wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2026 – 03:32 am BST

PDB ID	:	4Y28 / pdb_00004y28
Title	:	The structure of plant photosystem I super-complex at 2.8 angstrom resolution.
Authors	:	Mazor, Y.; Brovikov, A.; Nelson, N.
Deposited on	:	2015-02-09
Resolution	:	2.80 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:

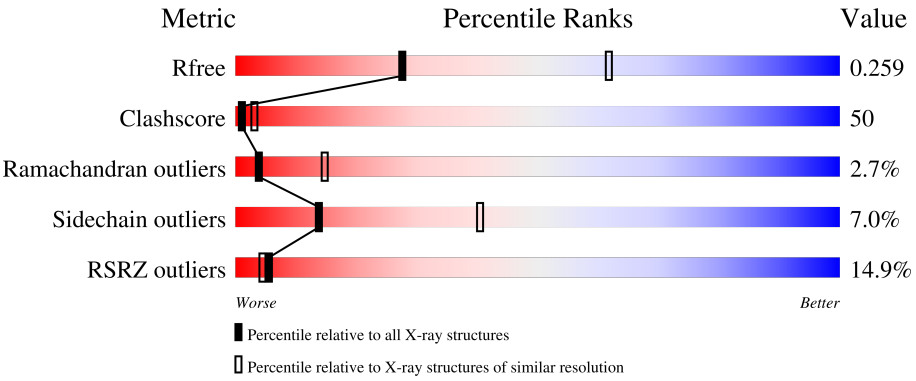
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	758	9% 73% 24%
2	B	733	9% 75% 24%
3	I	30	17% 37% 47% 13%
4	J	42	14% 36% 40% 17% 5%
5	F	154	11% 64% 28% 6%

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Mol	Chain	Length	Quality of chain
6	G	97	25% 33% 44% 13% 6%
7	L	167	21% 38% 41% 11% 5%
8	C	81	9% 56% 36% 7%
9	D	147	24% 41% 37% 14%
10	E	66	8% 45% 44% 9%
11	H	90	26% 49% 28% 12% 7%
12	K	129	14% 9% 26% 9% 56%
13	2	269	12% 18% 43% 12% 23%
14	4	252	9% 23% 43% 11% 21%
15	1	202	25% 27% 53% 14%
16	3	275	23% 12% 48% 15% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	1	1001	-	-	X	-
18	CLA	1	1003	-	-	X	-
18	CLA	1	1004	-	-	X	-
18	CLA	1	1008	-	-	X	-
18	CLA	2	2001	-	-	X	-
18	CLA	2	2002	-	-	X	-
18	CLA	2	2003	-	-	X	-
18	CLA	2	2004	-	-	X	-
18	CLA	2	2005	-	-	X	-
18	CLA	2	2006	-	-	X	-
18	CLA	2	2007	-	-	X	-
18	CLA	2	2012	-	-	X	-
18	CLA	2	2016	-	-	X	-
18	CLA	3	3001	-	-	X	-
18	CLA	3	3003	-	-	X	-
18	CLA	3	3006	-	-	X	-
18	CLA	3	3010	-	-	X	-
18	CLA	3	3012	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CLA	3	3013	-	-	X	-
18	CLA	4	4001	-	-	X	-
18	CLA	4	4006	-	-	X	-
18	CLA	4	4012	-	-	X	-
18	CLA	4	4016	-	-	X	-
18	CLA	G	1001	-	-	X	-
18	CLA	G	1002	-	-	X	-
18	CLA	G	1003	-	-	X	-
22	BCR	G	2011	-	-	X	-
22	BCR	L	6019	-	-	X	-
27	LUT	1	1501	X	-	X	-
27	LUT	1	1502	X	-	-	-
27	LUT	2	2501	X	-	X	-
27	LUT	2	2502	X	-	X	-
27	LUT	3	3501	X	-	X	-
27	LUT	3	3502	X	-	X	-
27	LUT	4	4501	X	-	X	-
27	LUT	4	4502	X	-	X	-
27	LUT	4	4503	X	-	X	-
27	LUT	I	6018	X	-	-	-
28	CHL	1	1009	X	-	X	-
28	CHL	3	3011	X	-	X	-

2 Entry composition (i)

There are 29 unique types of molecules in this entry. The entry contains 35653 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	742	Total	C	N	O	S	0	0	0
			5852	3833	997	1004	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ILE	LEU	engineered mutation	UNP P05310
A	22	LEU	VAL	engineered mutation	UNP P05310
A	117	ARG	GLY	engineered mutation	UNP P05310
A	220	GLY	ARG	engineered mutation	UNP P05310

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	732	Total	C	N	O	S	0	0	0
			5856	3851	995	996	14			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	5	LEU	ILE	engineered mutation	UNP P05311
B	115	ILE	ASN	engineered mutation	UNP P05311
B	273	MET	VAL	engineered mutation	UNP P05311
B	471	SER	THR	engineered mutation	UNP P05311
B	476	VAL	ILE	engineered mutation	UNP P05311
B	477	LEU	PRO	engineered mutation	UNP P05311
B	635	TYR	ILE	engineered mutation	UNP P05311

- Molecule 3 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	29	Total	C	N	O	S	0	0	0
			224	155	35	33	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	J	41	Total	C	N	O	0	0	0
			321	217	50	54			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	150	Total	C	N	O	S	0	0	0
			1187	770	207	208	2			

- Molecule 6 is a protein called photosystem I reaction center.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	G	91	Total	C	N	O	0	0	0
			689	444	117	128			

- Molecule 7 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	L	160	Total	C	N	O	S	0	0	0
			1197	791	190	215	1			

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	C	80	Total	C	N	O	S	0	0	0
			612	379	107	115	11			

- Molecule 9 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	141	Total	C	N	O	S	0	0	0
			1116	720	192	201	3			

- Molecule 10 is a protein called Photosystem I reaction center subunit IV A, chloroplastic.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	E	66	Total	C	N	O	0	0	0
			530	337	93	100			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	H	84	Total	C	N	O	0	0	0
			642	425	97	120			

- Molecule 12 is a protein called Photosystem I reaction center subunit X psaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	57	Total	C	N	O	S	0	0	0
			379	241	64	71	3			

- Molecule 13 is a protein called Type II chlorophyll a/b binding protein from photosystem I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	2	207	Total	C	N	O	S	0	0	0
			1613	1057	263	289	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	133	LEU	ASN	engineered mutation	UNP Q41038

- Molecule 14 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	4	198	Total	C	N	O	S	0	0	0
			1544	1007	252	282	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	128	ASP	ALA	engineered mutation	UNP Q9SQL2

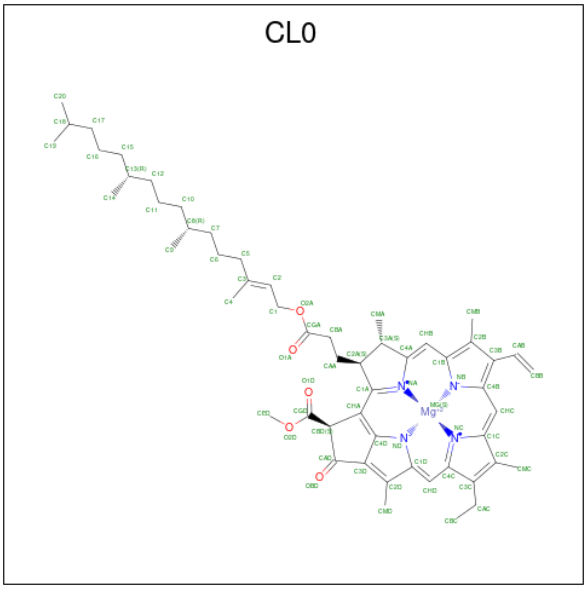
- Molecule 15 is a protein called Light-harvesting complex I chlorophyll A/B-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	1	194	Total	C	N	O	S	0	0	0
			1513	986	254	268	5			

- Molecule 16 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

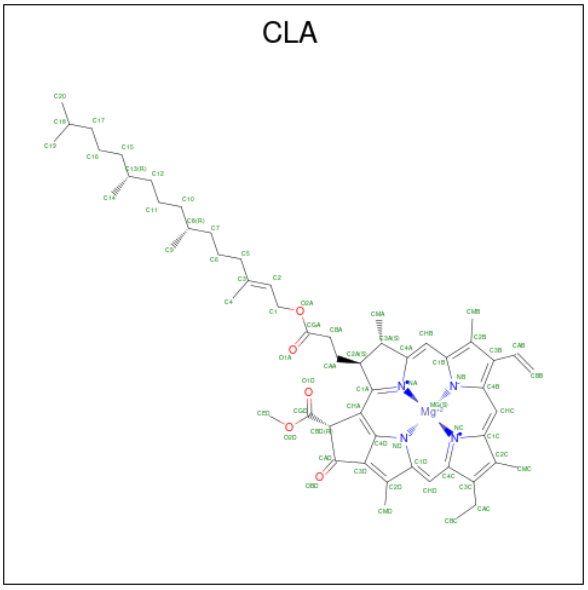
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	3	215	Total	C	N	O	S	0	0	0
			1619	1053	263	298	5			

- Molecule 17 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	J	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			45	35	1	4	5		
18	F	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	G	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	L	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	H	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	K	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	2	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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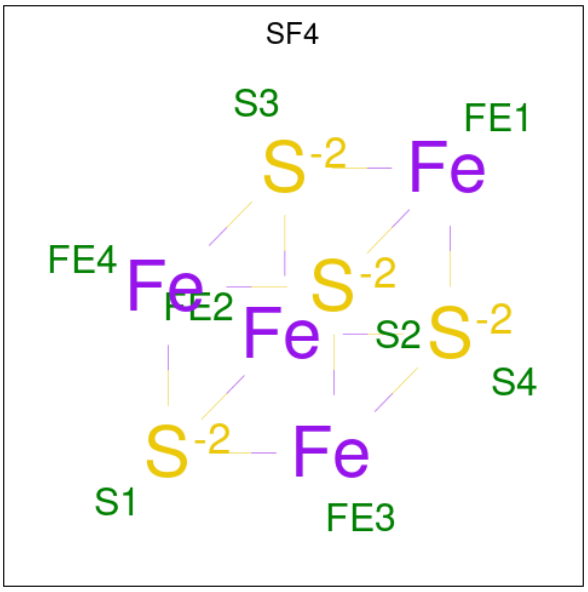
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	2	1	Total C Mg N 27 22 1 4	0	0
18	2	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 65 55 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 50 40 1 4 5	0	0
18	4	1	Total C Mg N O 60 50 1 4 5	0	0
18	4	1	Total C Mg N O 46 36 1 4 5	0	0
18	4	1	Total C Mg N O 65 55 1 4 5	0	0
18	4	1	Total C Mg N O 46 36 1 4 5	0	0
18	4	1	Total C Mg N O 65 55 1 4 5	0	0
18	1	1	Total C Mg N O 60 50 1 4 5	0	0
18	1	1	Total C Mg N O 46 36 1 4 5	0	0
18	1	1	Total C Mg N O 55 45 1 4 5	0	0
18	1	1	Total C Mg N O 65 55 1 4 5	0	0
18	1	1	Total C Mg N O 55 45 1 4 5	0	0
18	1	1	Total C Mg N O 50 40 1 4 5	0	0
18	1	1	Total C Mg N O 46 36 1 4 5	0	0

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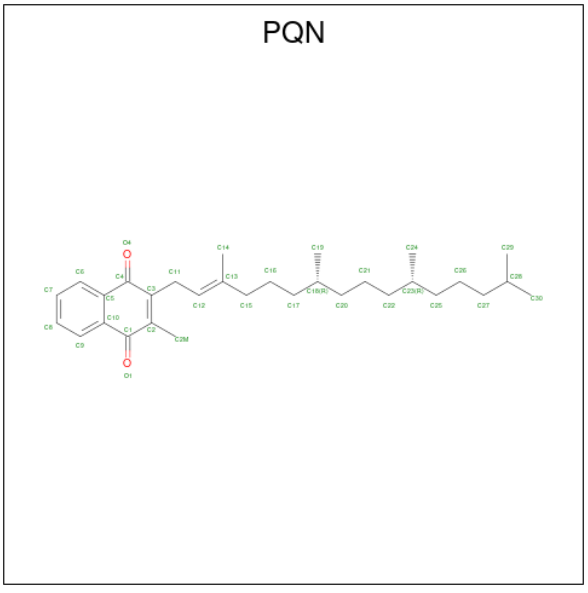
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	1	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			48	38	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
18	3	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
18	3	1	Total	C	Mg	N		0	0
			27	22	1	4			

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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



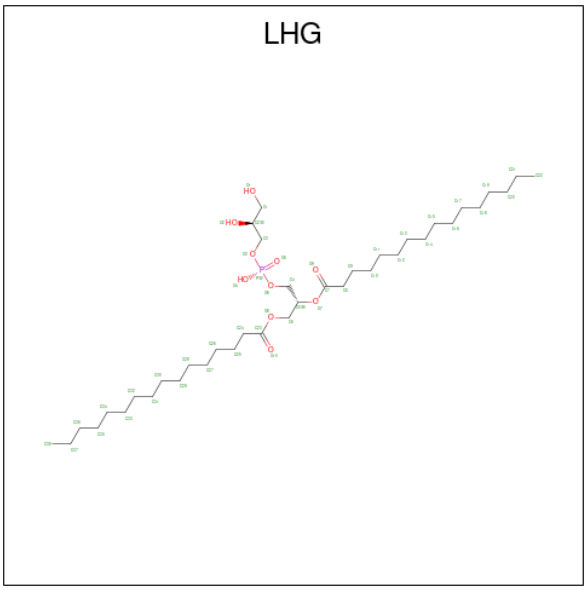
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	A	1	Total C O 33 31 2	0	0

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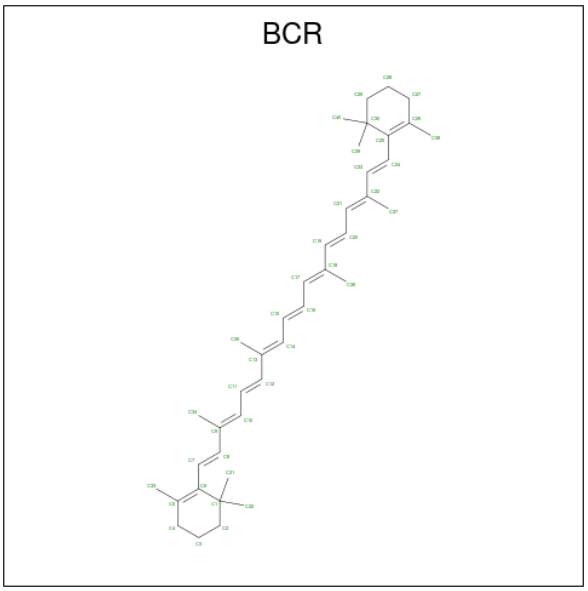
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	B	1	Total	C	O	0	0
			33	31	2		

- Molecule 21 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	O	P	0	0
			40	29	10	1		
21	A	1	Total	C	O	P	0	0
			49	38	10	1		
21	B	1	Total	C	O	P	0	0
			21	10	10	1		
21	2	1	Total	C	O	P	0	0
			24	13	10	1		
21	1	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



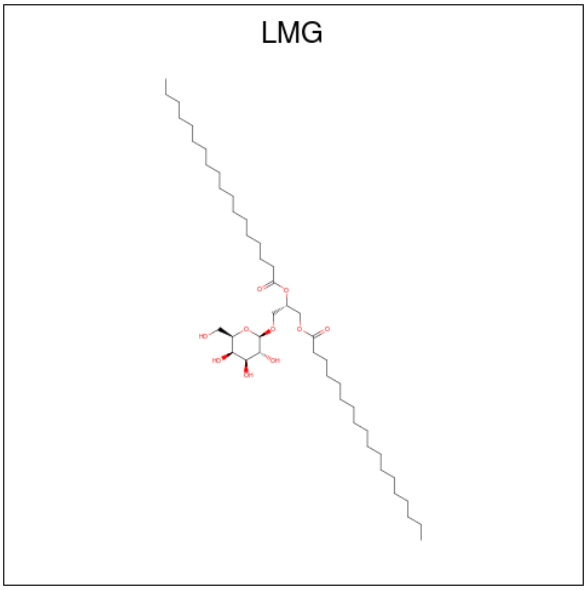
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	A	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total C 40 40	0	0
22	B	1	Total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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	F	1	Total C 40 40	0	0
22	F	1	Total C 40 40	0	0
22	G	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	L	1	Total C 40 40	0	0
22	K	1	Total C 40 40	0	0
22	3	1	Total C 40 40	0	0

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 38 28 10	0	0
23	J	1	Total C O 55 45 10	0	0
23	F	1	Total C O 23 13 10	0	0
23	F	1	Total C O 37 27 10	0	0

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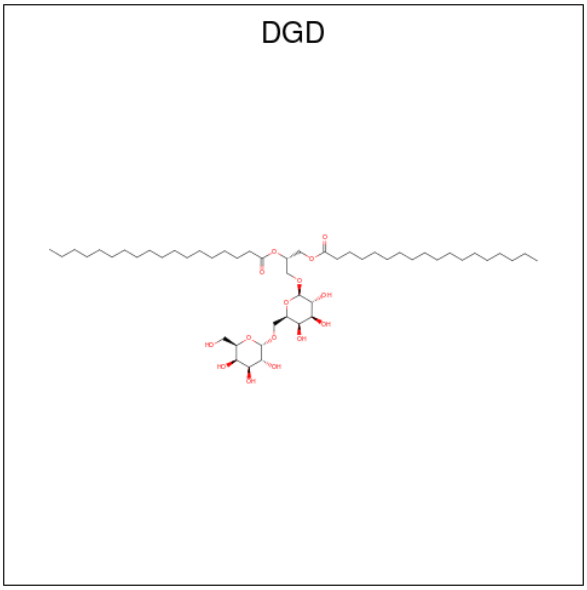
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	G	1	Total C O 41 31 10	0	0
23	2	1	Total C O 35 25 10	0	0
23	4	1	Total C O 35 25 10	0	0

- Molecule 24 is CALCIUM ION (CCD ID: CA) (formula: Ca).

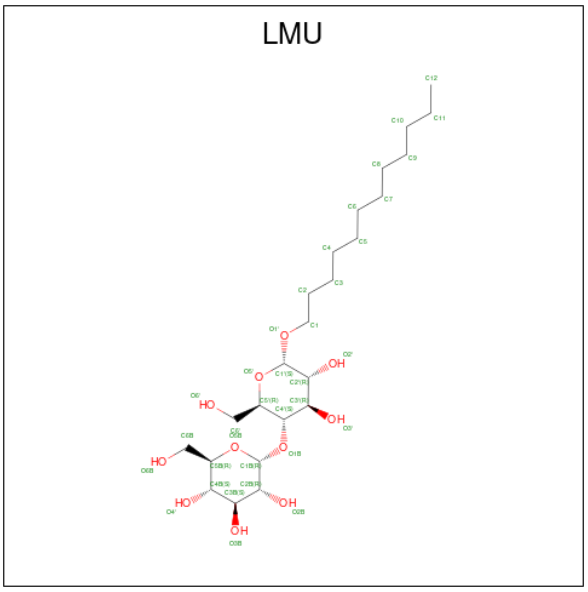
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	B	1	Total Ca 1 1	0	0

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



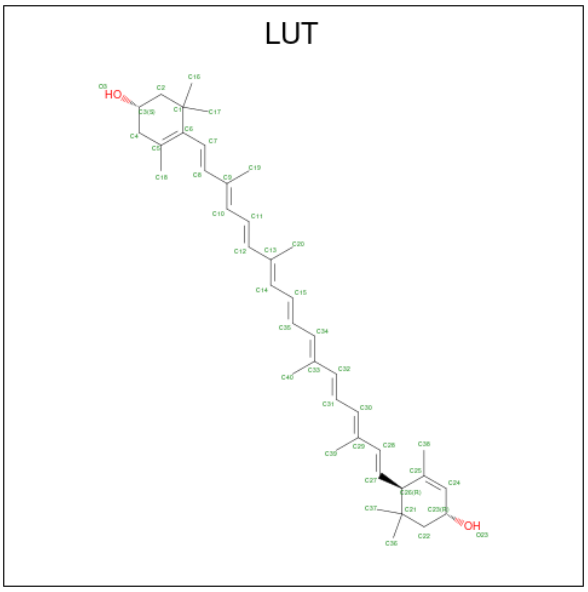
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	B	1	Total C O 61 46 15	0	0

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 27 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



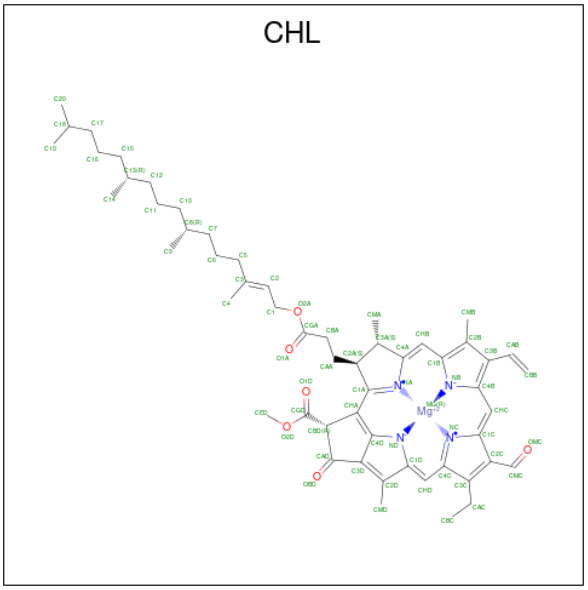
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	I	1	Total C O 42 40 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	2	1	Total C O 42 40 2	0	0
27	2	1	Total C O 42 40 2	0	0
27	4	1	Total C O 42 40 2	0	0
27	4	1	Total C O 42 40 2	0	0
27	4	1	Total C O 42 40 2	0	0
27	1	1	Total C O 42 40 2	0	0
27	1	1	Total C O 42 40 2	0	0
27	3	1	Total C O 42 40 2	0	0
27	3	1	Total C O 42 40 2	0	0

- Molecule 28 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



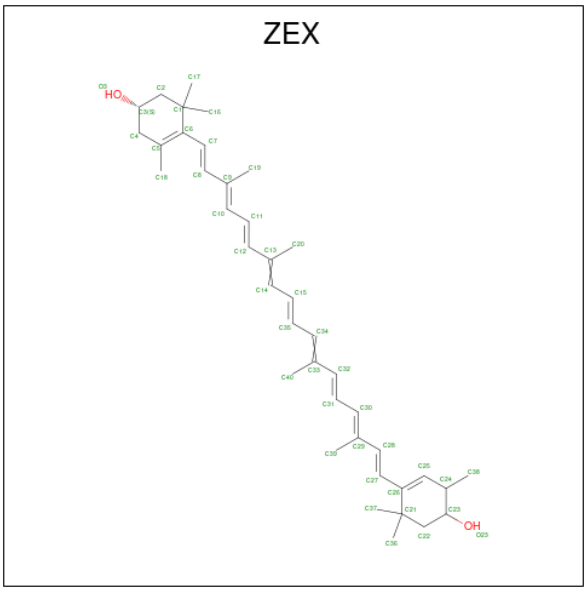
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	2	1	Total C Mg N O 47 36 1 4 6	0	0
28	2	1	Total C Mg N O 48 37 1 4 6	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	2	1	Total	C	Mg	N	O	0	0
			46	35	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
28	4	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		
28	1	1	Total	C	Mg	N	O	0	0
			47	36	1	4	6		
28	3	1	Total	C	Mg	N	O	0	0
			56	45	1	4	6		

- Molecule 29 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).

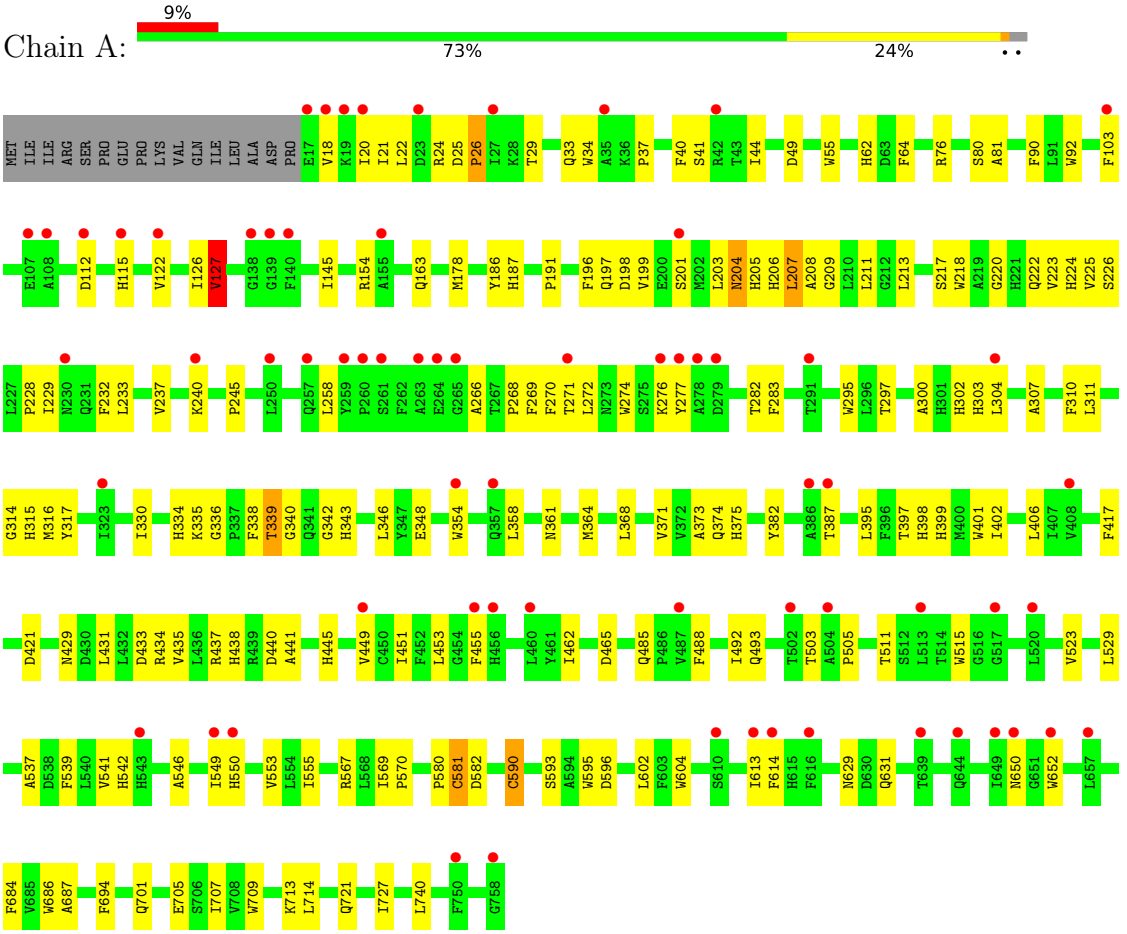


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	4	1	Total	C	O	0	0
			42	40	2		

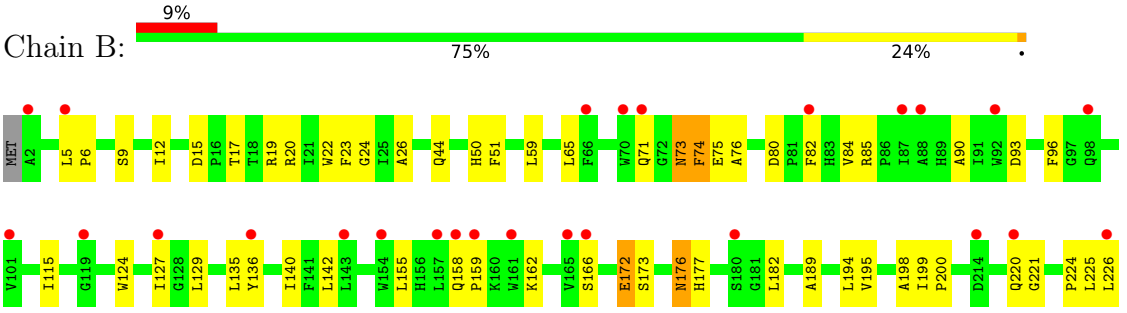
3 Residue-property plots (i)

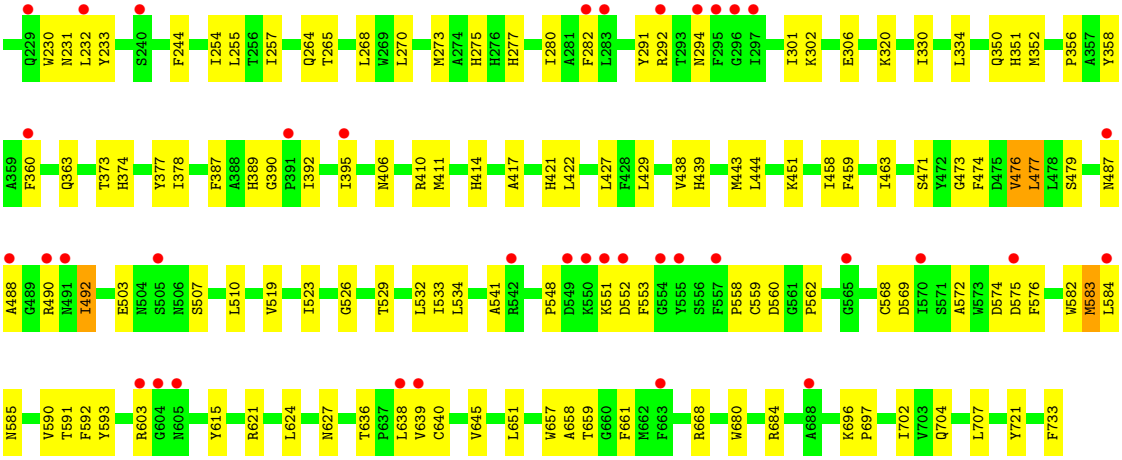
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



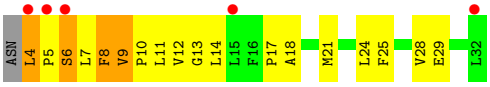
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





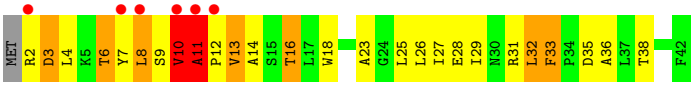
• Molecule 3: Photosystem I reaction center subunit VIII





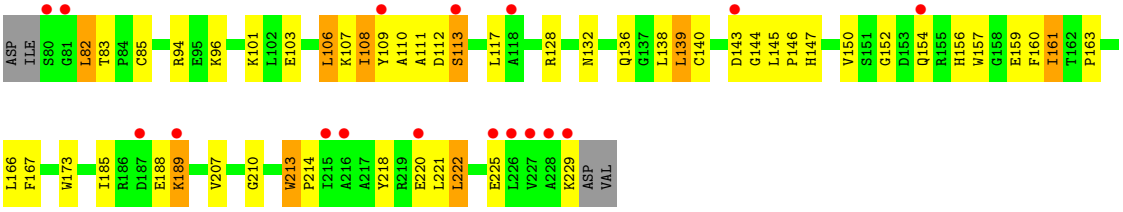
• Molecule 4: Photosystem I reaction center subunit IX





