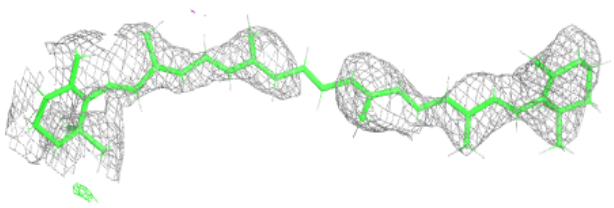


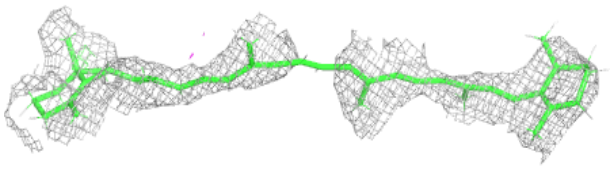


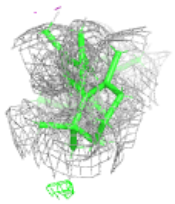


Electron density around BCR A 850:

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

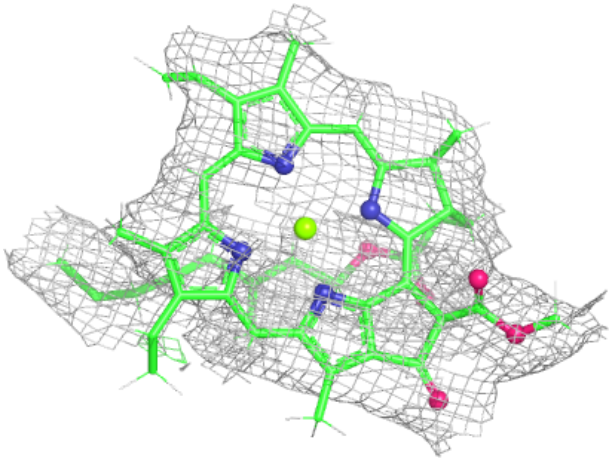


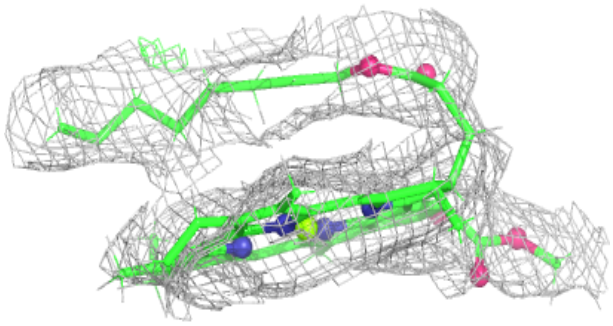




Electron density around CLA A 813:

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

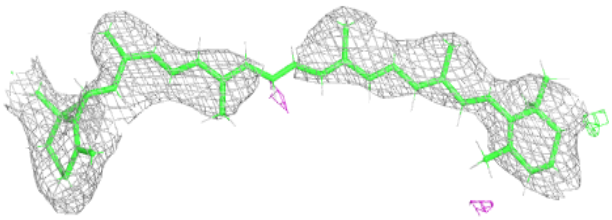


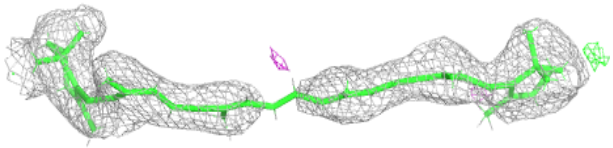


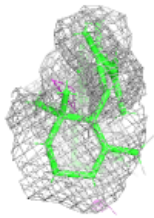


Electron density around BCR B 844:

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

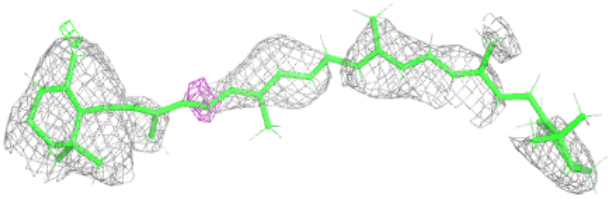


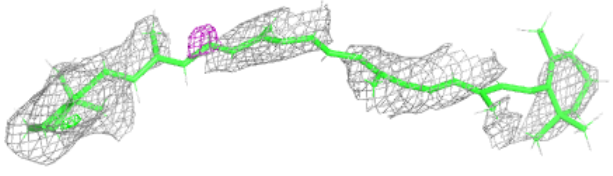


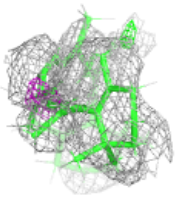


Electron density around BCR B 847:

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

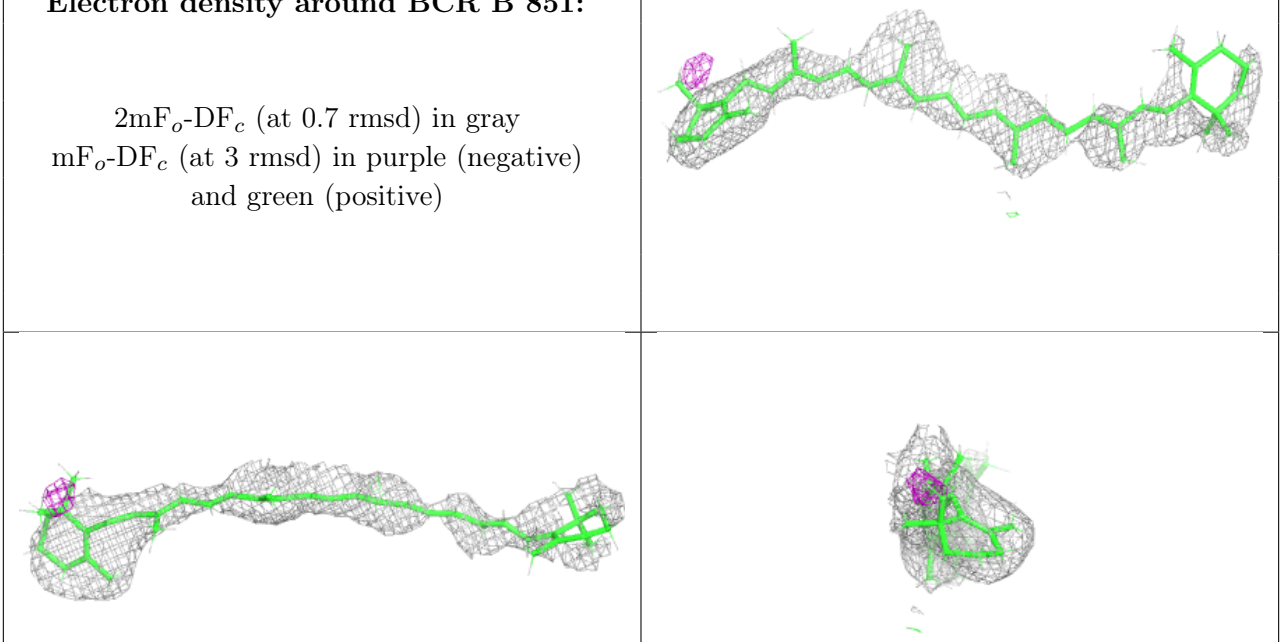






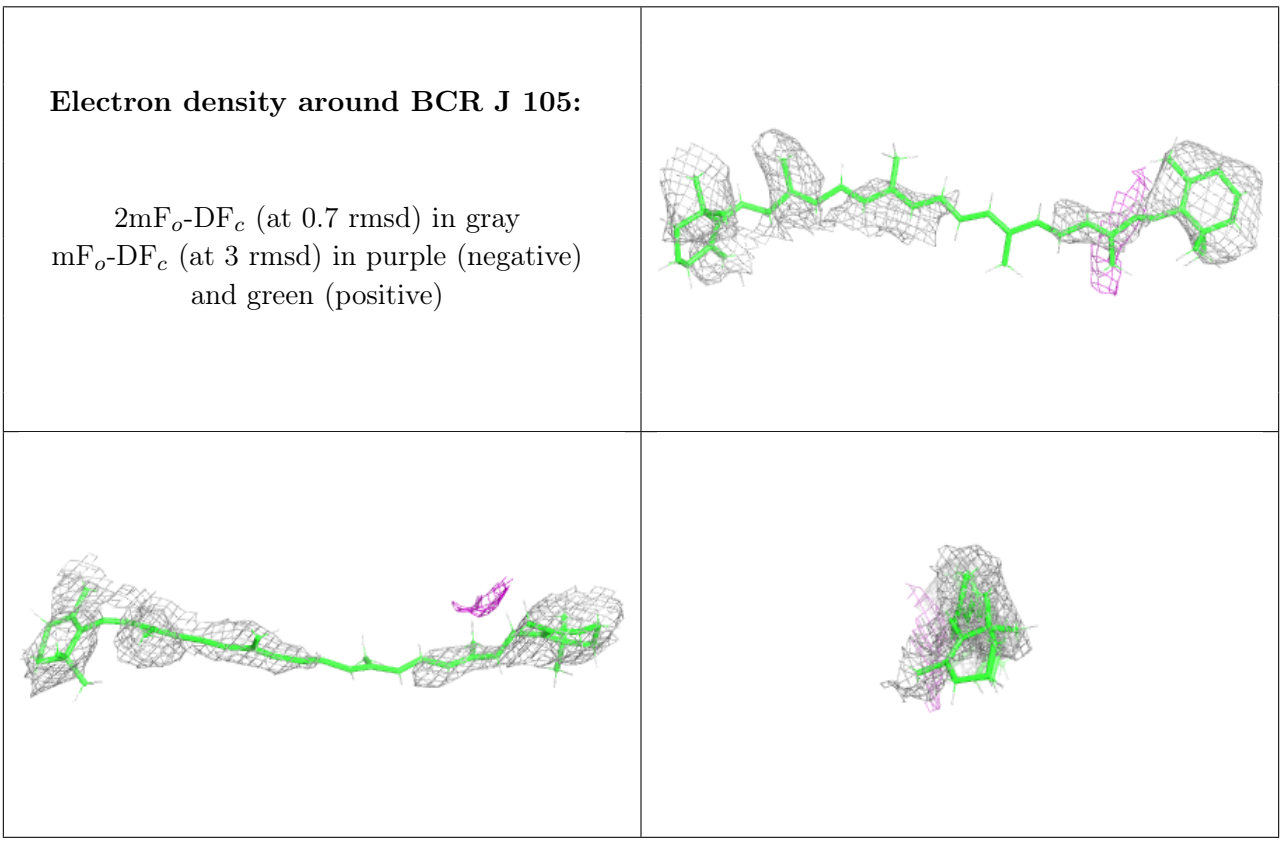
Electron density around BCR B 851:

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



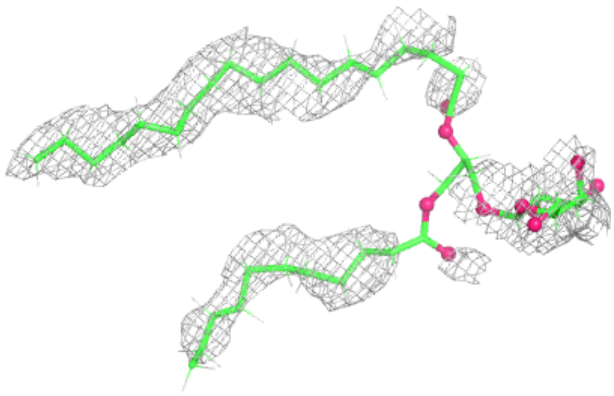
Electron density around BCR J 105:

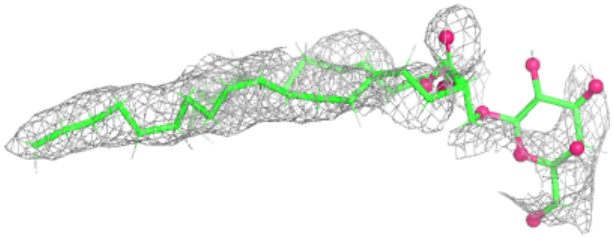
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

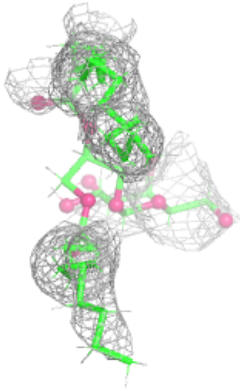


Electron density around LMG A 853:

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

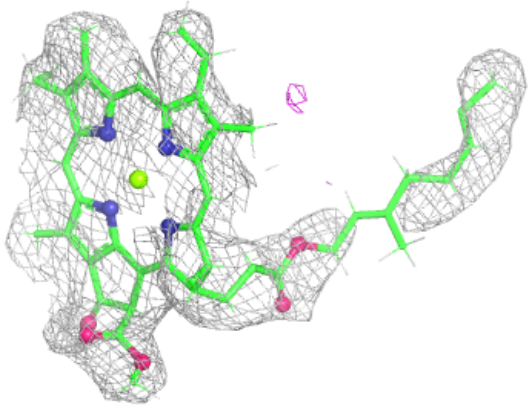


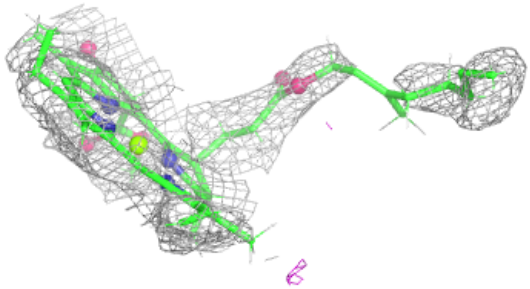


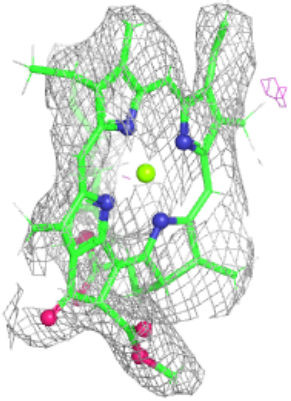


Electron density around CLA A 836:

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

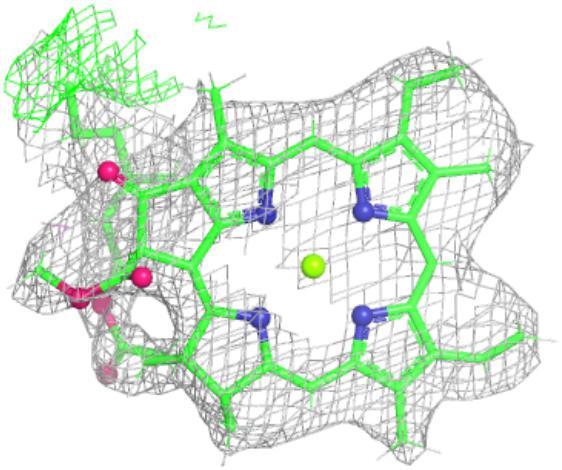


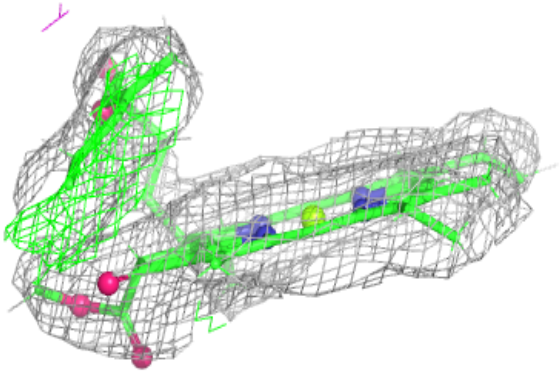


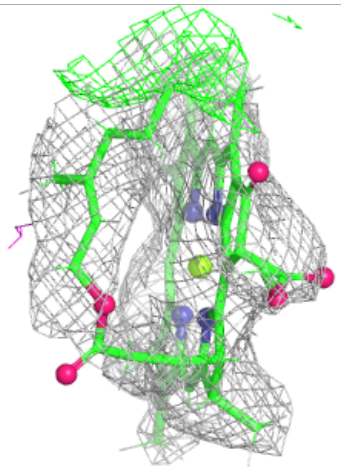


Electron density around CLA A 844:

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

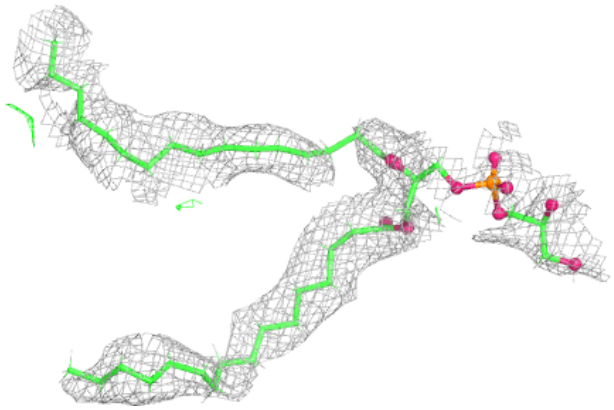


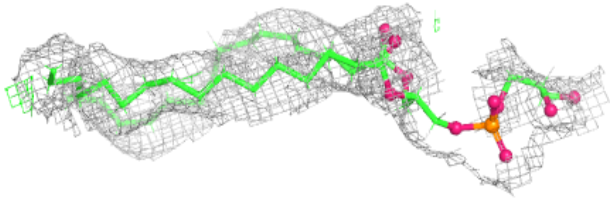


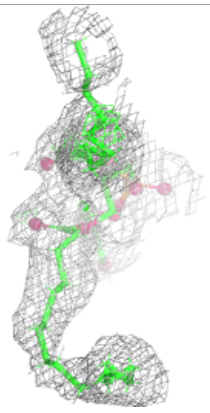


Electron density around LHG M 101:

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

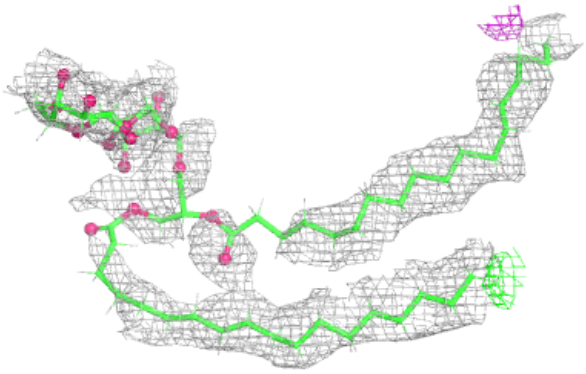


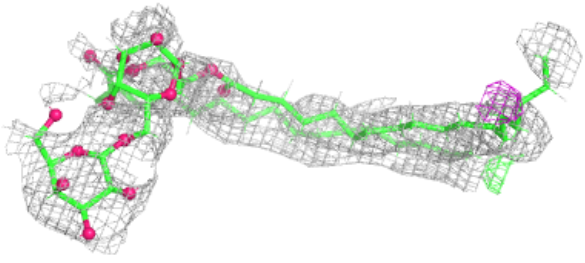


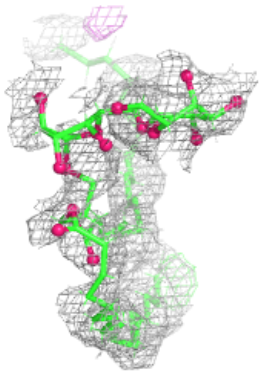


Electron density around DGD L 207:

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

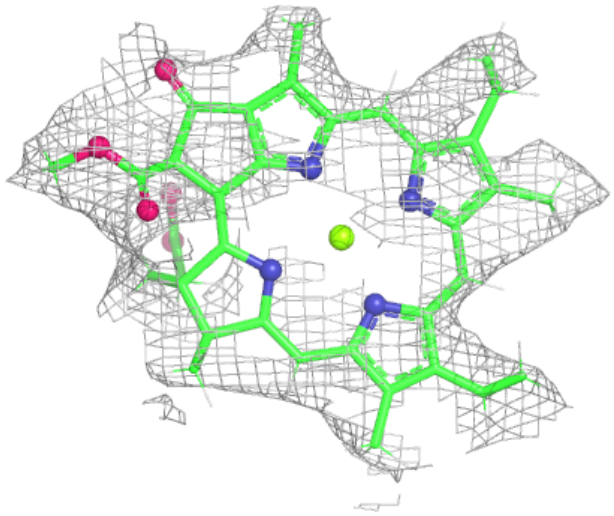


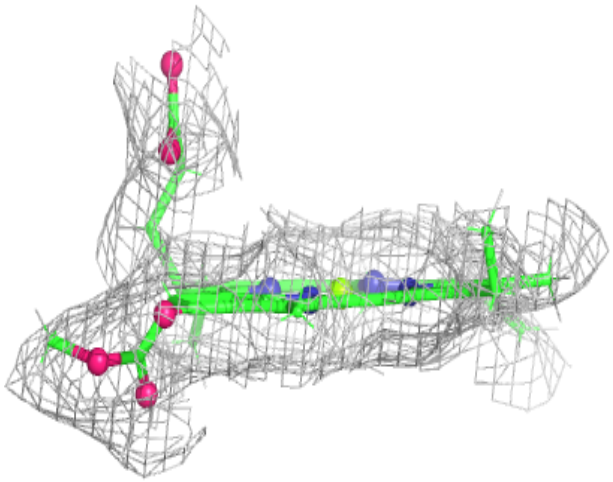


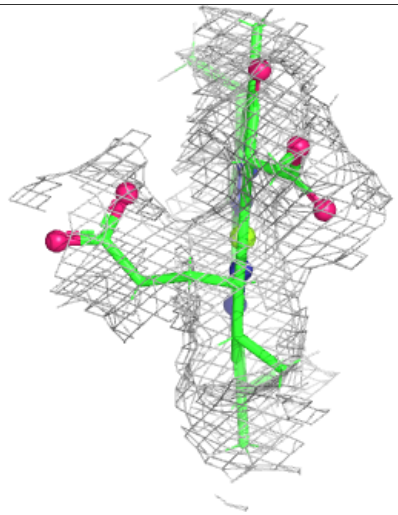


Electron density around CLA B 812:

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

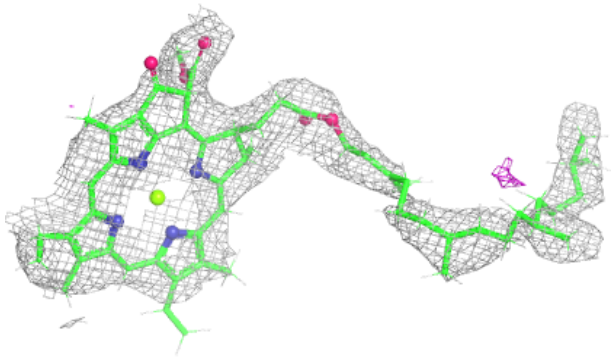


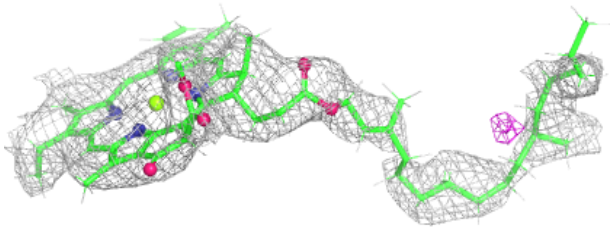


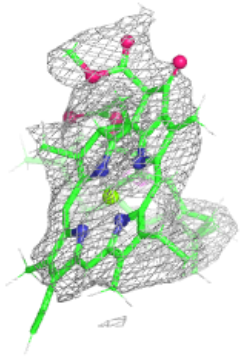


Electron density around CLA B 813:

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

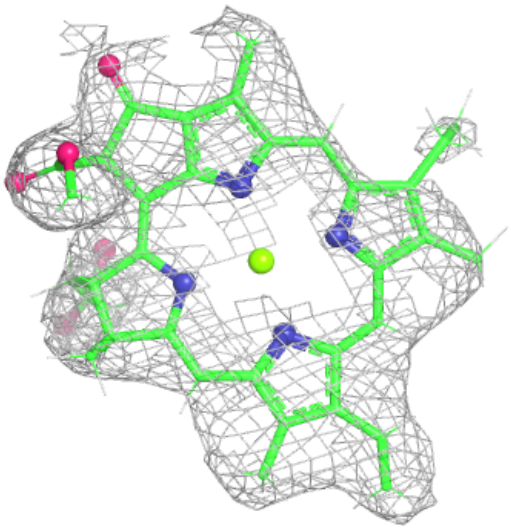


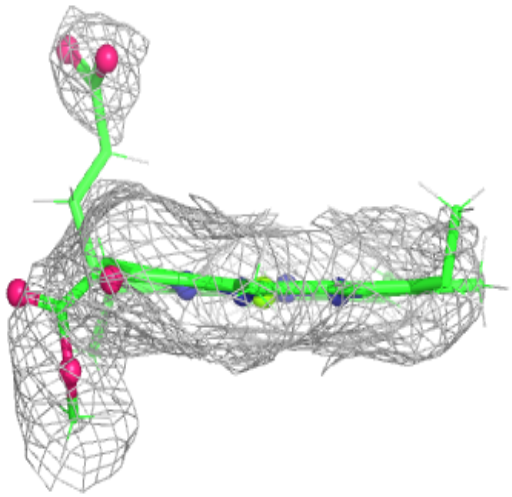


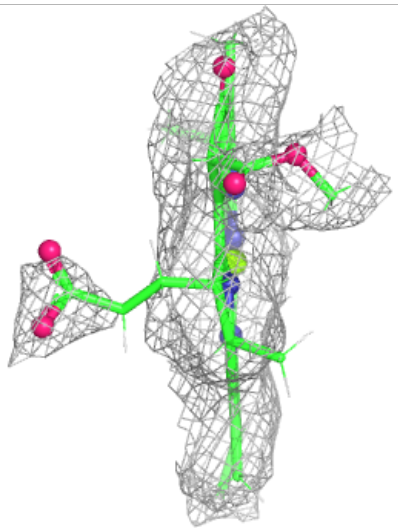


Electron density around CLA B 815:

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

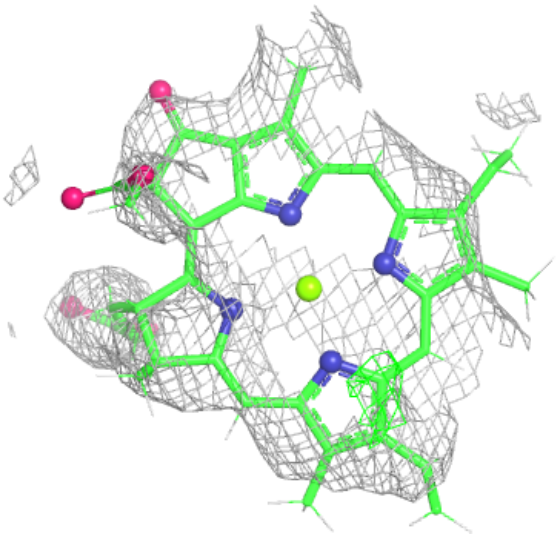


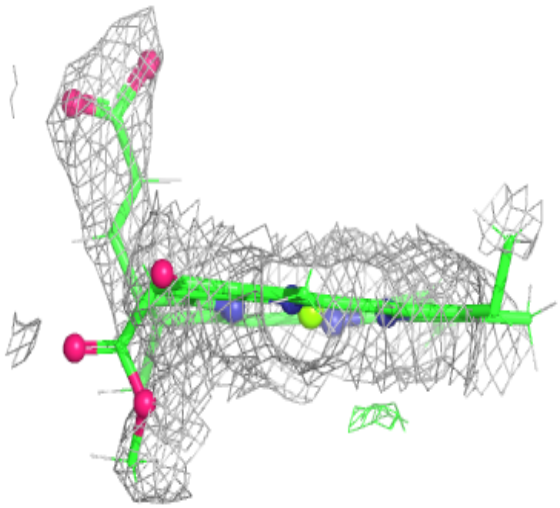


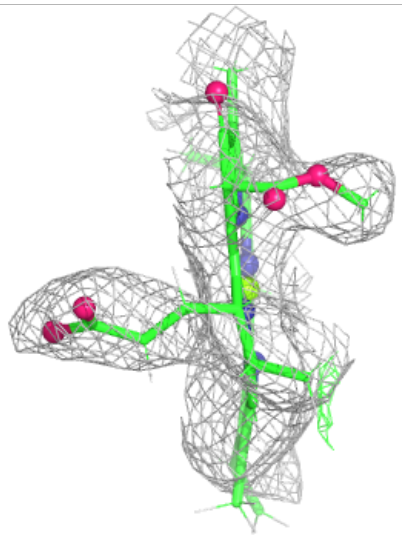


Electron density around CLA A 815:

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

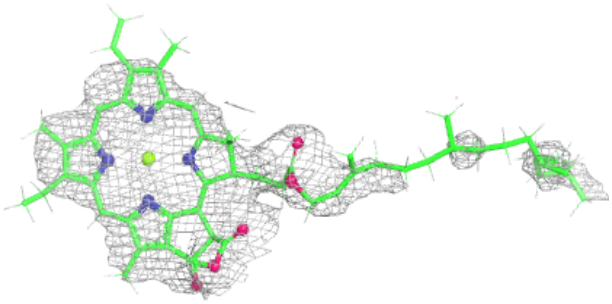


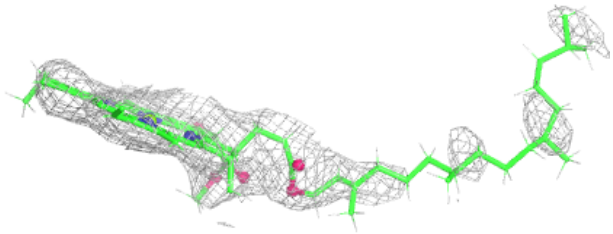


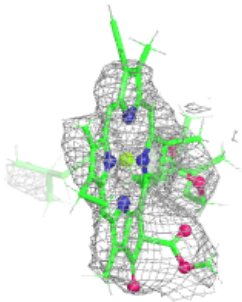


Electron density around CLA A 806:

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

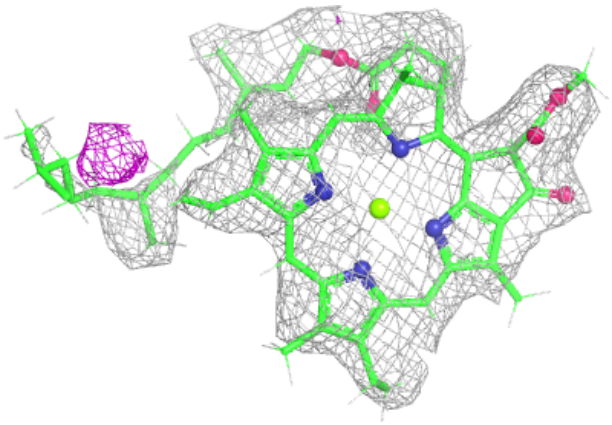


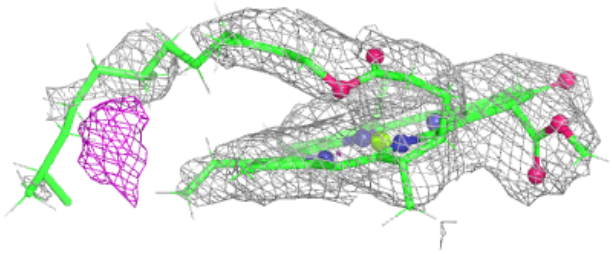




Electron density around CLA B 818:

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

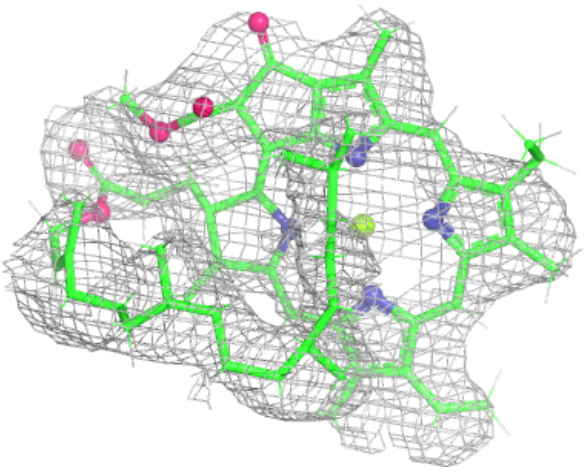


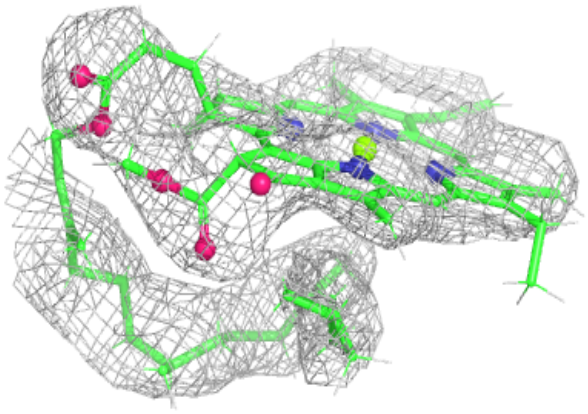


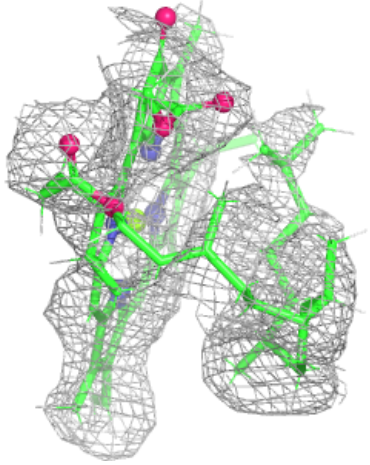


Electron density around CLA A 807:

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

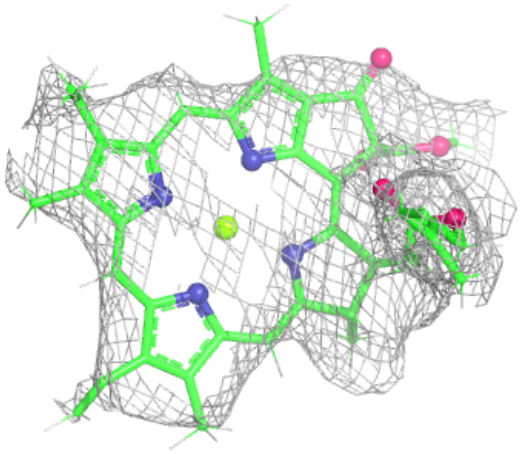


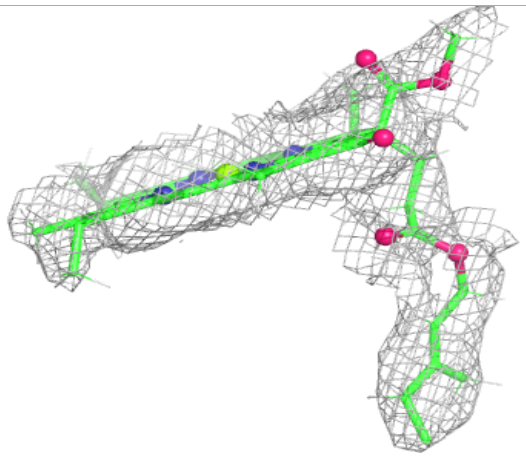


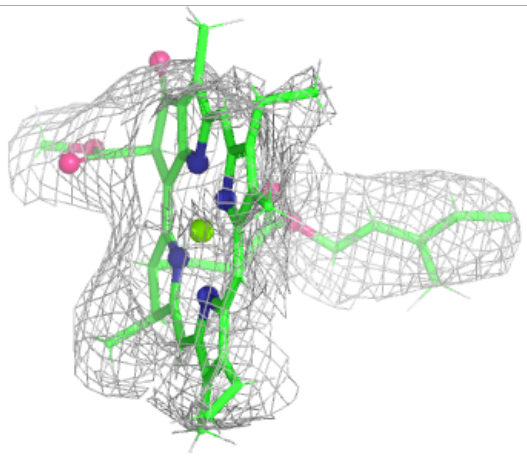


Electron density around CLA A 808:

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

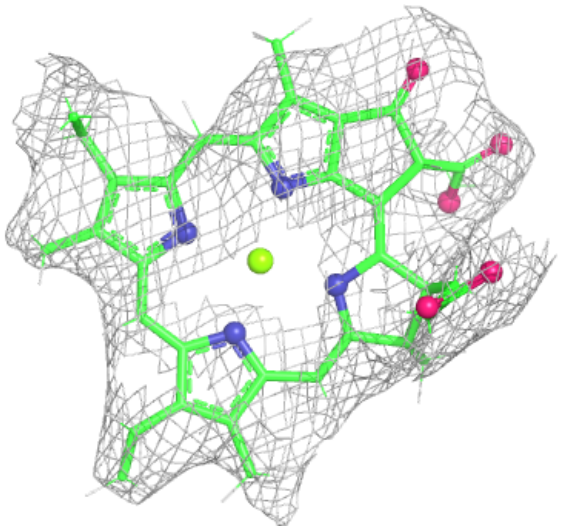


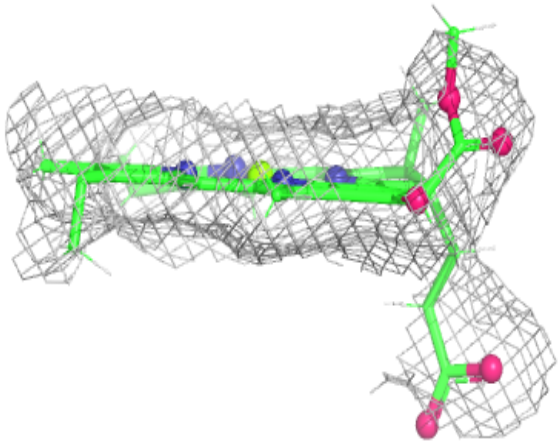


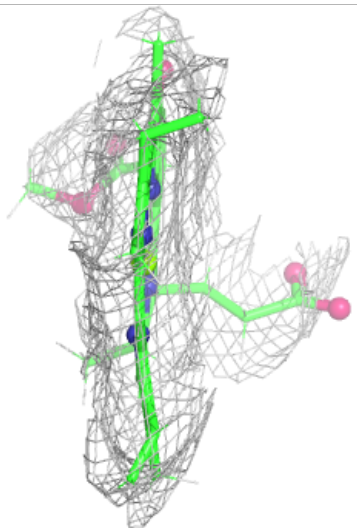


Electron density around CLA B 821:

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

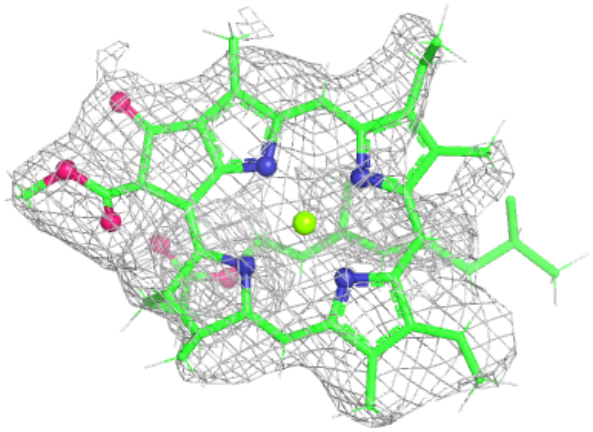


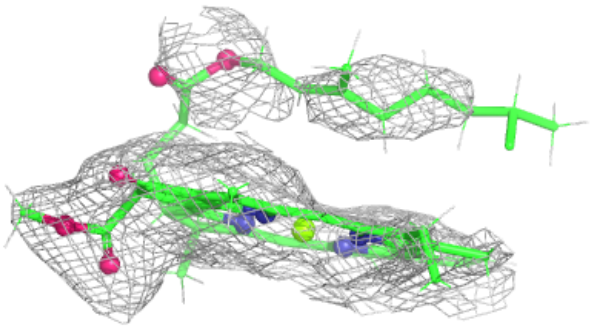


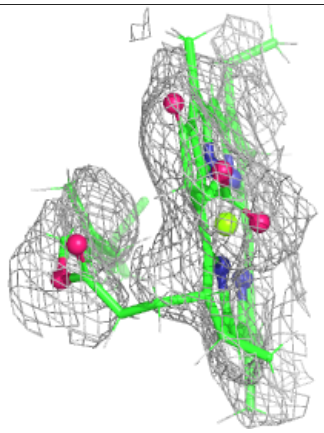


Electron density around CLA B 822:

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

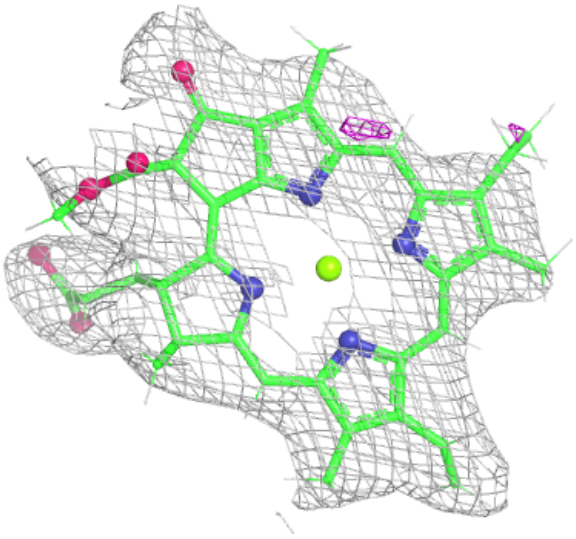


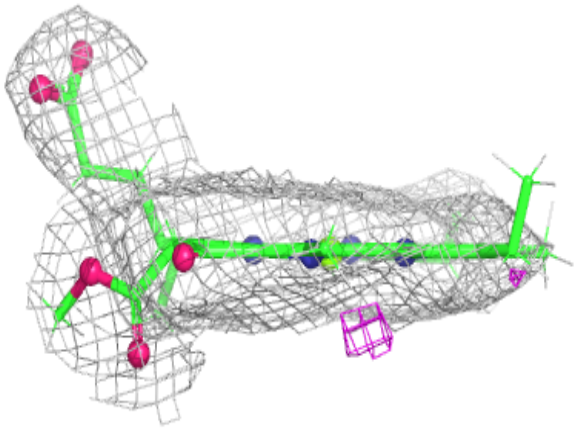


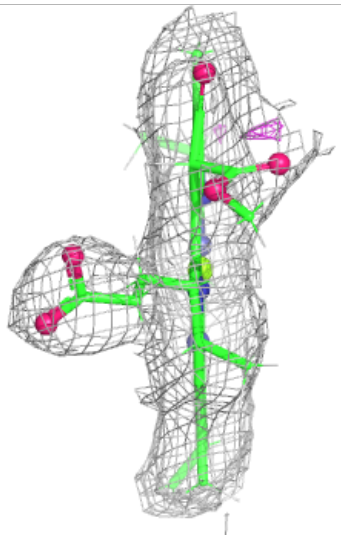


Electron density around CLA B 823:

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

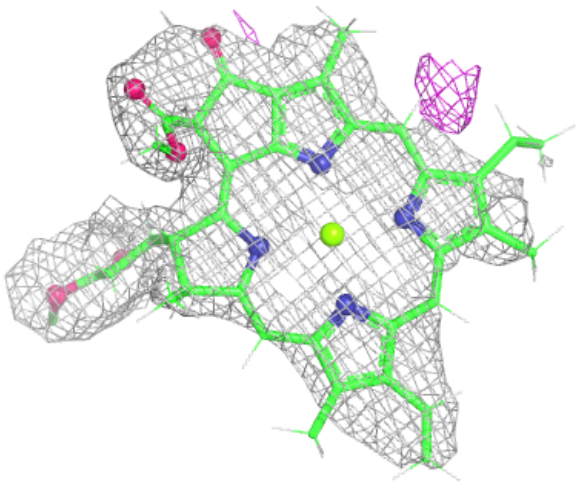


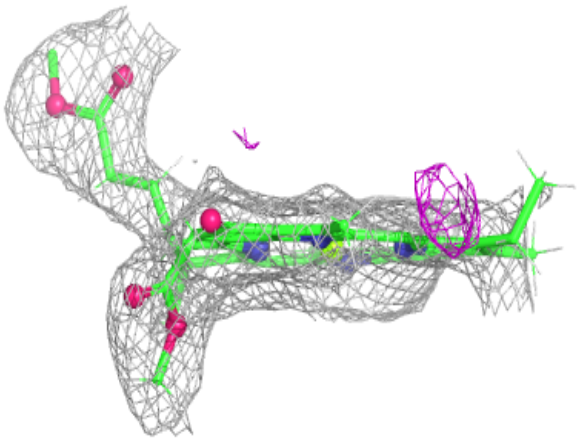


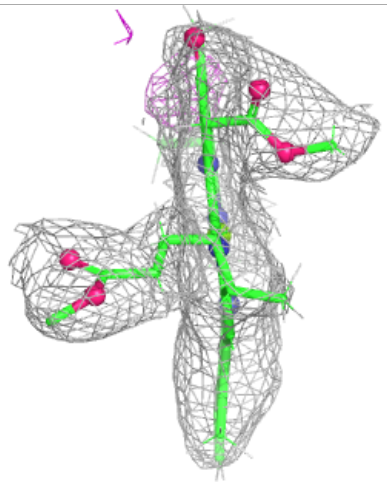


Electron density around CLA B 825:

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

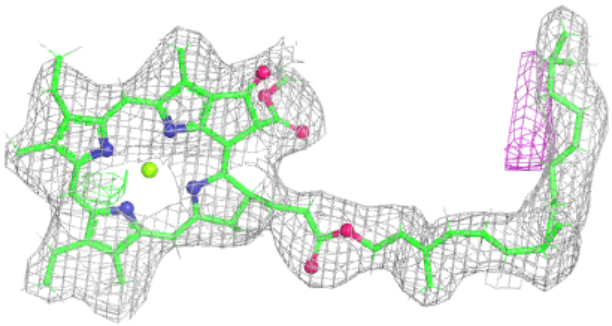


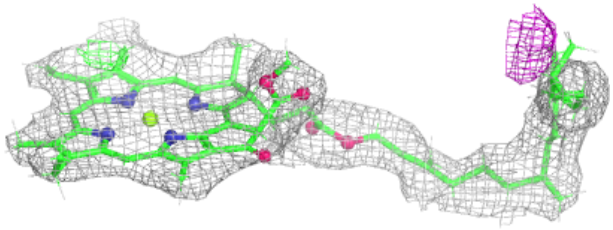


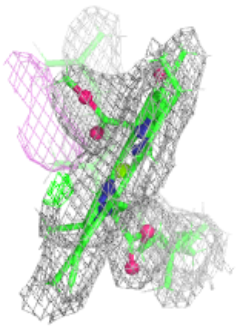


Electron density around CLA B 826:

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

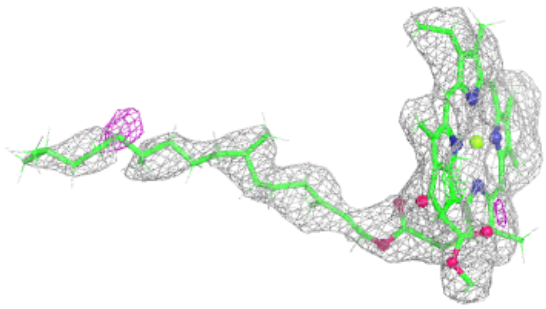


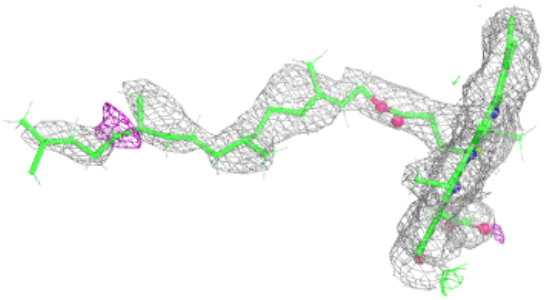


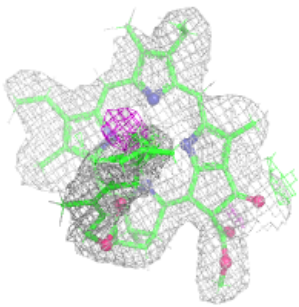


Electron density around CLA B 828:

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

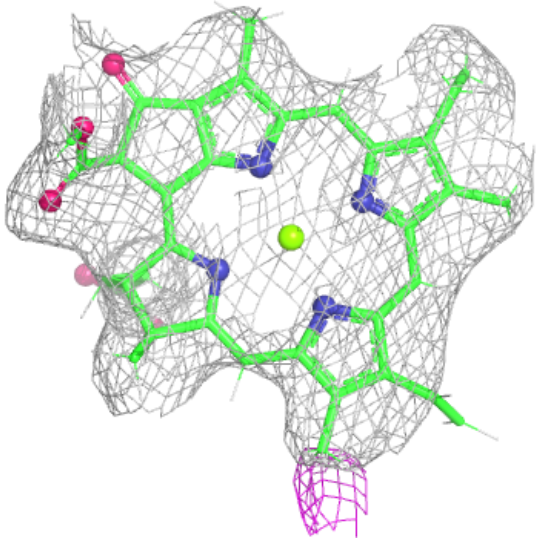


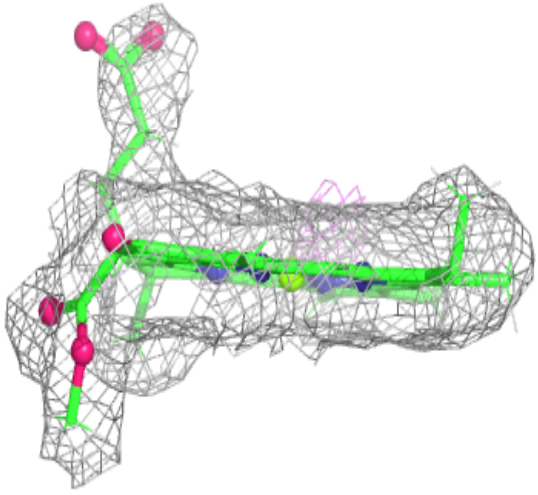


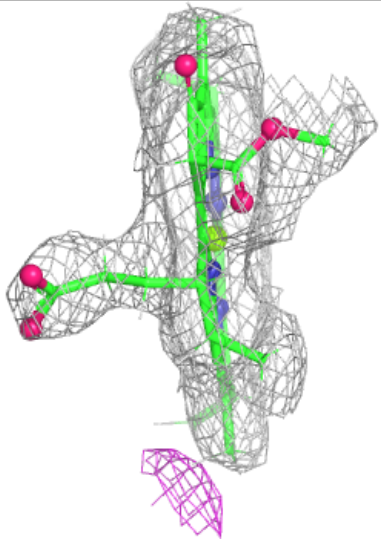


Electron density around CLA B 830:

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

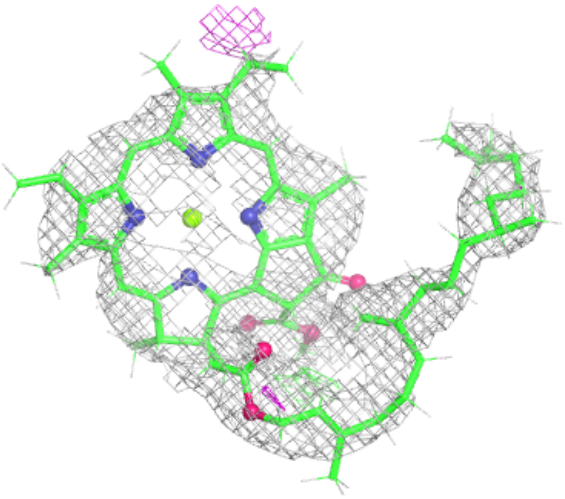


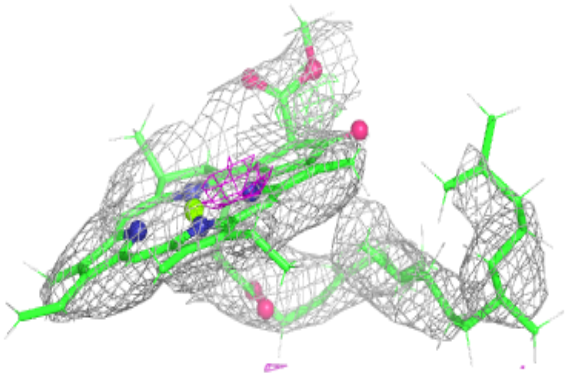


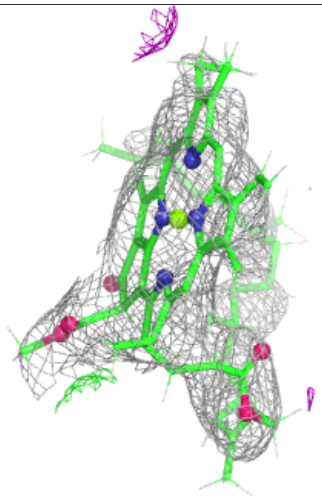


Electron density around CLA B 832:

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

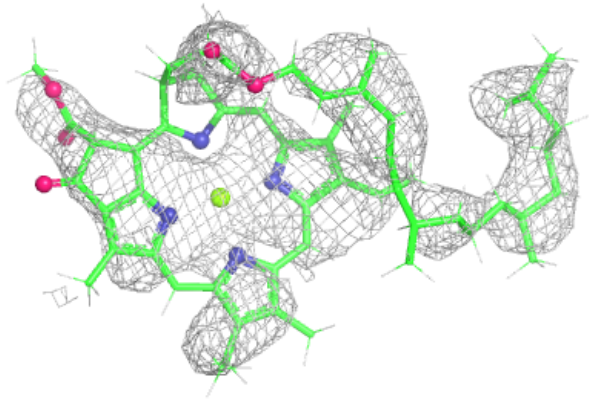


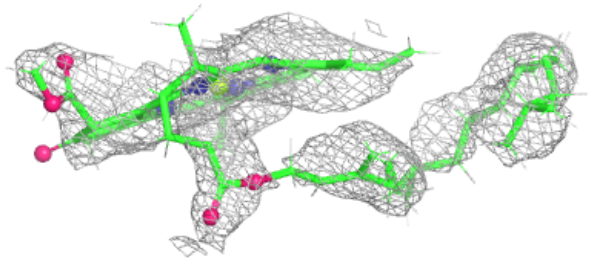


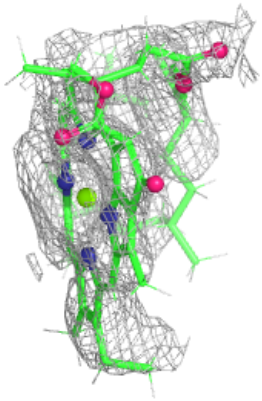


Electron density around CLA A 820:

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

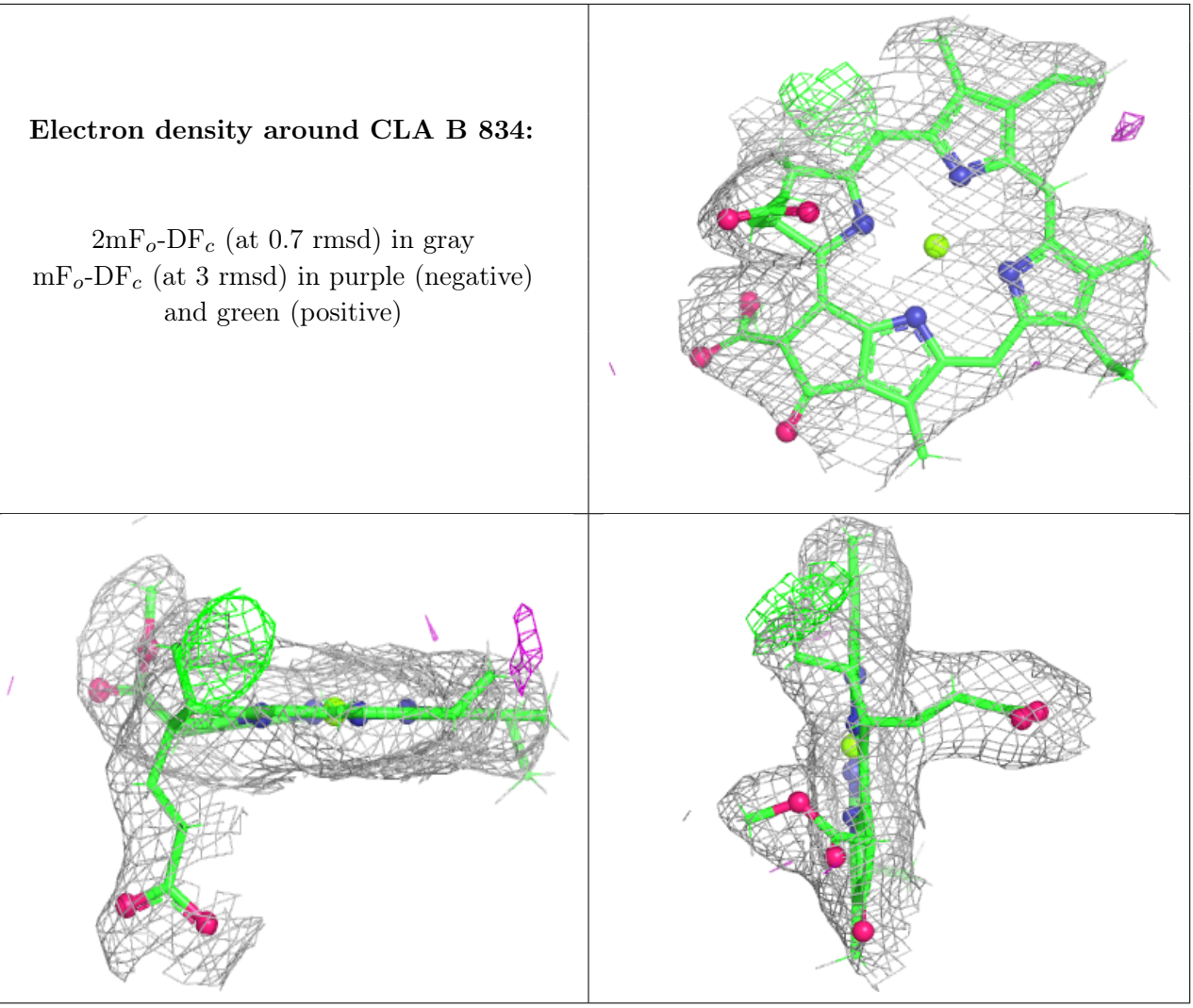






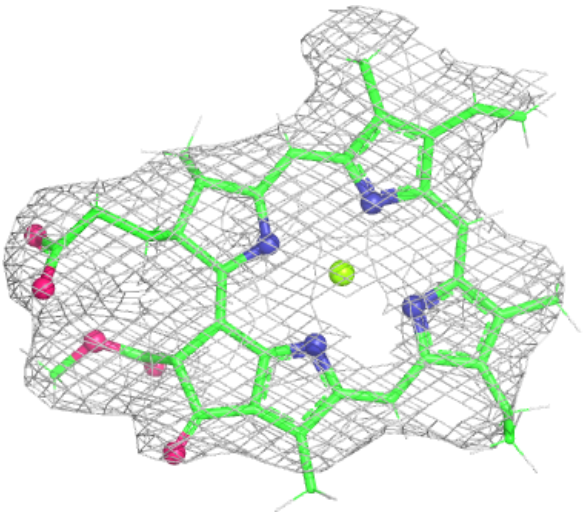
Electron density around CLA B 834:

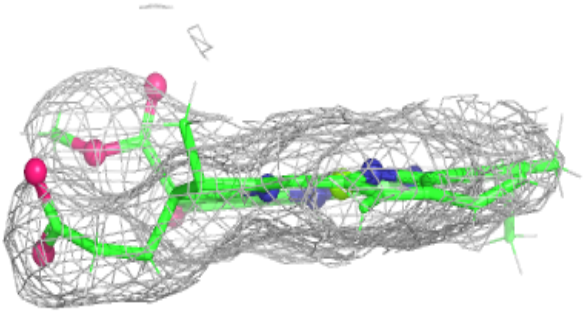
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 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)

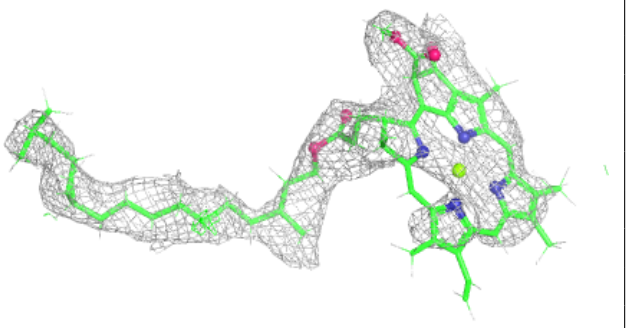


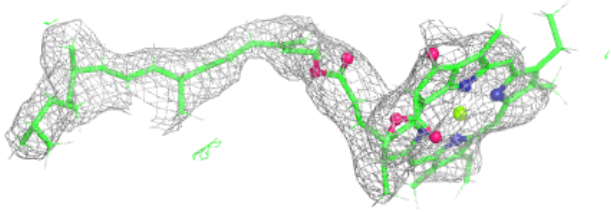




Electron density around CLA A 822:

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

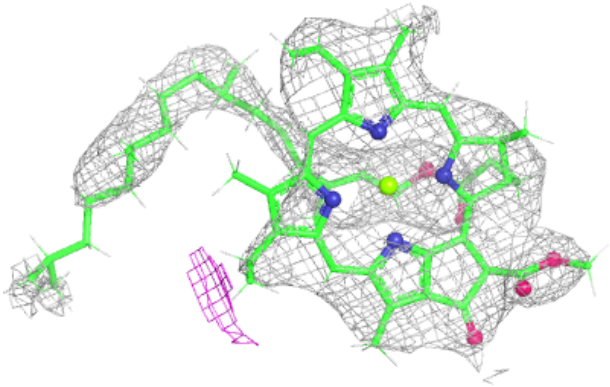


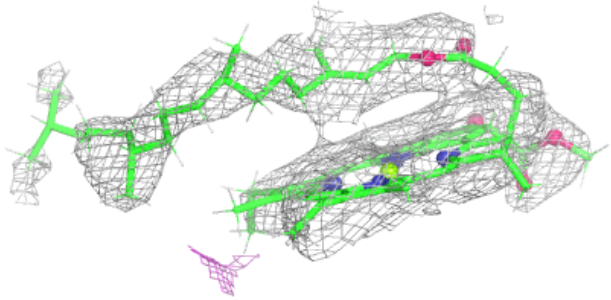




Electron density around CLA B 838:

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

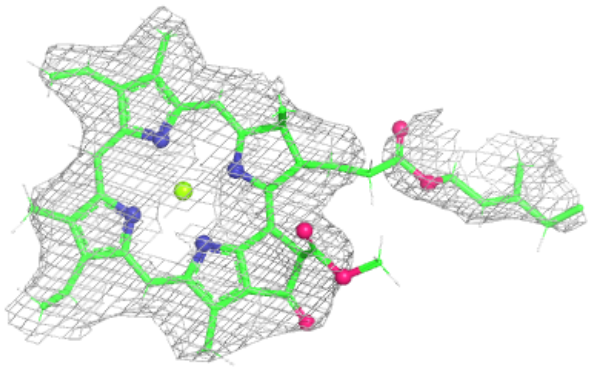


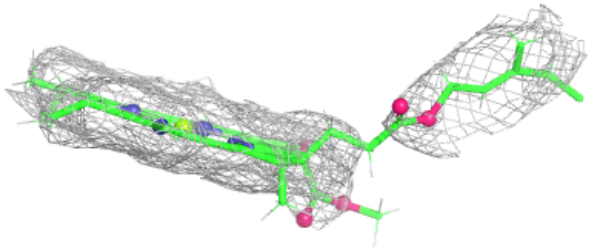


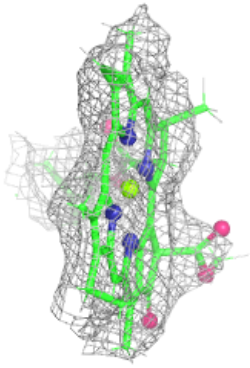


Electron density around CLA F 201:

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

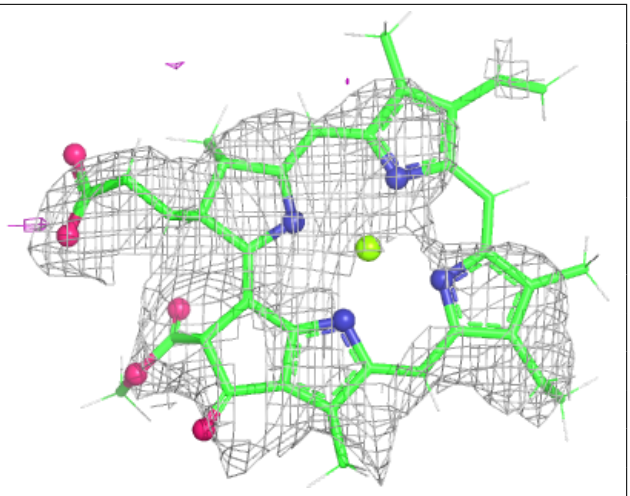


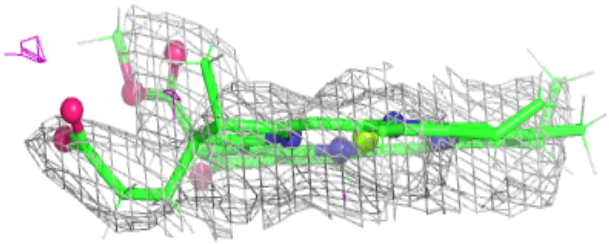


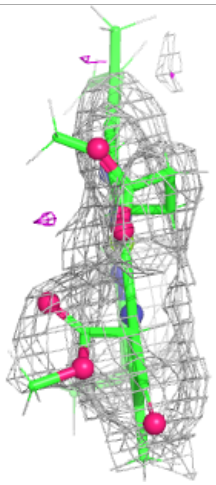


Electron density around CLA F 202:

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

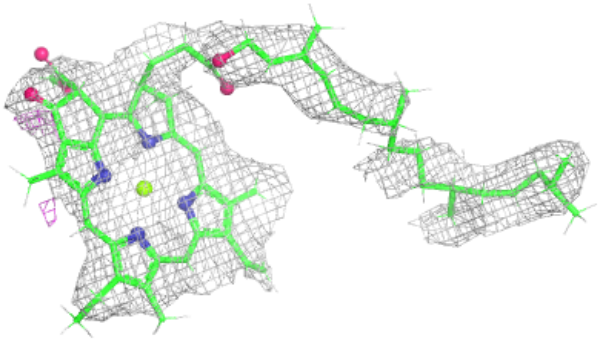


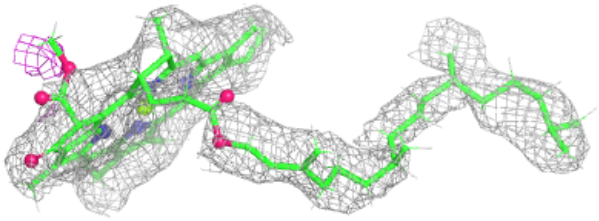


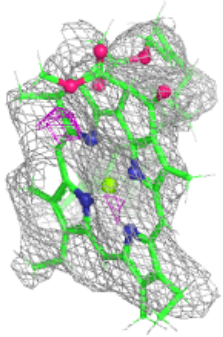


Electron density around CLA A 809:

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

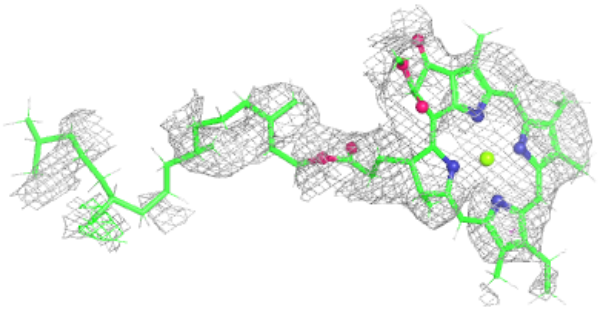


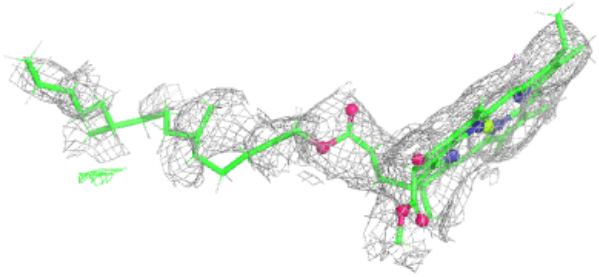


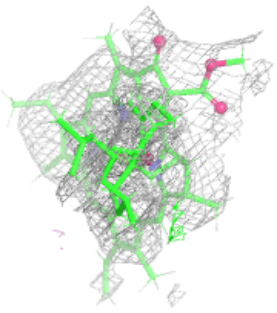


Electron density around CLA A 810:

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

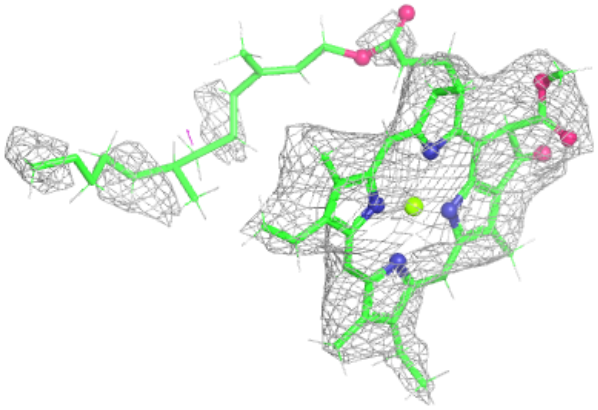


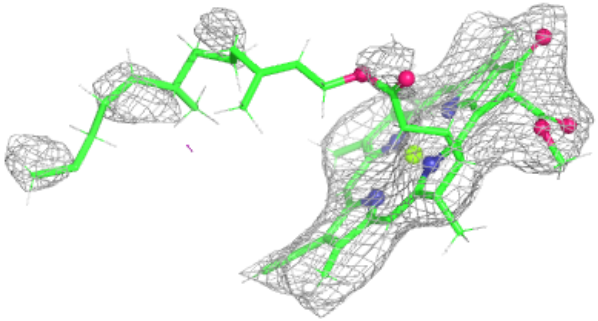


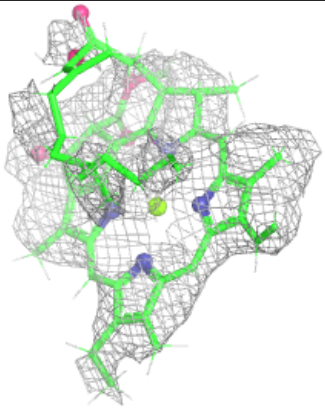


Electron density around CLA A 825:

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

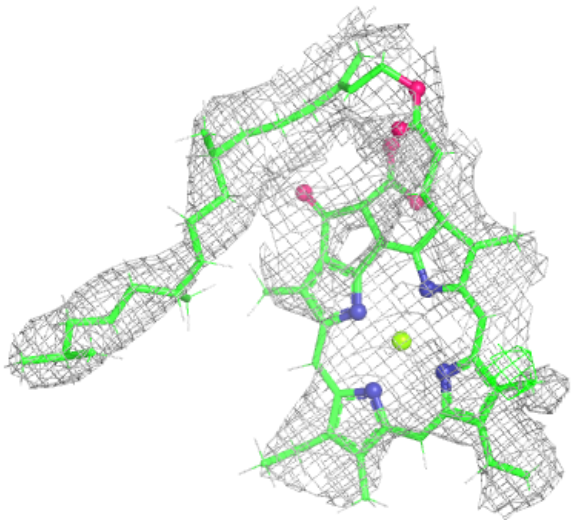


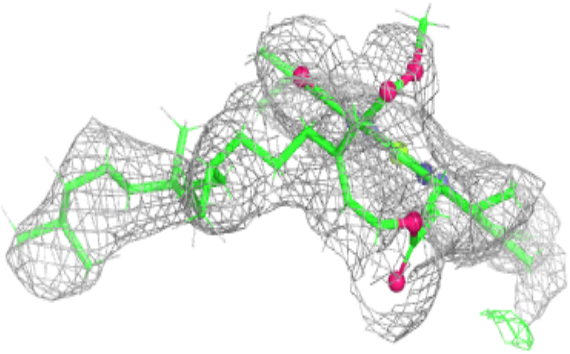




Electron density around CLA A 826:

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

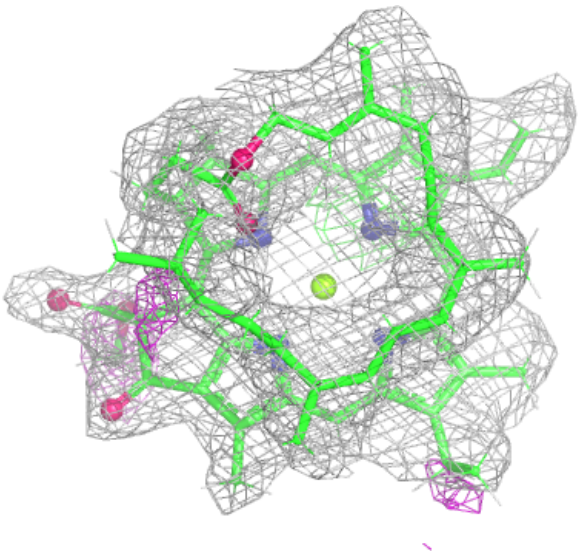


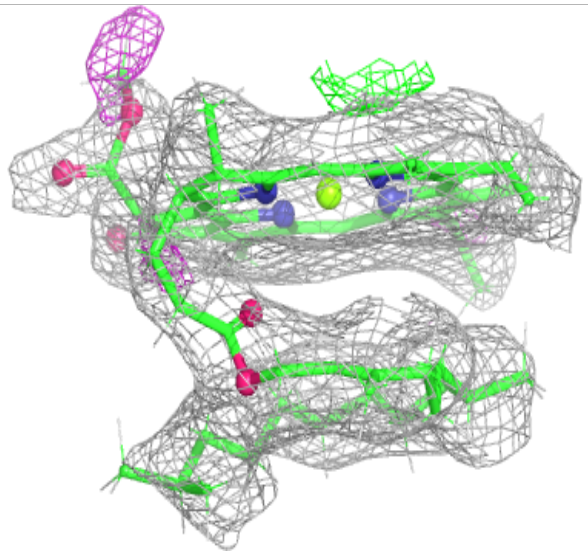


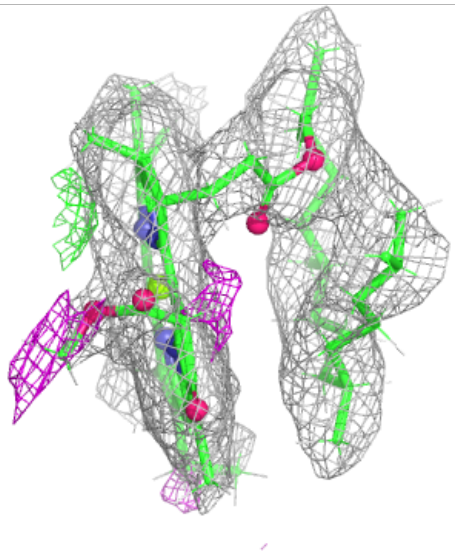


Electron density around CLA L 204:

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

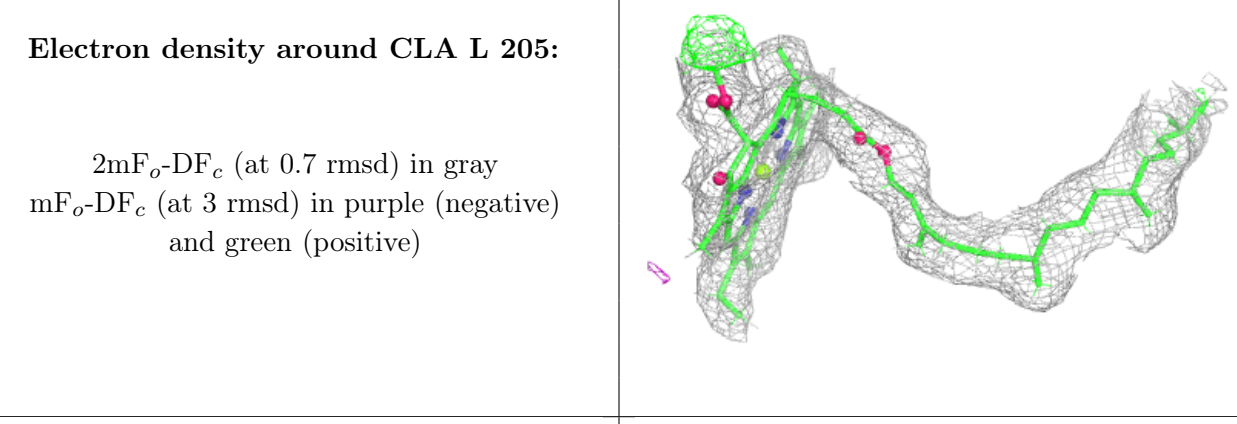






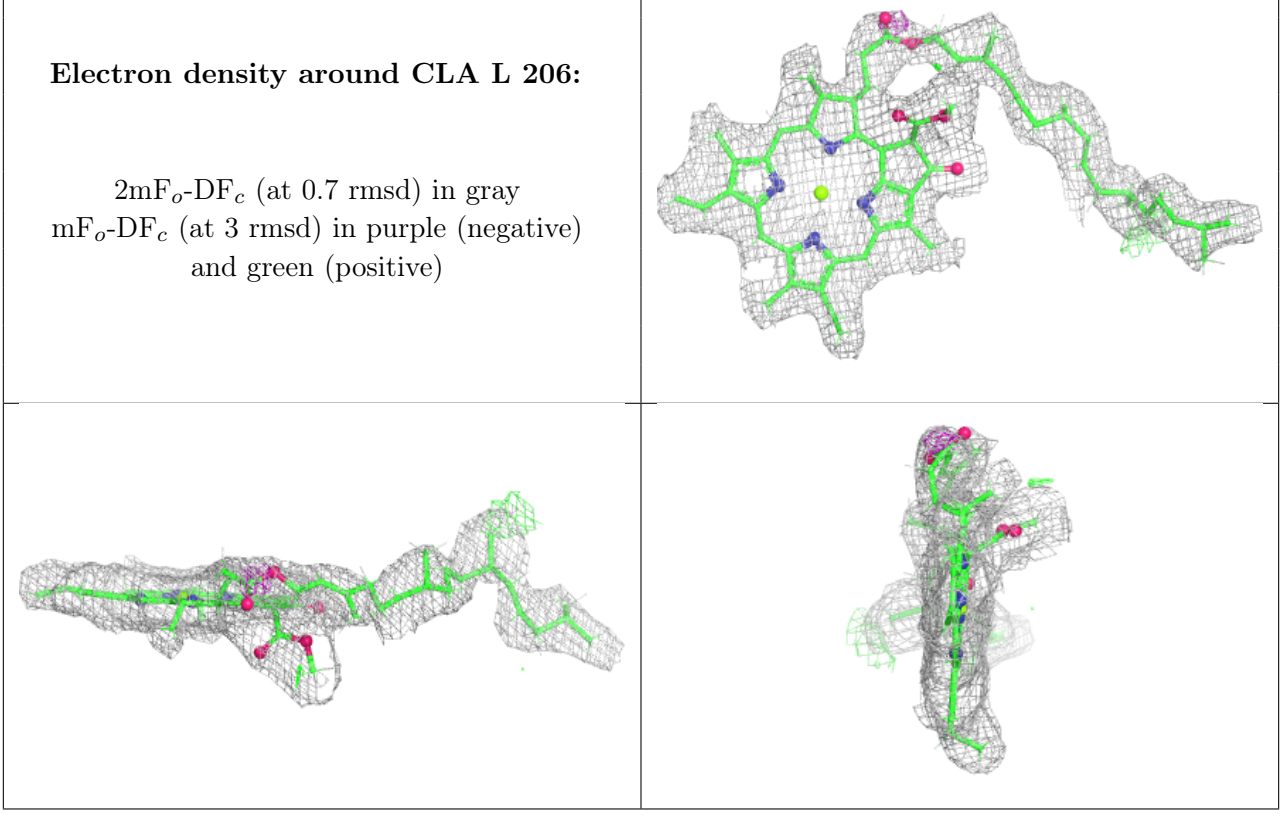
Electron density around CLA L 205:

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



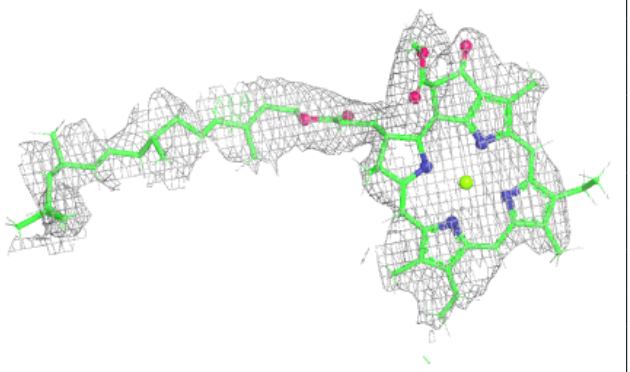
Electron density around CLA L 206:

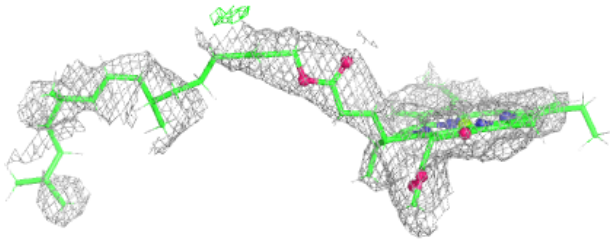
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

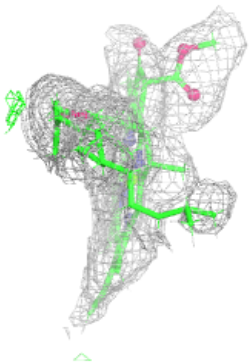


Electron density around CLA A 827:

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

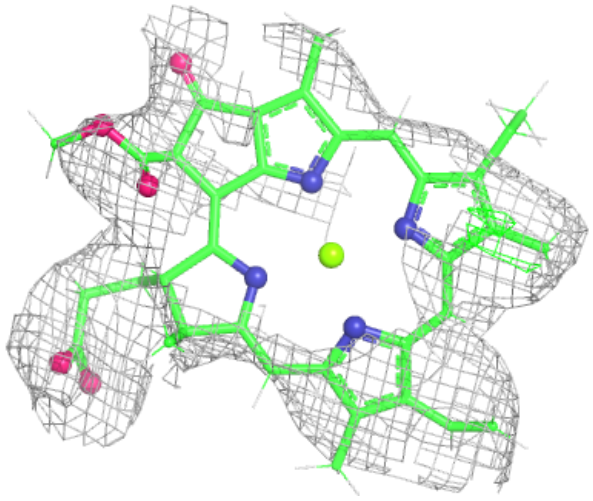


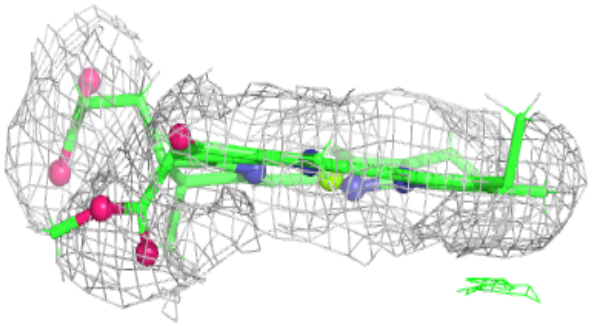


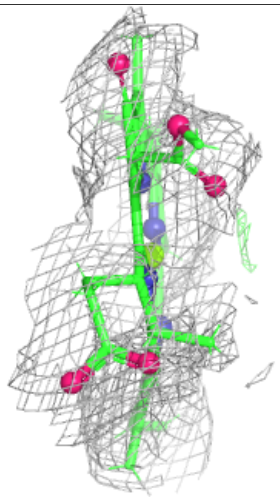


Electron density around CLA X 1701:

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

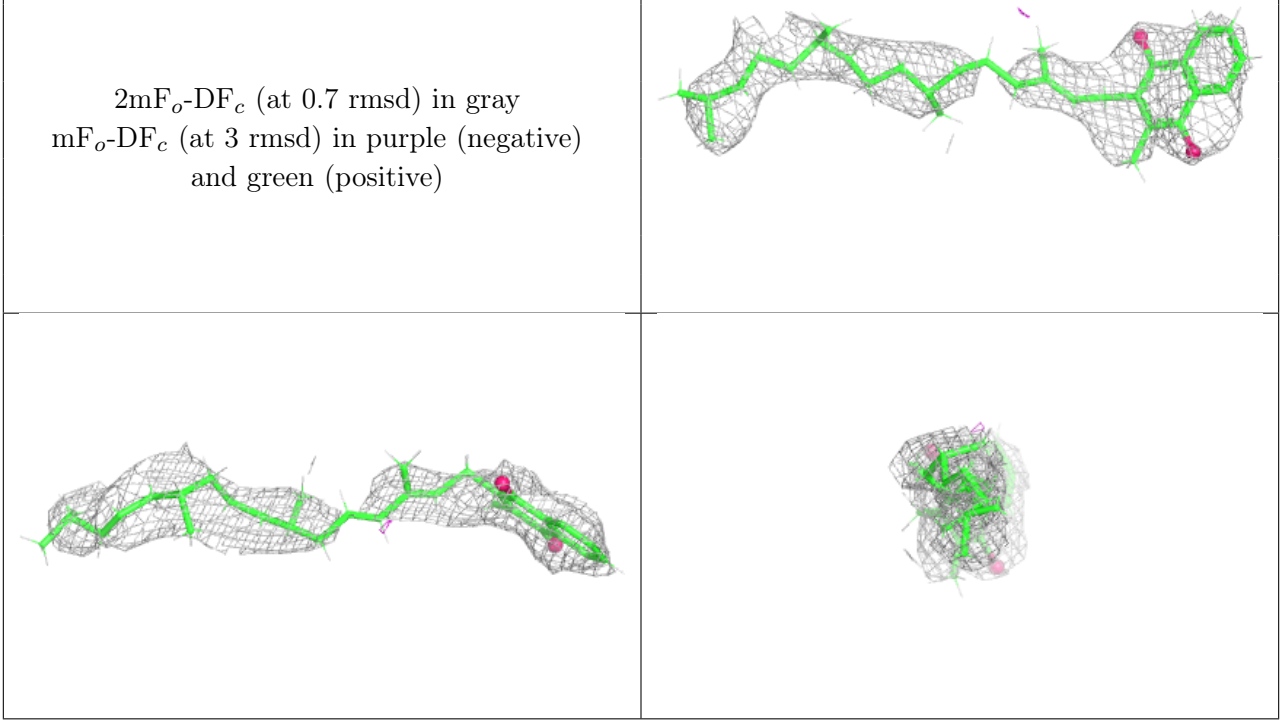






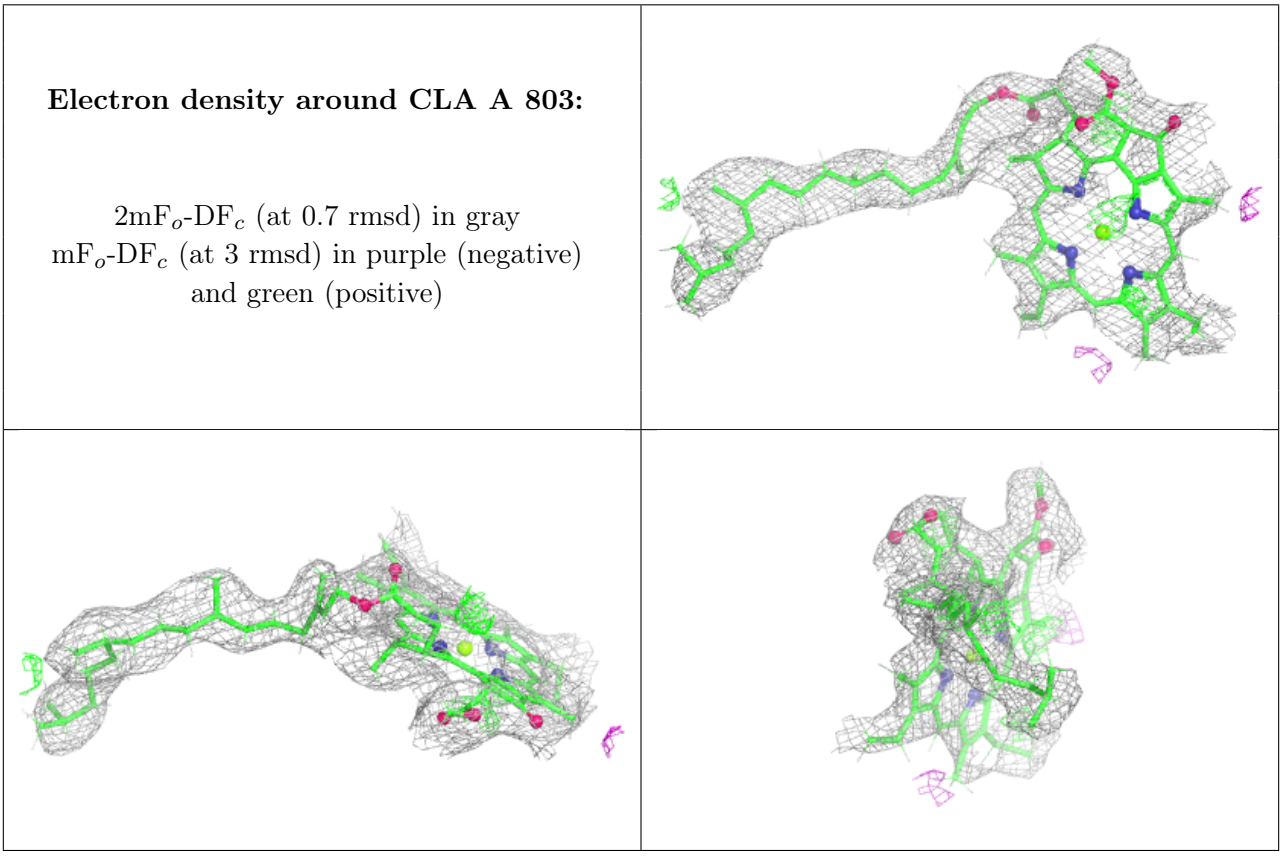
Electron density around PQN A 845:

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



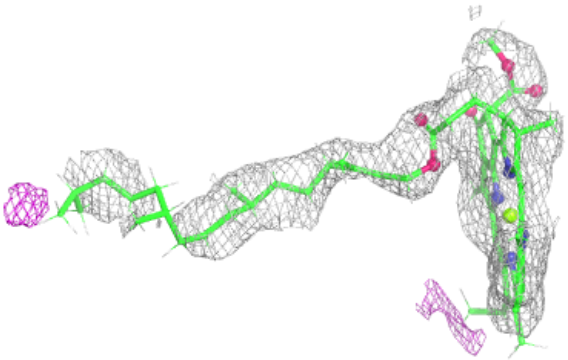
Electron density around CLA A 803:

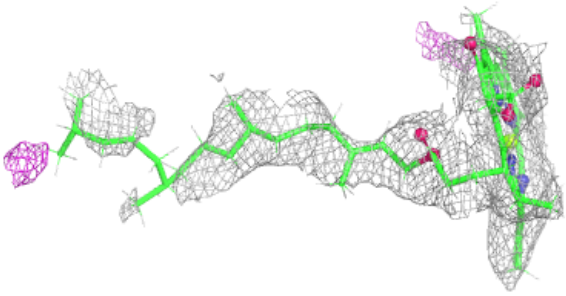
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

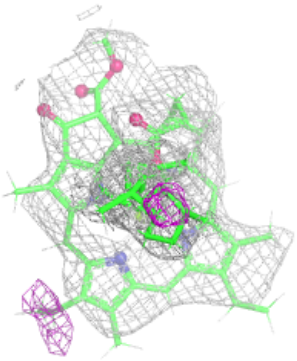


Electron density around CLA A 829:

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

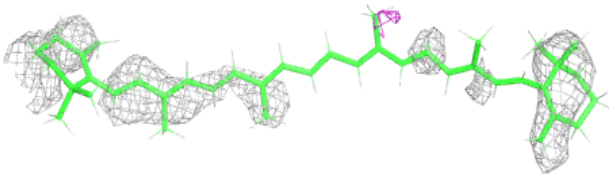


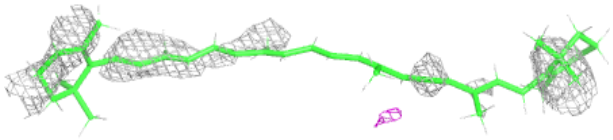


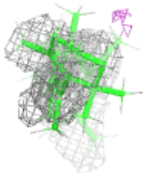


Electron density around BCR A 849:

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

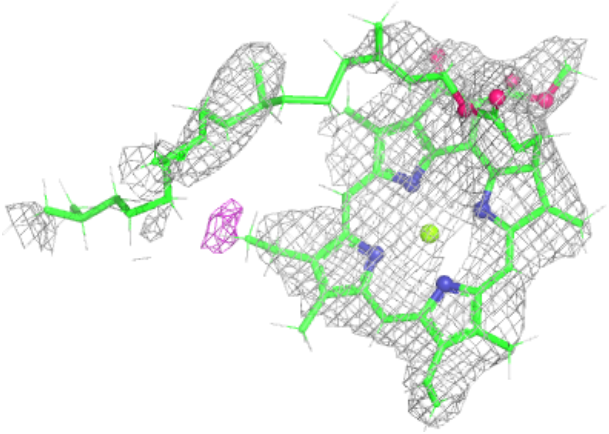


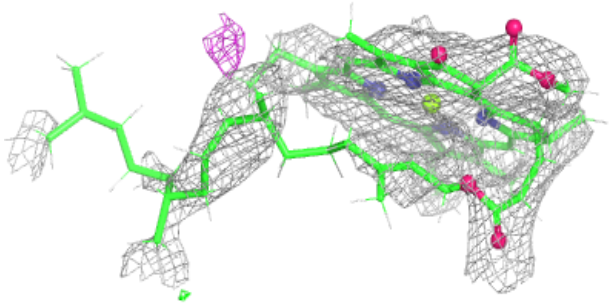


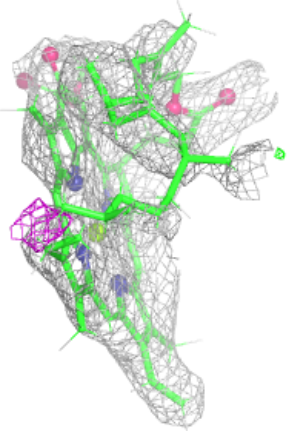


Electron density around CLA A 830:

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

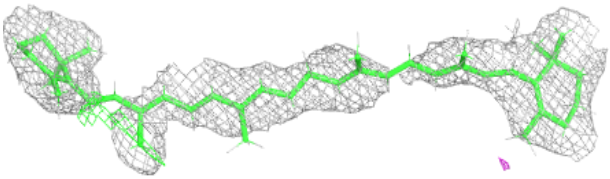


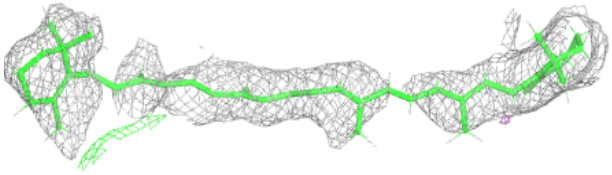


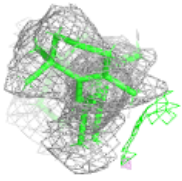


Electron density around BCR A 851:

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

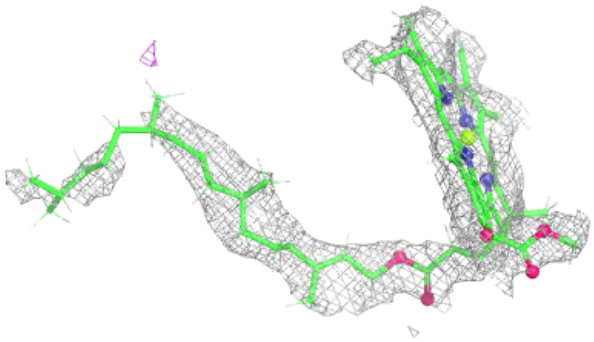


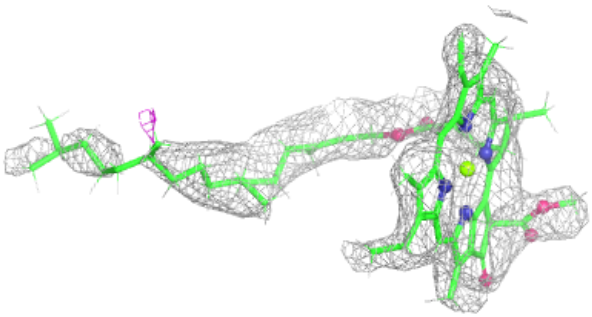


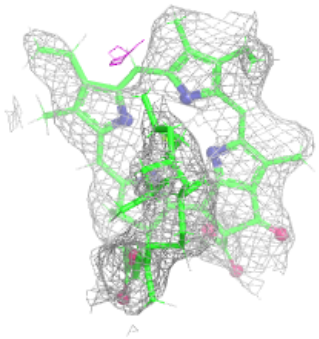


Electron density around CLA A 831:

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

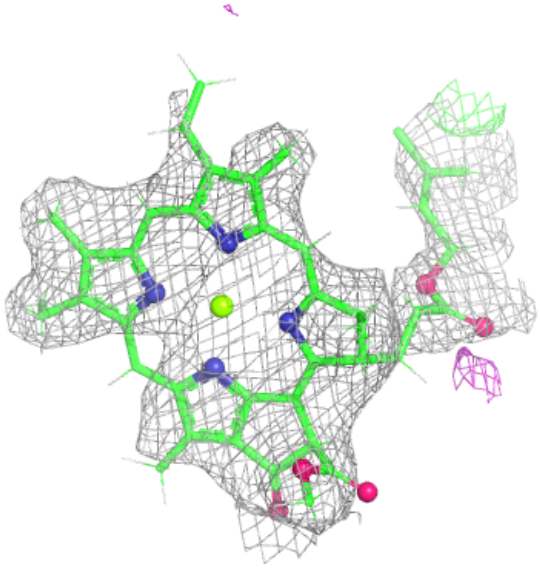


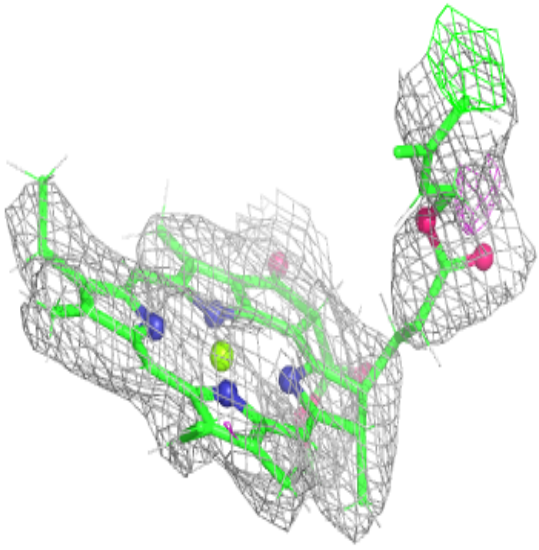


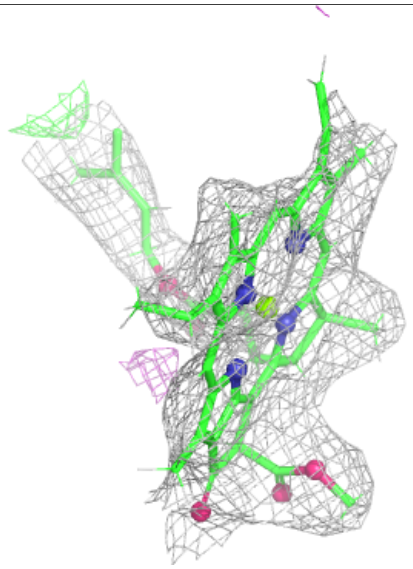


Electron density around CLA A 832:

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

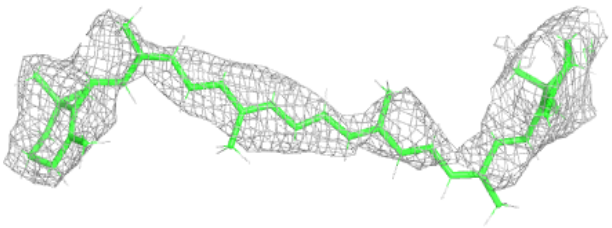


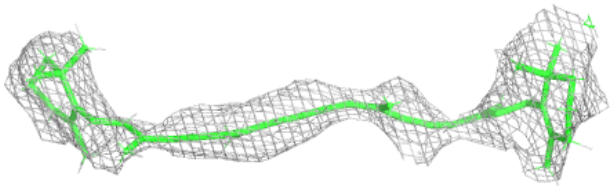


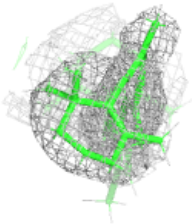


Electron density around BCR B 845:

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

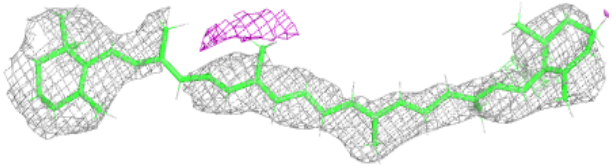


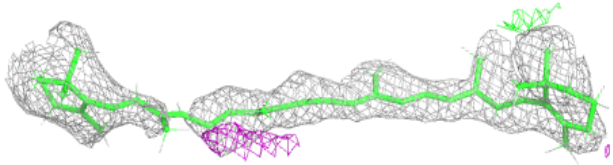


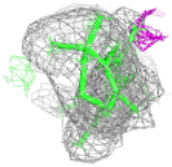


Electron density around BCR B 846:

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

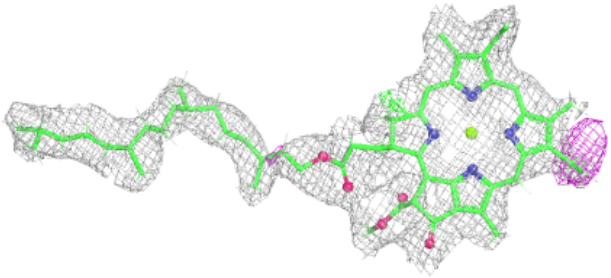


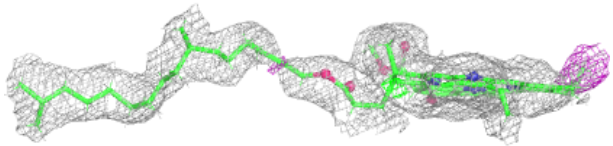


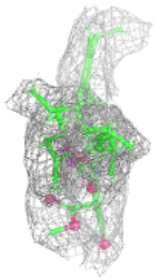


Electron density around CLA A 834:

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

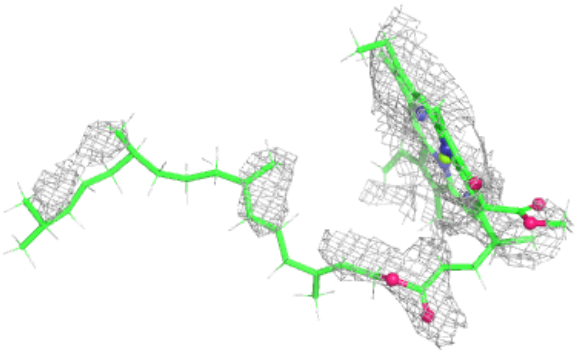


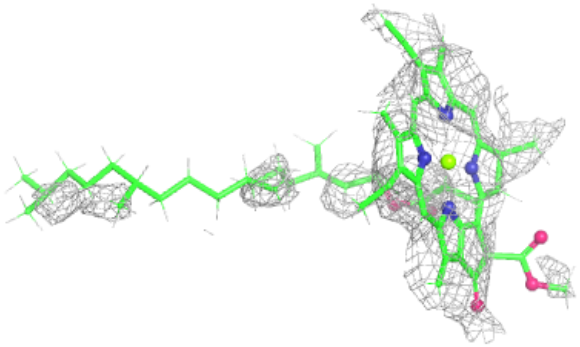


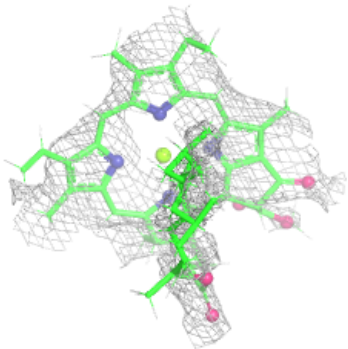


Electron density around CLA A 812:

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

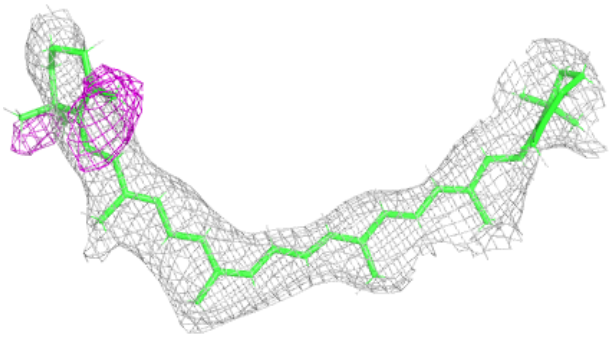


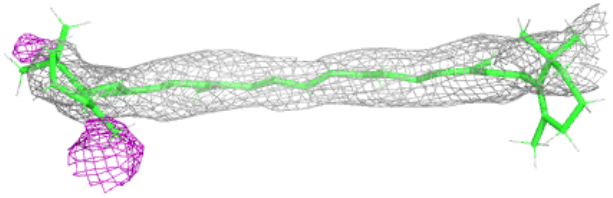


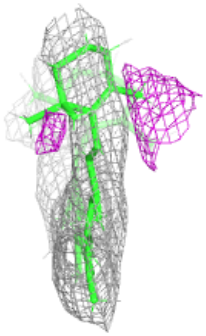


Electron density around BCR F 203:

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



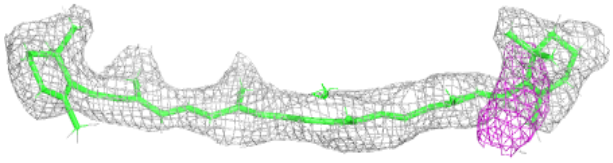


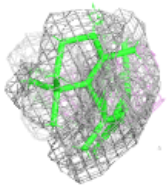


Electron density around BCR I 101:

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

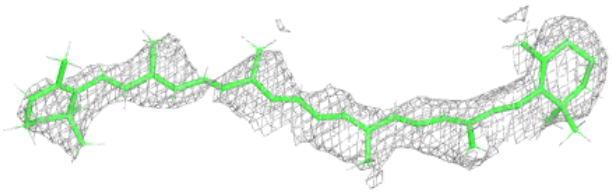


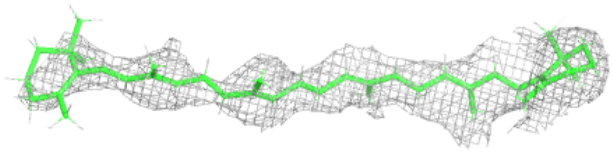


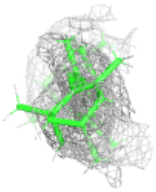


Electron density around BCR J 103:

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

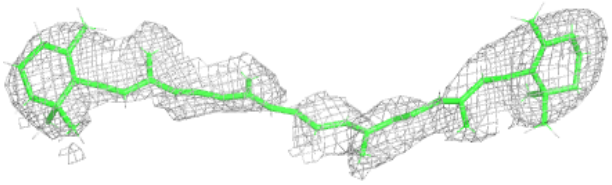


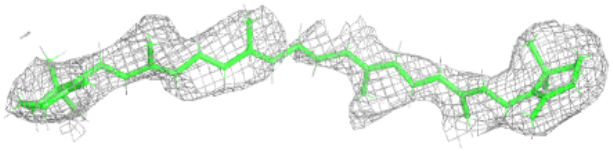


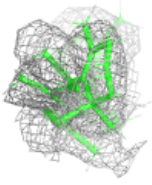


Electron density around BCR J 104:

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

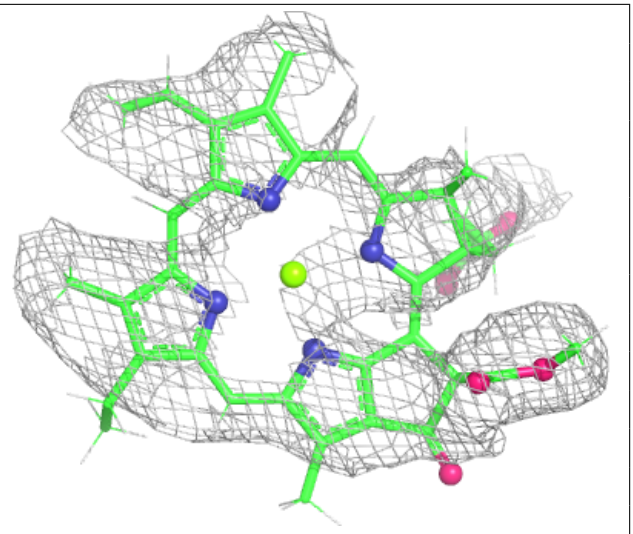


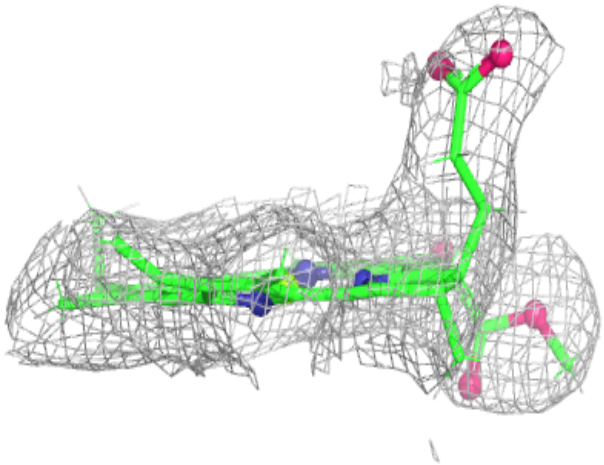


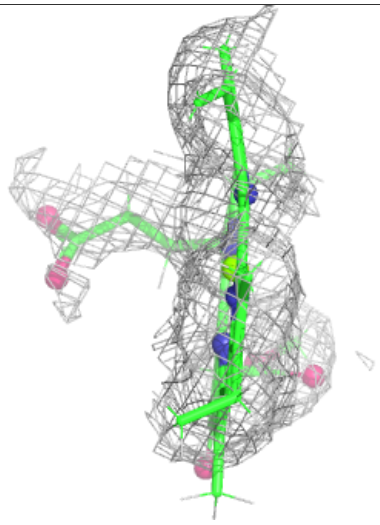


Electron density around CLA A 837:

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

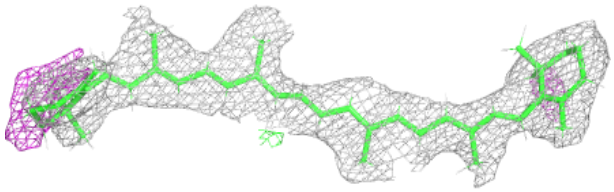


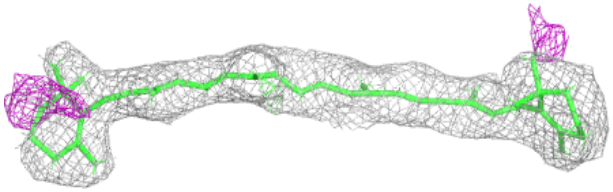


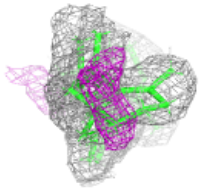


Electron density around BCR M 103:

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

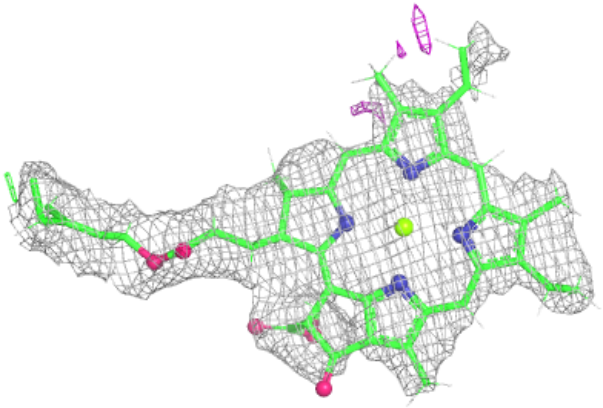


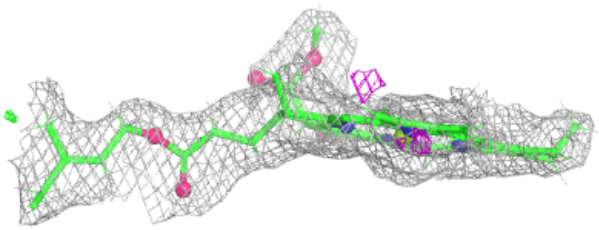




Electron density around CLA A 838:

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

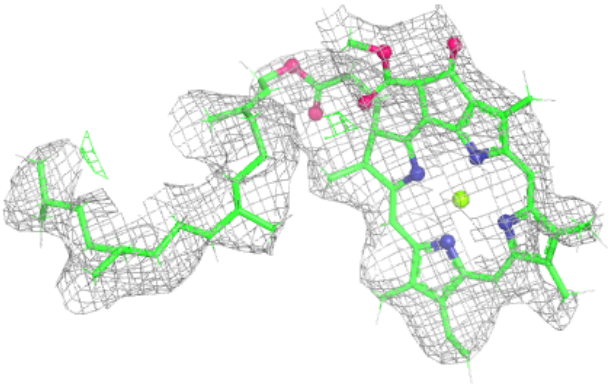


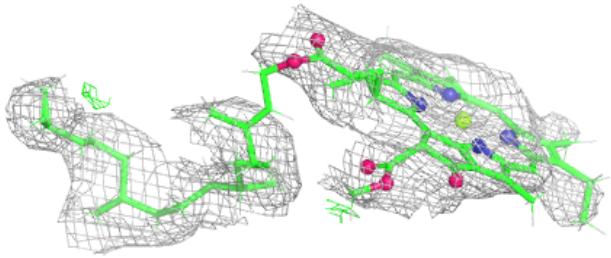


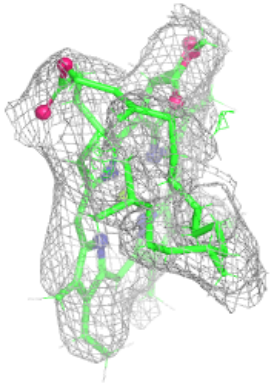


Electron density around CLA A 804:

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

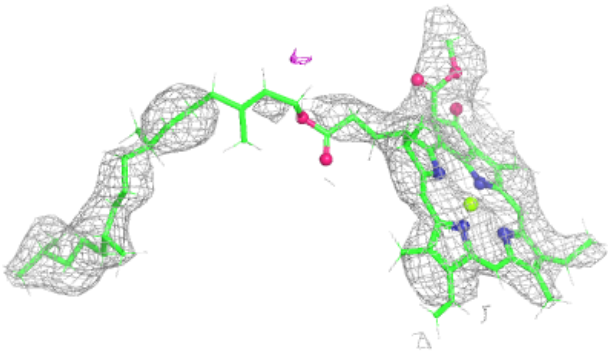


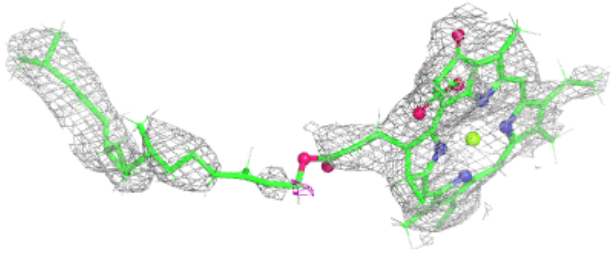




Electron density around CLA A 857:

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

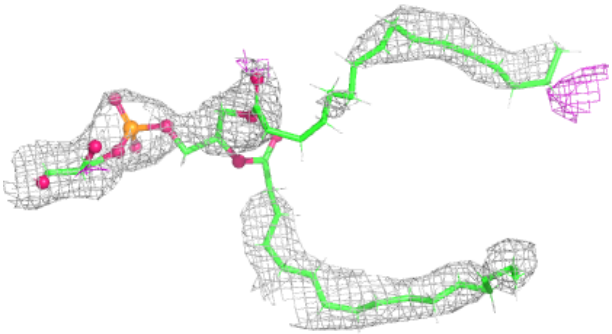


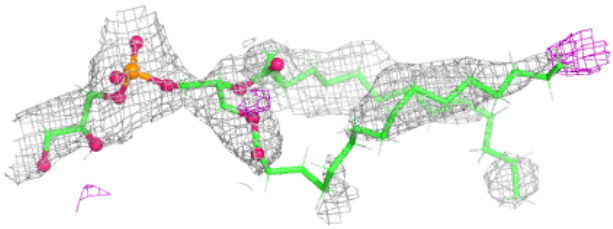


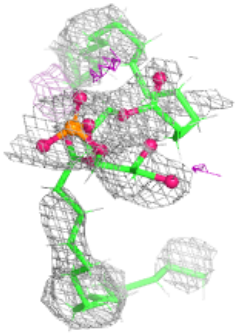


Electron density around LHG A 854:

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

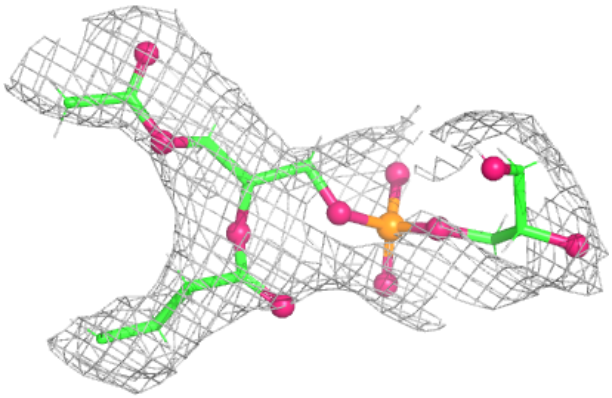


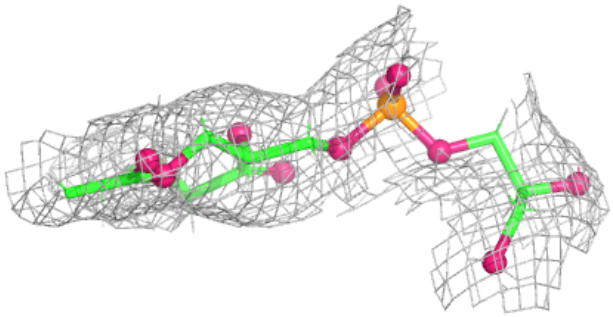


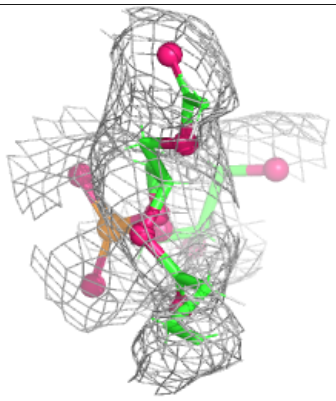


Electron density around LHG B 850:

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

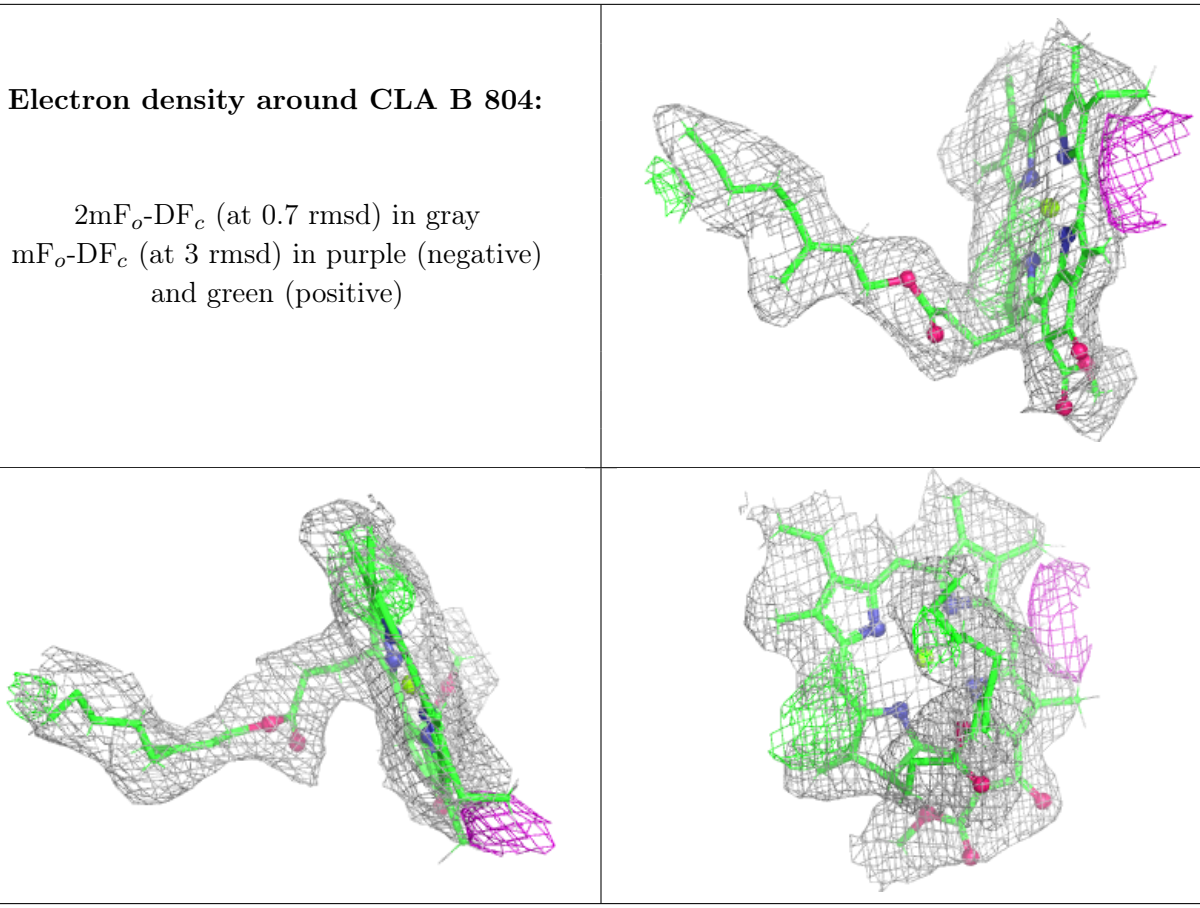






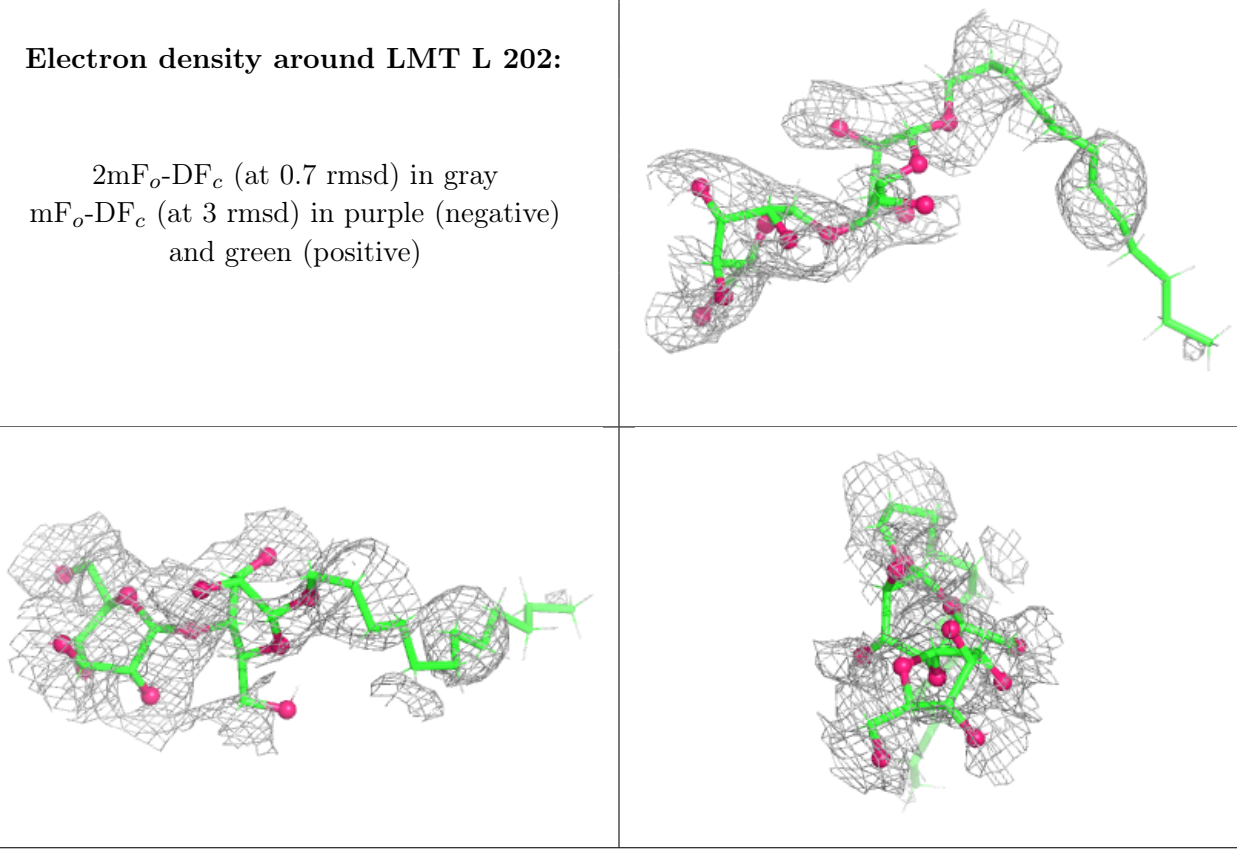
Electron density around CLA B 804:

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



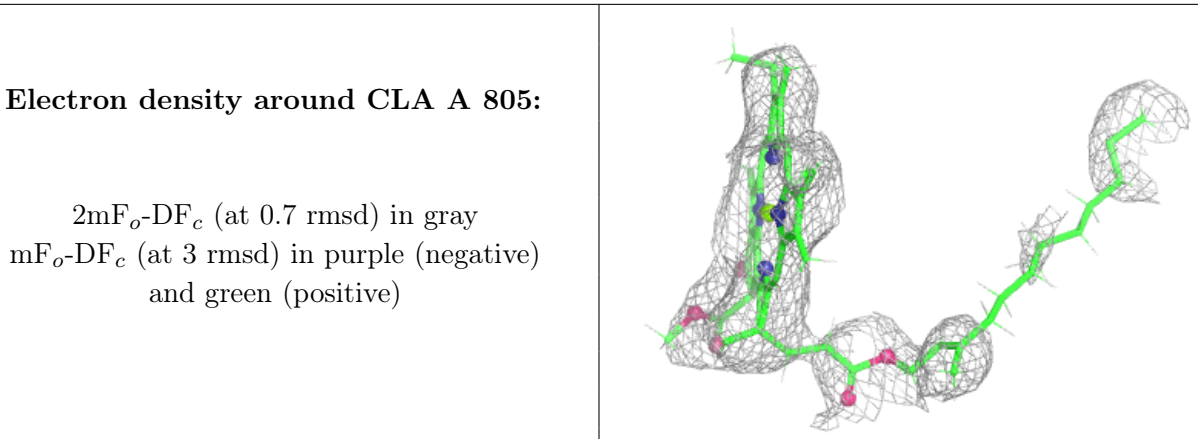
Electron density around LMT L 202:

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



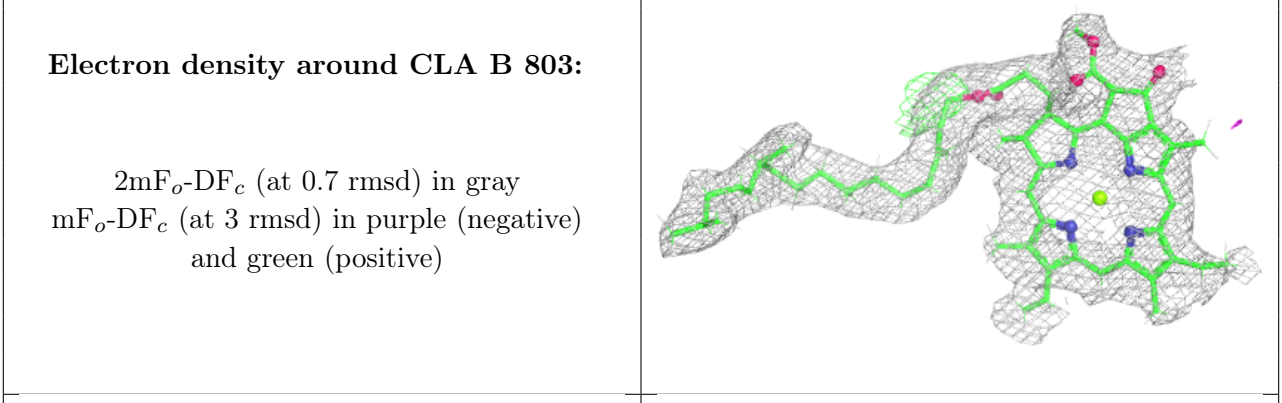
Electron density around CLA A 805:

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



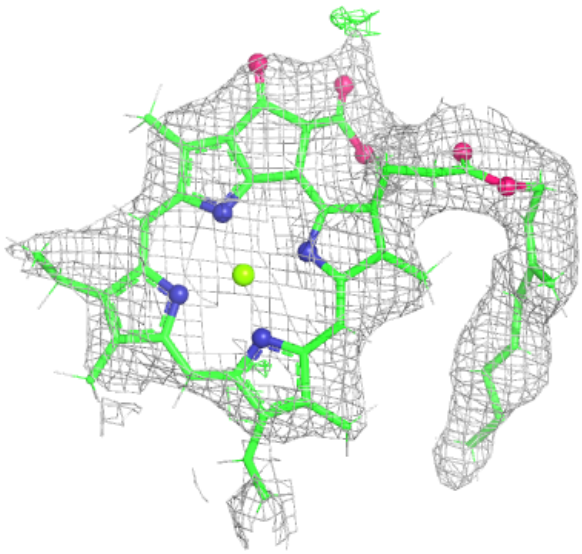
Electron density around CLA B 803:

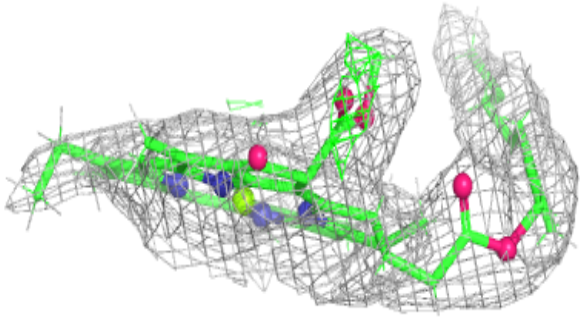
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

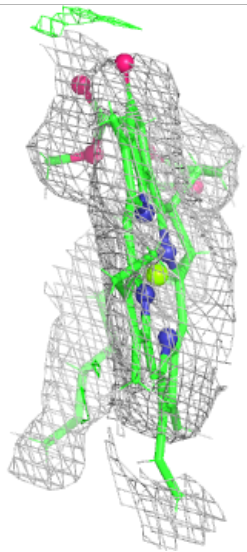


Electron density around CLA B 824:

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

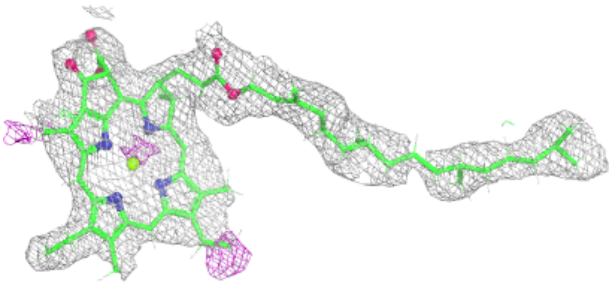


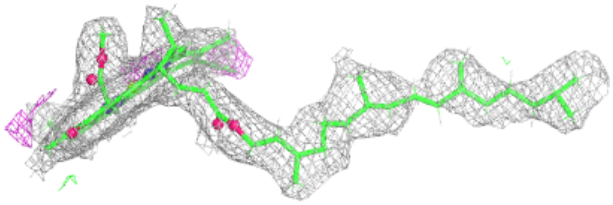


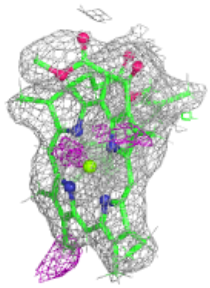


Electron density around CLA A 835:

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

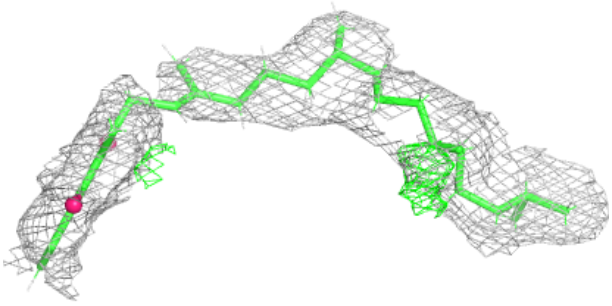


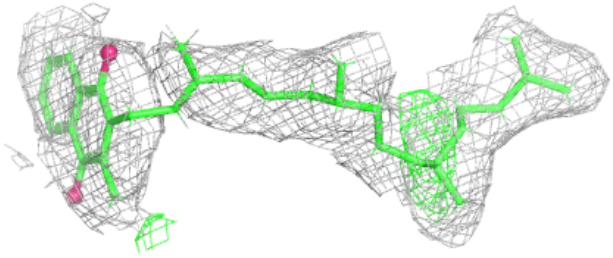




Electron density around PQN B 842:

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

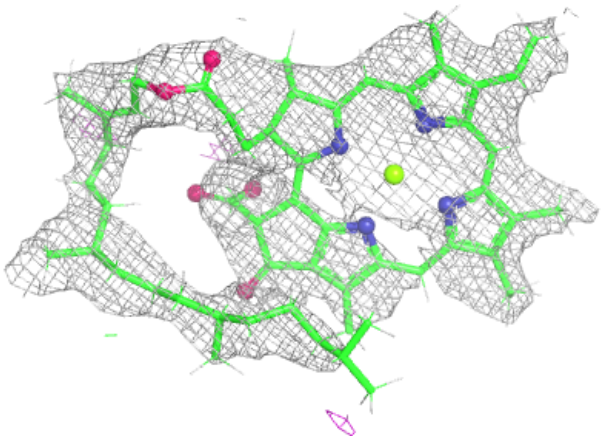


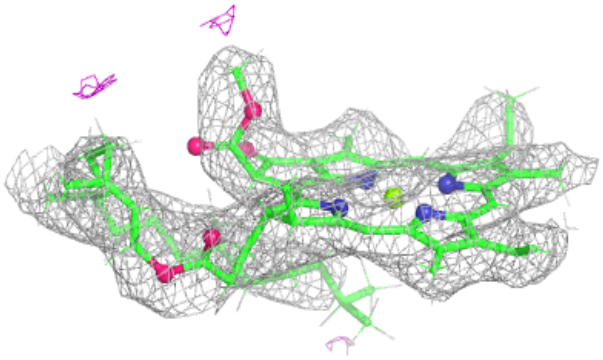


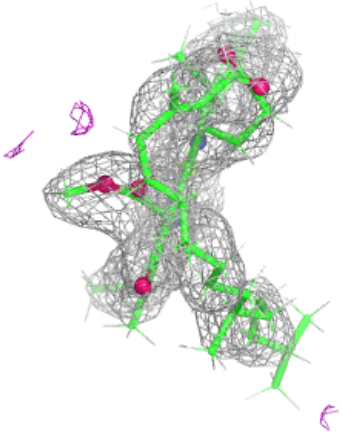


Electron density around CLA B 805:

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

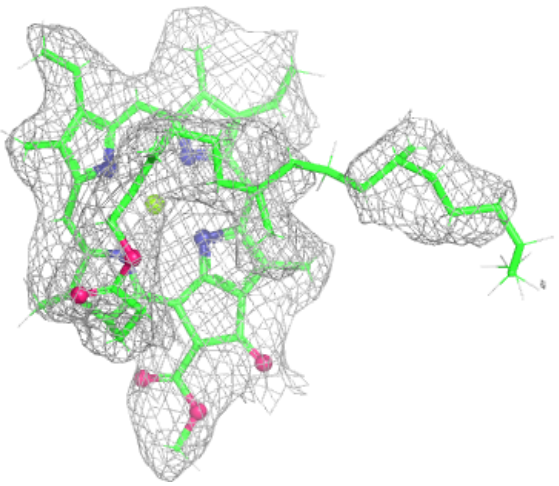


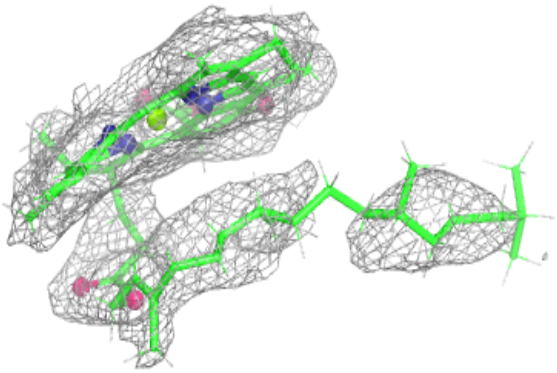


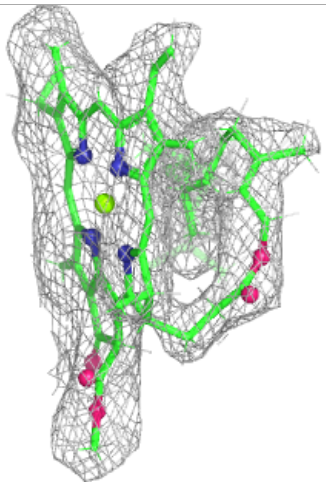


Electron density around CLA B 827:

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

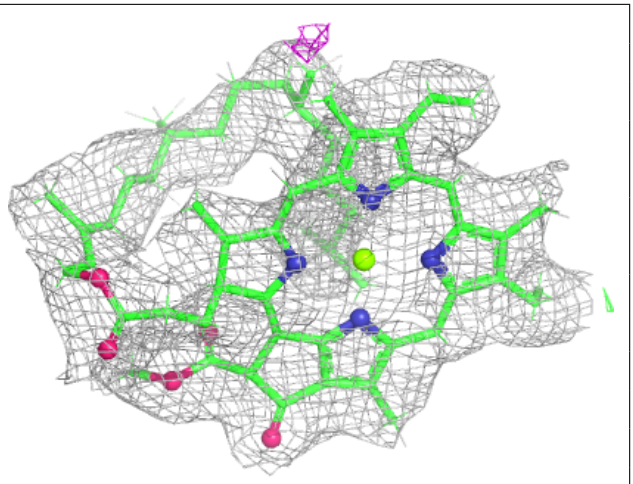


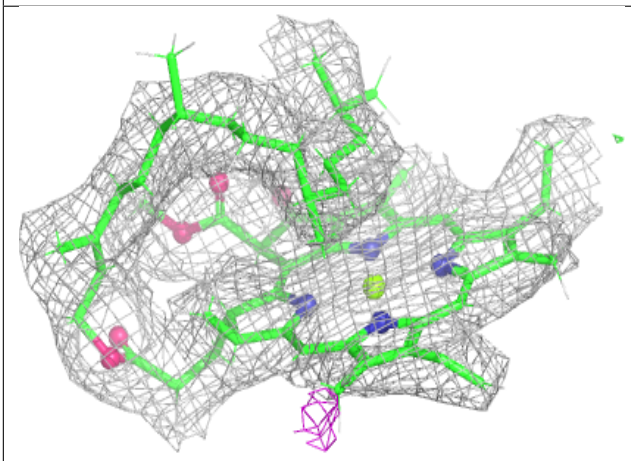


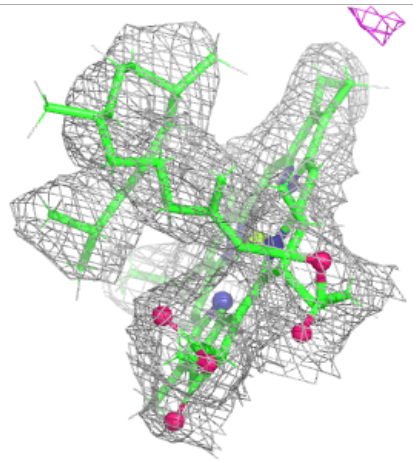


Electron density around CLA B 806:

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

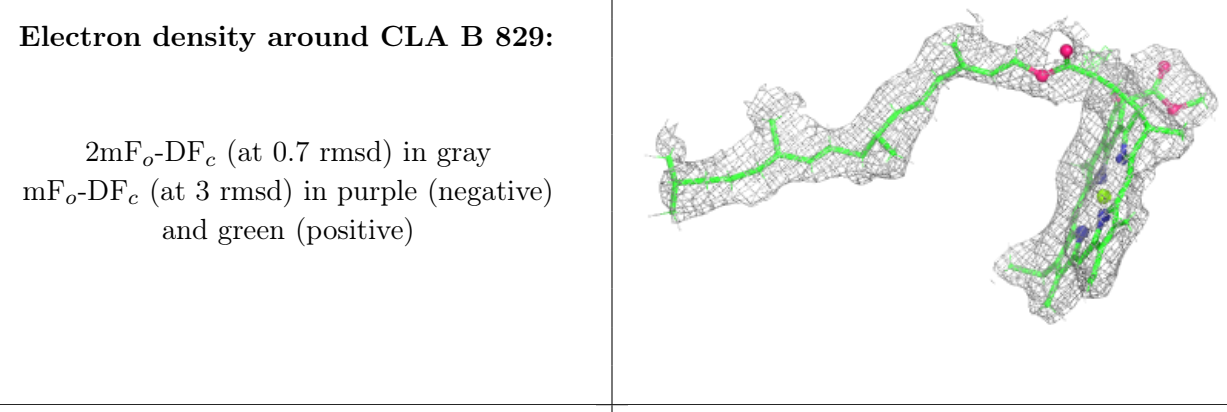






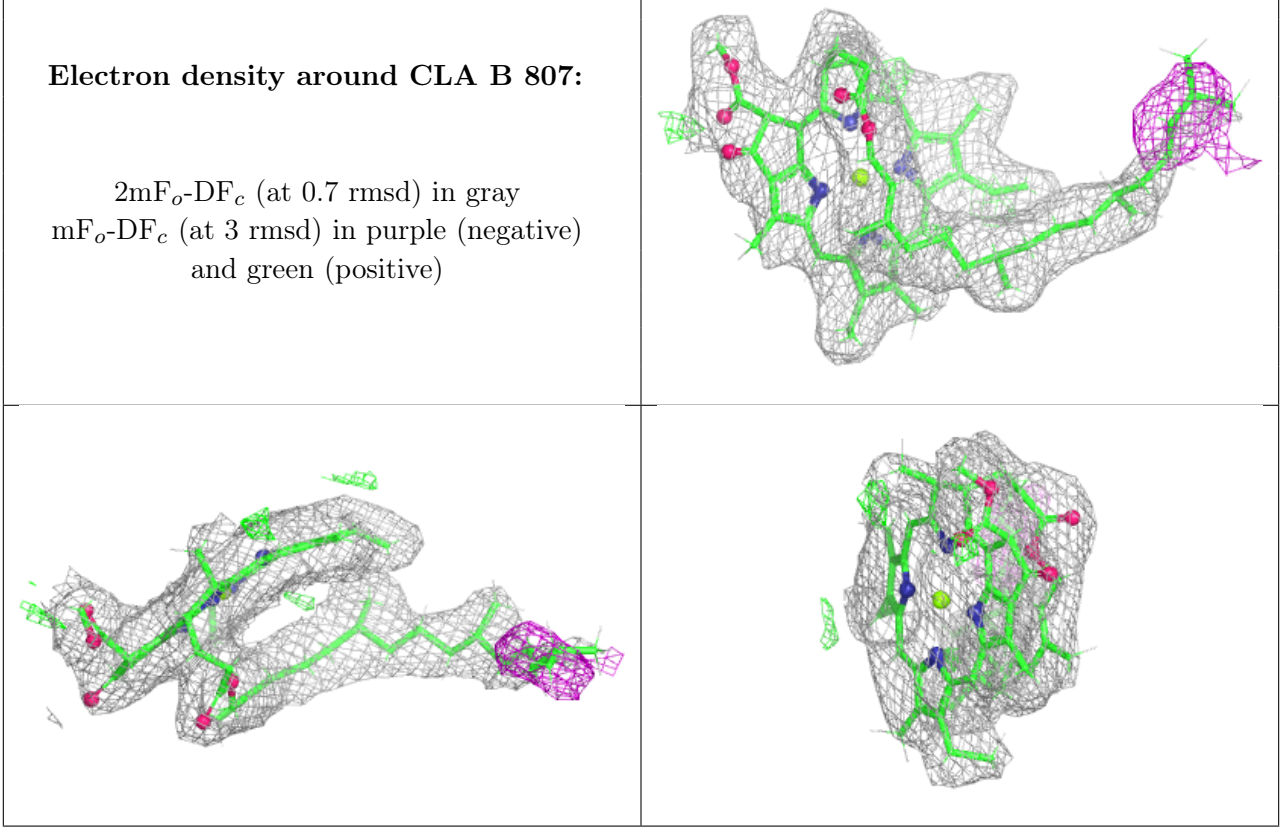
Electron density around CLA B 829:

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



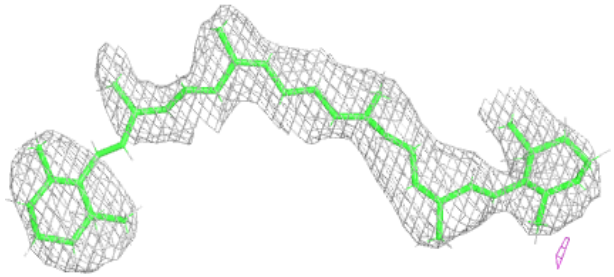
Electron density around CLA B 807:

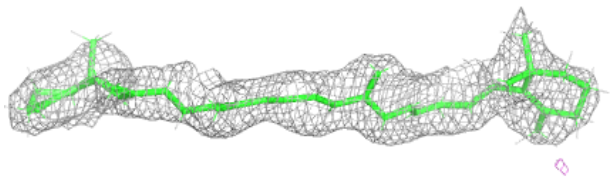
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

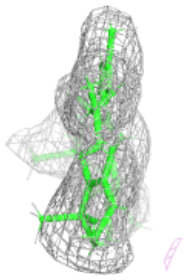


Electron density around BCR A 852:

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

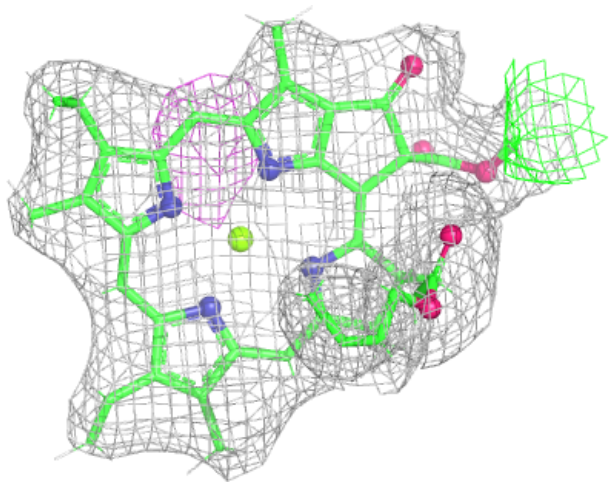


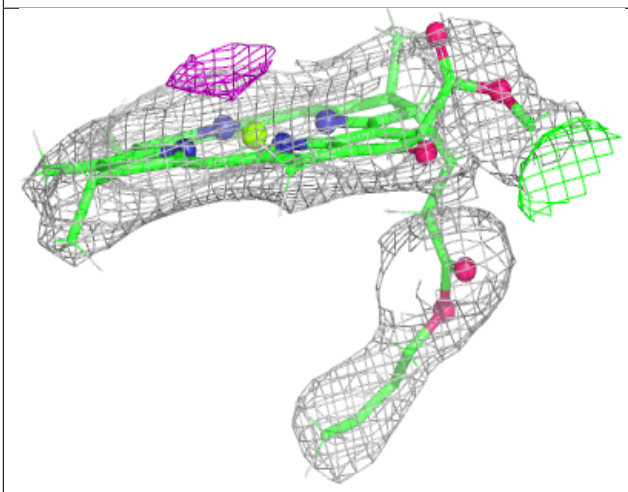


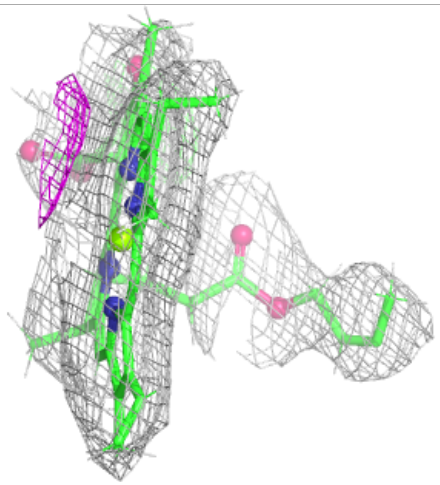


Electron density around CLA B 831:

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

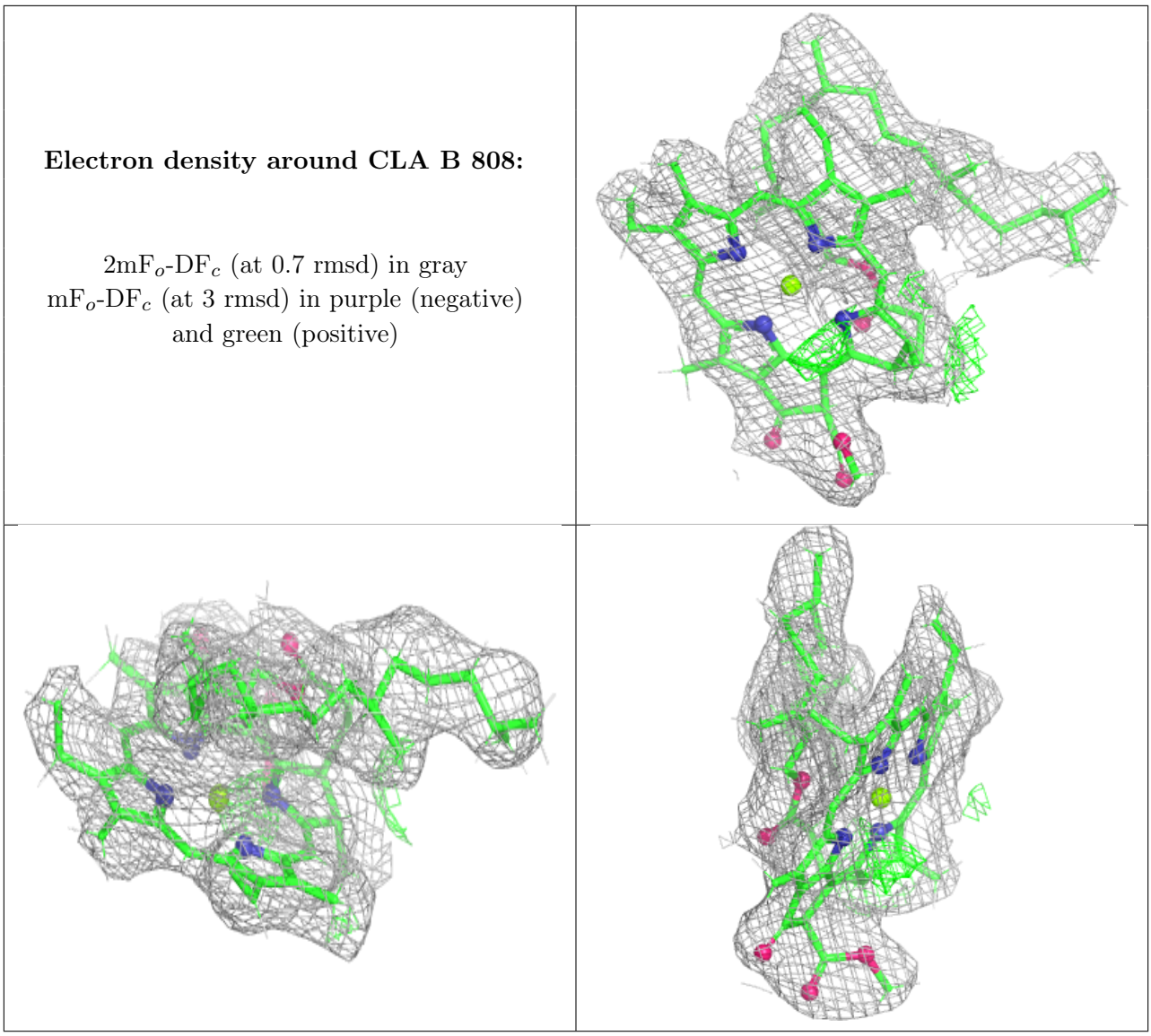






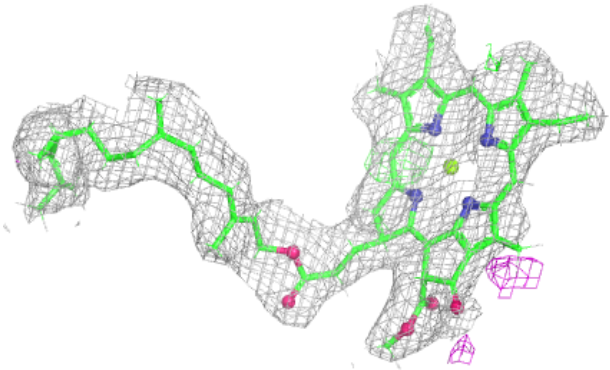
Electron density around CLA B 808:

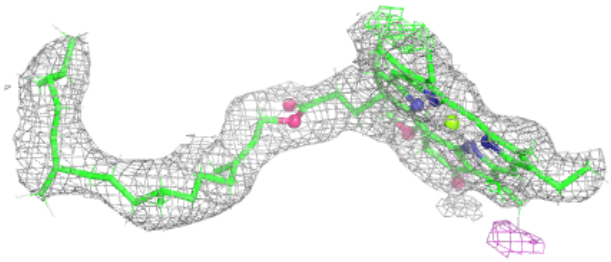
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

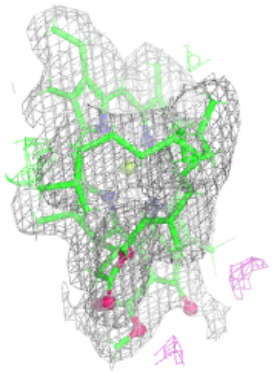


Electron density around CLA B 809:

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

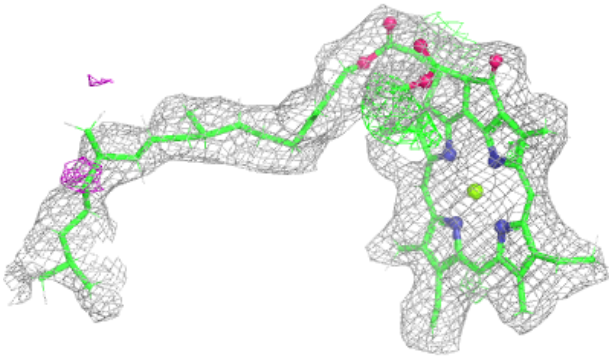


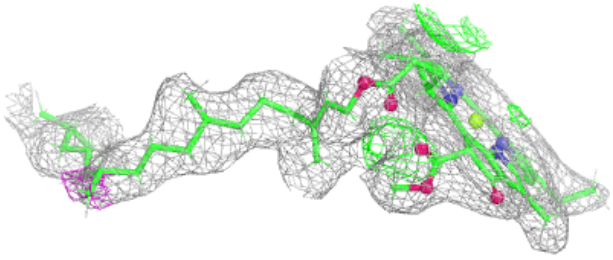


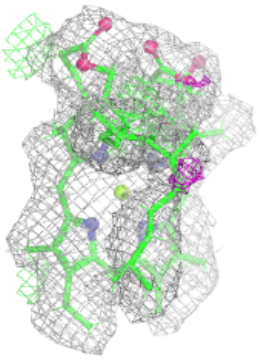


Electron density around CLA B 810:

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

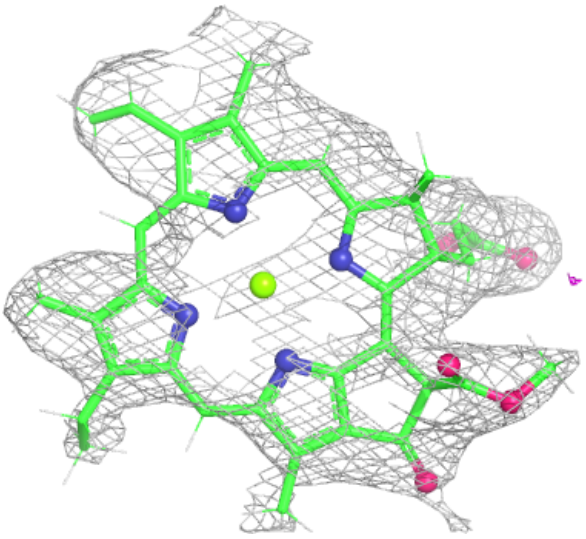


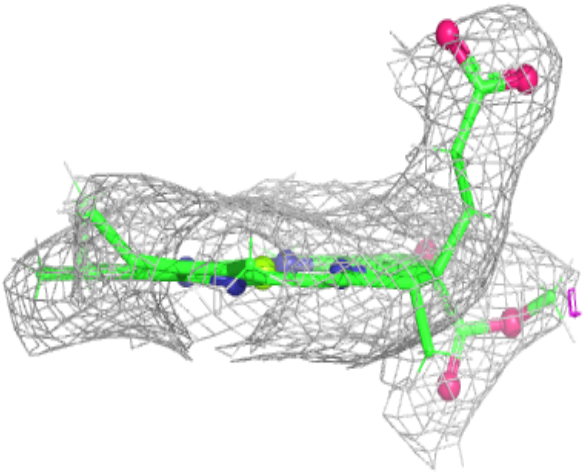


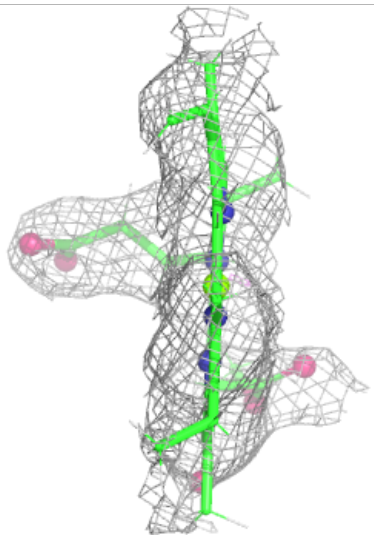


Electron density around CLA B 835:

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

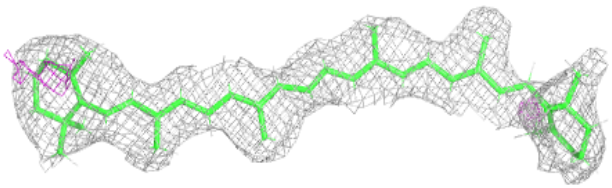


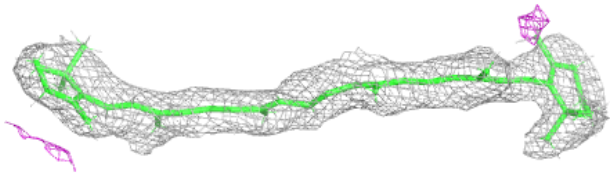


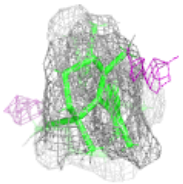


Electron density around BCR B 848:

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

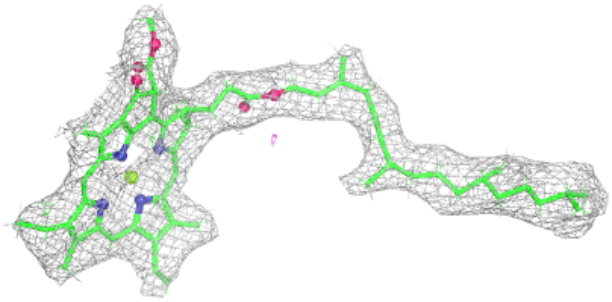


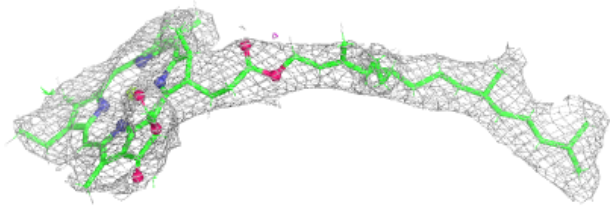


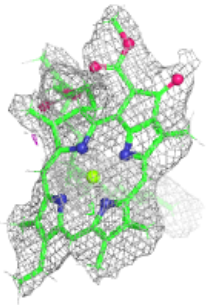


Electron density around CLA A 802:

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

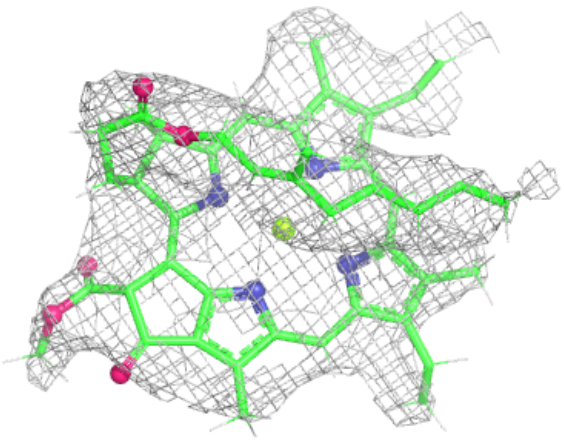


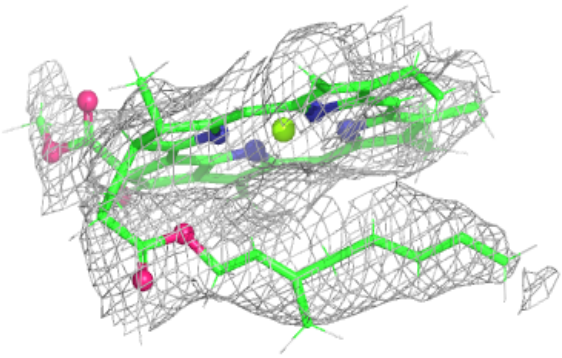


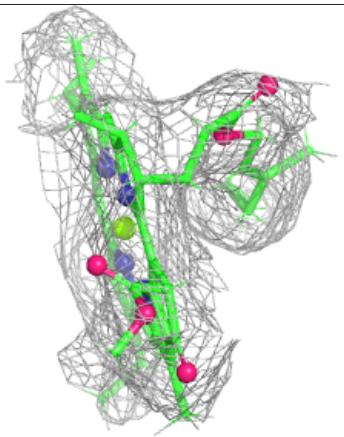


Electron density around CLA A 819:

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

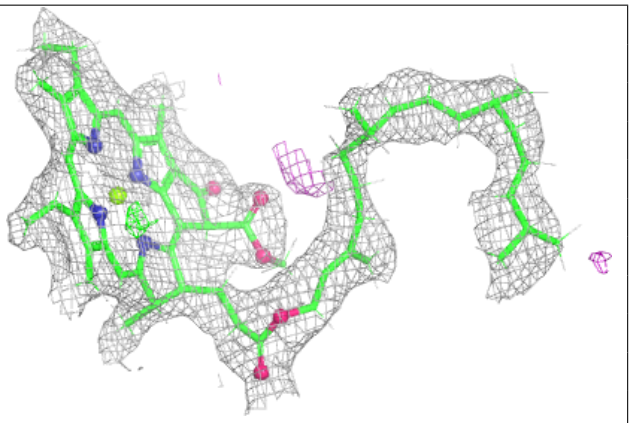


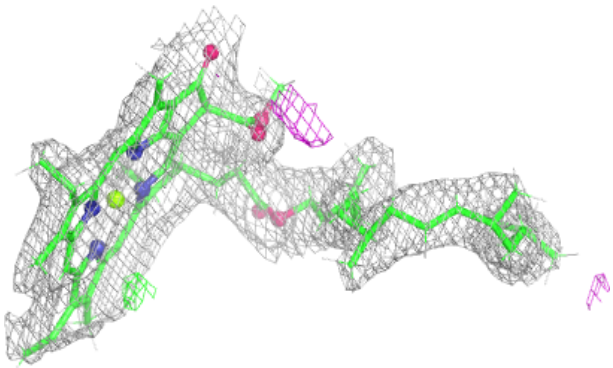


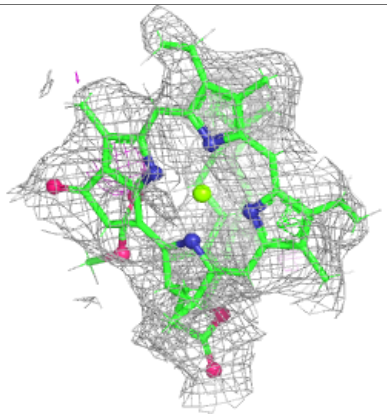


Electron density around CL0 A 801:

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

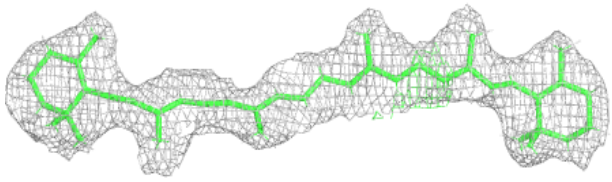


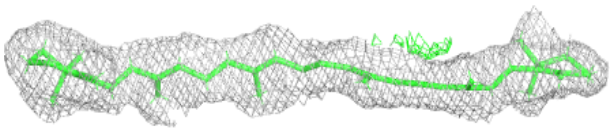


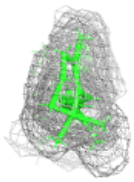


Electron density around BCR I 103:

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

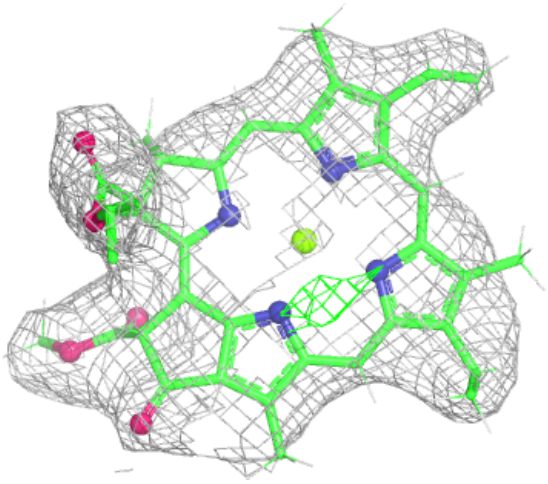


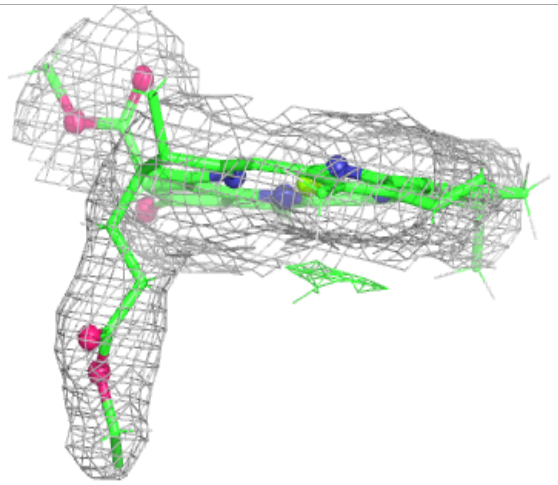


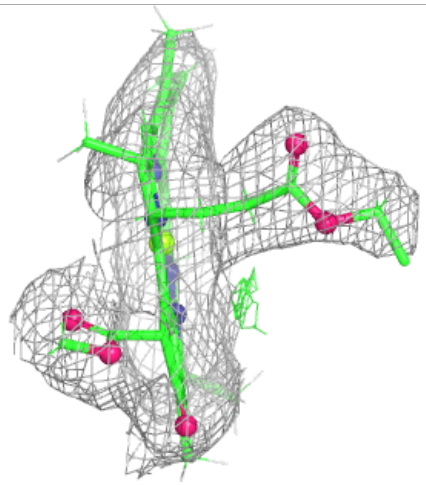


Electron density around CLA B 839:

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

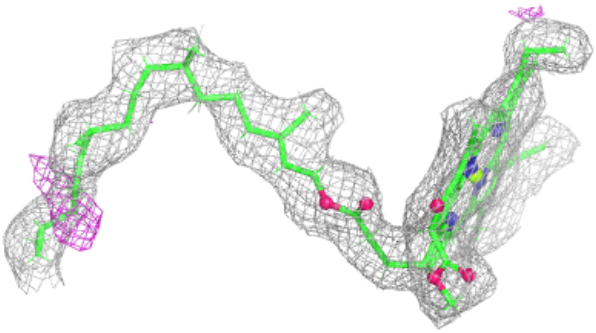


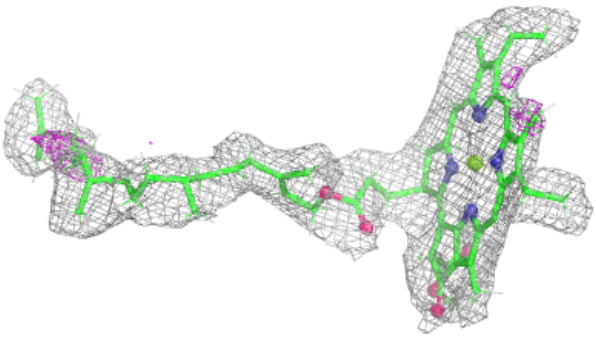


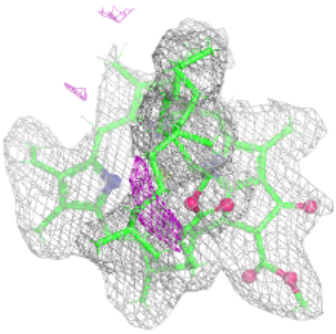


Electron density around CLA B 840:

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

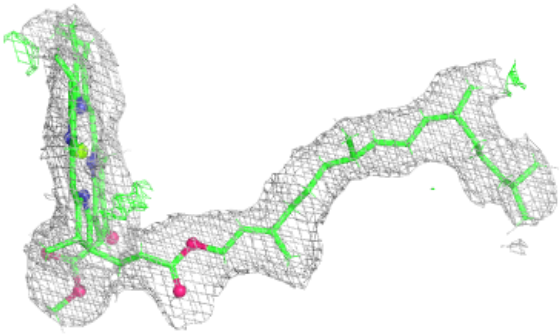


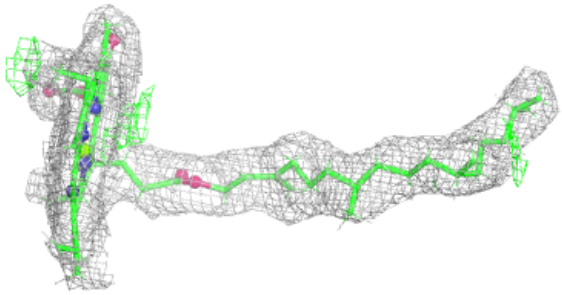


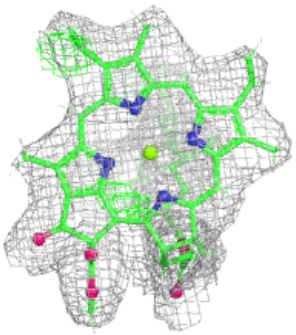


Electron density around CLA B 841:

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

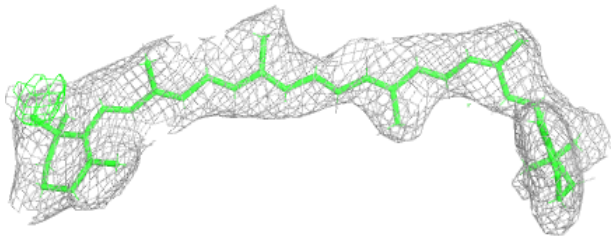


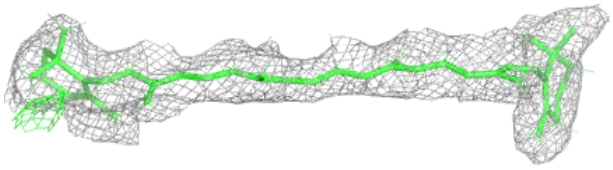


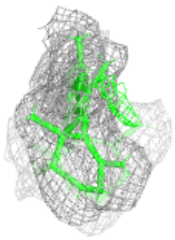


Electron density around BCR L 201:

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

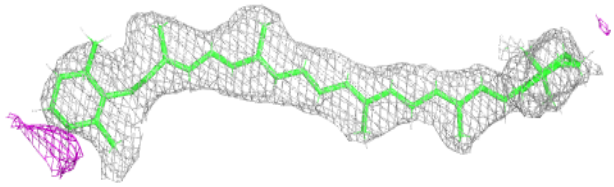


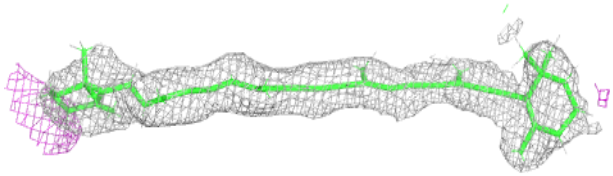


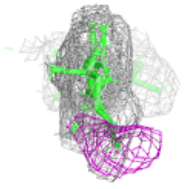


Electron density around BCR L 208:

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

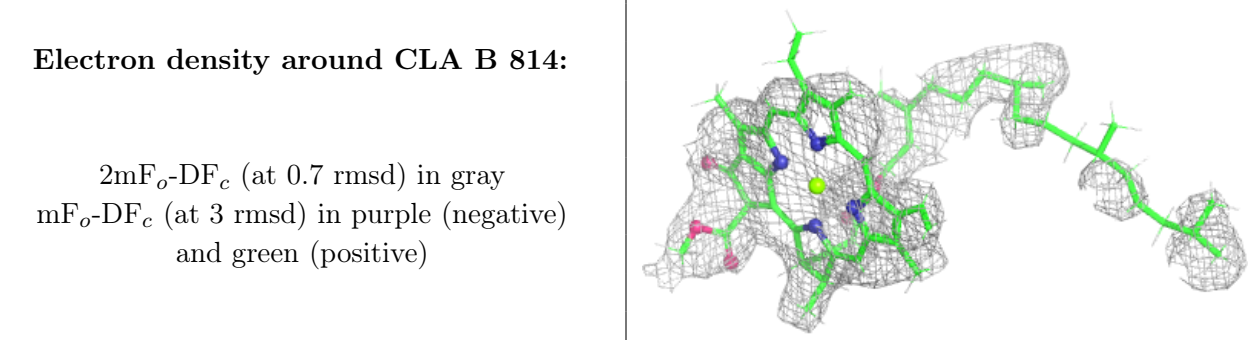


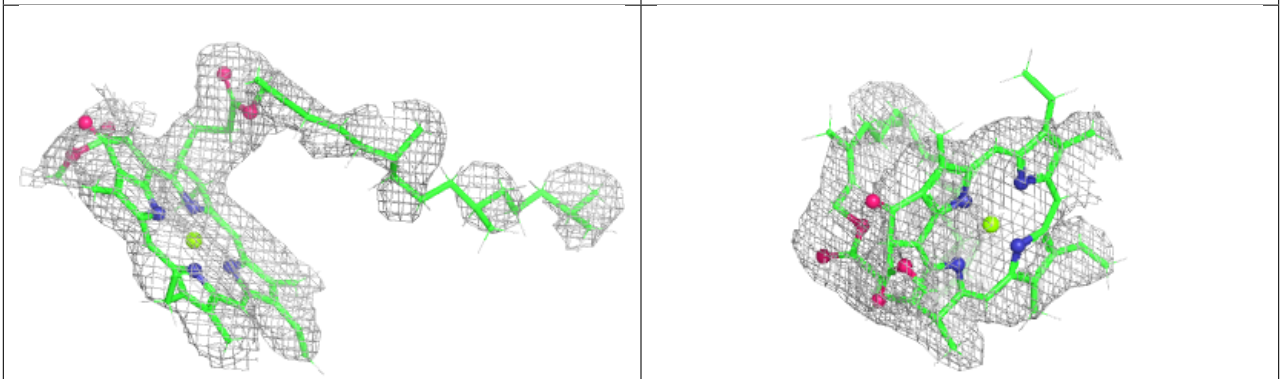




Electron density around CLA B 814:

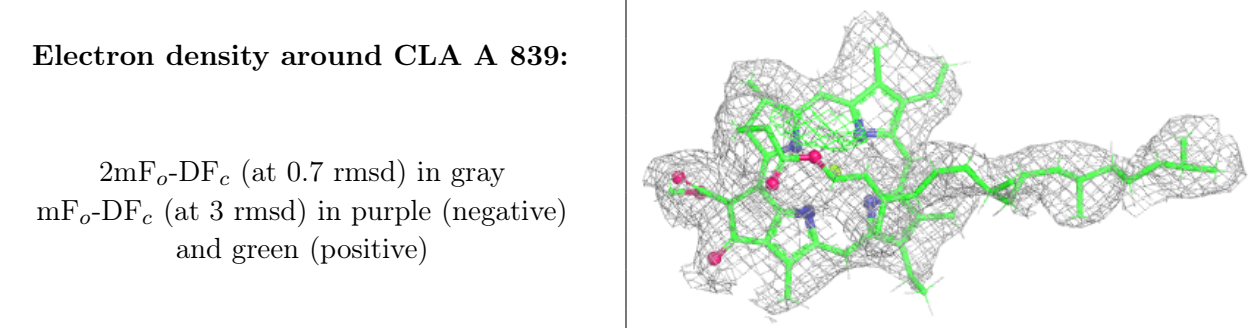
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

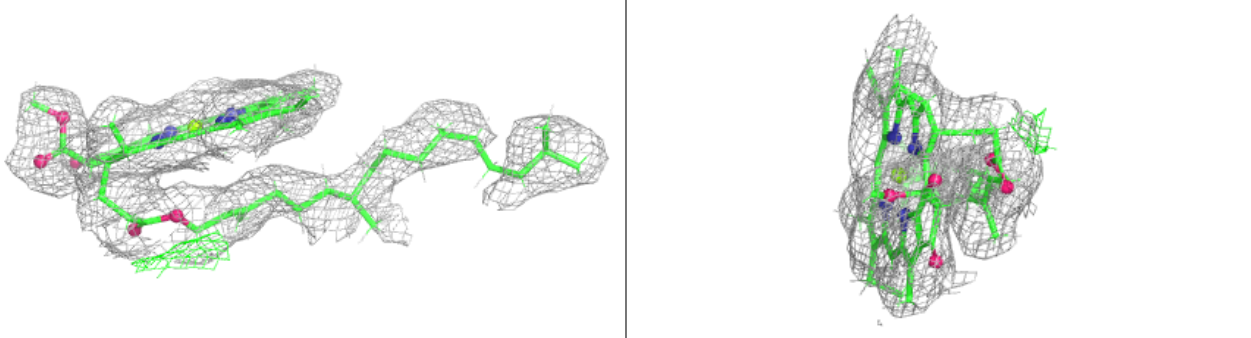




Electron density around CLA A 839:

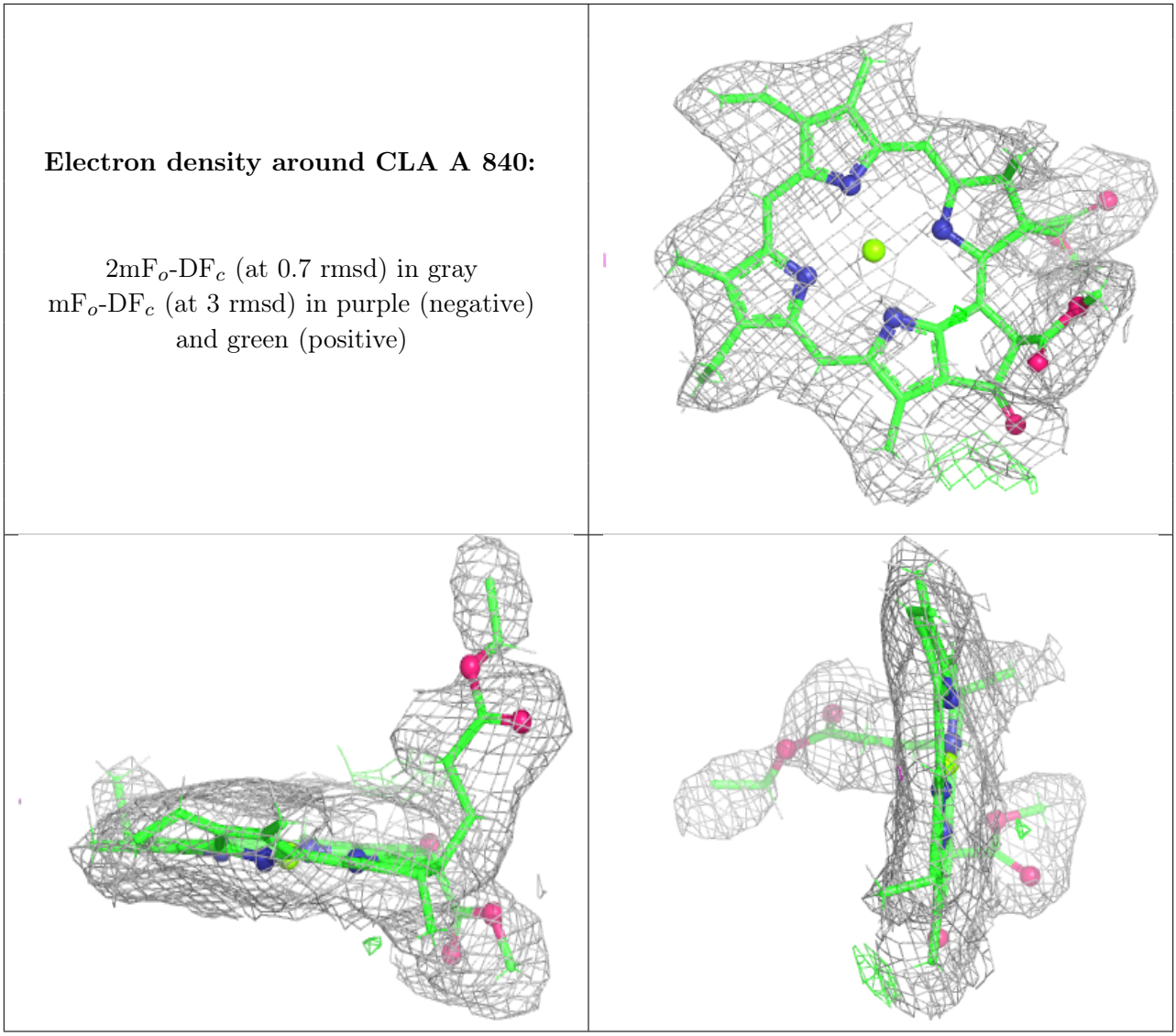
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





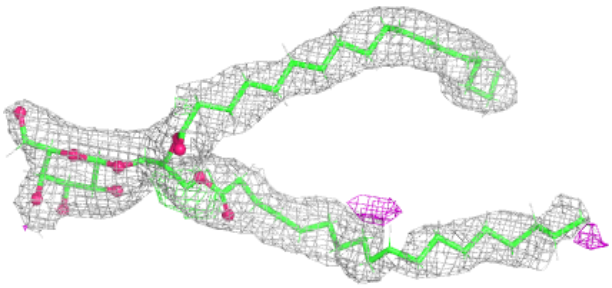
Electron density around CLA A 840:

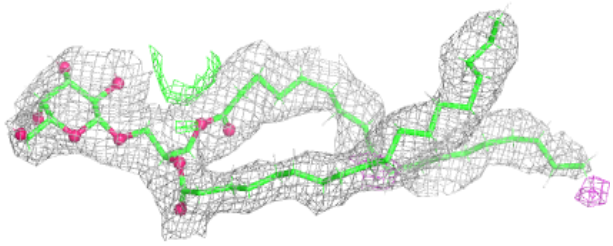
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

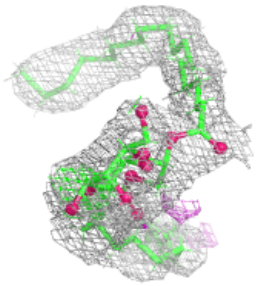


Electron density around LMG B 849:

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

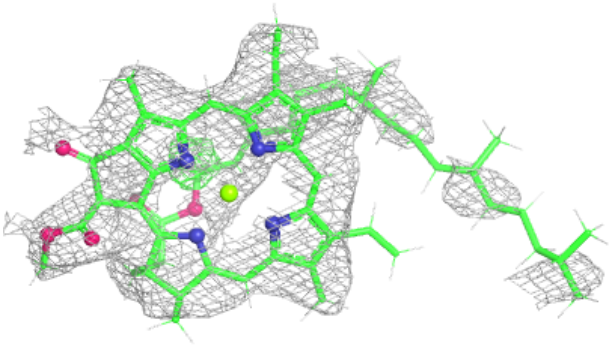


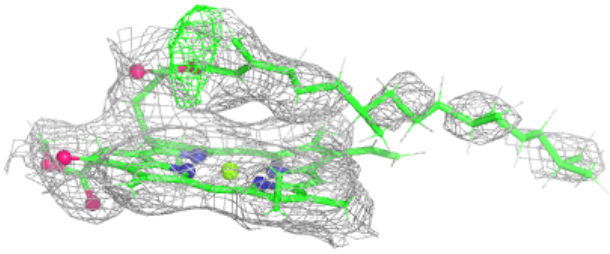


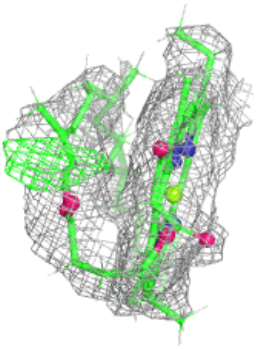


Electron density around CLA A 841:

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

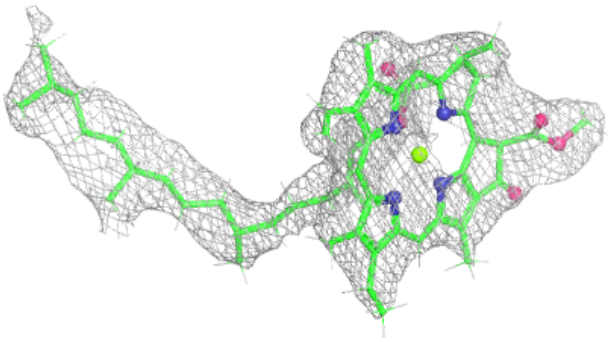


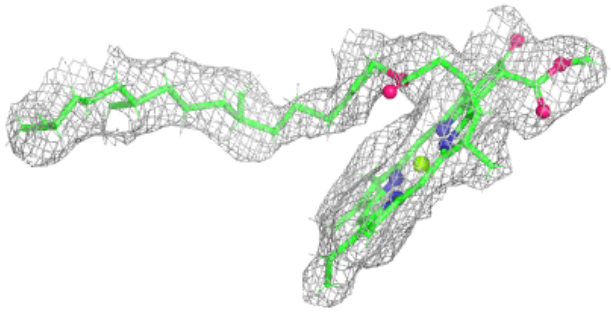


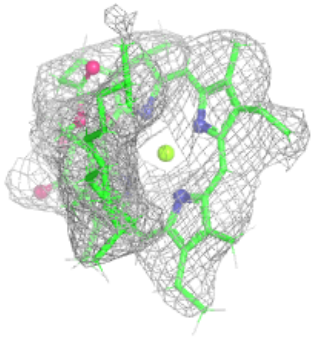


Electron density around CLA A 842:

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

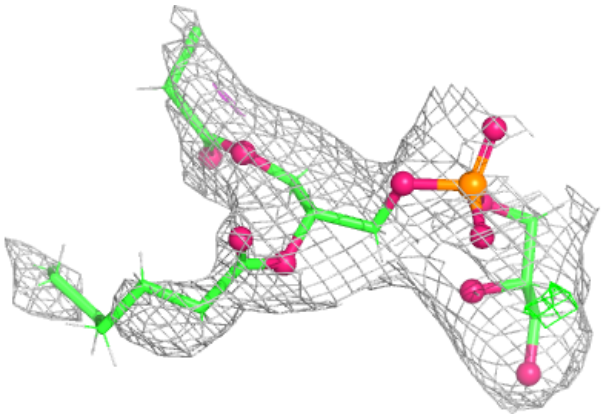


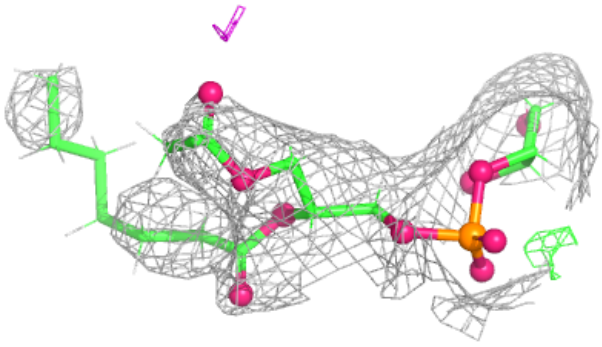


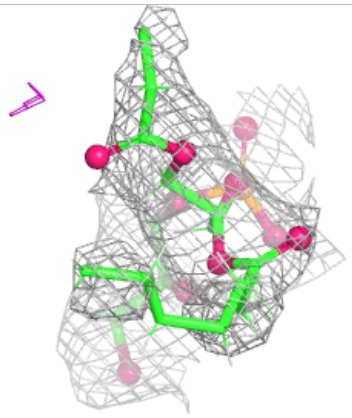


Electron density around LHG A 855:

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

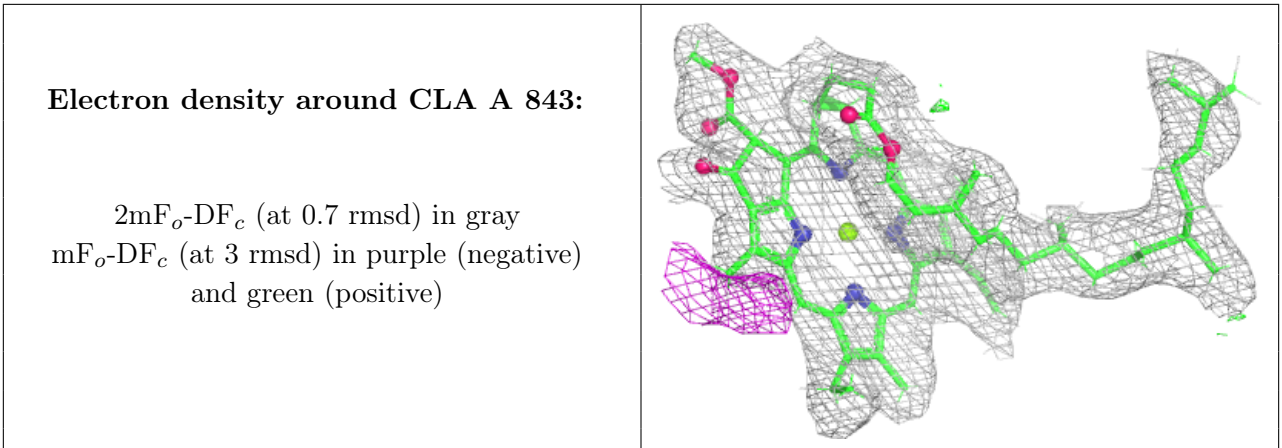






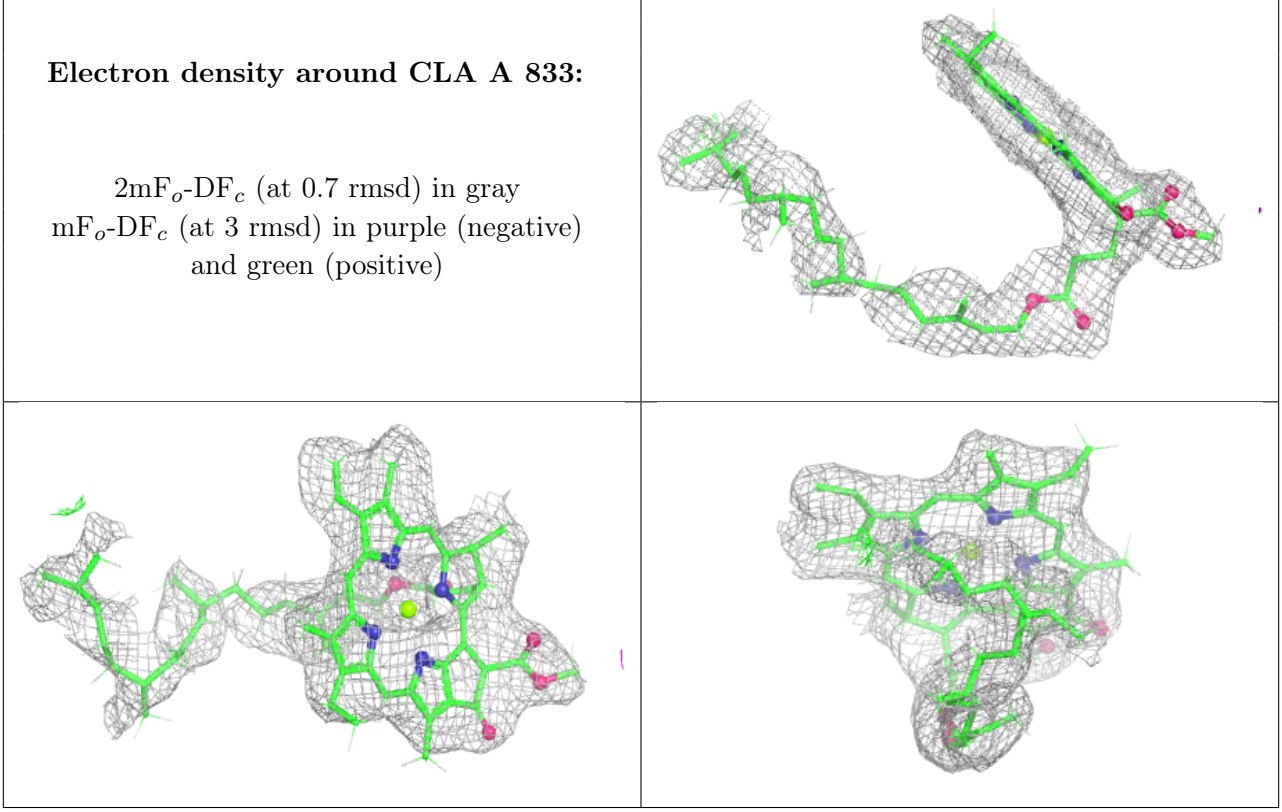
Electron density around CLA A 843:

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



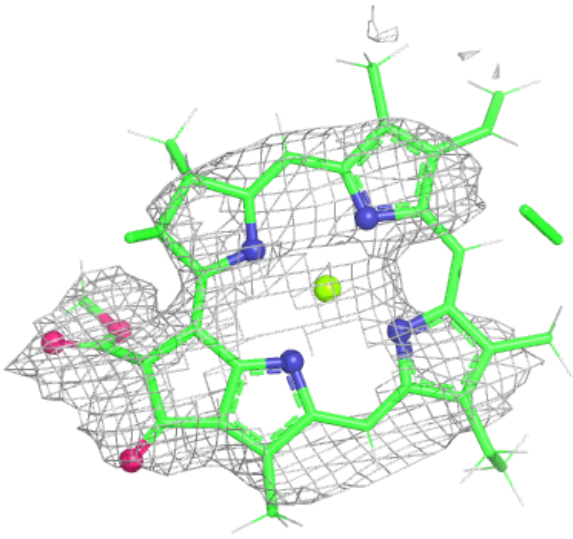
Electron density around CLA A 833:

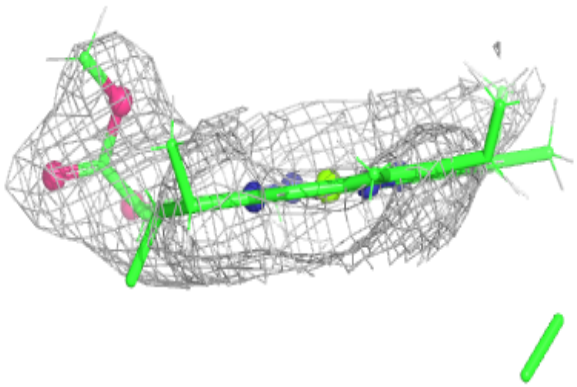
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

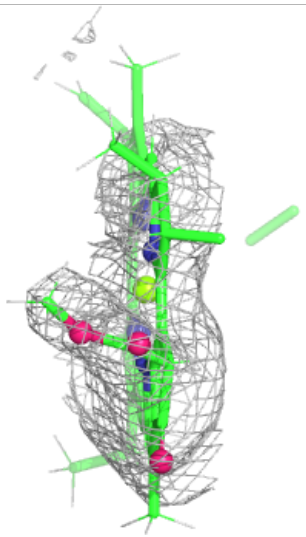


Electron density around CLA A 821:

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

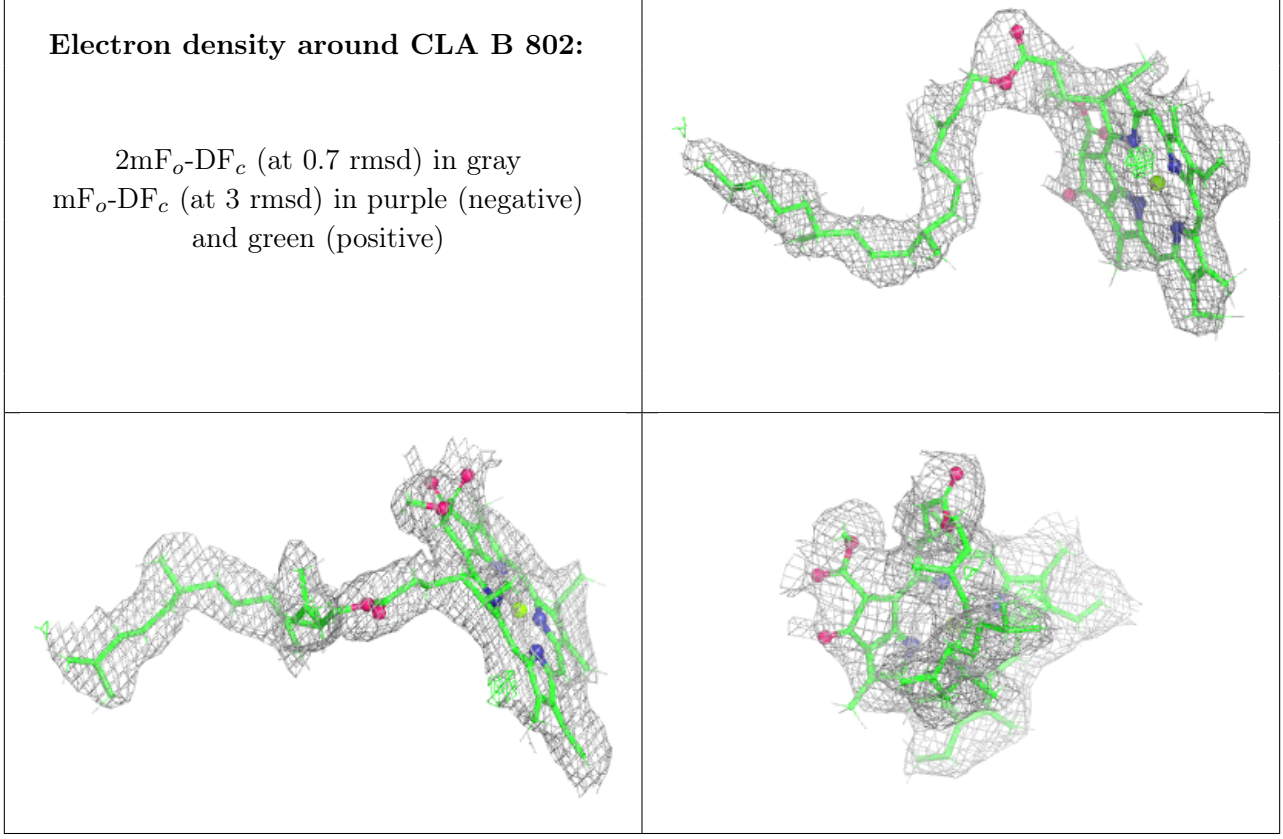






Electron density around CLA B 802:

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



6.5 Other polymers

There are no such residues in this entry.