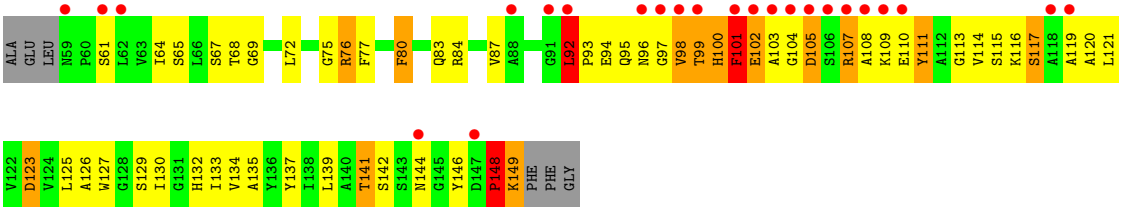
• Molecule 5: Photosystem I reaction center subunit III





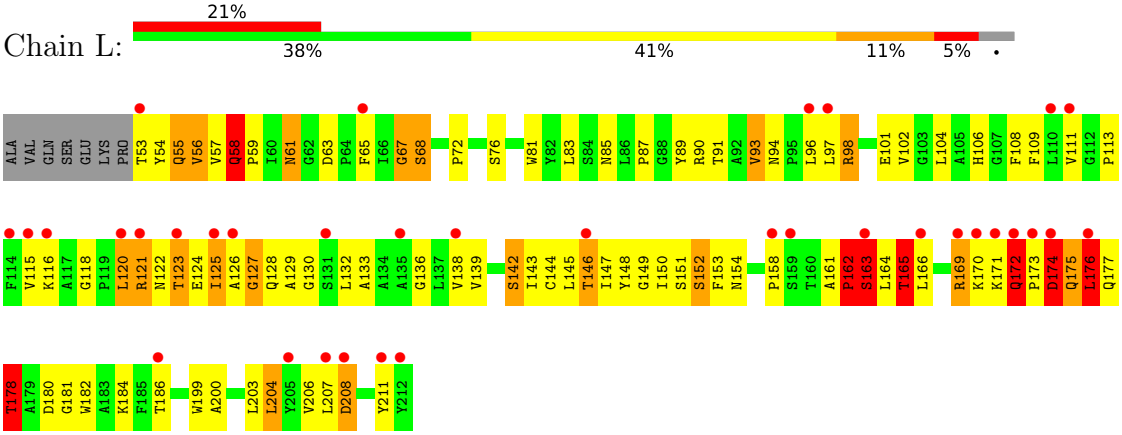
• Molecule 6: photosystem I reaction center





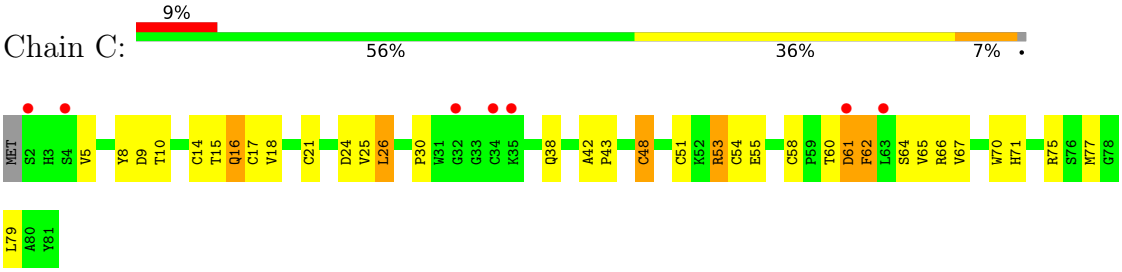
• Molecule 7: Putative uncharacterized protein

Chain L:



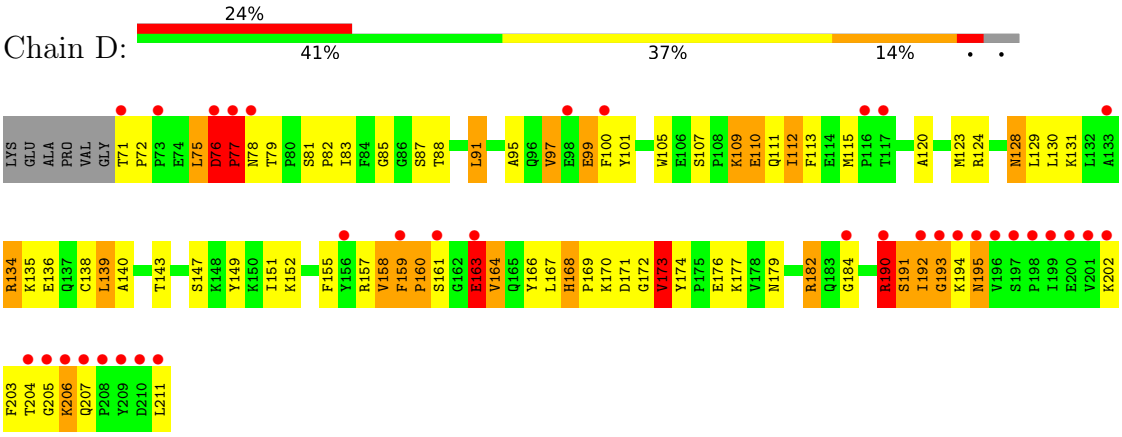
• Molecule 8: Photosystem I iron-sulfur center

Chain C:



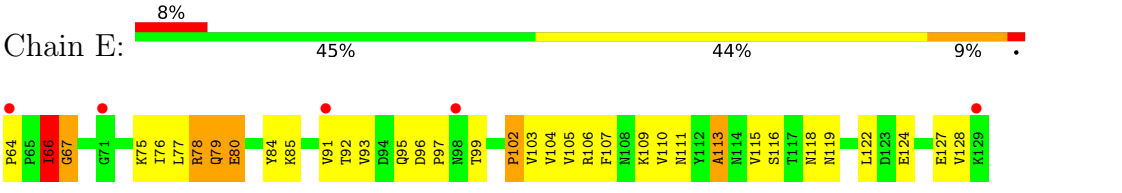
• Molecule 9: Photosystem I reaction center subunit II, chloroplastic

Chain D:



• Molecule 10: Photosystem I reaction center subunit IV A, chloroplastic

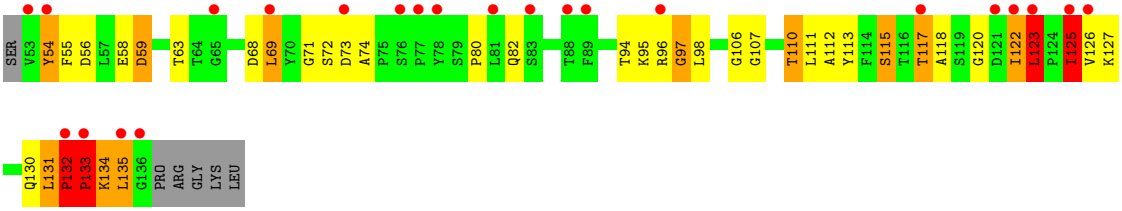
Chain E:



• Molecule 11: Photosystem I reaction center subunit VI

Chain H:

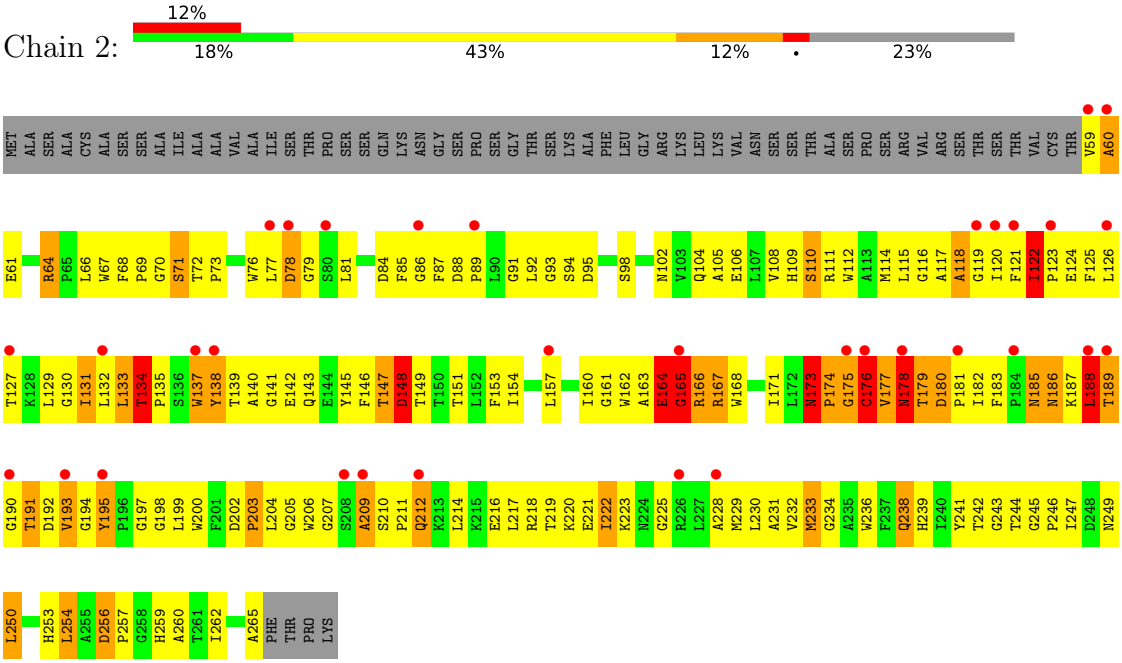




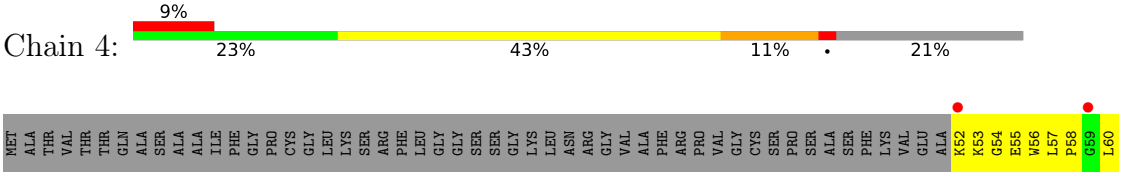
• Molecule 12: Photosystem I reaction center subunit X psaK

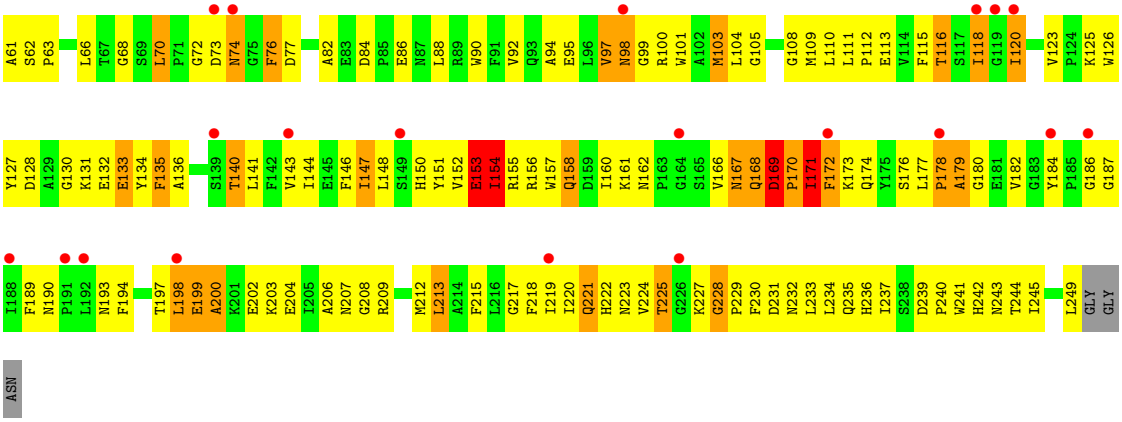


• Molecule 13: Type II chlorophyll a/b binding protein from photosystem I



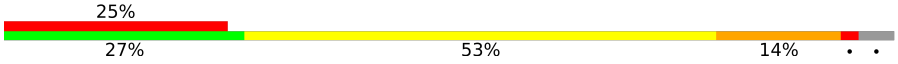
• Molecule 14: Chlorophyll a-b binding protein P4, chloroplastic

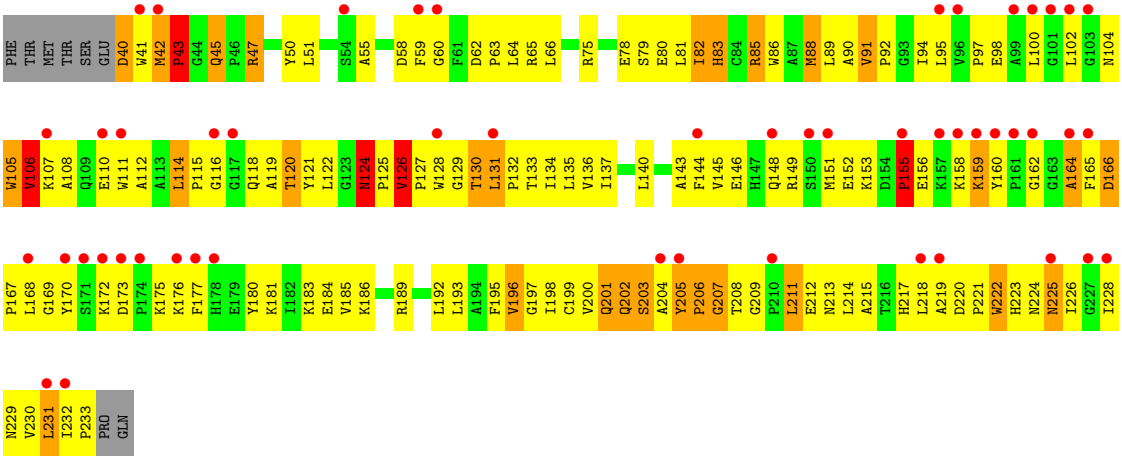




• Molecule 15: Light-harvesting complex I chlorophyll A/B-binding protein

Chain 1:

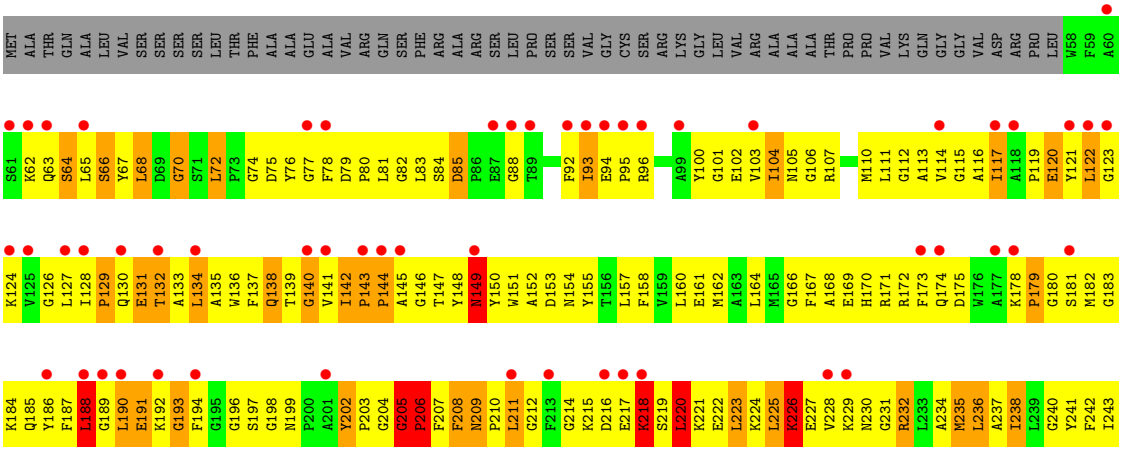


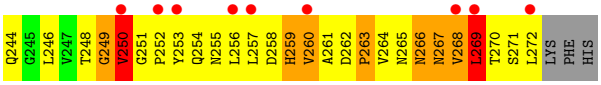


• Molecule 16: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:






Q244
G245
L246
V247
T248
G249
V250
G251
P252
Y253
Q254
N255
L256
L257
D258
H259
V260
A261
D262
P263
V264
N265
M266
N267
V268
L269
T270
S271
L272
LYS
PHE
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	189.00Å 201.90Å 213.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.80 48.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.65-2.80) 89.2 (48.65-2.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.259 , 0.268 0.246 , 0.259	Depositor DCC
R_{free} test set	3977 reflections (1.40%)	wwPDB-VP
Wilson B-factor (Å^2)	78.1	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 53.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	35653	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: SF4, CL0, CA, ZEX, BCR, LMG, LHG, CHL, CLA, DGD, LUT, LMU, PQN

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	0.30	0/6049	0.72	2/8253 (0.0%)
2	B	0.30	0/6067	0.72	3/8287 (0.0%)
3	I	1.37	0/230	1.42	3/313 (1.0%)
4	J	1.15	0/330	1.47	6/452 (1.3%)
5	F	0.85	0/1214	1.06	10/1638 (0.6%)
6	G	1.11	0/705	1.56	12/956 (1.3%)
7	L	1.05	0/1233	1.37	17/1690 (1.0%)
8	C	1.11	2/625 (0.3%)	1.14	5/846 (0.6%)
9	D	1.29	0/1146	1.53	24/1550 (1.5%)
10	E	1.14	0/542	1.46	11/737 (1.5%)
11	H	0.84	2/662 (0.3%)	1.31	14/902 (1.6%)
12	K	0.70	0/381	1.28	7/517 (1.4%)
13	2	1.31	3/1672 (0.2%)	1.56	41/2292 (1.8%)
14	4	1.31	3/1592 (0.2%)	1.45	34/2174 (1.6%)
15	1	1.17	1/1563 (0.1%)	1.50	32/2132 (1.5%)
16	3	1.16	5/1666 (0.3%)	1.60	46/2265 (2.0%)
All	All	0.86	16/25677 (0.1%)	1.16	267/35004 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	G	0	1
7	L	0	1
13	2	0	1
14	4	0	1
16	3	0	1
All	All	0	5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	164	GLU	C-O	-15.54	1.03	1.24
14	4	153	GLU	C-O	-14.60	1.03	1.23
14	4	154	ILE	C-N	9.56	1.47	1.33
16	3	205	GLY	C-O	-8.79	1.12	1.24
16	3	208	PHE	C-N	8.31	1.43	1.33

The worst 5 of 267 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	E	66	ILE	N-CA-C	16.27	126.04	110.42
6	G	100	HIS	N-CA-C	-15.45	83.33	108.52
7	L	174	ASP	N-CA-C	14.88	132.29	109.23
6	G	101	PHE	CA-C-N	14.51	149.25	121.54
6	G	101	PHE	C-N-CA	14.51	149.25	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	2	164	GLU	Mainchain
16	3	205	GLY	Mainchain
14	4	153	GLU	Mainchain
6	G	101	PHE	Peptide
7	L	98	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5852	0	5710	167	0
2	B	5856	0	5666	146	0
3	I	224	0	247	37	0
4	J	321	0	328	47	0
5	F	1187	0	1226	42	3
6	G	689	0	676	114	0
7	L	1197	0	1187	168	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	612	0	594	38	0
9	D	1116	0	1126	109	0
10	E	530	0	530	44	0
11	H	642	0	637	49	0
12	K	379	0	386	92	0
13	2	1613	0	1554	378	0
14	4	1544	0	1489	236	0
15	1	1513	0	1495	384	0
16	3	1619	0	1554	490	0
17	A	65	0	72	5	0
18	1	615	0	511	221	0
18	2	628	0	538	251	0
18	3	698	0	559	252	0
18	4	677	0	635	187	0
18	A	2583	0	2555	177	0
18	B	2519	0	2617	199	0
18	F	95	0	72	16	0
18	G	161	0	141	87	0
18	H	46	0	33	5	0
18	J	50	0	39	7	0
18	K	46	0	33	12	0
18	L	160	0	137	37	0
19	A	8	0	0	1	0
19	C	16	0	0	0	0
20	A	33	0	46	3	0
20	B	33	0	46	5	0
21	1	49	0	74	15	0
21	2	24	0	18	6	0
21	A	89	0	127	12	0
21	B	21	0	12	1	0
22	3	40	0	48	20	0
22	A	240	0	292	23	0
22	B	200	0	245	25	0
22	F	80	0	98	17	0
22	G	40	0	49	28	0
22	I	40	0	49	3	0
22	J	80	0	98	15	0
22	K	40	0	49	17	0
22	L	80	0	98	27	0
23	2	35	0	40	9	0
23	4	35	0	40	6	0
23	B	38	0	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	F	60	0	60	13	0
23	G	41	0	52	20	0
23	J	55	0	86	10	0
24	B	1	0	0	0	0
25	B	61	0	83	4	0
26	B	70	0	92	4	0
27	1	84	0	110	49	0
27	2	84	0	110	53	0
27	3	84	0	110	62	0
27	4	126	0	165	81	0
27	I	42	0	55	12	0
28	1	103	0	78	36	0
28	2	141	0	95	37	0
28	3	56	0	47	22	0
28	4	145	0	99	43	0
29	4	42	0	56	12	0
All	All	35653	0	35120	3545	3

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 50.

The worst 5 of 3545 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)
16:3:138:GLN:HB2	16:3:145:ALA:HB2	1.25	1.18
16:3:268:VAL:HG21	18:3:3003:CLA:H43	1.17	1.16
16:3:111:LEU:HD22	18:3:3006:CLA:CBB	1.74	1.15
16:3:127:LEU:HB2	18:3:3018:CLA:HBC1	1.29	1.15
7:L:85:ASN:HB3	18:L:1501:CLA:HAC1	1.26	1.14

All (3) 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)
5:F:96:LYS:CD	7:L:170:LYS:NZ[3_555]	1.69	0.51
5:F:96:LYS:CE	7:L:170:LYS:NZ[3_555]	1.86	0.34
5:F:96:LYS:CG	7:L:170:LYS:NZ[3_555]	1.99	0.21

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	740/758 (98%)	691 (93%)	45 (6%)	4 (0%)	24 55
2	B	730/733 (100%)	695 (95%)	30 (4%)	5 (1%)	18 47
3	I	27/30 (90%)	25 (93%)	1 (4%)	1 (4%)	2 9
4	J	39/42 (93%)	34 (87%)	3 (8%)	2 (5%)	1 5
5	F	148/154 (96%)	138 (93%)	8 (5%)	2 (1%)	9 30
6	G	89/97 (92%)	76 (85%)	8 (9%)	5 (6%)	1 4
7	L	158/167 (95%)	133 (84%)	15 (10%)	10 (6%)	1 3
8	C	78/81 (96%)	72 (92%)	6 (8%)	0	100 100
9	D	139/147 (95%)	116 (84%)	14 (10%)	9 (6%)	1 3
10	E	64/66 (97%)	57 (89%)	6 (9%)	1 (2%)	7 27
11	H	82/90 (91%)	65 (79%)	10 (12%)	7 (8%)	0 1
12	K	53/129 (41%)	49 (92%)	2 (4%)	2 (4%)	2 9
13	2	205/269 (76%)	184 (90%)	7 (3%)	14 (7%)	1 2
14	4	196/252 (78%)	174 (89%)	15 (8%)	7 (4%)	2 10
15	1	192/202 (95%)	168 (88%)	17 (9%)	7 (4%)	2 10
16	3	213/275 (78%)	189 (89%)	15 (7%)	9 (4%)	2 7
All	All	3153/3492 (90%)	2866 (91%)	202 (6%)	85 (3%)	4 15

5 of 85 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	VAL
3	I	6	SER
4	J	11	ALA
6	G	101	PHE
6	G	102	GLU

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	603/619 (97%)	590 (98%)	13 (2%)	45 78
2	B	599/600 (100%)	583 (97%)	16 (3%)	39 74
3	I	25/26 (96%)	23 (92%)	2 (8%)	11 34
4	J	33/35 (94%)	28 (85%)	5 (15%)	3 10
5	F	123/127 (97%)	114 (93%)	9 (7%)	13 38
6	G	71/76 (93%)	64 (90%)	7 (10%)	7 24
7	L	124/133 (93%)	105 (85%)	19 (15%)	3 10
8	C	69/70 (99%)	64 (93%)	5 (7%)	13 39
9	D	120/125 (96%)	107 (89%)	13 (11%)	6 21
10	E	59/59 (100%)	53 (90%)	6 (10%)	7 23
11	H	69/74 (93%)	63 (91%)	6 (9%)	9 30
12	K	38/99 (38%)	31 (82%)	7 (18%)	1 6
13	2	166/216 (77%)	149 (90%)	17 (10%)	7 23
14	4	161/202 (80%)	145 (90%)	16 (10%)	7 24
15	1	158/167 (95%)	139 (88%)	19 (12%)	5 17
16	3	159/213 (75%)	138 (87%)	21 (13%)	4 14
All	All	2577/2841 (91%)	2396 (93%)	181 (7%)	14 40

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	2	173	ASN
15	1	43	PRO
13	2	189	THR
14	4	140	THR
15	1	131	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 60 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	132	HIS
16	3	154	ASN
11	H	82	GLN
16	3	105	ASN
16	3	266	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 209 ligands modelled in this entry, 1 is monoatomic - leaving 208 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	$\#\|Z\| > 2$
22	BCR	L	6019	-	41,41,41	2.93	7 (17%)	56,56,56	6.55	24 (42%)
18	CLA	A	1134	-	59,63,73	2.58	22 (37%)	71,101,113	2.78	24 (33%)
18	CLA	4	4009	14	54,58,73	2.51	19 (35%)	65,95,113	2.90	24 (36%)
18	CLA	A	1121	1	59,63,73	2.57	23 (38%)	71,101,113	2.87	26 (36%)
18	CLA	A	1101	1	69,73,73	2.36	22 (31%)	83,113,113	2.66	23 (27%)
25	DGD	B	7101	-	62,62,67	0.91	1 (1%)	76,76,81	1.33	11 (14%)
18	CLA	A	1124	-	59,63,73	2.58	23 (38%)	71,101,113	2.88	25 (35%)
18	CLA	3	3007	-	54,58,73	2.58	20 (37%)	65,95,113	2.92	26 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
21	LHG	A	5003	18	39,39,48	1.04	2 (5%)	42,45,54	1.18	4 (9%)
21	LHG	A	7001	-	48,48,48	0.96	2 (4%)	51,54,54	1.13	4 (7%)
18	CLA	B	1205	2	69,73,73	2.36	22 (31%)	83,113,113	2.50	25 (30%)
18	CLA	B	1210	-	69,73,73	2.35	22 (31%)	83,113,113	2.60	26 (31%)
18	CLA	A	1139	-	69,73,73	2.38	23 (33%)	83,113,113	2.59	25 (30%)
22	BCR	J	6013	-	41,41,41	2.89	8 (19%)	56,56,56	6.55	30 (53%)
28	CHL	3	3011	-	60,64,74	1.75	9 (15%)	68,102,114	1.63	12 (17%)
23	LMG	4	4801	-	35,35,55	1.04	2 (5%)	43,43,63	1.63	10 (23%)
18	CLA	B	1222	-	69,73,73	2.35	22 (31%)	83,113,113	2.66	27 (32%)
22	BCR	K	2011	-	41,41,41	2.71	6 (14%)	56,56,56	6.74	27 (48%)
28	CHL	2	2011	-	52,56,74	1.89	9 (17%)	58,92,114	1.68	12 (20%)
22	BCR	I	6020	-	41,41,41	2.77	7 (17%)	56,56,56	6.64	20 (35%)
18	CLA	A	1129	1	54,58,73	2.69	22 (40%)	65,95,113	2.92	25 (38%)
18	CLA	A	1119	-	69,73,73	2.37	22 (31%)	83,113,113	2.56	25 (30%)
18	CLA	B	1202	-	69,73,73	2.35	22 (31%)	83,113,113	2.67	25 (30%)
27	LUT	1	1501	-	42,43,43	2.50	4 (9%)	51,60,60	2.31	14 (27%)
22	BCR	B	6004	-	41,41,41	2.78	6 (14%)	56,56,56	6.67	29 (51%)
18	CLA	B	1012	-	69,73,73	2.36	22 (31%)	83,113,113	2.54	24 (28%)
17	CL0	A	1011	1	69,73,73	2.39	22 (31%)	83,113,113	2.57	26 (31%)
18	CLA	B	1212	-	59,63,73	2.55	23 (38%)	71,101,113	2.83	25 (35%)
18	CLA	B	1215	2	64,68,73	2.48	23 (35%)	77,107,113	2.67	23 (29%)
18	CLA	A	1151	21	54,58,73	2.73	23 (42%)	65,95,113	2.88	22 (33%)
18	CLA	1	1006	-	54,58,73	2.59	21 (38%)	65,95,113	2.93	25 (38%)
18	CLA	A	1103	1	69,73,73	2.35	23 (33%)	83,113,113	2.63	26 (31%)
18	CLA	B	1021	2	69,73,73	2.36	21 (30%)	83,113,113	2.65	24 (28%)
29	ZEX	4	4505	-	42,43,43	1.08	3 (7%)	55,60,60	2.17	19 (34%)
18	CLA	A	1120	1	64,68,73	2.46	22 (34%)	77,107,113	2.72	23 (29%)
18	CLA	A	1123	-	69,73,73	2.37	23 (33%)	83,113,113	2.61	25 (30%)
23	LMG	G	2021	-	41,41,55	0.95	2 (4%)	49,49,63	1.16	5 (10%)
18	CLA	B	1228	2	64,68,73	2.47	22 (34%)	77,107,113	2.67	23 (29%)
18	CLA	A	1116	1	64,68,73	2.46	22 (34%)	77,107,113	2.77	24 (31%)
18	CLA	2	2006	-	59,63,73	2.49	21 (35%)	71,101,113	2.79	24 (33%)
18	CLA	B	1219	2	64,68,73	2.47	23 (35%)	77,107,113	2.61	23 (29%)
18	CLA	B	1223	2	69,73,73	2.34	22 (31%)	83,113,113	2.63	26 (31%)
18	CLA	B	1207	-	69,73,73	2.36	23 (33%)	83,113,113	2.63	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	A	1106	1	69,73,73	2.37	23 (33%)	83,113,113	2.62	24 (28%)
18	CLA	B	1023	-	69,73,73	2.37	22 (31%)	83,113,113	2.60	26 (31%)
18	CLA	B	1238	-	69,73,73	2.38	23 (33%)	83,113,113	2.58	22 (26%)
23	LMG	F	5001	-	23,23,55	1.24	3 (13%)	31,31,63	1.72	6 (19%)
22	BCR	A	6008	-	41,41,41	2.83	6 (14%)	56,56,56	6.57	26 (46%)
22	BCR	F	6014	-	41,41,41	3.05	7 (17%)	56,56,56	6.69	23 (41%)
18	CLA	J	1302	4	54,58,73	2.71	23 (42%)	65,95,113	2.96	25 (38%)
22	BCR	3	3503	-	41,41,41	2.95	9 (21%)	56,56,56	6.43	31 (55%)
27	LUT	4	4502	-	42,43,43	2.38	3 (7%)	51,60,60	1.95	15 (29%)
18	CLA	A	1136	1	60,64,73	2.54	23 (38%)	72,102,113	2.79	27 (37%)
18	CLA	B	1230	2	62,66,73	2.47	19 (30%)	74,104,113	2.86	24 (32%)
18	CLA	A	1132	1	69,73,73	2.38	23 (33%)	83,113,113	2.62	26 (31%)
18	CLA	A	1105	1	55,59,73	2.69	22 (40%)	66,96,113	2.89	28 (42%)
18	CLA	3	3001	16	54,58,73	2.57	21 (38%)	65,95,113	3.01	24 (36%)
18	CLA	1	1007	21	50,54,73	2.65	19 (38%)	60,90,113	3.11	24 (40%)
18	CLA	B	1235	2	69,73,73	2.36	22 (31%)	83,113,113	2.67	24 (28%)
18	CLA	B	1206	2	69,73,73	2.38	22 (31%)	83,113,113	2.57	25 (30%)
21	LHG	2	2801	-	23,23,48	1.32	2 (8%)	26,29,54	1.21	4 (15%)
22	BCR	A	6017	-	41,41,41	2.67	6 (14%)	56,56,56	7.12	27 (48%)
18	CLA	A	1013	-	69,73,73	2.36	23 (33%)	83,113,113	2.62	24 (28%)
18	CLA	B	1232	-	59,63,73	2.58	23 (38%)	71,101,113	2.77	23 (32%)
18	CLA	G	1001	-	59,63,73	2.44	19 (32%)	71,101,113	2.85	30 (42%)
18	CLA	B	1231	2	64,68,73	2.49	22 (34%)	77,107,113	2.64	25 (32%)
28	CHL	1	1009	-	60,64,74	1.46	8 (13%)	68,102,114	1.44	11 (16%)
18	CLA	K	1001	-	50,54,73	2.73	20 (40%)	60,90,113	3.10	23 (38%)
22	BCR	B	6009	-	41,41,41	2.81	6 (14%)	56,56,56	6.39	23 (41%)
23	LMG	J	5001	-	55,55,55	0.88	2 (3%)	63,63,63	1.44	7 (11%)
18	CLA	4	4001	14	64,68,73	2.33	20 (31%)	77,107,113	2.77	28 (36%)
22	BCR	G	2011	-	41,41,41	3.05	7 (17%)	56,56,56	6.73	29 (51%)
27	LUT	3	3502	-	42,43,43	2.39	3 (7%)	51,60,60	2.28	17 (33%)
28	CHL	1	1010	15	51,55,74	1.54	6 (11%)	57,91,114	1.55	8 (14%)
18	CLA	3	3008	16	52,56,73	2.51	19 (36%)	62,92,113	3.35	28 (45%)
18	CLA	A	1140	1	69,73,73	2.39	23 (33%)	83,113,113	2.57	25 (30%)
18	CLA	B	1213	2	64,68,73	2.46	21 (32%)	77,107,113	2.68	23 (29%)
18	CLA	A	1126	1	69,73,73	2.38	23 (33%)	83,113,113	2.62	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	2	2002	13	50,54,73	2.66	19 (38%)	60,90,113	2.96	26 (43%)
18	CLA	3	3004	16	64,68,73	2.35	19 (29%)	77,107,113	2.69	24 (31%)
18	CLA	A	1128	1	69,73,73	2.36	22 (31%)	83,113,113	2.47	22 (26%)
18	CLA	B	1203	2	69,73,73	2.33	22 (31%)	83,113,113	2.62	24 (28%)
18	CLA	2	2003	13	59,63,73	2.39	20 (33%)	71,101,113	2.96	25 (35%)
18	CLA	A	1109	1	69,73,73	2.37	21 (30%)	83,113,113	2.61	24 (28%)
18	CLA	A	1131	1	69,73,73	2.37	23 (33%)	83,113,113	2.57	23 (27%)
27	LUT	4	4501	-	42,43,43	2.44	3 (7%)	51,60,60	2.19	16 (31%)
20	PQN	A	5001	-	34,34,34	1.62	2 (5%)	42,45,45	1.19	3 (7%)
18	CLA	4	4002	-	54,58,73	2.55	18 (33%)	65,95,113	2.92	29 (44%)
18	CLA	L	1503	-	54,58,73	2.57	20 (37%)	65,95,113	2.92	24 (36%)
18	CLA	B	1218	2	69,73,73	2.37	22 (31%)	83,113,113	2.64	24 (28%)
18	CLA	2	2008	13	54,58,73	2.49	19 (35%)	65,95,113	3.25	32 (49%)
18	CLA	3	3010	-	64,68,73	2.35	19 (29%)	77,107,113	2.72	25 (32%)
18	CLA	A	1102	1	54,58,73	2.67	22 (40%)	65,95,113	2.86	23 (35%)
18	CLA	A	1125	1	64,68,73	2.42	22 (34%)	77,107,113	2.70	26 (33%)
18	CLA	A	1114	-	50,54,73	2.85	21 (42%)	60,90,113	2.83	23 (38%)
22	BCR	A	6007	-	41,41,41	2.75	7 (17%)	56,56,56	6.52	23 (41%)
22	BCR	A	6002	-	41,41,41	2.74	6 (14%)	56,56,56	6.45	22 (39%)
18	CLA	B	1239	2	69,73,73	2.37	23 (33%)	83,113,113	2.59	24 (28%)
18	CLA	A	1117	-	69,73,73	2.37	22 (31%)	83,113,113	2.56	23 (27%)
18	CLA	B	1236	2	59,63,73	2.57	22 (37%)	71,101,113	2.84	24 (33%)
18	CLA	B	1227	-	69,73,73	2.37	23 (33%)	83,113,113	2.62	26 (31%)
22	BCR	A	6011	-	41,41,41	2.89	6 (14%)	56,56,56	6.72	24 (42%)
18	CLA	2	2019	-	28,35,73	3.30	16 (57%)	32,60,113	3.10	15 (46%)
22	BCR	L	6020	-	41,41,41	2.83	7 (17%)	56,56,56	6.55	29 (51%)
18	CLA	2	2009	13	54,58,73	2.58	21 (38%)	65,95,113	2.92	25 (38%)
22	BCR	B	6005	-	41,41,41	2.71	6 (14%)	56,56,56	6.79	23 (41%)
23	LMG	F	5002	-	37,37,55	1.07	2 (5%)	45,45,63	1.27	5 (11%)
18	CLA	A	1104	-	69,73,73	2.38	23 (33%)	83,113,113	2.63	25 (30%)
18	CLA	B	1229	2	69,73,73	2.37	23 (33%)	83,113,113	2.63	25 (30%)
26	LMU	B	8001	-	36,36,36	0.49	0	47,47,47	1.18	5 (10%)
22	BCR	J	6012	-	41,41,41	2.91	8 (19%)	56,56,56	6.56	29 (51%)
18	CLA	2	2016	13	54,58,73	2.62	19 (35%)	65,95,113	3.49	32 (49%)
18	CLA	1	1001	15	64,68,73	2.33	19 (29%)	77,107,113	2.76	23 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	4	4017	-	69,73,73	2.25	20 (28%)	83,113,113	2.62	27 (32%)
18	CLA	A	1115	1	50,54,73	2.85	23 (46%)	60,90,113	2.82	21 (35%)
18	CLA	3	3006	-	54,58,73	2.56	20 (37%)	65,95,113	2.97	26 (40%)
27	LUT	4	4503	-	42,43,43	2.41	3 (7%)	51,60,60	2.42	15 (29%)
27	LUT	3	3501	-	42,43,43	2.34	1 (2%)	51,60,60	2.37	19 (37%)
18	CLA	1	1005	15	59,63,73	2.42	20 (33%)	71,101,113	2.88	28 (39%)
18	CLA	1	1002	15	50,54,73	2.63	19 (38%)	60,90,113	3.02	24 (40%)
21	LHG	1	1801	18	48,48,48	0.91	2 (4%)	51,54,54	1.20	5 (9%)
27	LUT	1	1502	-	42,43,43	2.47	4 (9%)	51,60,60	2.21	18 (35%)
18	CLA	A	1110	-	59,63,73	2.59	23 (38%)	71,101,113	2.73	24 (33%)
18	CLA	2	2004	13	69,73,73	2.40	19 (27%)	83,113,113	2.60	27 (32%)
19	SF4	A	3001	2,1	0,12,12	-	-	-		
18	CLA	A	1108	-	50,54,73	2.86	23 (46%)	60,90,113	2.85	22 (36%)
18	CLA	3	3003	16	64,68,73	2.37	20 (31%)	77,107,113	2.73	27 (35%)
18	CLA	A	1118	1	50,54,73	2.82	21 (42%)	60,90,113	2.90	22 (36%)
21	LHG	B	5004	18	20,20,48	1.34	2 (10%)	23,26,54	1.53	3 (13%)
28	CHL	4	4011	-	55,59,74	1.79	8 (14%)	62,96,114	1.65	11 (17%)
22	BCR	B	6010	-	41,41,41	2.73	6 (14%)	56,56,56	6.56	23 (41%)
18	CLA	1	1003	15	59,63,73	2.43	22 (37%)	71,101,113	2.84	28 (39%)
18	CLA	B	1234	-	64,68,73	2.48	23 (35%)	77,107,113	2.72	26 (33%)
22	BCR	A	6003	-	41,41,41	2.79	6 (14%)	56,56,56	6.48	20 (35%)
18	CLA	4	4005	14	64,68,73	2.31	19 (29%)	77,107,113	2.82	31 (40%)
18	CLA	3	3005	-	59,63,73	2.47	19 (32%)	71,101,113	2.86	27 (38%)
18	CLA	B	1221	-	69,73,73	2.38	23 (33%)	83,113,113	2.64	27 (32%)
28	CHL	4	4013	-	51,55,74	1.84	9 (17%)	57,91,114	1.68	11 (19%)
18	CLA	3	3018	16	54,58,73	2.57	21 (38%)	65,95,113	3.03	27 (41%)
26	LMU	B	8002	-	36,36,36	0.45	0	47,47,47	1.06	3 (6%)
18	CLA	H	1000	11	50,54,73	2.84	22 (44%)	60,90,113	2.85	22 (36%)
28	CHL	2	2010	-	51,55,74	1.81	9 (17%)	57,91,114	1.63	10 (17%)
18	CLA	A	1130	1	54,58,73	2.70	23 (42%)	65,95,113	2.91	22 (33%)
18	CLA	B	1224	-	69,73,73	2.36	22 (31%)	83,113,113	2.61	25 (30%)
18	CLA	A	1122	1	69,73,73	2.37	22 (31%)	83,113,113	2.55	24 (28%)
18	CLA	4	4006	-	54,58,73	2.51	19 (35%)	65,95,113	2.80	25 (38%)
18	CLA	3	3013	-	50,54,73	2.77	20 (40%)	60,90,113	2.66	22 (36%)
23	LMG	B	5005	-	38,38,55	1.08	2 (5%)	46,46,63	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	BCR	F	6016	-	41,41,41	3.07	9 (21%)	56,56,56	6.70	24 (42%)
18	CLA	B	1209	2	50,54,73	2.85	22 (44%)	60,90,113	2.86	20 (33%)
18	CLA	1	1004	15	69,73,73	2.25	20 (28%)	83,113,113	2.65	25 (30%)
18	CLA	B	1217	-	50,54,73	2.84	23 (46%)	60,90,113	2.84	21 (35%)
18	CLA	B	1225	2	69,73,73	2.39	23 (33%)	83,113,113	2.53	23 (27%)
18	CLA	1	1013	-	50,54,73	2.74	21 (42%)	60,90,113	2.93	22 (36%)
18	CLA	L	1501	7	54,58,73	2.59	18 (33%)	65,95,113	2.93	28 (43%)
18	CLA	G	1003	-	64,68,73	2.37	21 (32%)	77,107,113	2.74	27 (35%)
23	LMG	2	2802	-	35,35,55	1.08	2 (5%)	43,43,63	1.33	7 (16%)
20	PQN	B	5002	-	34,34,34	1.69	2 (5%)	42,45,45	1.07	3 (7%)
18	CLA	A	1138	1	69,73,73	2.40	23 (33%)	83,113,113	2.51	26 (31%)
18	CLA	1	1014	15	50,54,73	2.69	19 (38%)	60,90,113	3.03	25 (41%)
18	CLA	B	1220	2	69,73,73	2.38	23 (33%)	83,113,113	2.52	25 (30%)
22	BCR	B	6006	-	41,41,41	2.79	6 (14%)	56,56,56	6.86	28 (50%)
27	LUT	I	6018	-	42,43,43	2.46	1 (2%)	51,60,60	2.21	18 (35%)
18	CLA	4	4012	14	69,73,73	2.23	19 (27%)	83,113,113	2.69	29 (34%)
18	CLA	A	1127	-	69,73,73	2.38	22 (31%)	83,113,113	2.53	23 (27%)
28	CHL	2	2013	-	50,54,74	1.47	6 (12%)	56,90,114	1.53	9 (16%)
18	CLA	A	1137	1	59,63,73	2.56	23 (38%)	71,101,113	2.74	24 (33%)
18	CLA	3	3012	16	54,58,73	2.52	19 (35%)	65,95,113	3.09	26 (40%)
18	CLA	2	2001	13	64,68,73	2.31	19 (29%)	77,107,113	2.79	29 (37%)
27	LUT	2	2501	-	42,43,43	2.43	1 (2%)	51,60,60	2.11	14 (27%)
18	CLA	3	3017	16	50,54,73	2.74	20 (40%)	60,90,113	2.84	23 (38%)
28	CHL	4	4010	-	51,55,74	1.97	11 (21%)	57,91,114	1.90	13 (22%)
18	CLA	B	1204	2	59,63,73	2.59	22 (37%)	71,101,113	2.79	23 (32%)
18	CLA	2	2012	13	59,63,73	2.41	19 (32%)	71,101,113	2.86	27 (38%)
18	CLA	B	1216	-	69,73,73	2.38	23 (33%)	83,113,113	2.57	25 (30%)
18	CLA	A	1107	1	69,73,73	2.38	23 (33%)	83,113,113	2.61	25 (30%)
18	CLA	1	1008	15	50,54,73	2.66	19 (38%)	60,90,113	2.92	26 (43%)
18	CLA	4	4003	14	69,73,73	2.27	21 (30%)	83,113,113	2.61	26 (31%)
19	SF4	C	3003	8	0,12,12	-	-	-		
18	CLA	A	1111	-	64,68,73	2.45	22 (34%)	77,107,113	2.67	26 (33%)
27	LUT	2	2502	-	42,43,43	2.47	3 (7%)	51,60,60	2.10	16 (31%)
18	CLA	A	1135	-	55,59,73	2.66	22 (40%)	66,96,113	2.91	24 (36%)
18	CLA	F	1302	5	54,58,73	2.62	21 (38%)	65,95,113	2.92	23 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	CLA	4	4007	-	64,68,73	2.29	19 (29%)	77,107,113	2.84	26 (33%)
18	CLA	B	1240	21	69,73,73	2.36	22 (31%)	83,113,113	2.63	27 (32%)
18	CLA	F	1301	-	49,53,73	2.64	20 (40%)	59,89,113	2.88	21 (35%)
18	CLA	A	1113	1	50,54,73	2.84	22 (44%)	60,90,113	2.85	23 (38%)
18	CLA	1	1011	-	54,58,73	2.55	20 (37%)	65,95,113	2.95	27 (41%)
18	CLA	B	1226	2	69,73,73	2.34	22 (31%)	83,113,113	2.49	23 (27%)
18	CLA	B	1201	2	54,58,73	2.67	23 (42%)	65,95,113	2.87	26 (40%)
18	CLA	4	4008	14	50,54,73	2.61	20 (40%)	60,90,113	3.25	28 (46%)
19	SF4	C	3002	8	0,12,12	-	-	-		
18	CLA	2	2005	-	59,63,73	2.50	21 (35%)	71,101,113	2.73	26 (36%)
18	CLA	G	1002	-	50,54,73	2.74	22 (44%)	60,90,113	2.91	25 (41%)
18	CLA	2	2007	-	64,68,73	2.38	22 (34%)	77,107,113	2.67	24 (31%)
18	CLA	3	3002	-	50,54,73	2.68	21 (42%)	60,90,113	2.98	28 (46%)
18	CLA	A	1022	-	69,73,73	2.39	21 (30%)	83,113,113	2.54	26 (31%)
18	CLA	B	1211	2	69,73,73	2.36	21 (30%)	83,113,113	2.69	29 (34%)
18	CLA	A	1237	-	64,68,73	2.45	22 (34%)	77,107,113	2.80	25 (32%)
18	CLA	B	1214	-	63,67,73	2.49	22 (34%)	75,105,113	2.75	25 (33%)
18	CLA	B	1208	2	59,63,73	2.59	22 (37%)	71,101,113	2.82	24 (33%)
18	CLA	A	1133	1	59,63,73	2.56	23 (38%)	71,101,113	2.78	24 (33%)
18	CLA	3	3019	-	28,35,73	3.43	16 (57%)	32,60,113	3.02	14 (43%)
18	CLA	A	1112	-	69,73,73	2.37	23 (33%)	83,113,113	2.61	24 (28%)
18	CLA	L	1502	7	64,68,73	2.36	20 (31%)	77,107,113	2.75	27 (35%)
18	CLA	1	1012	15	54,58,73	2.57	20 (37%)	65,95,113	2.88	26 (40%)
18	CLA	4	4016	-	50,54,73	2.74	21 (42%)	60,90,113	2.90	25 (41%)
18	CLA	4	4004	14	64,68,73	2.35	18 (28%)	77,107,113	2.72	27 (35%)

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
22	BCR	L	6019	-	-	11/29/63/63	0/2/2/2
18	CLA	A	1134	-	-	17/27/103/115	-
18	CLA	4	4009	14	-	4/21/97/115	-
18	CLA	A	1121	1	-	17/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1101	1	-	15/39/115/115	-
25	DGD	B	7101	-	-	23/50/90/95	0/2/2/2
18	CLA	A	1124	-	-	12/27/103/115	-
18	CLA	3	3007	-	-	8/21/97/115	-
21	LHG	A	5003	18	-	21/44/44/53	-
21	LHG	A	7001	-	-	30/53/53/53	-
18	CLA	B	1205	2	-	12/39/115/115	-
18	CLA	B	1210	-	-	15/39/115/115	-
18	CLA	A	1139	-	-	14/39/115/115	-
22	BCR	J	6013	-	-	13/29/63/63	0/2/2/2
28	CHL	3	3011	-	1/1/13/21	6/29/105/117	-
23	LMG	4	4801	-	-	16/30/50/70	0/1/1/1
18	CLA	B	1222	-	-	16/39/115/115	-
22	BCR	K	2011	-	-	11/29/63/63	0/2/2/2
28	CHL	2	2011	-	-	2/20/96/117	-
22	BCR	I	6020	-	-	10/29/63/63	0/2/2/2
18	CLA	A	1129	1	-	11/21/97/115	-
18	CLA	A	1119	-	-	26/39/115/115	-
18	CLA	B	1202	-	-	18/39/115/115	-
27	LUT	1	1501	-	1/1/12/27	8/29/67/67	0/2/2/2
22	BCR	B	6004	-	-	10/29/63/63	0/2/2/2
18	CLA	B	1012	-	-	17/39/115/115	-
17	CL0	A	1011	1	-	8/39/115/115	-
18	CLA	B	1212	-	-	9/27/103/115	-
18	CLA	B	1215	2	-	15/33/109/115	-
18	CLA	A	1151	21	-	13/21/97/115	-
18	CLA	1	1006	-	-	10/21/97/115	-
18	CLA	A	1103	1	-	23/39/115/115	-
18	CLA	B	1021	2	-	14/39/115/115	-
29	ZEX	4	4505	-	-	2/29/67/67	0/2/2/2
18	CLA	A	1120	1	-	18/33/109/115	-
18	CLA	A	1123	-	-	16/39/115/115	-
23	LMG	G	2021	-	-	24/36/56/70	0/1/1/1
18	CLA	B	1228	2	-	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1116	1	-	18/33/109/115	-
18	CLA	2	2006	-	-	12/27/103/115	-
18	CLA	B	1223	2	-	16/39/115/115	-
18	CLA	B	1219	2	-	19/33/109/115	-
18	CLA	B	1207	-	-	19/39/115/115	-
18	CLA	A	1106	1	-	14/39/115/115	-
18	CLA	B	1023	-	-	12/39/115/115	-
18	CLA	B	1238	-	-	17/39/115/115	-
23	LMG	F	5001	-	-	9/16/36/70	0/1/1/1
22	BCR	A	6008	-	-	9/29/63/63	0/2/2/2
22	BCR	F	6014	-	-	12/29/63/63	0/2/2/2
27	LUT	4	4502	-	1/1/12/27	8/29/67/67	0/2/2/2
18	CLA	J	1302	4	-	13/21/97/115	-
22	BCR	3	3503	-	-	14/29/63/63	0/2/2/2
18	CLA	A	1136	1	-	11/29/105/115	-
18	CLA	B	1230	2	-	18/31/107/115	-
18	CLA	A	1132	1	-	15/39/115/115	-
18	CLA	A	1105	1	-	12/23/99/115	-
18	CLA	3	3001	16	-	6/21/97/115	-
18	CLA	1	1007	21	-	10/17/93/115	-
18	CLA	B	1235	2	-	19/39/115/115	-
18	CLA	B	1206	2	-	15/39/115/115	-
21	LHG	2	2801	-	-	15/28/28/53	-
22	BCR	A	6017	-	-	10/29/63/63	0/2/2/2
18	CLA	A	1013	-	-	13/39/115/115	-
28	CHL	1	1009	-	1/1/13/21	8/29/105/117	-
18	CLA	B	1232	-	-	7/27/103/115	-
18	CLA	B	1231	2	-	13/33/109/115	-
18	CLA	G	1001	-	-	18/27/103/115	-
18	CLA	K	1001	-	-	11/17/93/115	-
22	BCR	B	6009	-	-	7/29/63/63	0/2/2/2
23	LMG	J	5001	-	-	36/50/70/70	0/1/1/1
18	CLA	4	4001	14	-	15/33/109/115	-
22	BCR	G	2011	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LUT	3	3502	-	1/1/12/27	8/29/67/67	0/2/2/2
28	CHL	1	1010	15	-	5/19/95/117	-
18	CLA	3	3008	16	-	12/19/95/115	-
18	CLA	A	1140	1	-	18/39/115/115	-
18	CLA	B	1213	2	-	13/33/109/115	-
18	CLA	A	1126	1	-	17/39/115/115	-
18	CLA	2	2002	13	-	8/17/93/115	-
18	CLA	3	3004	16	-	10/33/109/115	-
18	CLA	A	1128	1	-	13/39/115/115	-
18	CLA	B	1203	2	-	16/39/115/115	-
18	CLA	2	2003	13	-	13/27/103/115	-
18	CLA	A	1109	1	-	11/39/115/115	-
18	CLA	A	1131	1	-	14/39/115/115	-
27	LUT	4	4501	-	1/1/12/27	4/29/67/67	0/2/2/2
20	PQN	A	5001	-	-	10/23/43/43	0/2/2/2
18	CLA	4	4002	-	-	7/21/97/115	-
18	CLA	L	1503	-	-	7/21/97/115	-
18	CLA	B	1218	2	-	17/39/115/115	-
18	CLA	2	2008	13	-	9/21/97/115	-
18	CLA	3	3010	-	-	17/33/109/115	-
18	CLA	A	1102	1	-	7/21/97/115	-
18	CLA	A	1125	1	-	21/33/109/115	-
18	CLA	A	1114	-	-	6/17/93/115	-
22	BCR	A	6007	-	-	6/29/63/63	0/2/2/2
22	BCR	A	6002	-	-	11/29/63/63	0/2/2/2
18	CLA	B	1239	2	-	20/39/115/115	-
18	CLA	A	1117	-	-	13/39/115/115	-
18	CLA	B	1236	2	-	12/27/103/115	-
18	CLA	B	1227	-	-	13/39/115/115	-
22	BCR	A	6011	-	-	18/29/63/63	0/2/2/2
22	BCR	L	6020	-	-	9/29/63/63	0/2/2/2
18	CLA	2	2009	13	-	7/21/97/115	-
22	BCR	B	6005	-	-	13/29/63/63	0/2/2/2
23	LMG	F	5002	-	-	15/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1104	-	-	18/39/115/115	-
18	CLA	B	1229	2	-	17/39/115/115	-
26	LMU	B	8001	-	-	8/21/61/61	0/2/2/2
22	BCR	J	6012	-	-	11/29/63/63	0/2/2/2
18	CLA	2	2016	13	-	9/21/97/115	-
18	CLA	1	1001	15	-	16/33/109/115	-
18	CLA	4	4017	-	-	19/39/115/115	-
18	CLA	A	1115	1	-	8/17/93/115	-
27	LUT	4	4503	-	1/1/12/27	10/29/67/67	0/2/2/2
18	CLA	3	3006	-	-	6/21/97/115	-
27	LUT	3	3501	-	1/1/12/27	5/29/67/67	0/2/2/2
18	CLA	1	1005	15	-	10/27/103/115	-
18	CLA	1	1002	15	-	6/17/93/115	-
21	LHG	1	1801	18	-	24/53/53/53	-
27	LUT	1	1502	-	1/1/12/27	3/29/67/67	0/2/2/2
18	CLA	A	1110	-	-	10/27/103/115	-
18	CLA	2	2004	13	-	13/39/115/115	-
19	SF4	A	3001	2,1	-	-	0/6/5/5
18	CLA	A	1108	-	-	6/17/93/115	-
18	CLA	3	3003	16	-	12/33/109/115	-
18	CLA	A	1118	1	-	10/17/93/115	-
21	LHG	B	5004	18	-	15/23/23/53	-
28	CHL	4	4011	-	-	3/23/99/117	-
22	BCR	B	6010	-	-	10/29/63/63	0/2/2/2
18	CLA	1	1003	15	-	9/27/103/115	-
18	CLA	B	1234	-	-	13/33/109/115	-
22	BCR	A	6003	-	-	13/29/63/63	0/2/2/2
18	CLA	4	4005	14	-	14/33/109/115	-
18	CLA	3	3005	-	-	17/27/103/115	-
18	CLA	B	1221	-	-	21/39/115/115	-
28	CHL	4	4013	-	-	4/19/95/117	-
18	CLA	3	3018	16	-	7/21/97/115	-
26	LMU	B	8002	-	-	14/21/61/61	0/2/2/2
18	CLA	H	1000	11	-	12/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CHL	2	2010	-	-	3/19/95/117	-
18	CLA	A	1130	1	-	7/21/97/115	-
18	CLA	B	1224	-	-	23/39/115/115	-
18	CLA	A	1122	1	-	26/39/115/115	-
18	CLA	4	4006	-	-	6/21/97/115	-
18	CLA	3	3013	-	-	13/17/93/115	-
23	LMG	B	5005	-	-	17/33/53/70	0/1/1/1
22	BCR	F	6016	-	-	8/29/63/63	0/2/2/2
18	CLA	B	1209	2	-	5/17/93/115	-
18	CLA	1	1004	15	-	20/39/115/115	-
18	CLA	B	1217	-	-	10/17/93/115	-
18	CLA	B	1225	2	-	18/39/115/115	-
18	CLA	1	1013	-	-	10/17/93/115	-
18	CLA	L	1501	7	-	9/21/97/115	-
18	CLA	G	1003	-	-	15/33/109/115	-
23	LMG	2	2802	-	-	12/30/50/70	0/1/1/1
20	PQN	B	5002	-	-	13/23/43/43	0/2/2/2
18	CLA	A	1138	1	-	19/39/115/115	-
18	CLA	1	1014	15	-	9/17/93/115	-
18	CLA	B	1220	2	-	18/39/115/115	-
22	BCR	B	6006	-	-	10/29/63/63	0/2/2/2
27	LUT	I	6018	-	1/1/12/27	3/29/67/67	0/2/2/2
18	CLA	4	4012	14	-	19/39/115/115	-
18	CLA	A	1127	-	-	19/39/115/115	-
28	CHL	2	2013	-	-	4/17/93/117	-
18	CLA	A	1137	1	-	12/27/103/115	-
18	CLA	3	3012	16	-	8/21/97/115	-
27	LUT	2	2501	-	1/1/12/27	3/29/67/67	0/2/2/2
18	CLA	2	2001	13	-	18/33/109/115	-
18	CLA	3	3017	16	-	9/17/93/115	-
28	CHL	4	4010	-	-	4/19/95/117	-
18	CLA	B	1204	2	-	14/27/103/115	-
18	CLA	2	2012	13	-	9/27/103/115	-
18	CLA	B	1216	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	1107	1	-	16/39/115/115	-
18	CLA	1	1008	15	-	9/17/93/115	-
18	CLA	4	4003	14	-	17/39/115/115	-
19	SF4	C	3003	8	-	-	0/6/5/5
18	CLA	A	1111	-	-	13/33/109/115	-
27	LUT	2	2502	-	1/1/12/27	4/29/67/67	0/2/2/2
18	CLA	A	1135	-	-	6/23/99/115	-
18	CLA	F	1302	5	-	10/21/97/115	-
18	CLA	4	4007	-	-	14/33/109/115	-
18	CLA	B	1240	21	-	19/39/115/115	-
18	CLA	F	1301	-	-	2/15/91/115	-
18	CLA	A	1113	1	-	13/17/93/115	-
18	CLA	1	1011	-	-	10/21/97/115	-
18	CLA	B	1226	2	-	19/39/115/115	-
18	CLA	B	1201	2	-	10/21/97/115	-
18	CLA	4	4008	14	-	12/17/93/115	-
19	SF4	C	3002	8	-	-	0/6/5/5
18	CLA	2	2005	-	-	16/27/103/115	-
18	CLA	G	1002	-	-	8/17/93/115	-
18	CLA	2	2007	-	-	13/33/109/115	-
18	CLA	3	3002	-	-	6/17/93/115	-
18	CLA	A	1022	-	-	14/39/115/115	-
18	CLA	B	1211	2	-	11/39/115/115	-
18	CLA	A	1237	-	-	15/33/109/115	-
18	CLA	B	1214	-	-	12/32/108/115	-
18	CLA	A	1133	1	-	12/27/103/115	-
18	CLA	B	1208	2	-	15/27/103/115	-
18	CLA	A	1112	-	-	16/39/115/115	-
18	CLA	L	1502	7	-	17/33/109/115	-
18	CLA	1	1012	15	-	10/21/97/115	-
18	CLA	4	4016	-	-	13/17/93/115	-
18	CLA	4	4004	14	-	12/33/109/115	-

The worst 5 of 3404 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	2	2502	LUT	C24-C25	14.89	1.51	1.33
27	I	6018	LUT	C24-C25	14.89	1.51	1.33
27	2	2501	LUT	C24-C25	14.81	1.51	1.33
27	1	1501	LUT	C24-C25	14.74	1.51	1.33
27	1	1502	LUT	C24-C25	14.31	1.51	1.33

The worst 5 of 4558 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	A	6017	BCR	C16-C17-C18	29.85	169.91	127.31
22	G	2011	BCR	C16-C17-C18	27.95	167.20	127.31
22	B	6005	BCR	C16-C17-C18	27.71	166.86	127.31
22	K	2011	BCR	C16-C17-C18	27.60	166.70	127.31
22	I	6020	BCR	C16-C17-C18	27.15	166.06	127.31

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	I	6018	LUT	C26
27	2	2501	LUT	C26
27	2	2502	LUT	C26
27	4	4501	LUT	C26
27	4	4502	LUT	C26

5 of 2537 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1013	CLA	CHA-CBD-CGD-O1D
18	A	1151	CLA	C2B-C3B-CAB-CBB
18	A	1151	CLA	C4B-C3B-CAB-CBB
18	A	1151	CLA	CHA-CBD-CGD-O1D
18	A	1151	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

204 monomers are involved in 1868 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	L	6019	BCR	22	0
18	A	1134	CLA	2	0
18	4	4009	CLA	9	0
18	A	1121	CLA	4	0
18	A	1101	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	7101	DGD	4	0
18	A	1124	CLA	4	0
18	3	3007	CLA	4	0
21	A	5003	LHG	6	0
21	A	7001	LHG	6	0
18	B	1205	CLA	7	0
18	B	1210	CLA	7	0
18	A	1139	CLA	4	0
22	J	6013	BCR	8	0
28	3	3011	CHL	22	0
23	4	4801	LMG	6	0
18	B	1222	CLA	8	0
22	K	2011	BCR	17	0
28	2	2011	CHL	5	0
22	I	6020	BCR	3	0
18	A	1119	CLA	6	0
18	B	1202	CLA	7	0
27	1	1501	LUT	32	0
22	B	6004	BCR	9	0
18	B	1012	CLA	5	0
17	A	1011	CL0	5	0
18	B	1212	CLA	5	0
18	B	1215	CLA	5	0
18	A	1151	CLA	3	0
18	1	1006	CLA	7	0
18	A	1103	CLA	5	0
18	B	1021	CLA	7	0
29	4	4505	ZEX	12	0
18	A	1120	CLA	2	0
18	A	1123	CLA	6	0
23	G	2021	LMG	20	0
18	B	1228	CLA	3	0
18	A	1116	CLA	7	0
18	2	2006	CLA	22	0
18	B	1219	CLA	2	0
18	B	1223	CLA	4	0
18	B	1207	CLA	11	0
18	A	1106	CLA	11	0
18	B	1023	CLA	7	0
18	B	1238	CLA	7	0
23	F	5001	LMG	7	0
22	A	6008	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	F	6014	BCR	8	0
18	J	1302	CLA	7	0
22	3	3503	BCR	20	0
27	4	4502	LUT	28	0
18	A	1136	CLA	6	0
18	B	1230	CLA	8	0
18	A	1132	CLA	6	0
18	A	1105	CLA	4	0
18	3	3001	CLA	21	0
18	1	1007	CLA	7	0
18	B	1235	CLA	6	0
18	B	1206	CLA	4	0
21	2	2801	LHG	6	0
22	A	6017	BCR	8	0
18	A	1013	CLA	7	0
18	B	1232	CLA	3	0
18	G	1001	CLA	34	0
18	B	1231	CLA	3	0
28	1	1009	CHL	28	0
18	K	1001	CLA	12	0
22	B	6009	BCR	6	0
23	J	5001	LMG	10	0
18	4	4001	CLA	24	0
22	G	2011	BCR	28	0
27	3	3502	LUT	23	0
28	1	1010	CHL	8	0
18	3	3008	CLA	17	0
18	A	1140	CLA	3	0
18	B	1213	CLA	5	0
18	A	1126	CLA	9	0
18	2	2002	CLA	34	0
18	3	3004	CLA	16	0
18	A	1128	CLA	11	0
18	B	1203	CLA	2	0
18	2	2003	CLA	29	0
18	A	1109	CLA	6	0
18	A	1131	CLA	1	0
27	4	4501	LUT	21	0
20	A	5001	PQN	3	0
18	4	4002	CLA	11	0
18	L	1503	CLA	11	0
18	B	1218	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	2	2008	CLA	14	0
18	3	3010	CLA	35	0
18	A	1102	CLA	3	0
18	A	1125	CLA	4	0
18	A	1114	CLA	1	0
22	A	6007	BCR	3	0
22	A	6002	BCR	4	0
18	B	1239	CLA	5	0
18	A	1117	CLA	4	0
18	B	1236	CLA	6	0
18	B	1227	CLA	7	0
22	A	6011	BCR	4	0
22	L	6020	BCR	5	0
18	2	2009	CLA	16	0
22	B	6005	BCR	3	0
23	F	5002	LMG	6	0
18	A	1104	CLA	3	0
18	B	1229	CLA	5	0
26	B	8001	LMU	1	0
22	J	6012	BCR	7	0
18	2	2016	CLA	37	0
18	1	1001	CLA	48	0
18	4	4017	CLA	11	0
18	A	1115	CLA	1	0
18	3	3006	CLA	37	0
27	4	4503	LUT	32	0
27	3	3501	LUT	39	0
18	1	1005	CLA	16	0
18	1	1002	CLA	17	0
21	1	1801	LHG	15	0
27	1	1502	LUT	17	0
18	A	1110	CLA	10	0
18	2	2004	CLA	24	0
19	A	3001	SF4	1	0
18	A	1108	CLA	2	0
18	3	3003	CLA	49	0
18	A	1118	CLA	3	0
21	B	5004	LHG	1	0
28	4	4011	CHL	20	0
22	B	6010	BCR	1	0
18	1	1003	CLA	32	0
18	B	1234	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	6003	BCR	2	0
18	4	4005	CLA	13	0
18	3	3005	CLA	14	0
18	B	1221	CLA	10	0
28	4	4013	CHL	19	0
18	3	3018	CLA	20	0
26	B	8002	LMU	3	0
18	H	1000	CLA	5	0
28	2	2010	CHL	18	0
18	A	1130	CLA	2	0
18	B	1224	CLA	6	0
18	A	1122	CLA	7	0
18	4	4006	CLA	21	0
18	3	3013	CLA	24	0
23	B	5005	LMG	3	0
22	F	6016	BCR	9	0
18	B	1209	CLA	3	0
18	1	1004	CLA	26	0
18	B	1217	CLA	1	0
18	B	1225	CLA	3	0
18	1	1013	CLA	13	0
18	L	1501	CLA	13	0
18	G	1003	CLA	30	0
23	2	2802	LMG	9	0
20	B	5002	PQN	5	0
18	A	1138	CLA	7	0
18	1	1014	CLA	14	0
18	B	1220	CLA	10	0
22	B	6006	BCR	6	0
27	I	6018	LUT	12	0
18	4	4012	CLA	24	0
18	A	1127	CLA	5	0
28	2	2013	CHL	17	0
18	A	1137	CLA	3	0
18	3	3012	CLA	31	0
18	2	2001	CLA	36	0
27	2	2501	LUT	21	0
18	3	3017	CLA	11	0
28	4	4010	CHL	7	0
18	B	1204	CLA	9	0
18	2	2012	CLA	22	0
18	B	1216	CLA	4	0

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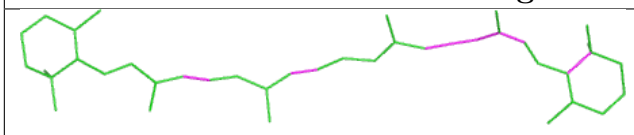
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	1107	CLA	2	0
18	1	1008	CLA	33	0
18	4	4003	CLA	13	0
18	A	1111	CLA	7	0
27	2	2502	LUT	32	0
18	A	1135	CLA	3	0
18	F	1302	CLA	11	0
18	4	4007	CLA	20	0
18	B	1240	CLA	6	0
18	F	1301	CLA	5	0
18	A	1113	CLA	3	0
18	1	1011	CLA	15	0
18	B	1226	CLA	7	0
18	B	1201	CLA	1	0
18	4	4008	CLA	15	0
18	2	2005	CLA	21	0
18	G	1002	CLA	23	0
18	2	2007	CLA	24	0
18	3	3002	CLA	8	0
18	A	1022	CLA	5	0
18	B	1211	CLA	8	0
18	A	1237	CLA	4	0
18	B	1214	CLA	4	0
18	B	1208	CLA	6	0
18	A	1133	CLA	3	0
18	3	3019	CLA	1	0
18	A	1112	CLA	10	0
18	L	1502	CLA	13	0
18	1	1012	CLA	16	0
18	4	4016	CLA	26	0
18	4	4004	CLA	17	0

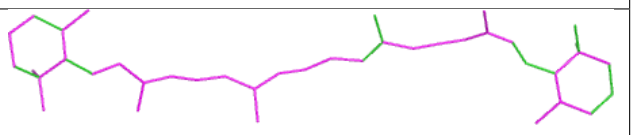
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

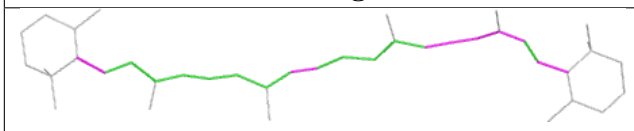
Ligand BCR L 6019



Bond lengths



Bond angles

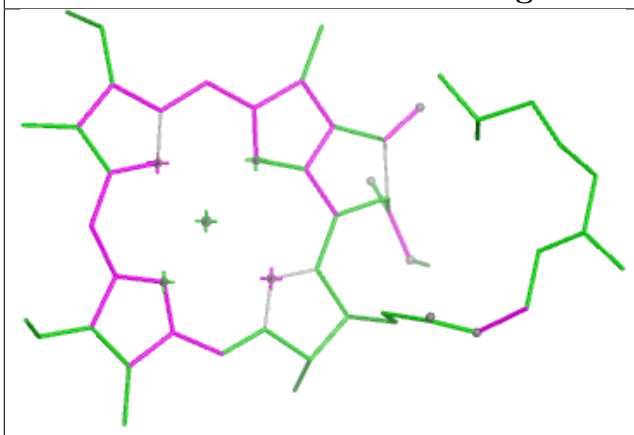


Torsions

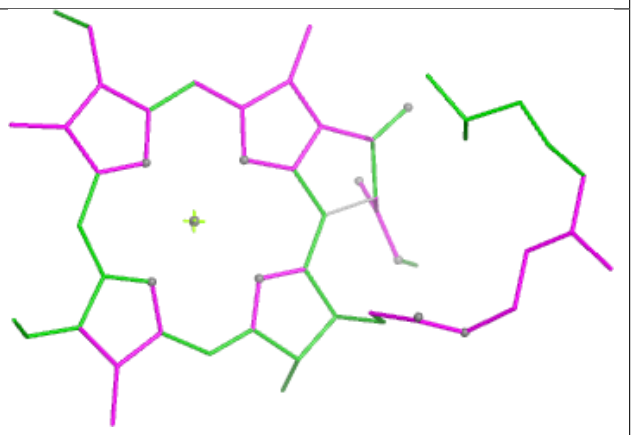


Rings

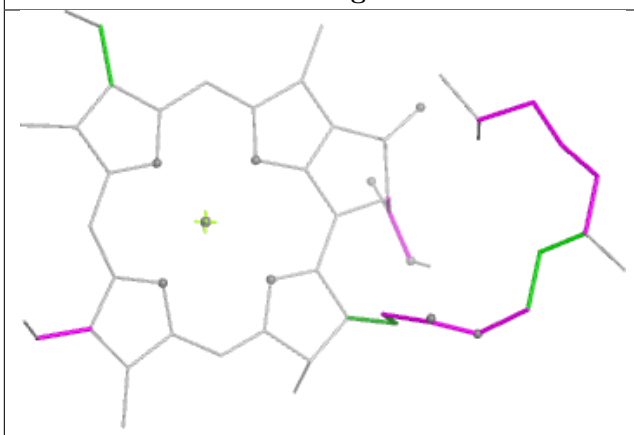
Ligand CLA A 1134



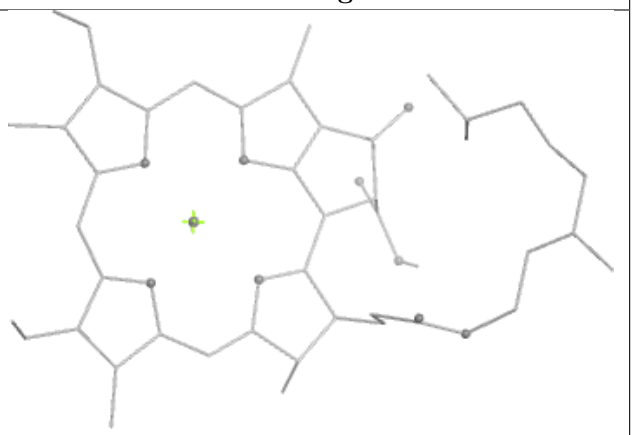
Bond lengths



Bond angles

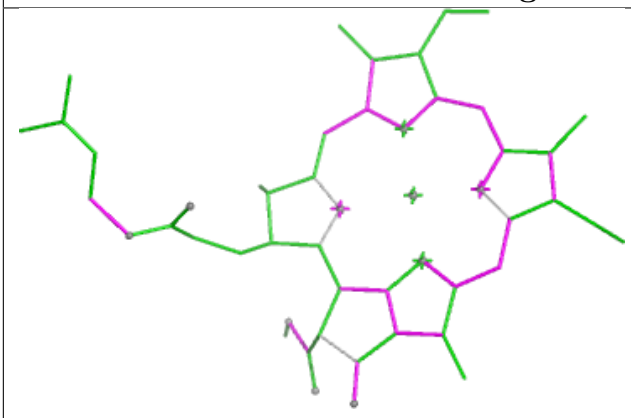


Torsions

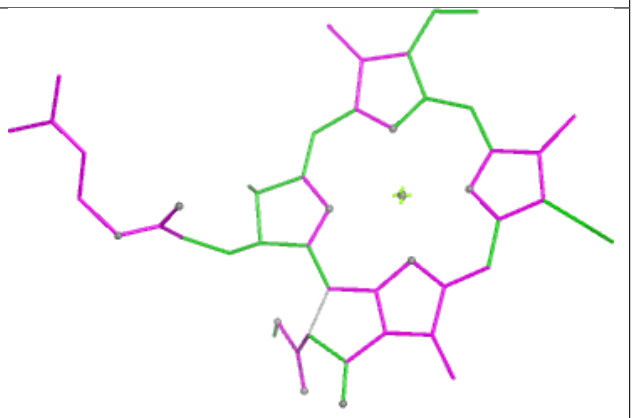


Rings

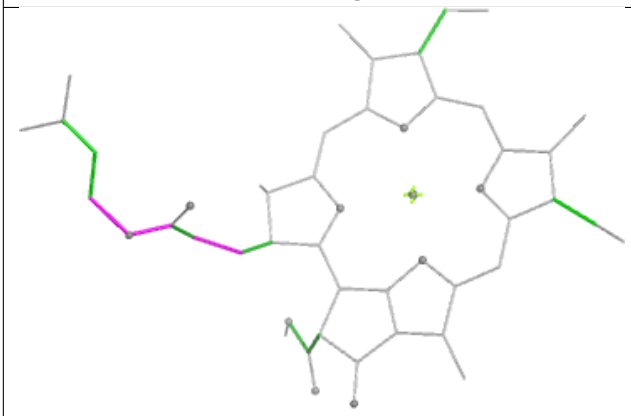
Ligand CLA 4 4009



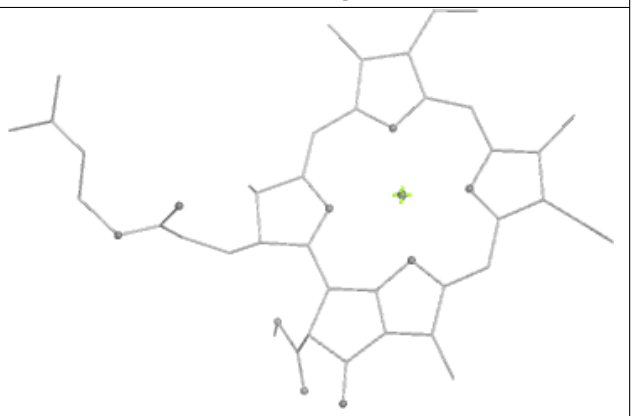
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Bond angles

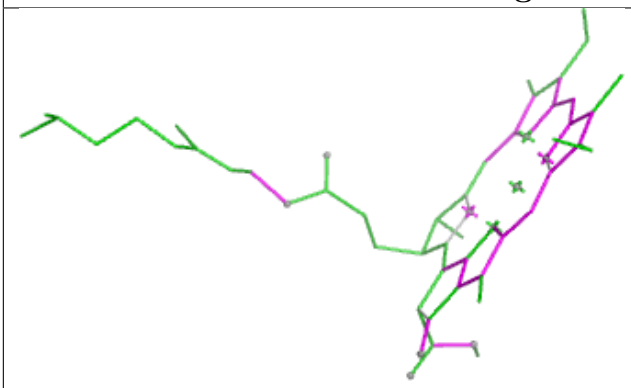


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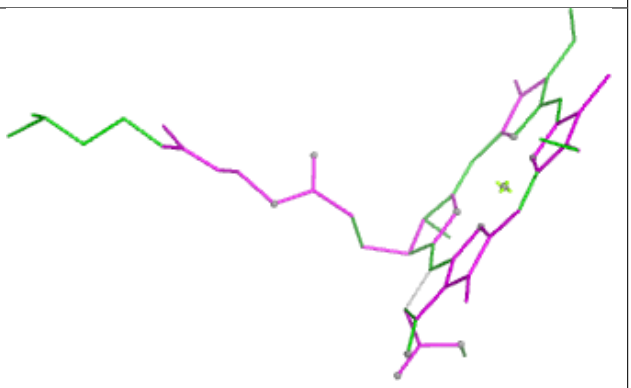


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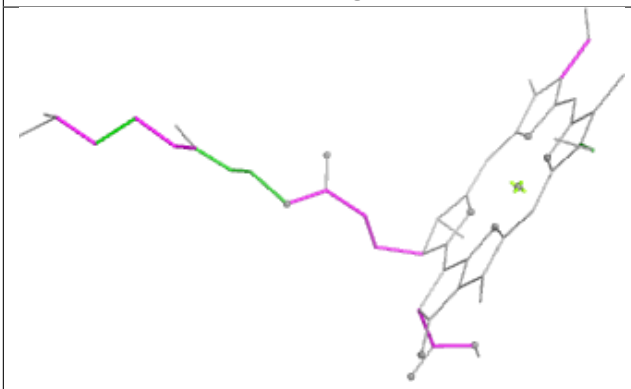
Ligand CLA A 1121



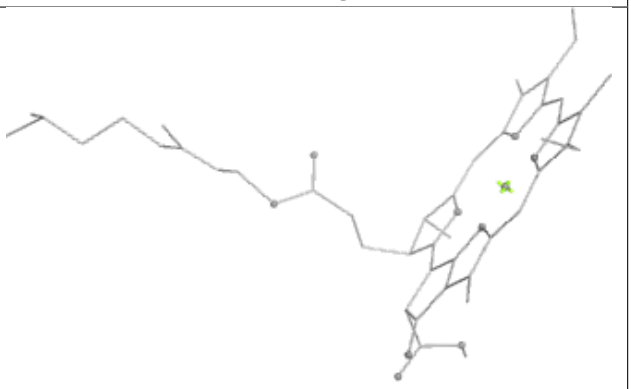
Bond lengths



Bond angles

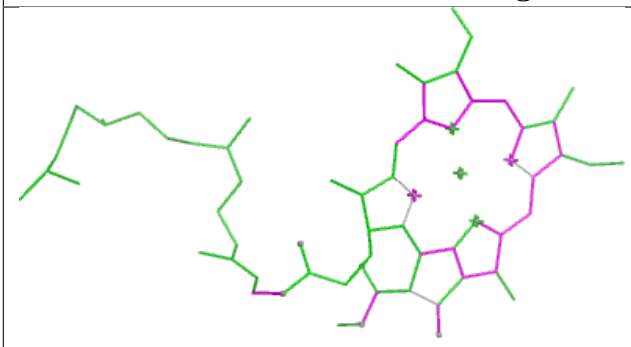


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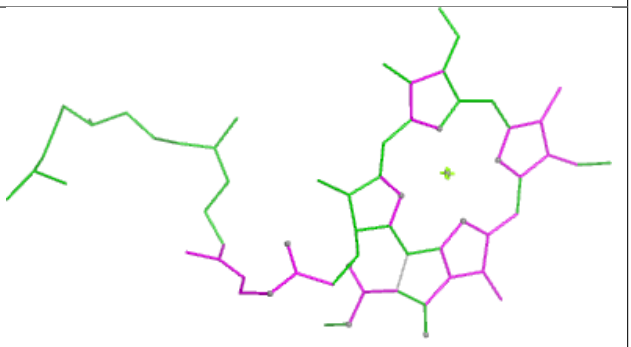


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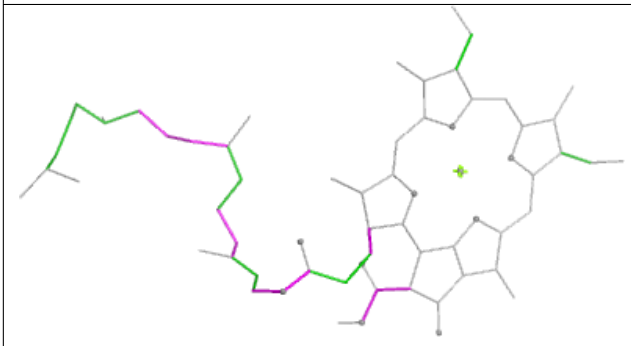
Ligand CLA A 1101



Bond lengths



Bond angles

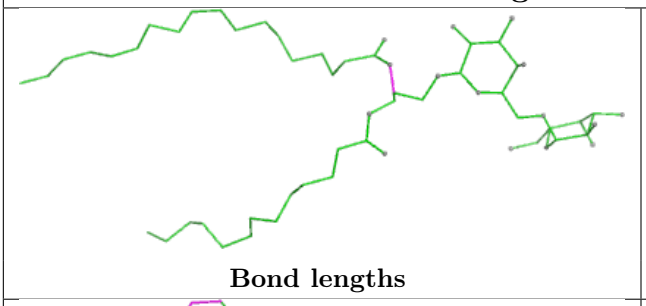


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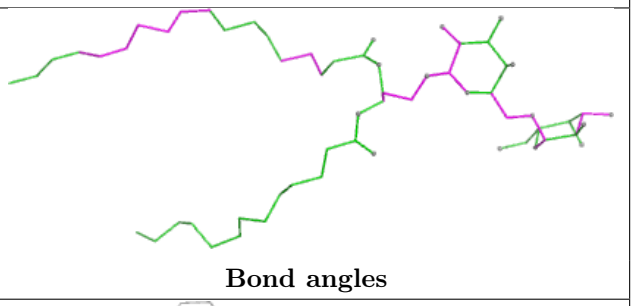


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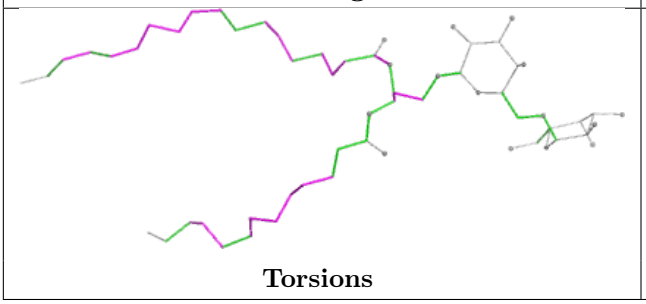
Ligand DGD B 7101



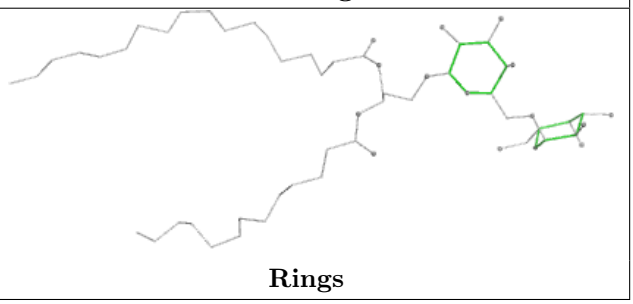
Bond lengths



Bond angles

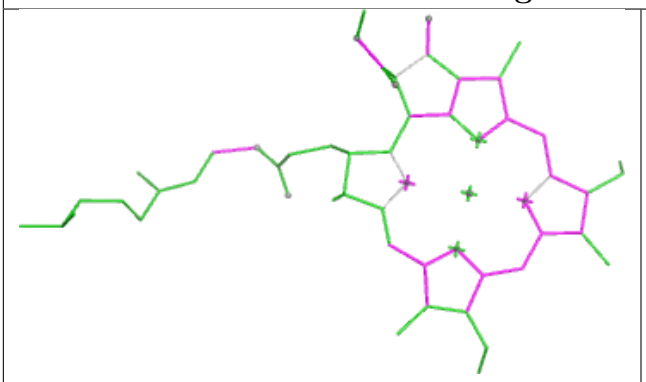


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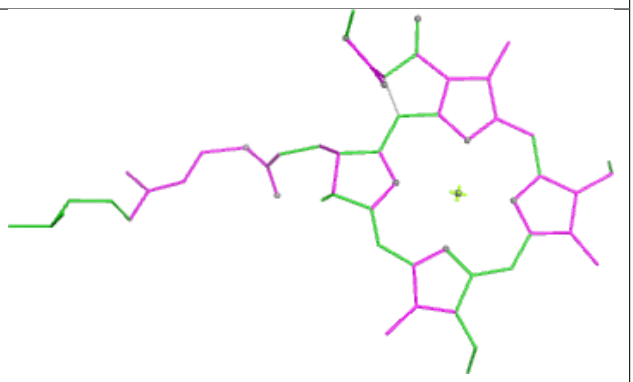


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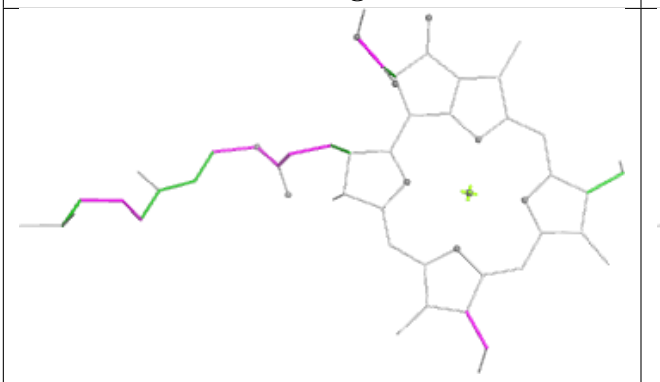
Ligand CLA A 1124



Bond lengths



Bond angles

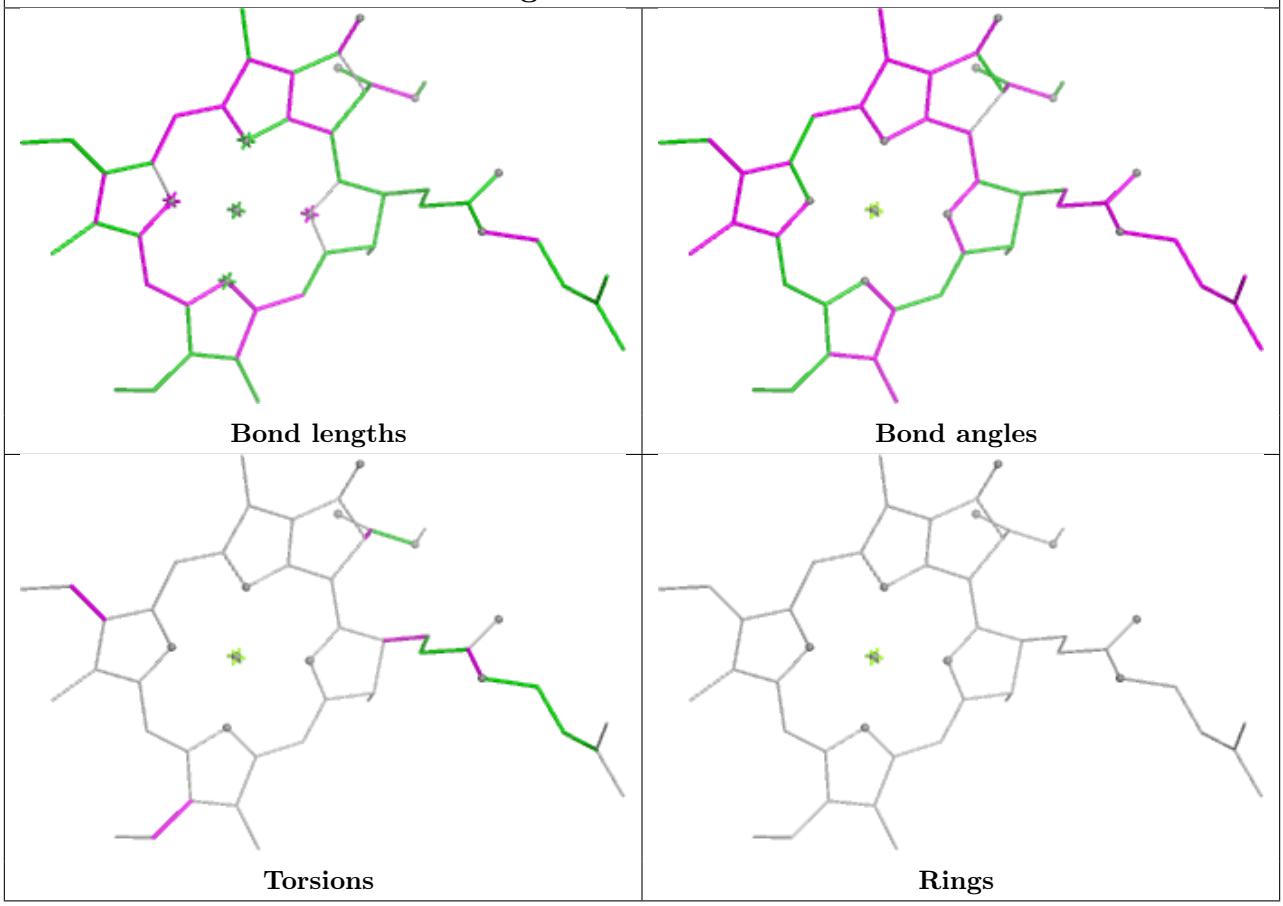


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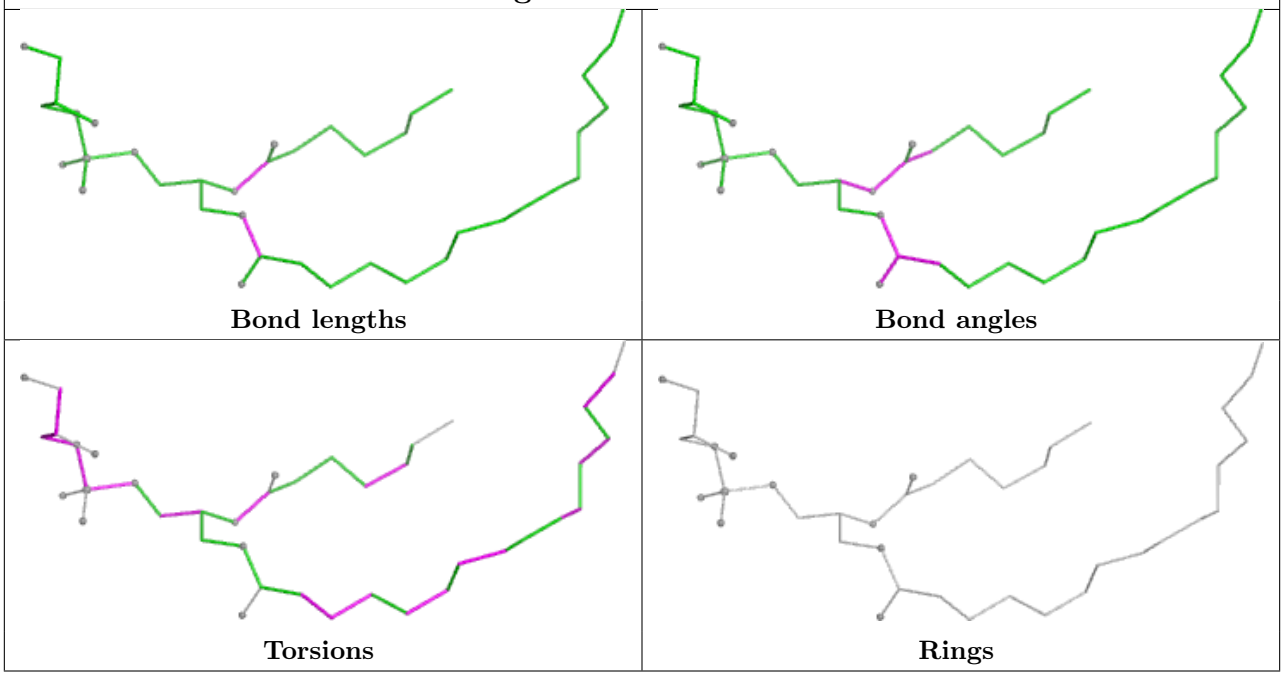


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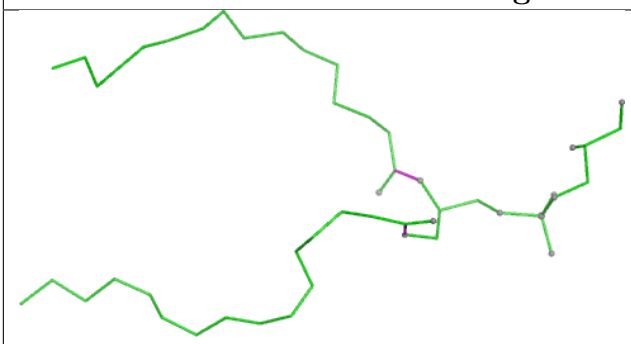
Ligand CLA 3 3007



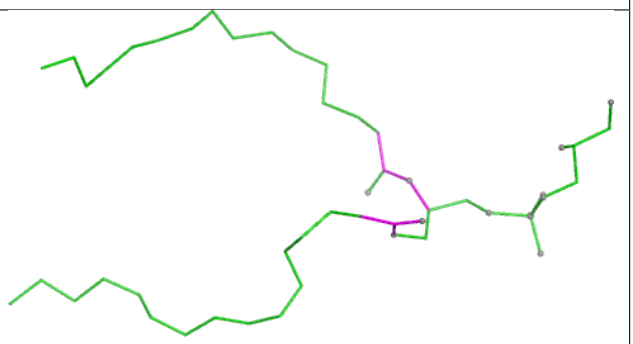
Ligand LHG A 5003



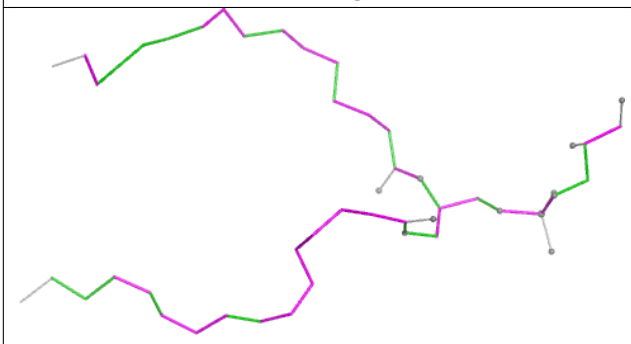
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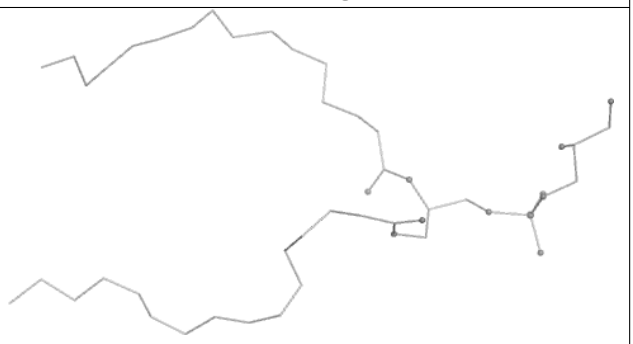
Bond lengths



Bond angles

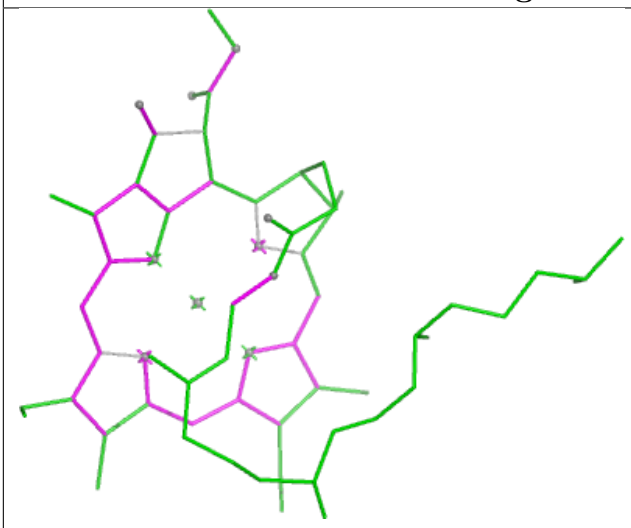


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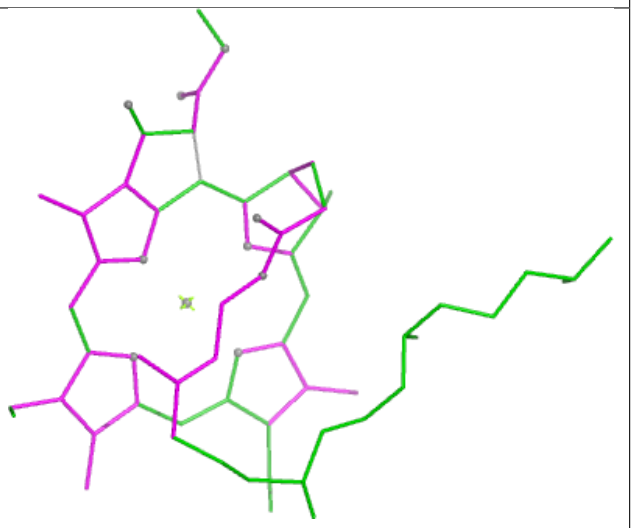


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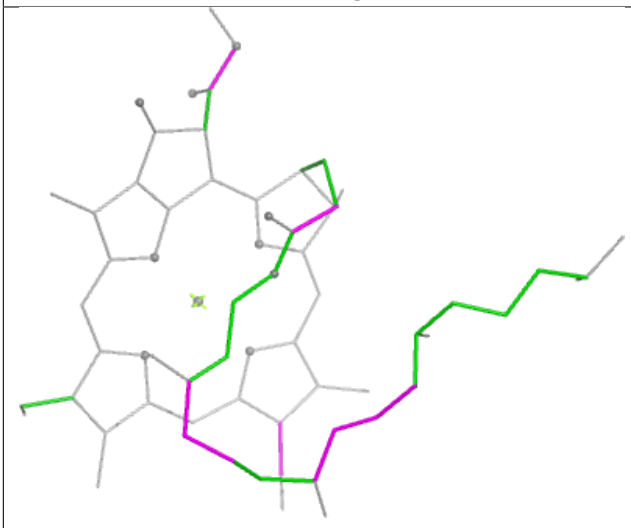
Ligand CLA B 1205



Bond lengths



Bond angles

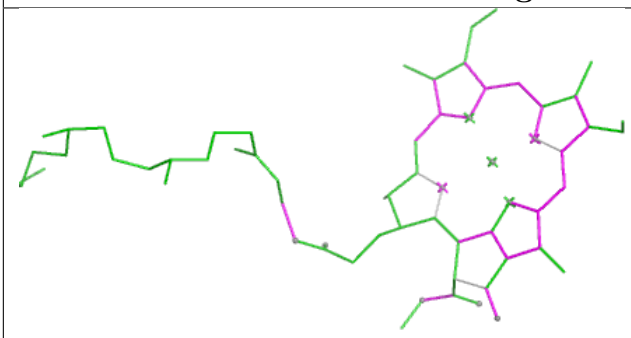


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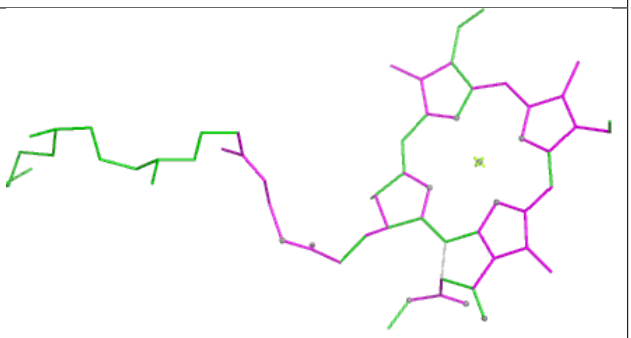


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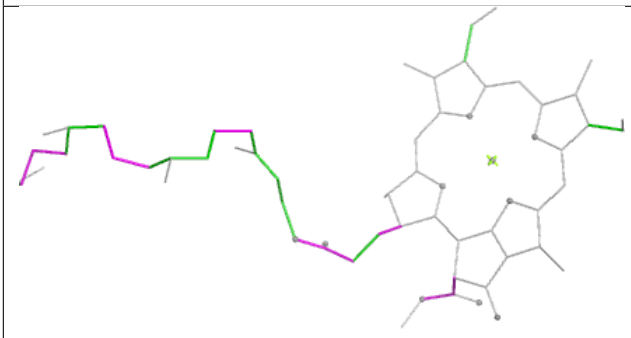
Ligand CLA B 1210



Bond lengths



Bond angles

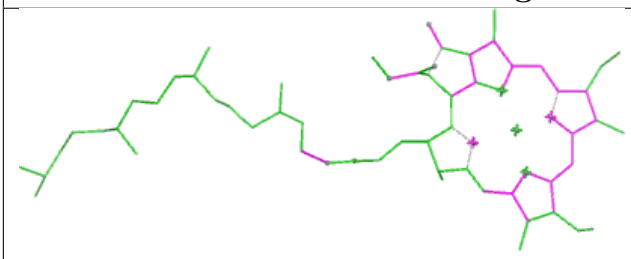


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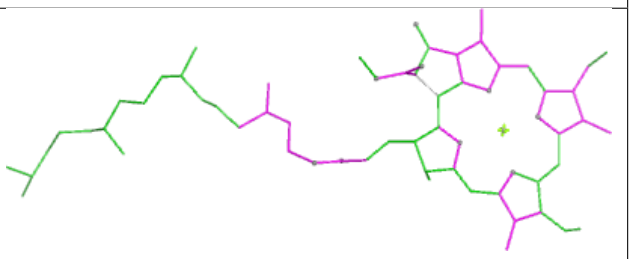


Rings

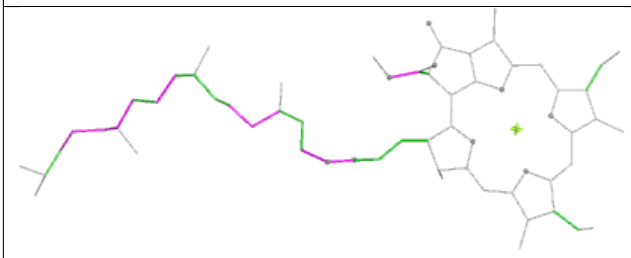
Ligand CLA A 1139



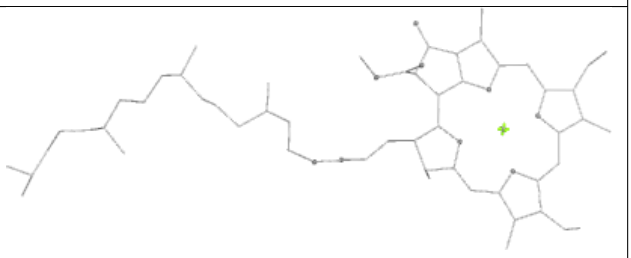
Bond lengths



Bond angles

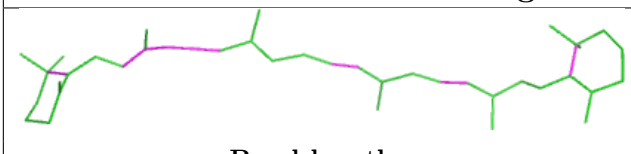


Torsions



Rings

Ligand BCR J 6013



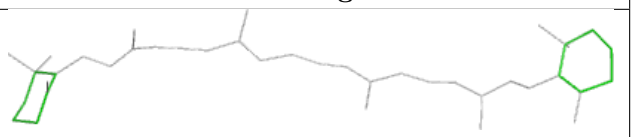
Bond lengths



Bond angles

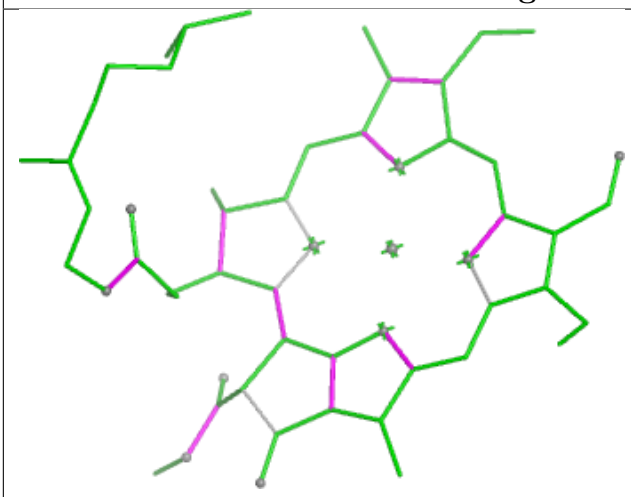


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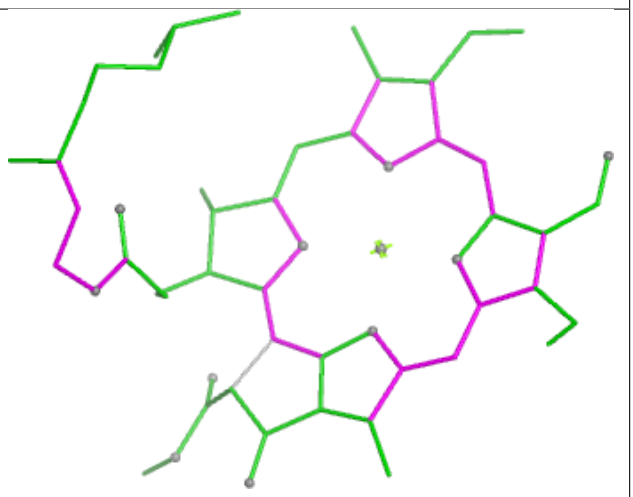


Rings

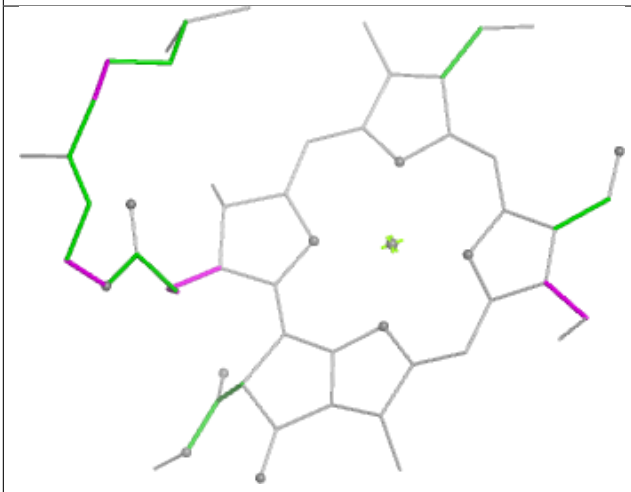
Ligand CHL 3 3011



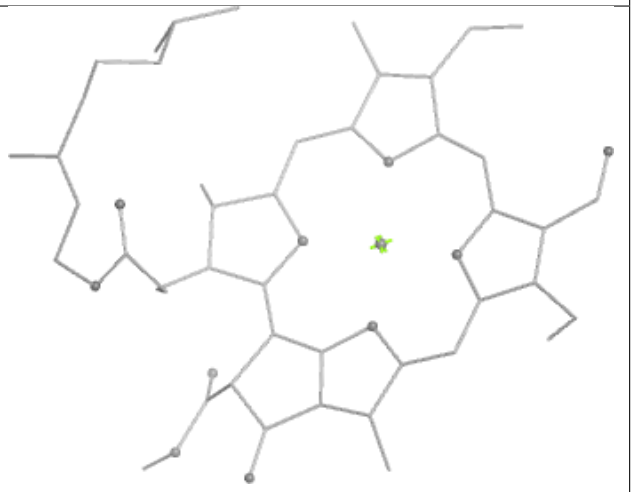
Bond lengths



Bond angles

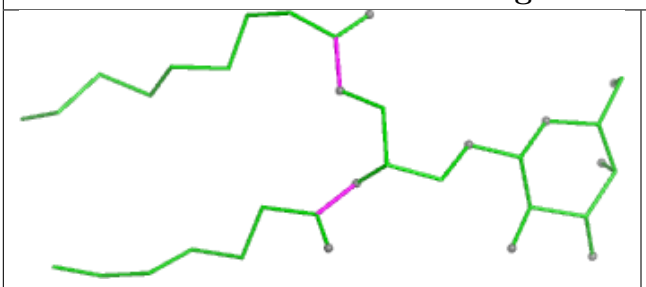


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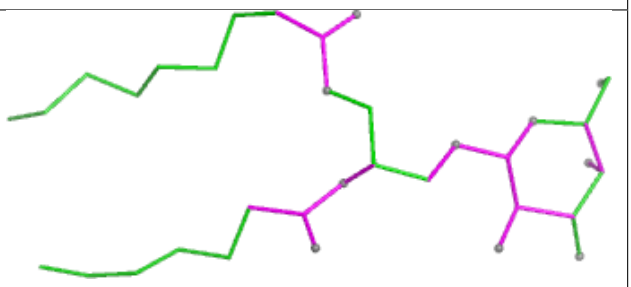


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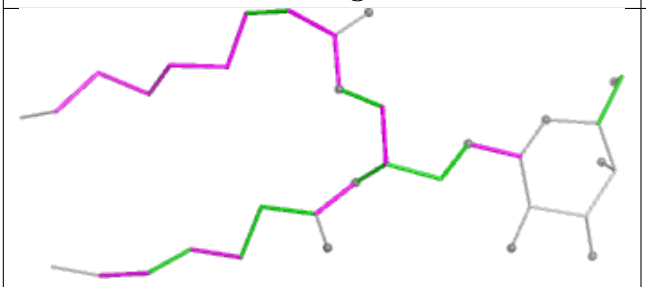
Ligand LMG 4 4801



Bond lengths



Bond angles

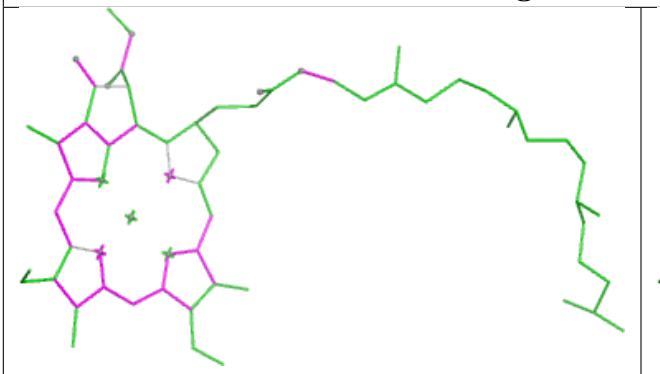


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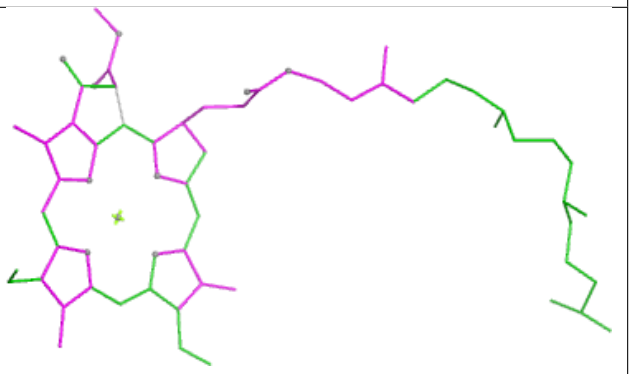


Rings

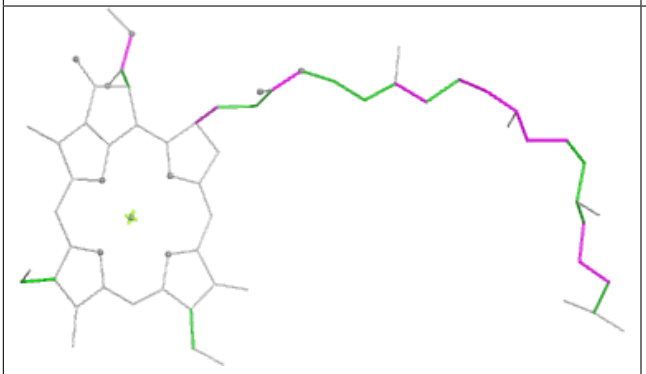
Ligand CLA B 1222



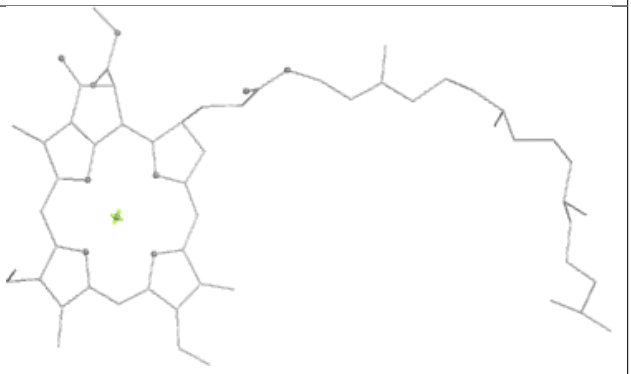
Bond lengths



Bond angles

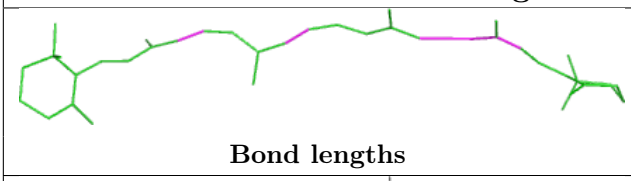


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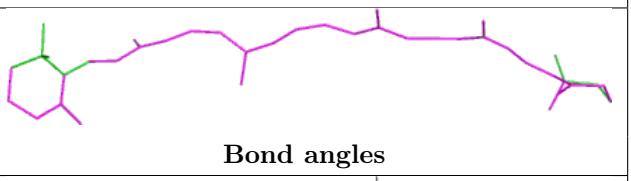


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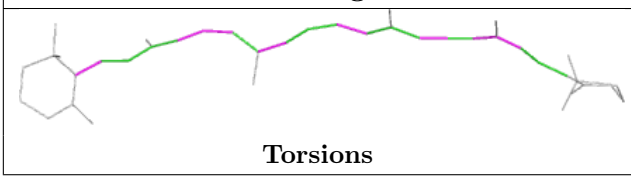
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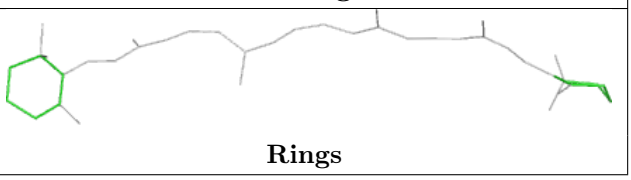
Bond lengths



Bond angles

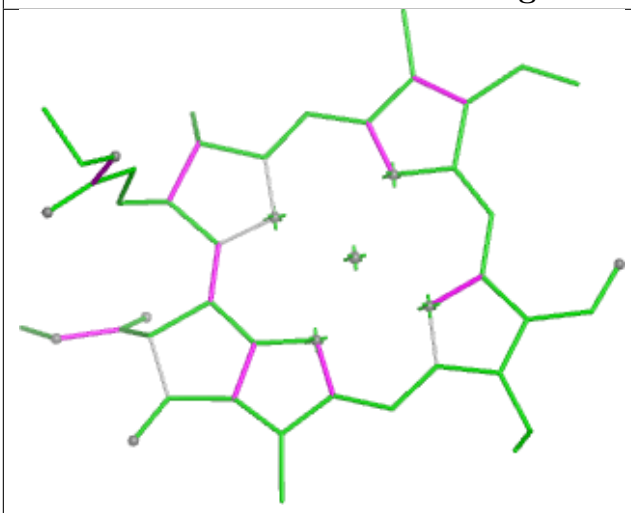


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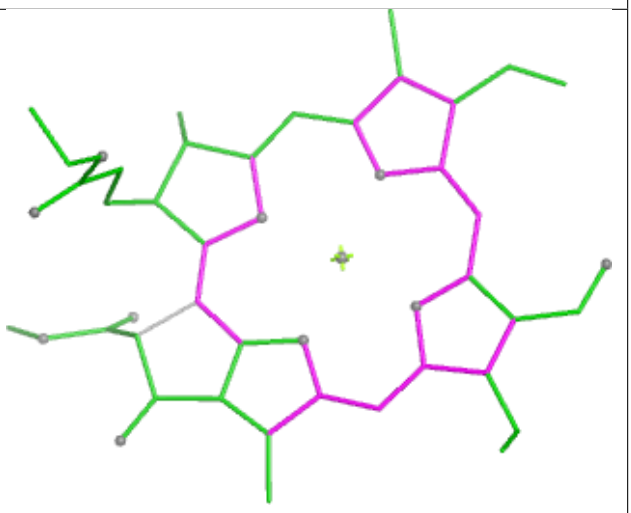


Rings

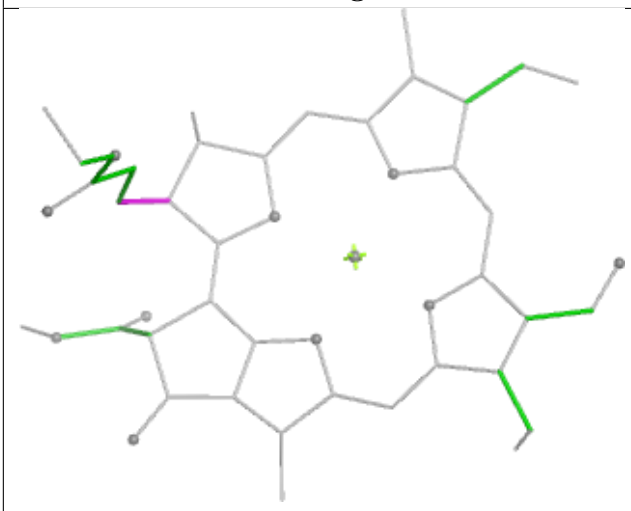
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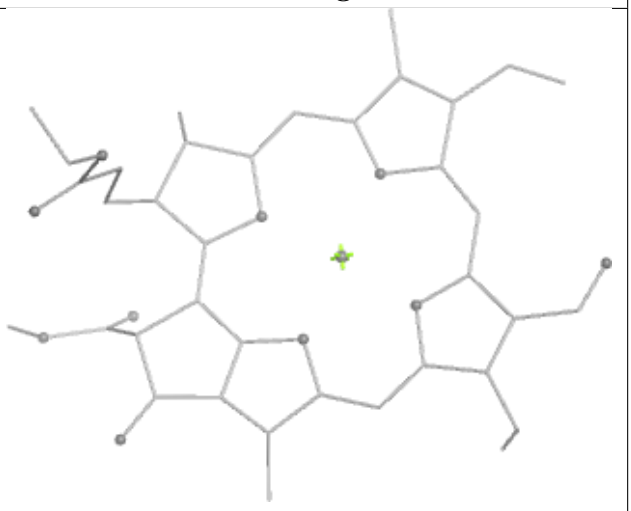
Bond lengths



Bond angles

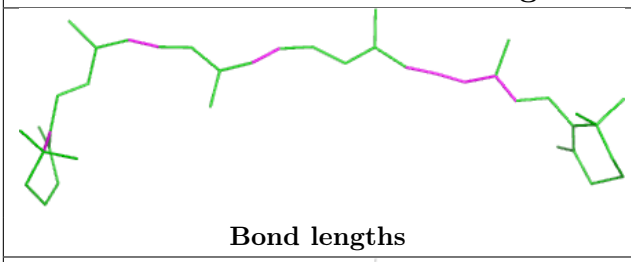


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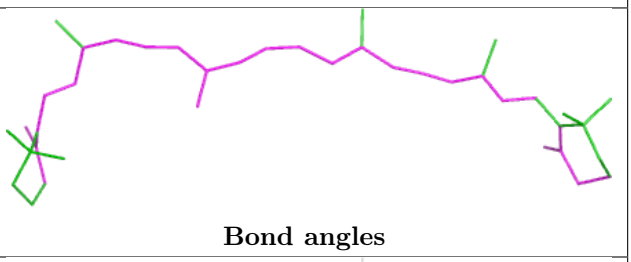


Rings

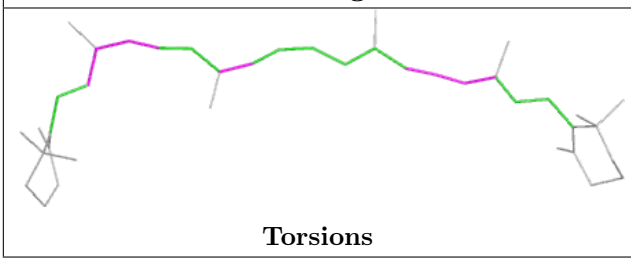
Ligand BCR I 6020



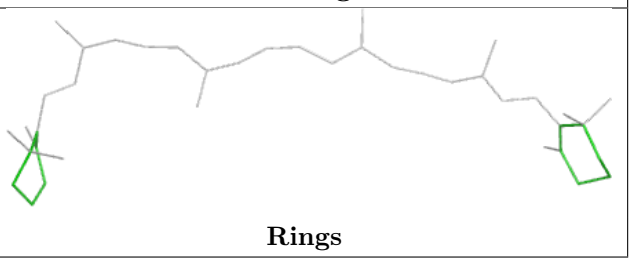
Bond lengths



Bond angles

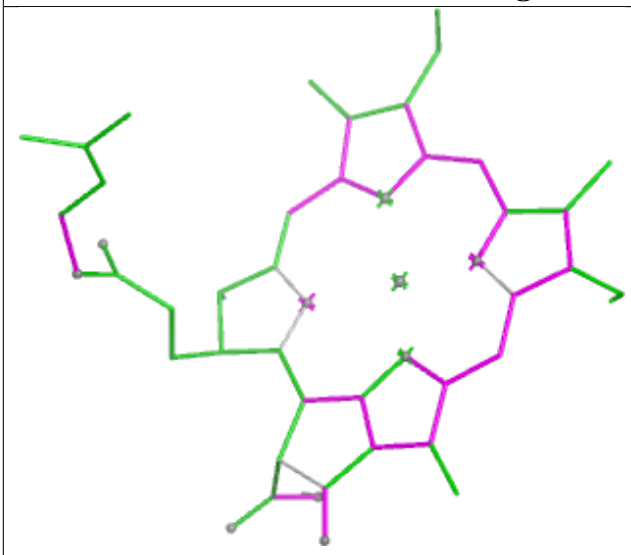


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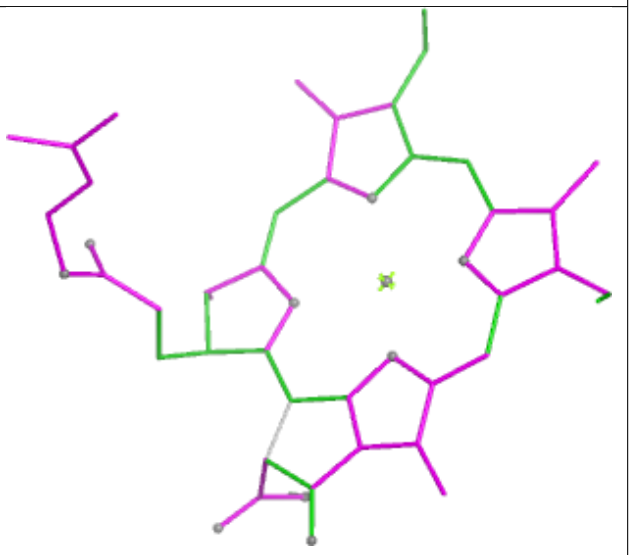


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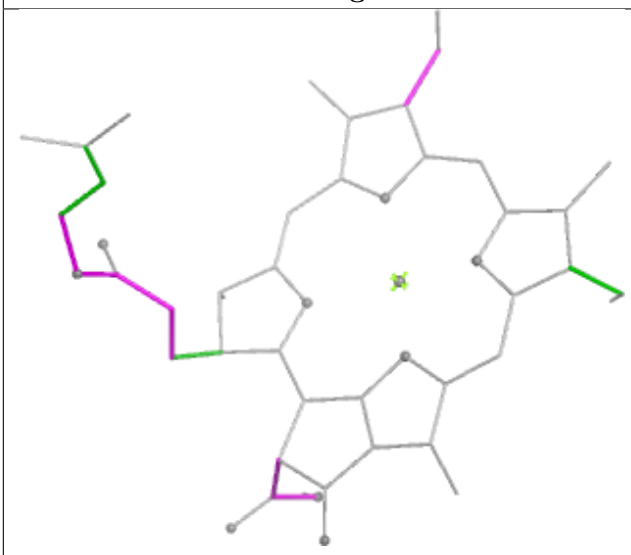
Ligand CLA A 1129



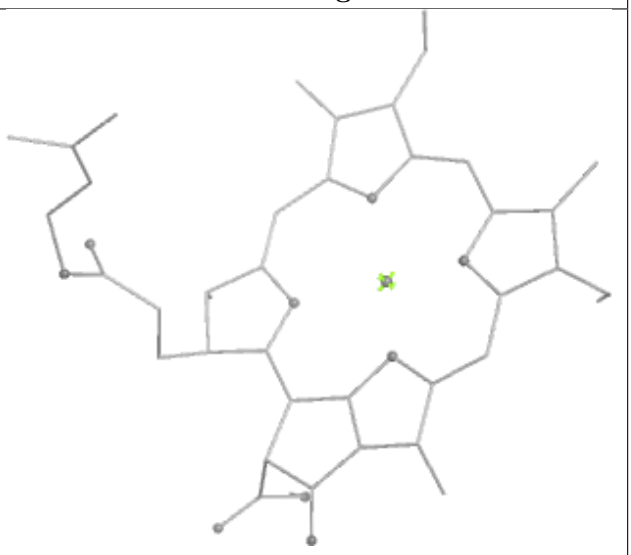
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Bond angles

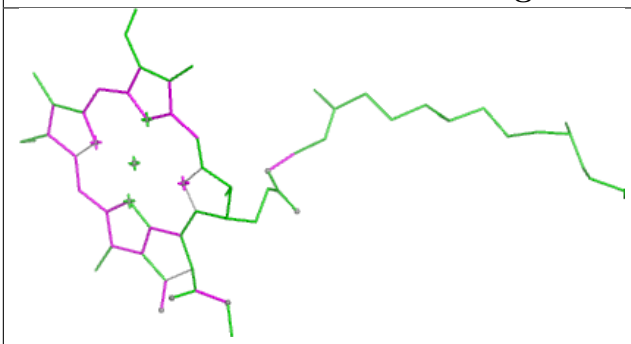


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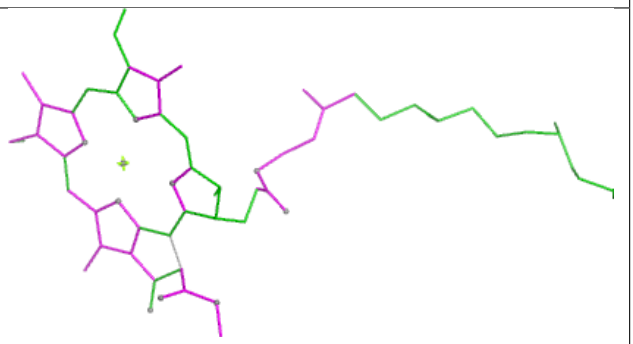


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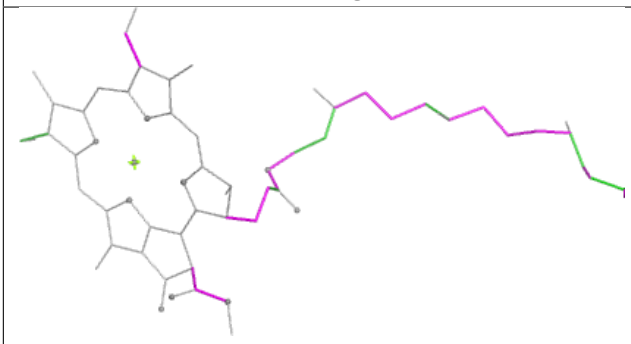
Ligand CLA A 1119



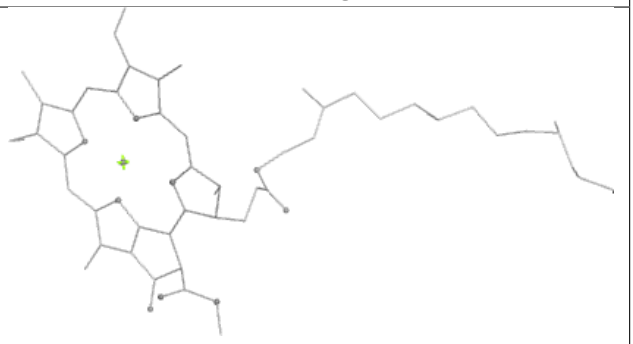
Bond lengths



Bond angles

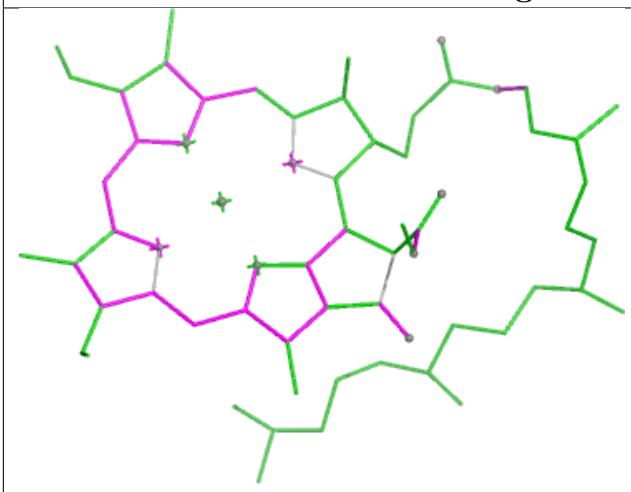


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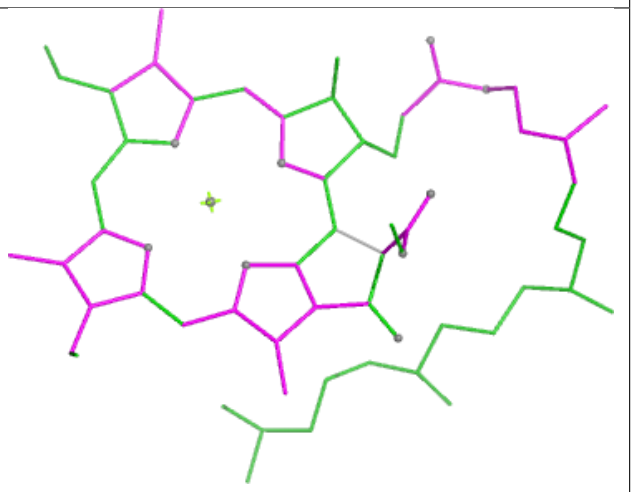


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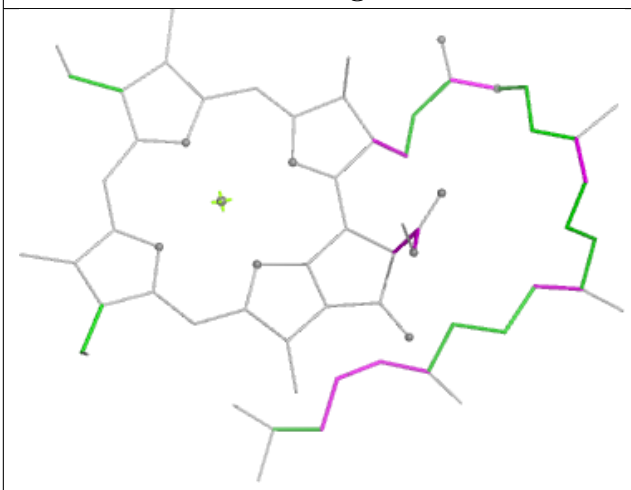
Ligand CLA B 1202



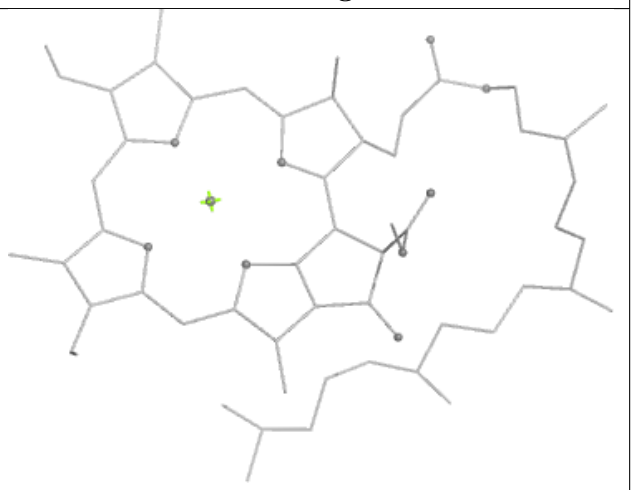
Bond lengths



Bond angles



Torsions

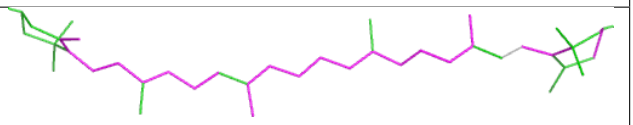


Rings

Ligand LUT 1 1501



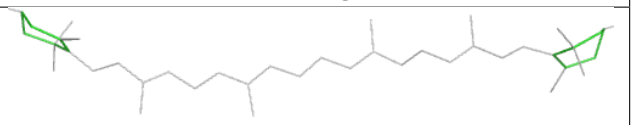
Bond lengths



Bond angles

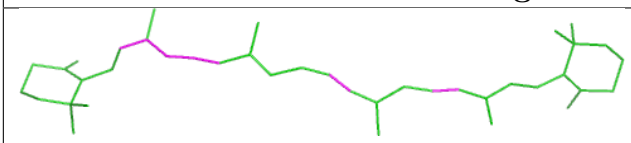


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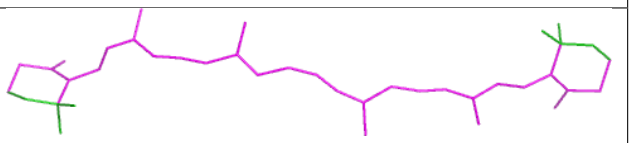


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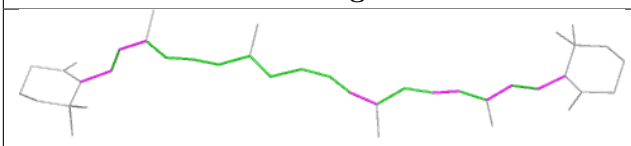
Ligand BCR B 6004



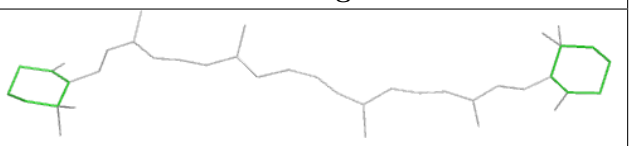
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Bond angles

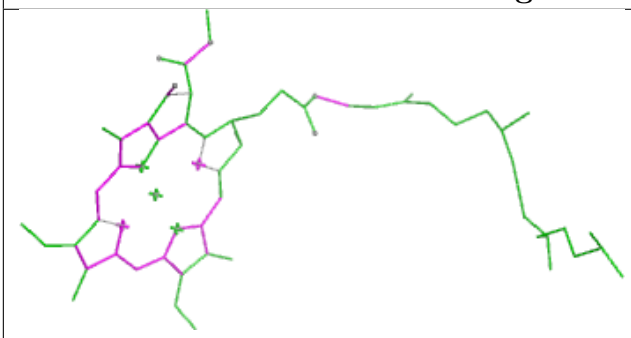


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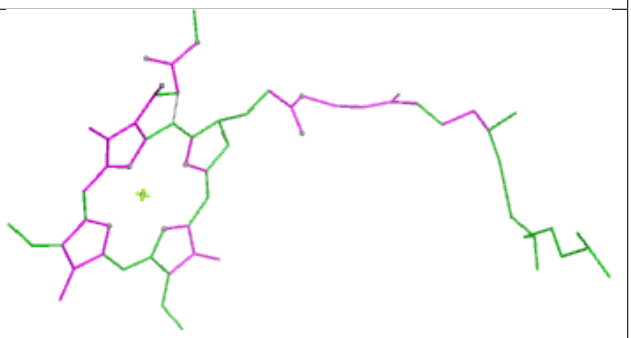


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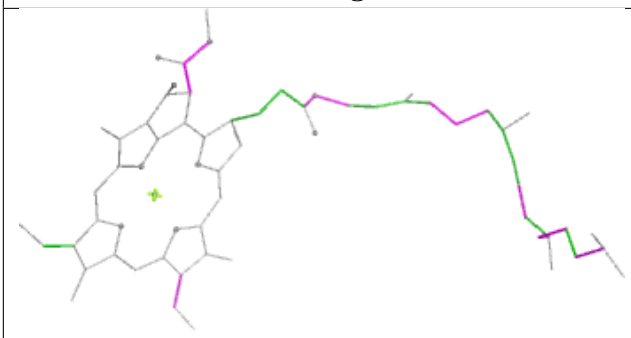
Ligand CLA B 1012



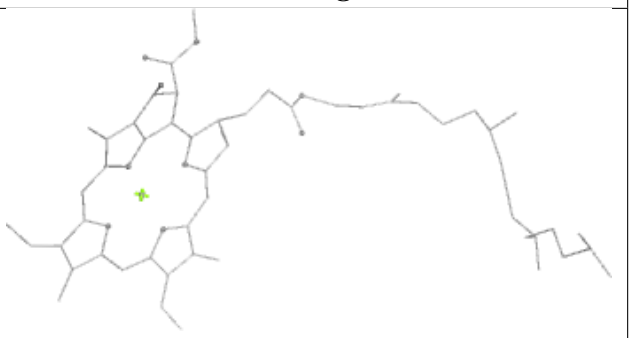
Bond lengths



Bond angles

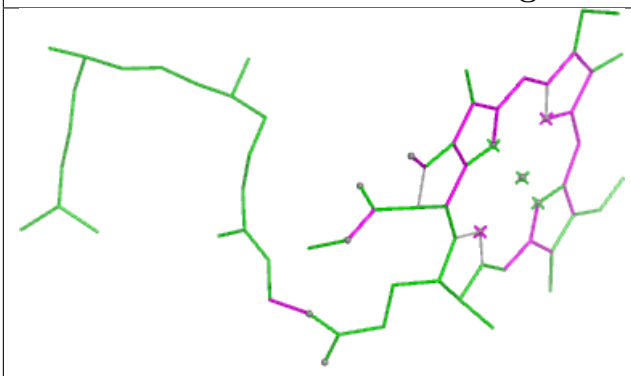


Torsions



Rings

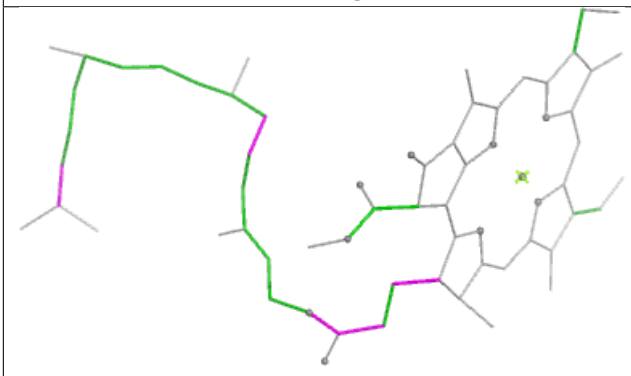
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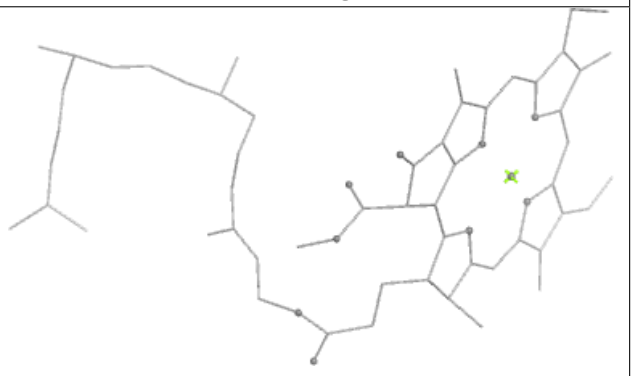
Bond lengths



Bond angles

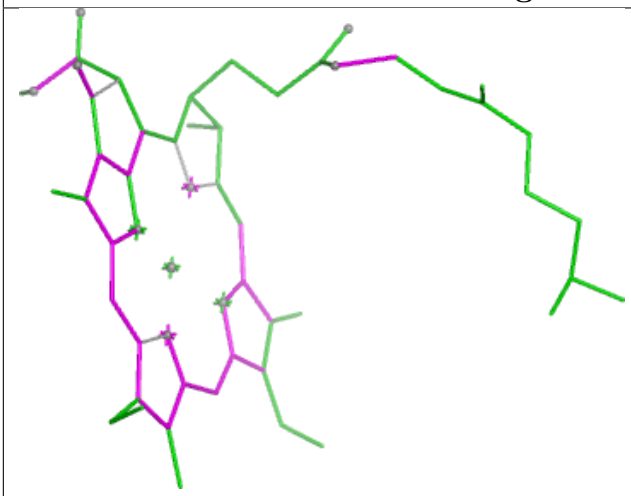


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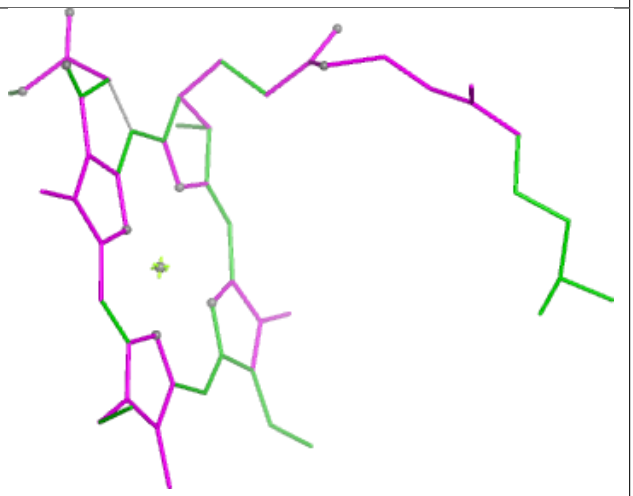


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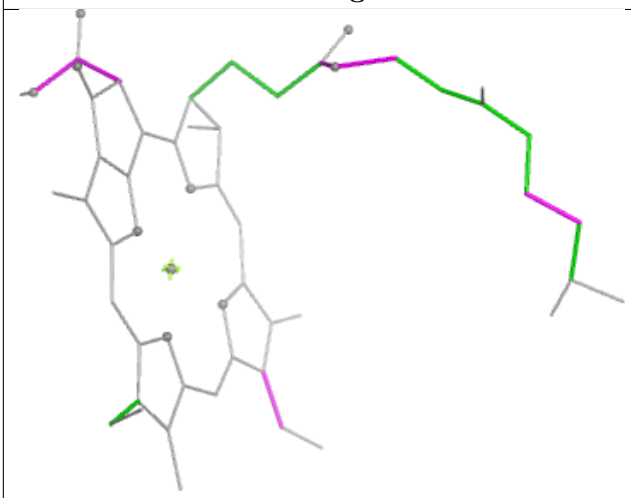
Ligand CLA B 1212



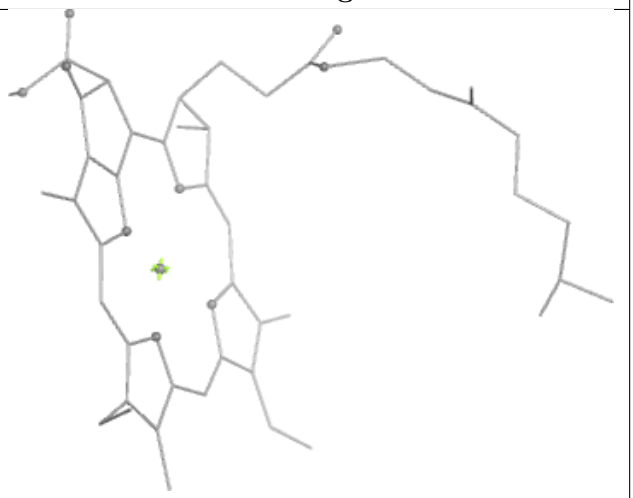
Bond lengths



Bond angles

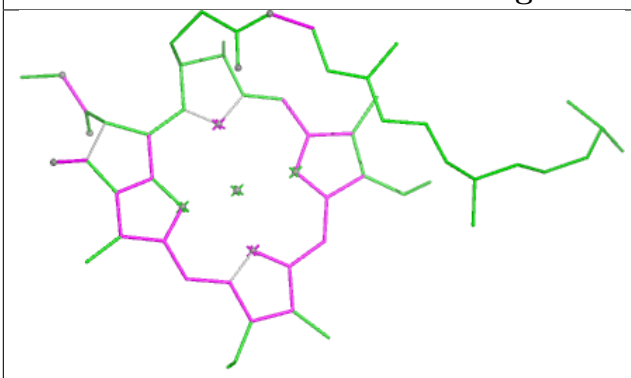


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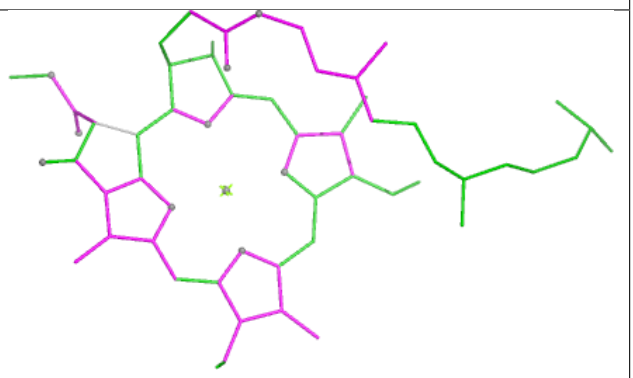


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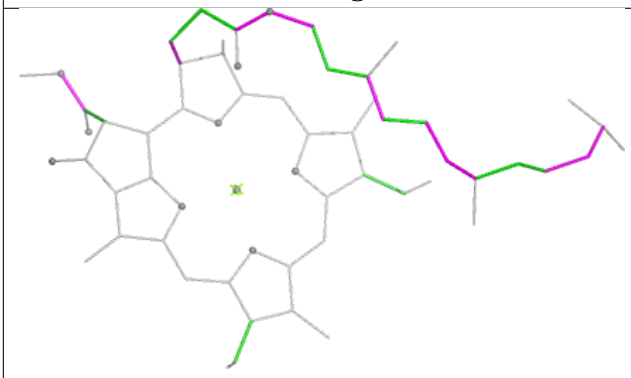
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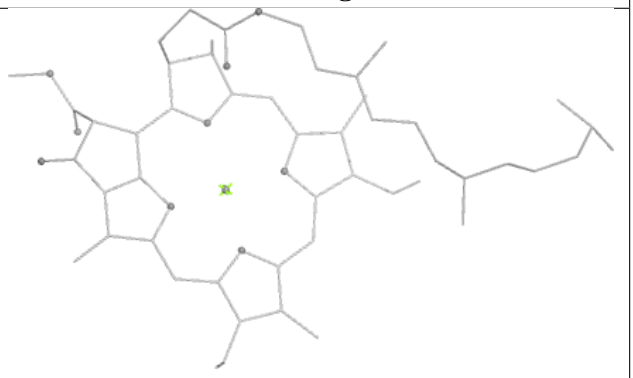
Bond lengths



Bond angles

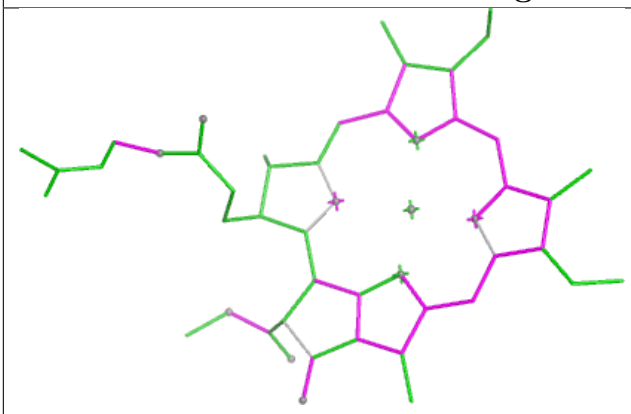


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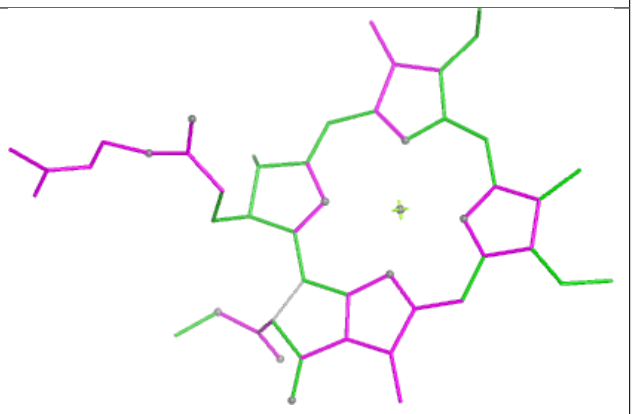


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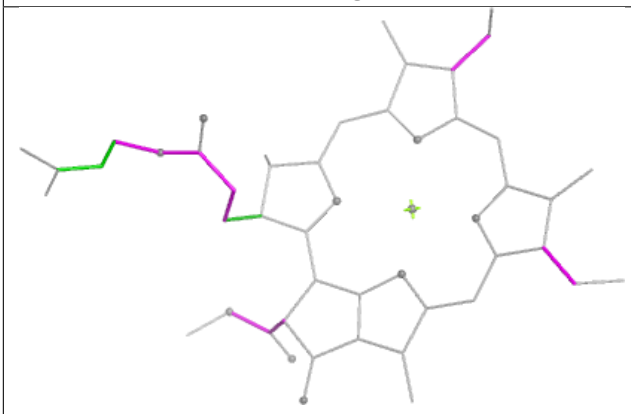
Ligand CLA A 1151



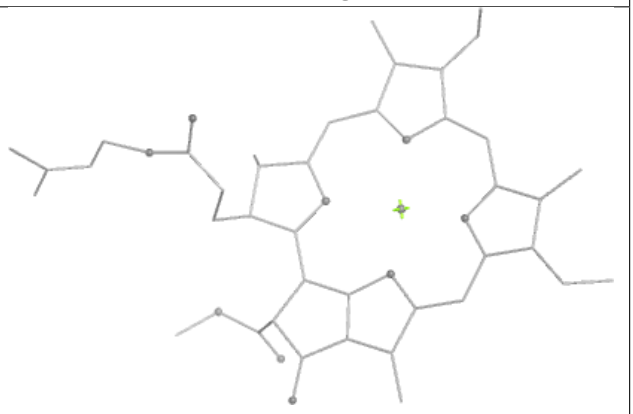
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Bond angles

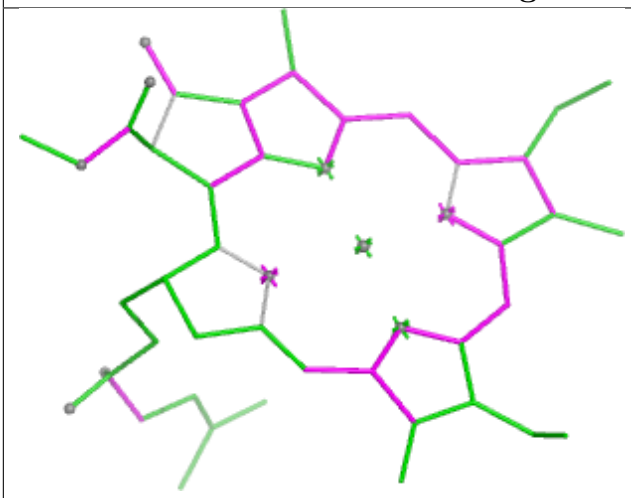


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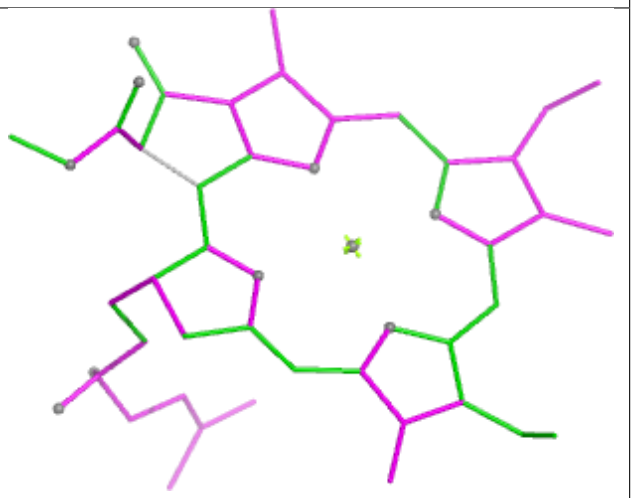


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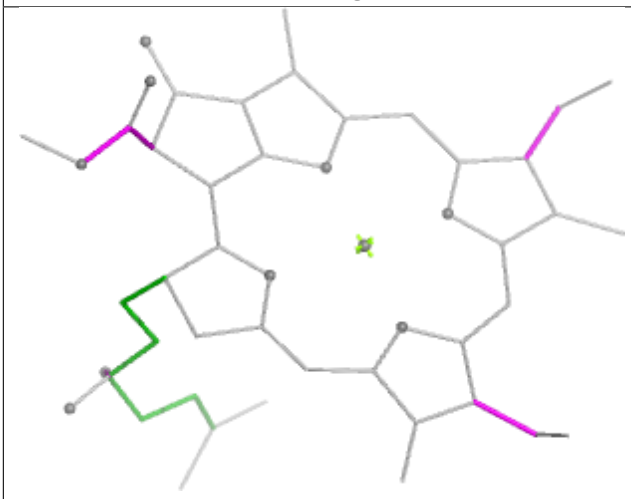
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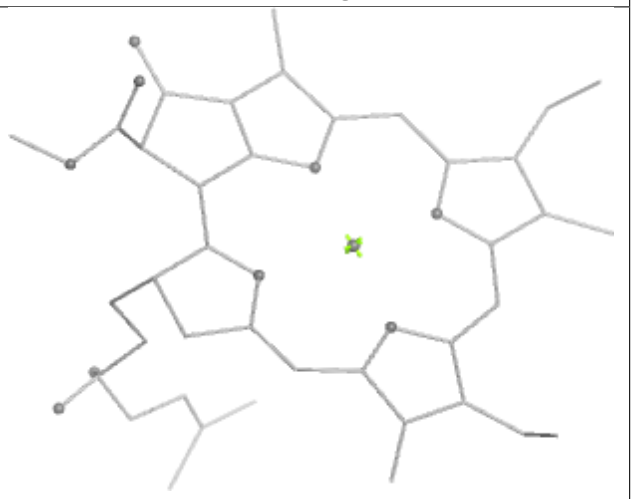
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Bond angles

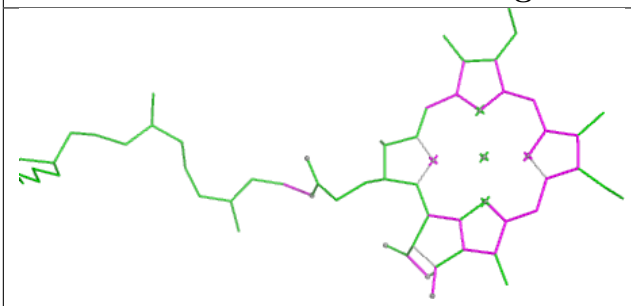


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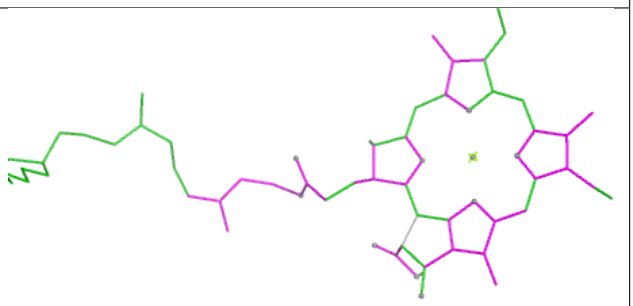


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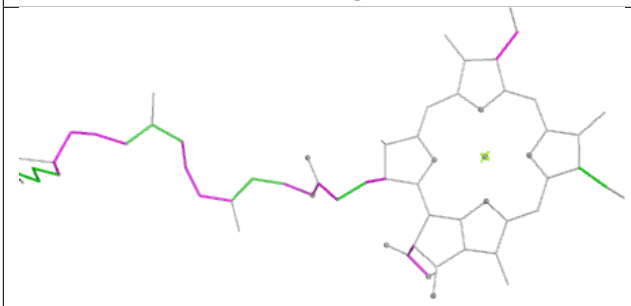
Ligand CLA A 1103



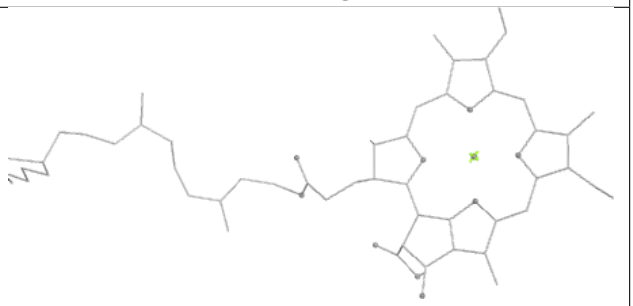
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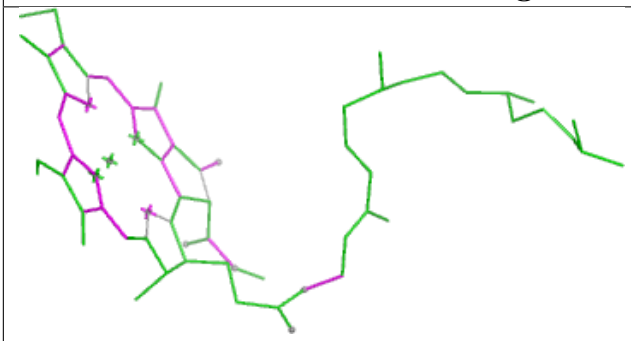


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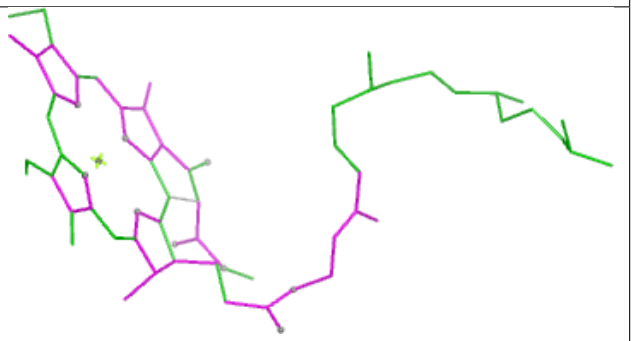


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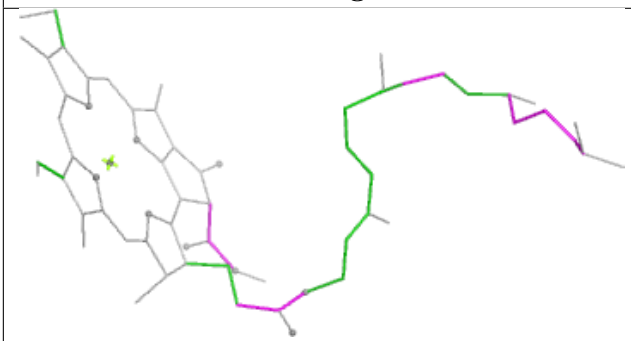
Ligand CLA B 1021



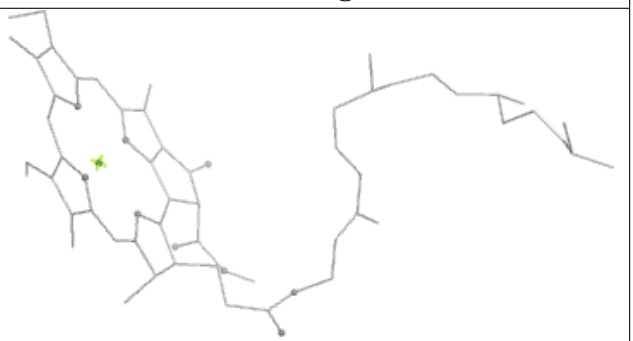
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Bond angles

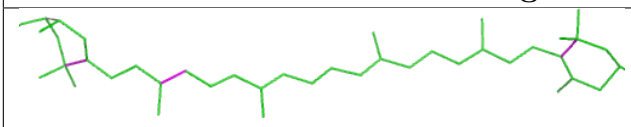


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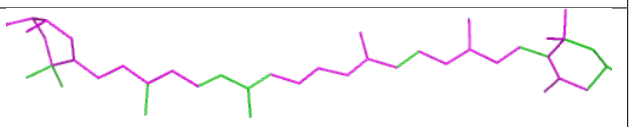


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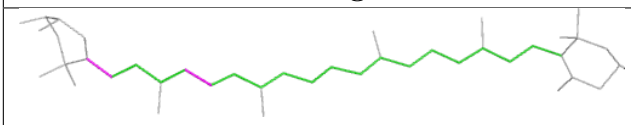
Ligand ZEX 4 4505



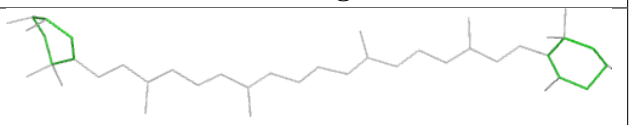
Bond lengths



Bond angles

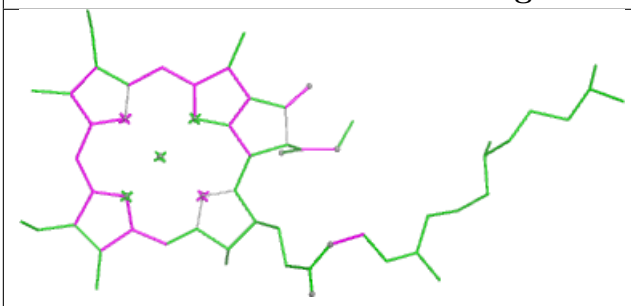


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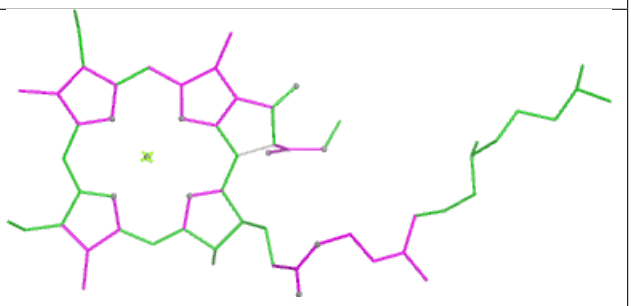


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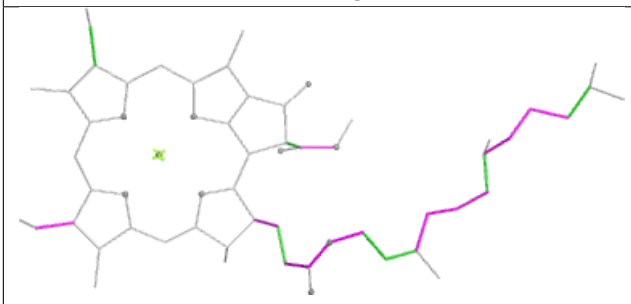
Ligand CLA A 1120



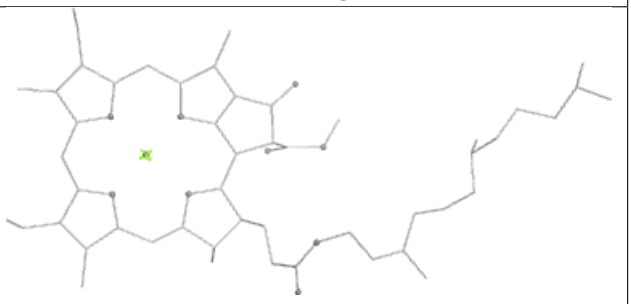
Bond lengths



Bond angles

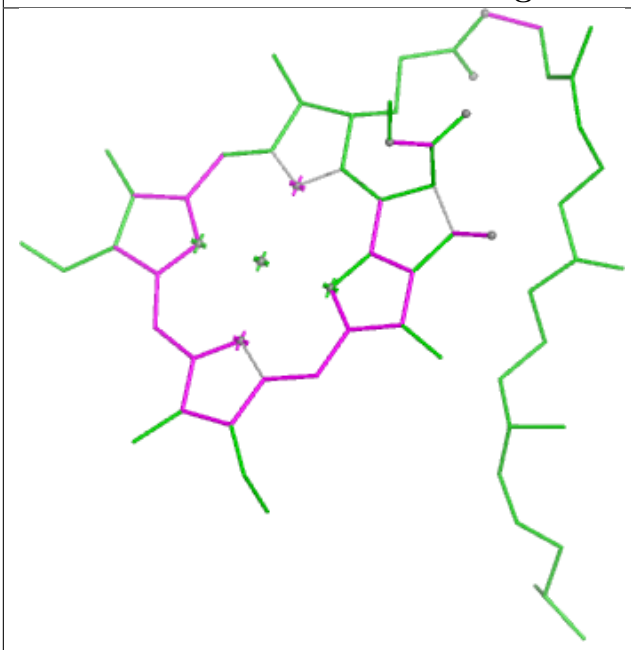


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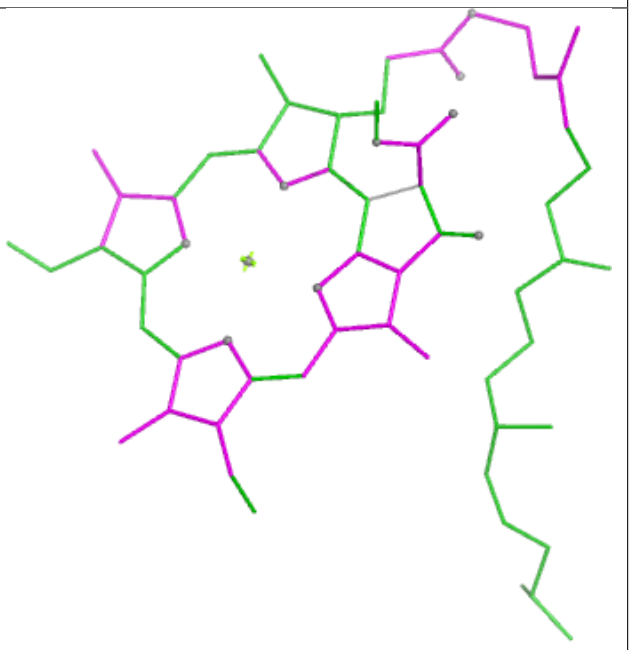


Rings

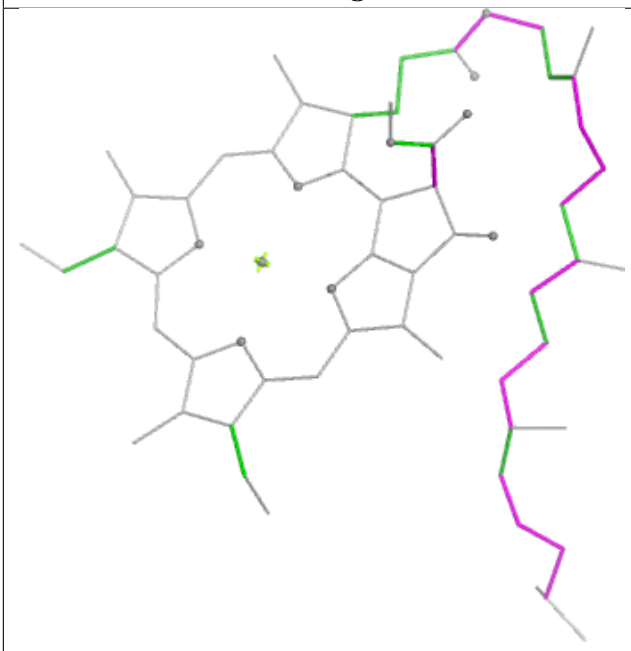
Ligand CLA A 1123



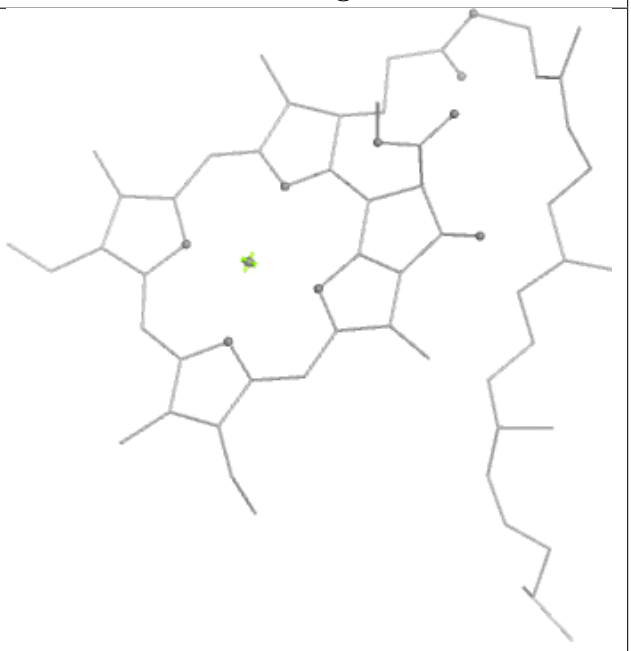
Bond lengths



Bond angles



Torsions

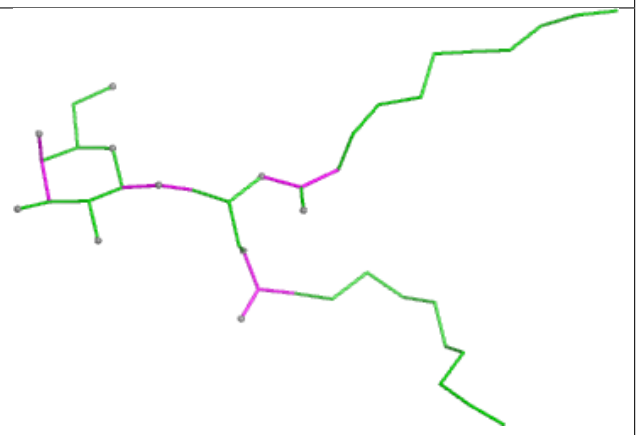


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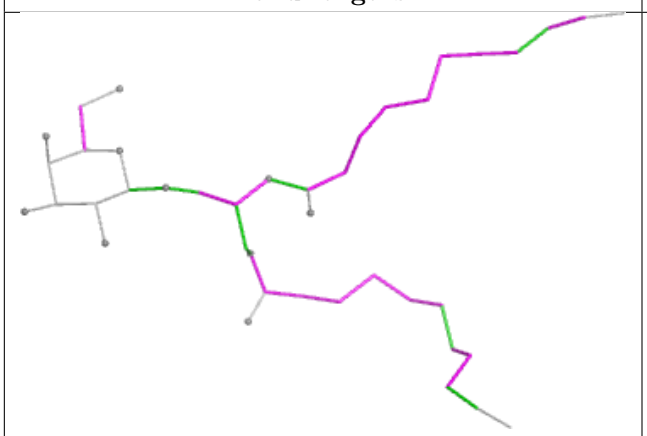
Ligand LMG G 2021



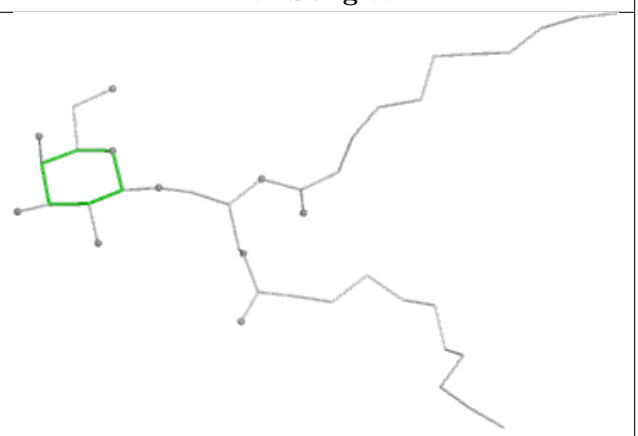
Bond lengths



Bond angles

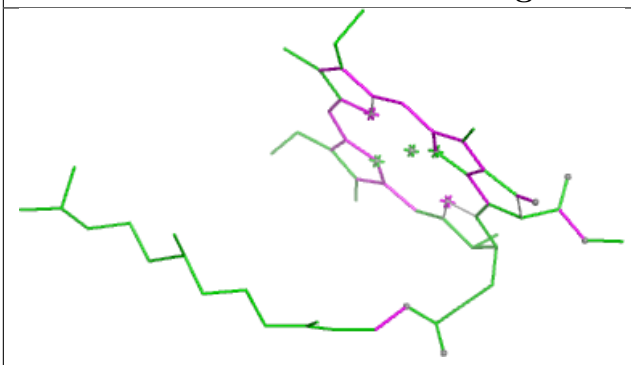


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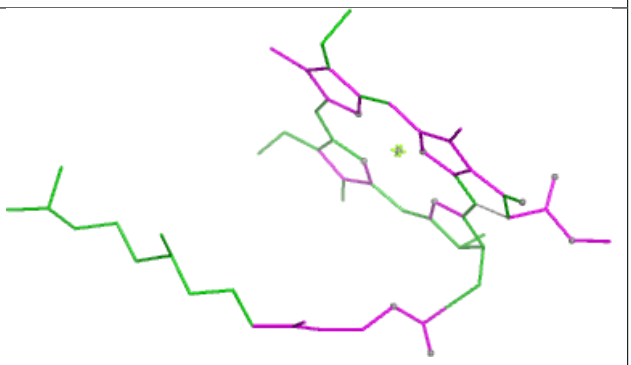


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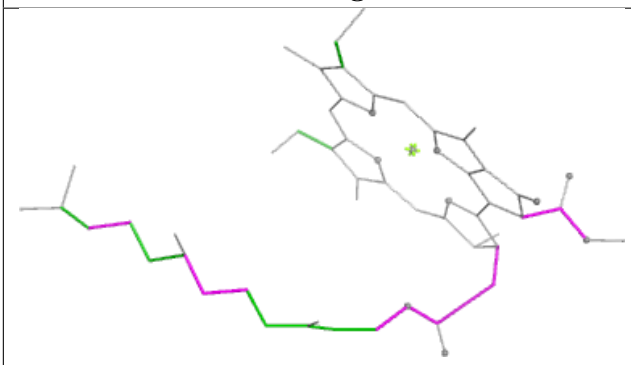
Ligand CLA B 1228



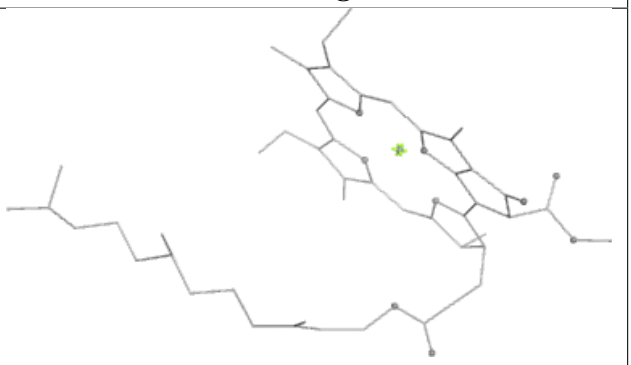
Bond lengths



Bond angles

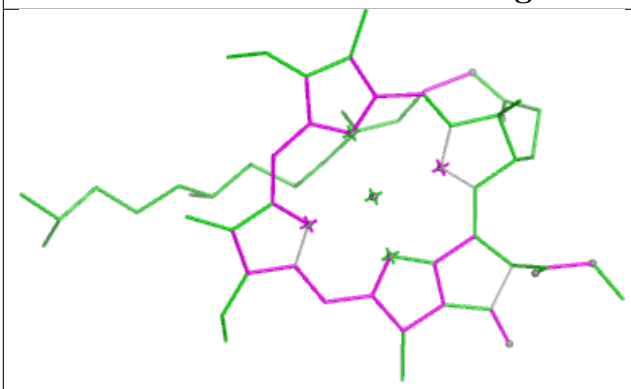


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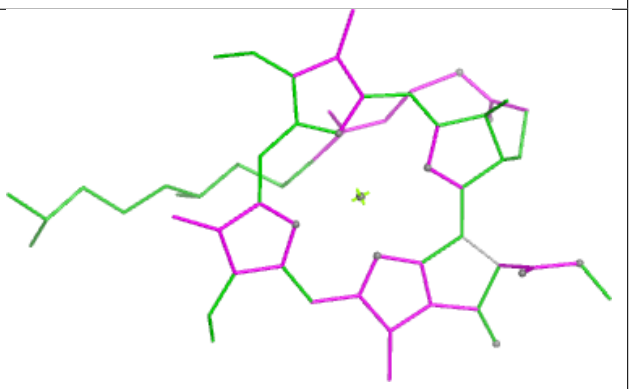


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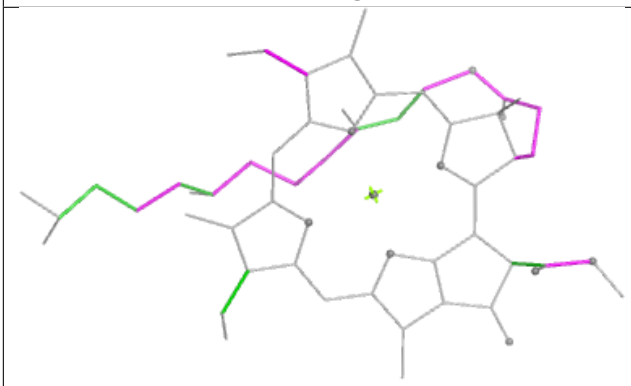
Ligand CLA A 1116



Bond lengths



Bond angles

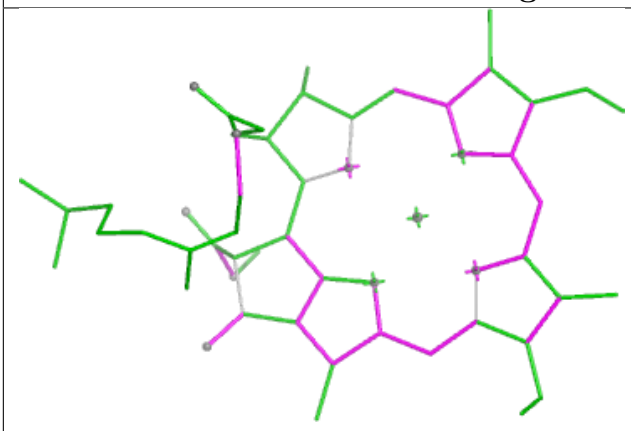


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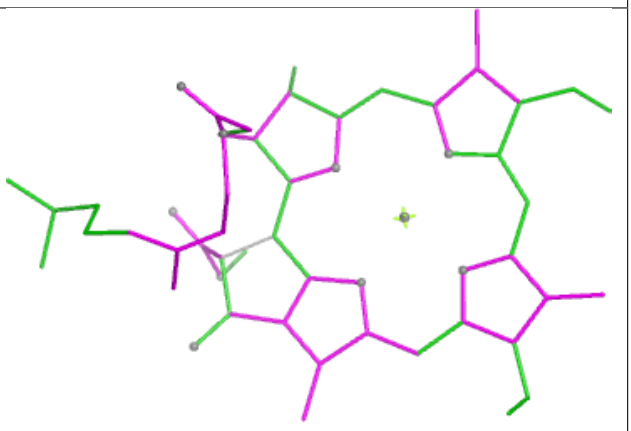


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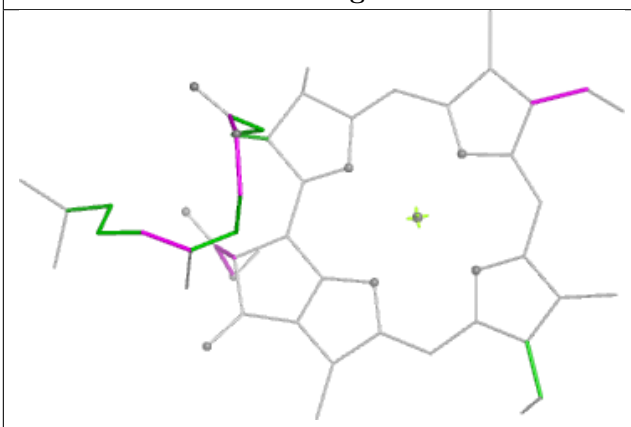
Ligand CLA 2 2006



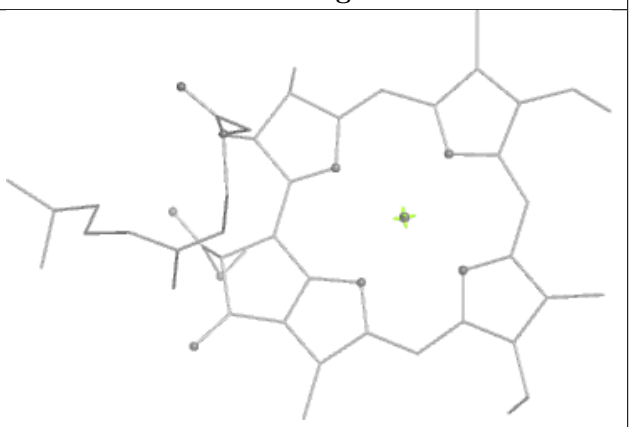
Bond lengths



Bond angles

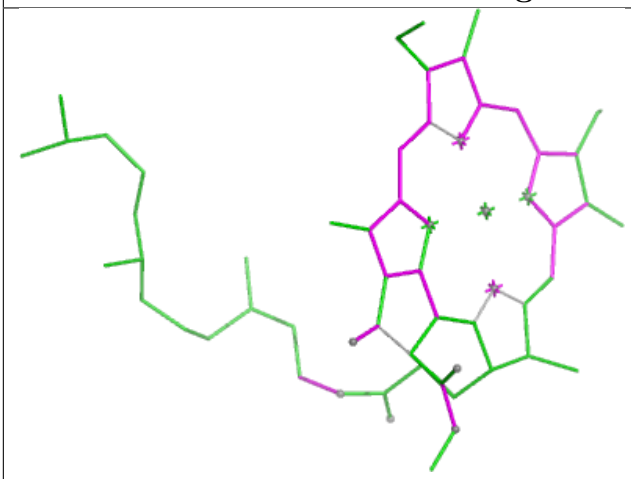


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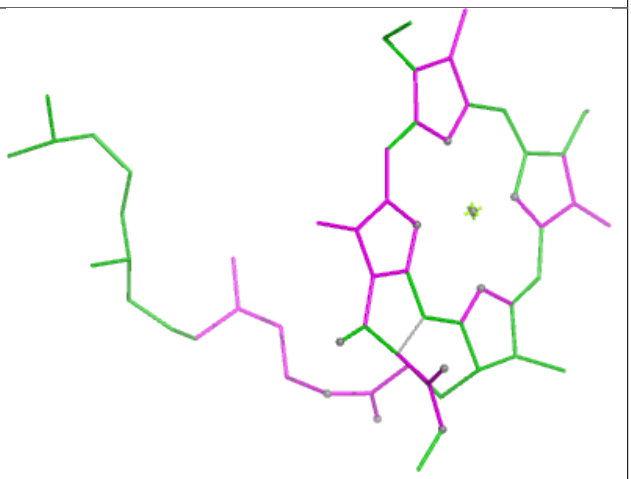


Rings

Ligand CLA B 1219



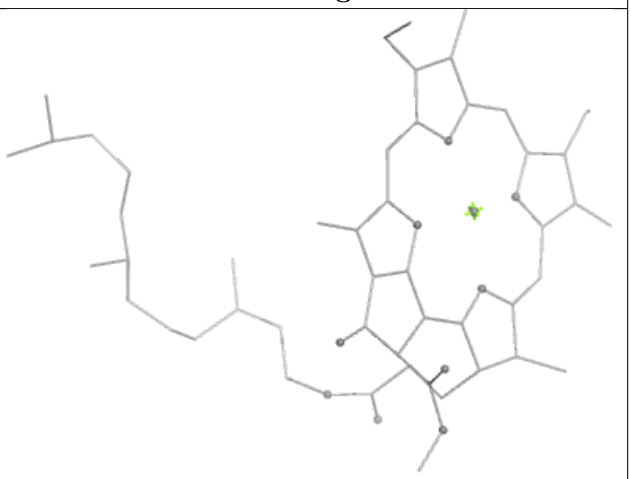
Bond lengths



Bond angles

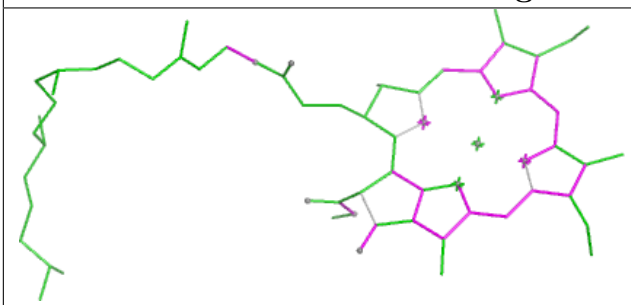


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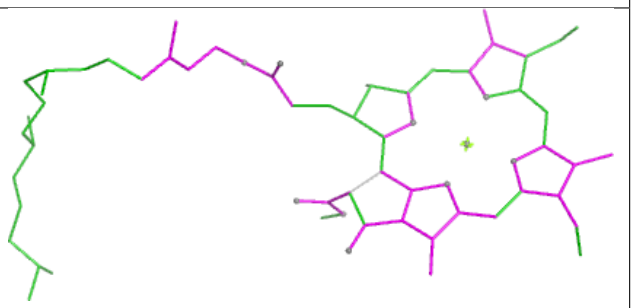


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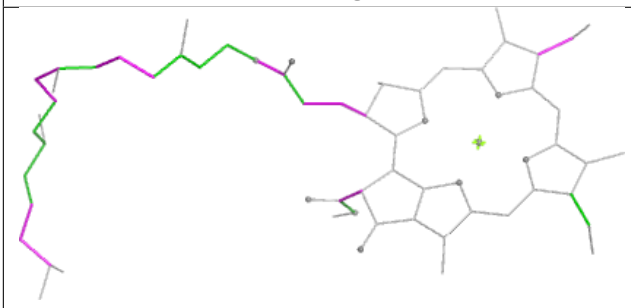
Ligand CLA B 1223



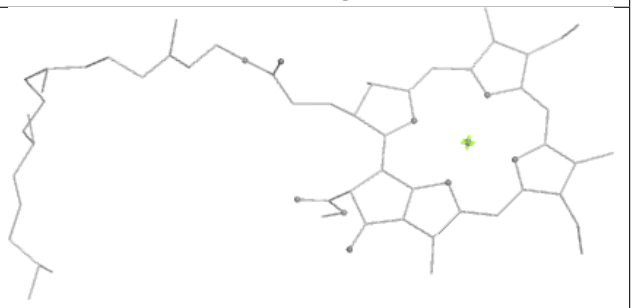
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Bond angles

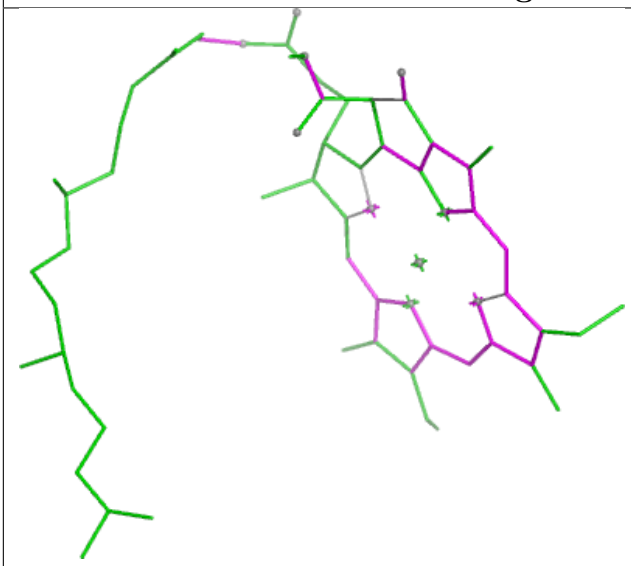


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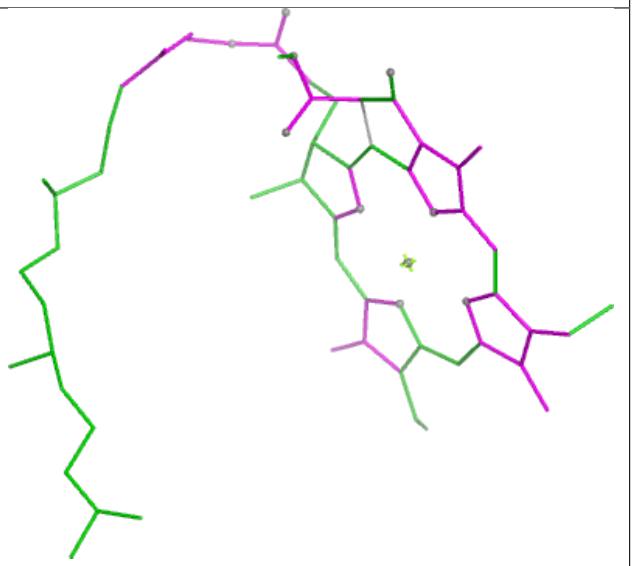


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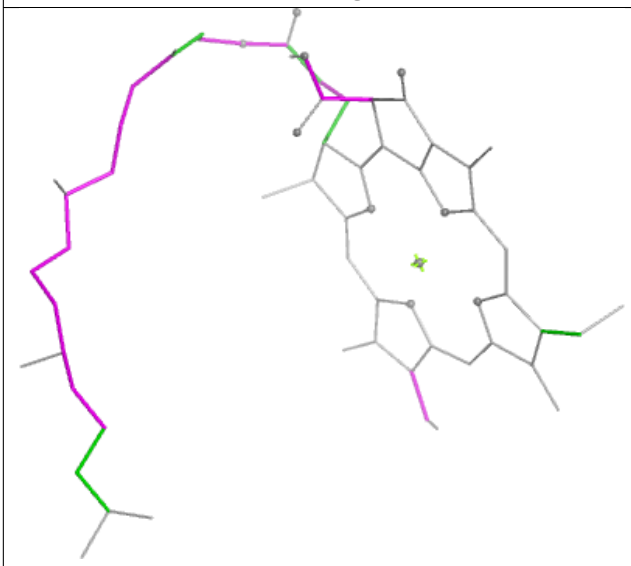
Ligand CLA B 1207



Bond lengths



Bond angles

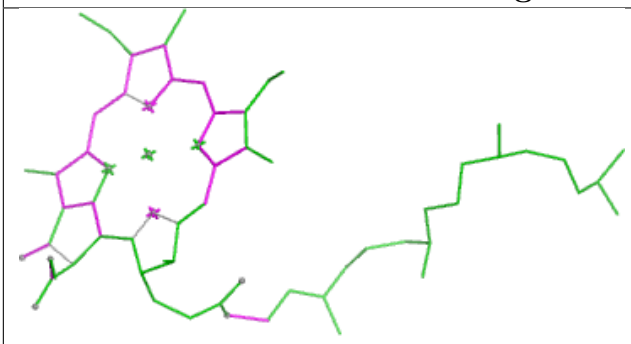


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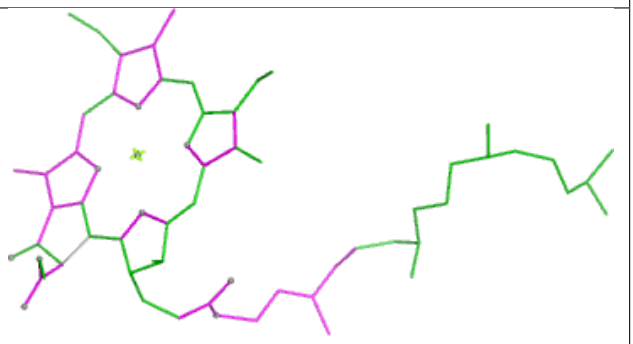


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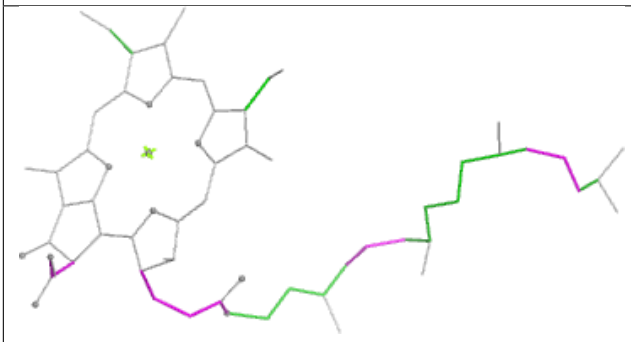
Ligand CLA A 1106



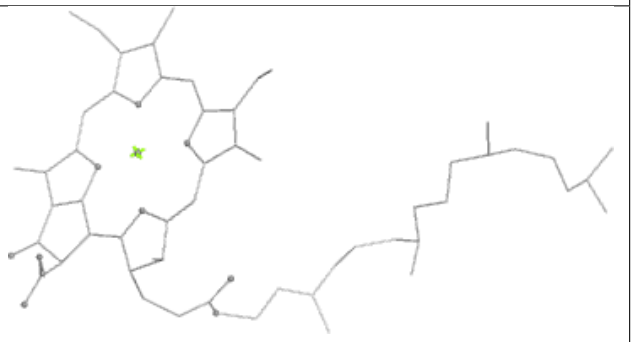
Bond lengths



Bond angles

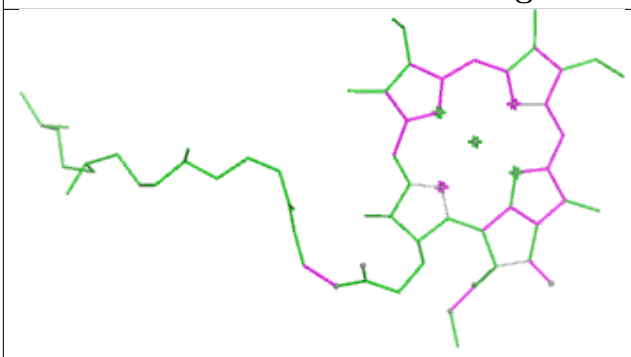


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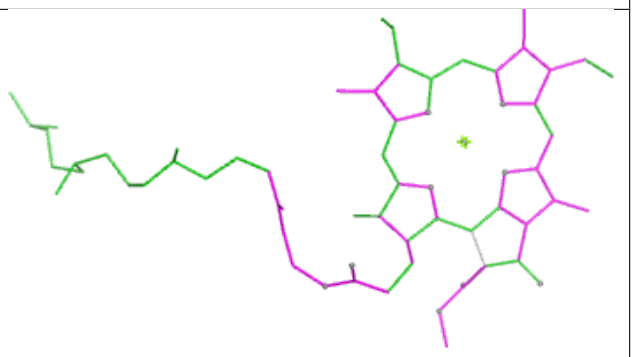


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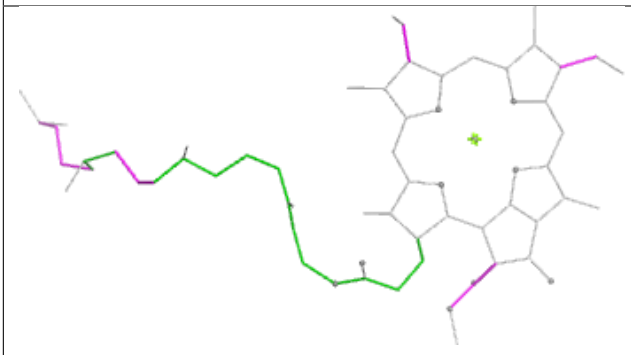
Ligand CLA B 1023



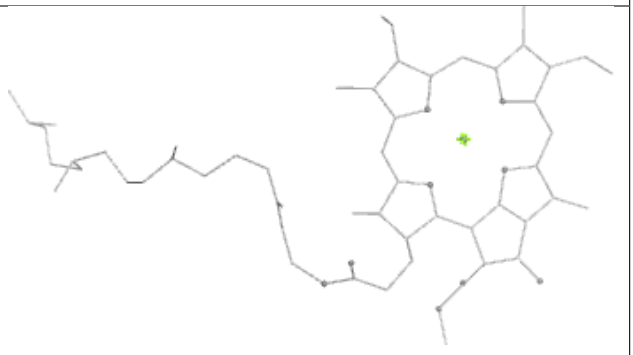
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Bond angles

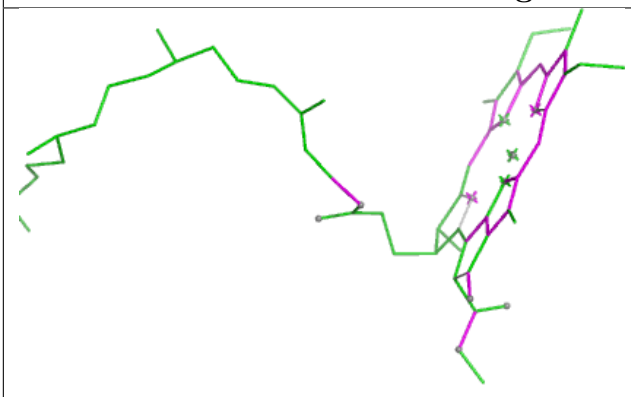


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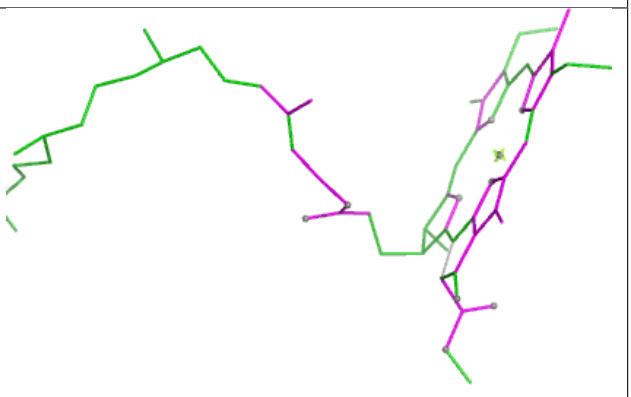


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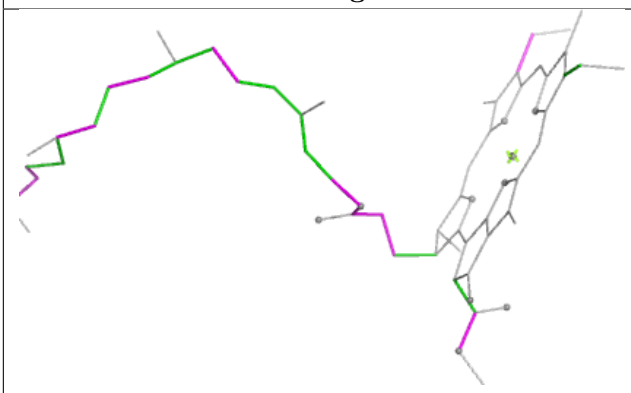
Ligand CLA B 1238



Bond lengths



Bond angles

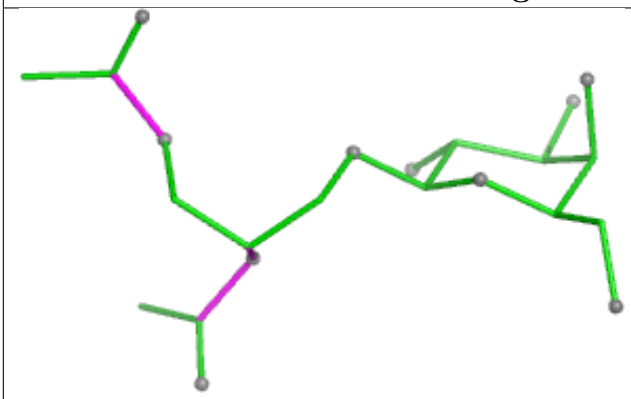


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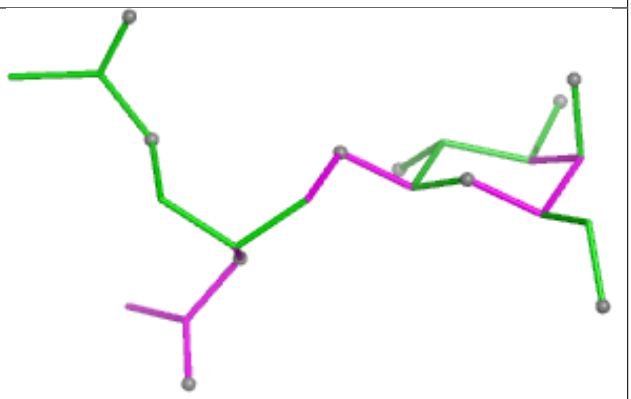


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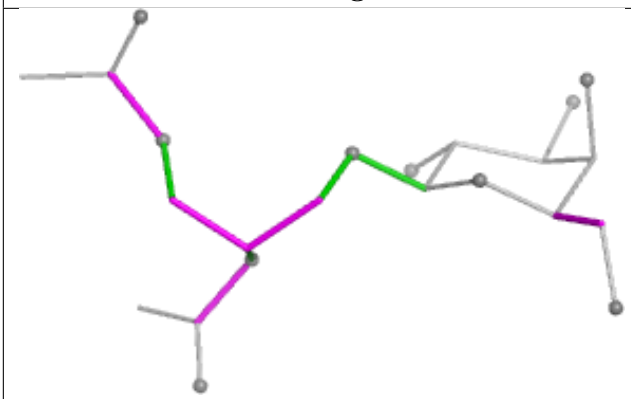
Ligand LMG F 5001



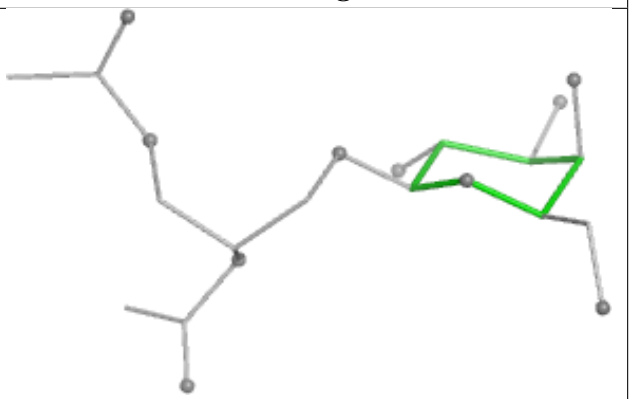
Bond lengths



Bond angles

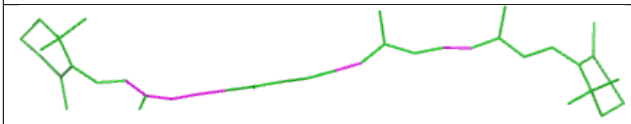


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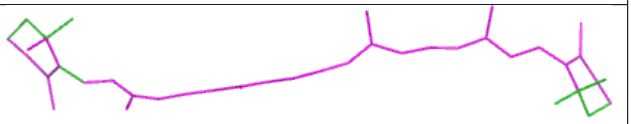


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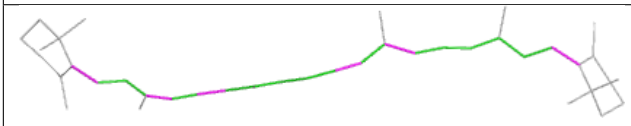
Ligand BCR A 6008



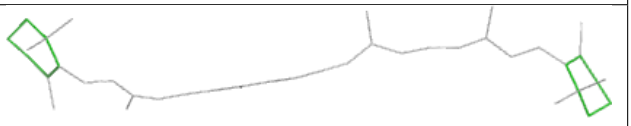
Bond lengths



Bond angles

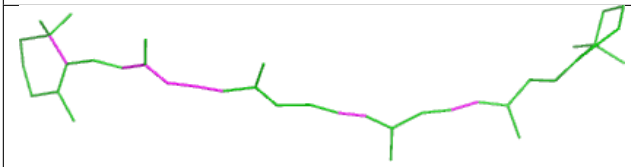


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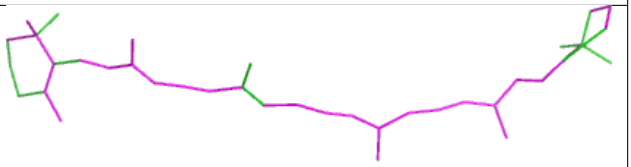


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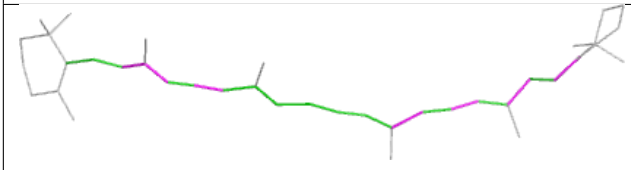
Ligand BCR F 6014



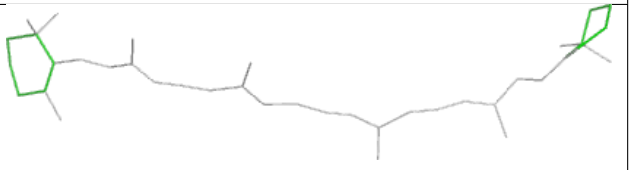
Bond lengths



Bond angles

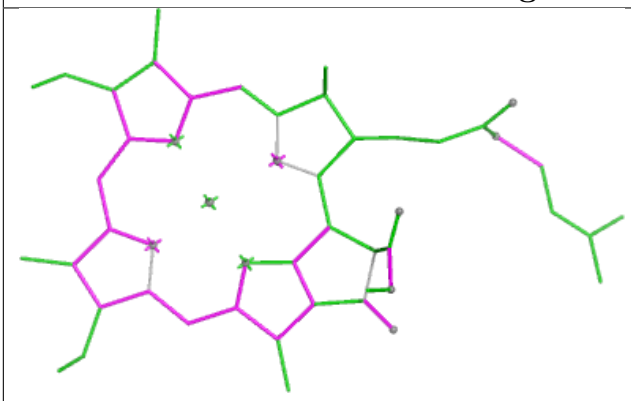


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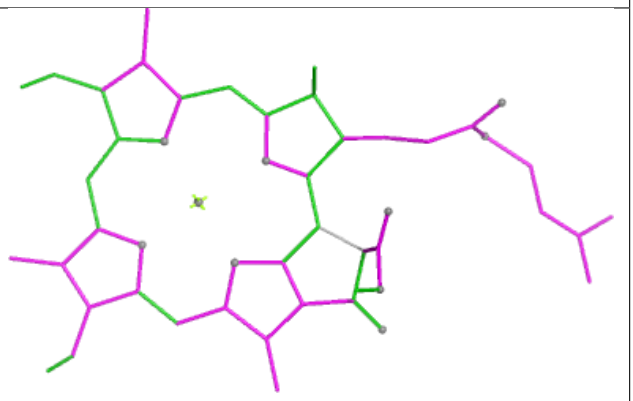


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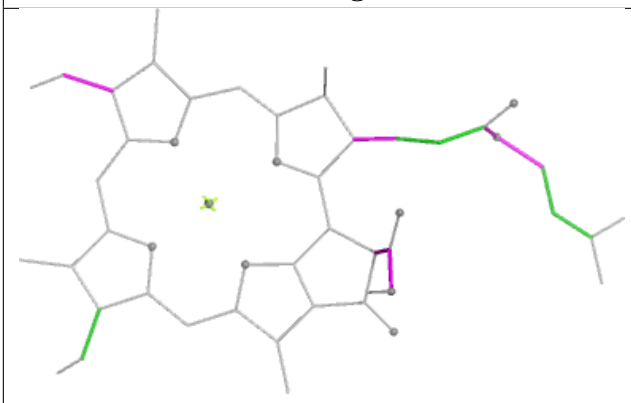
Ligand CLA J 1302



Bond lengths



Bond angles

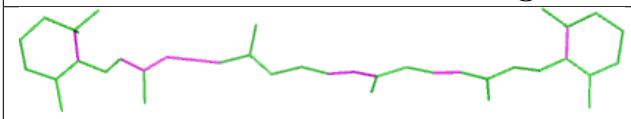


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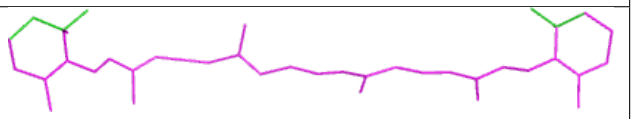


Rings

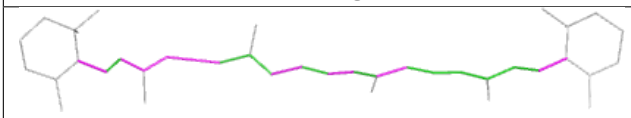
Ligand BCR 3 3503



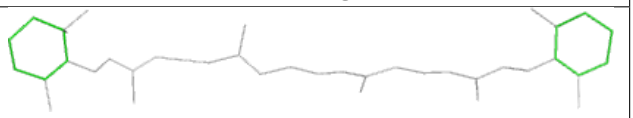
Bond lengths



Bond angles

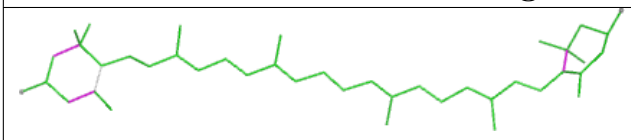


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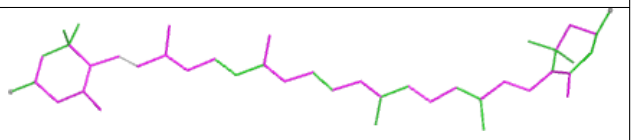


Rings

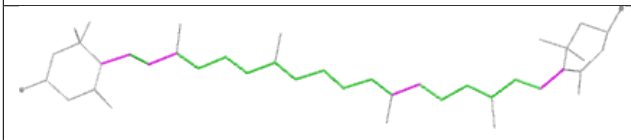
Ligand LUT 4 4502



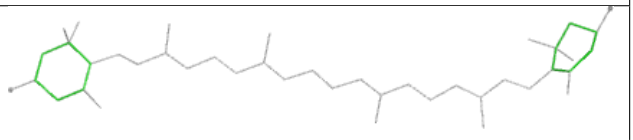
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Bond angles

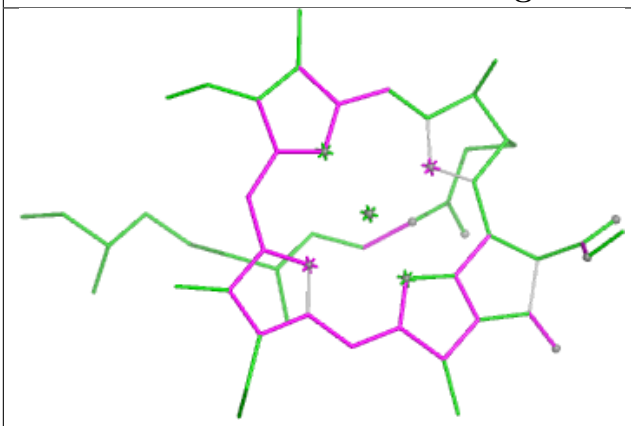


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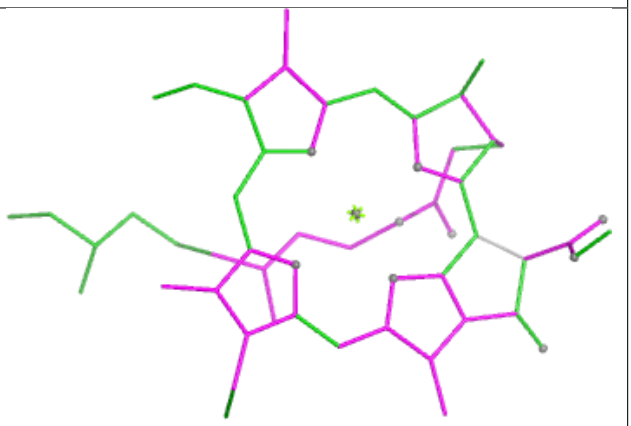


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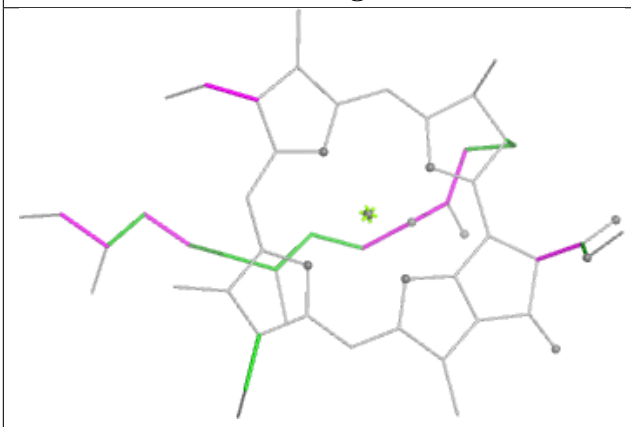
Ligand CLA A 1136



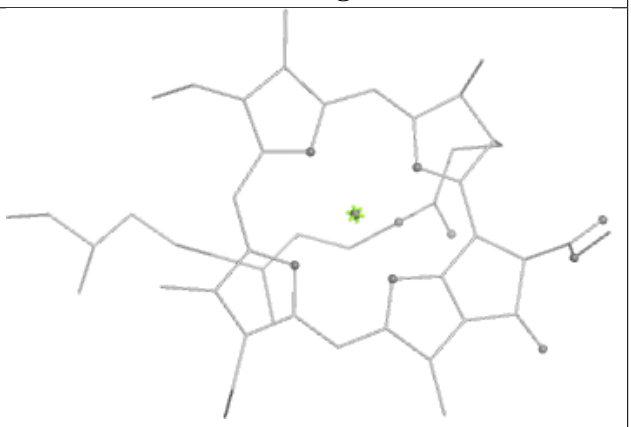
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Bond angles

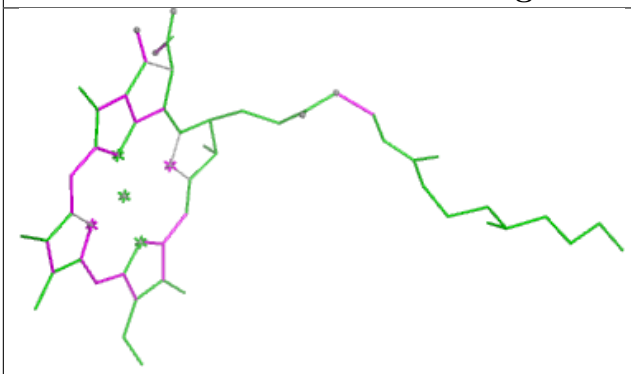


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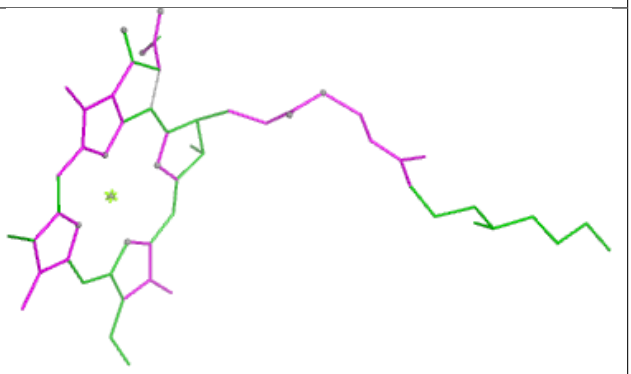


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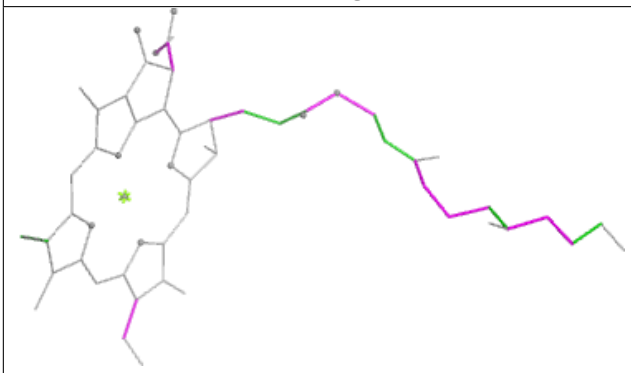
Ligand CLA B 1230



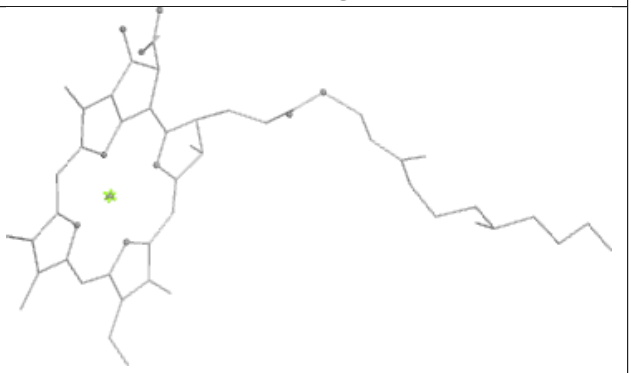
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Bond angles

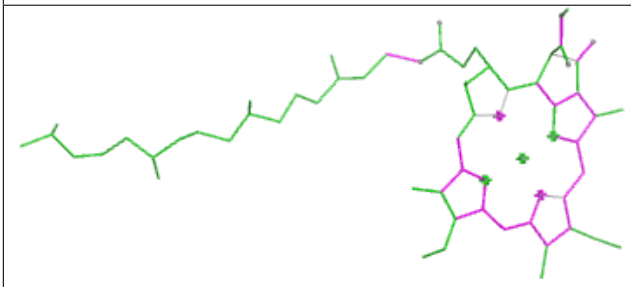


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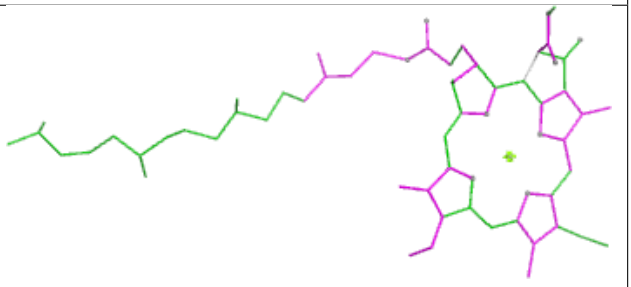


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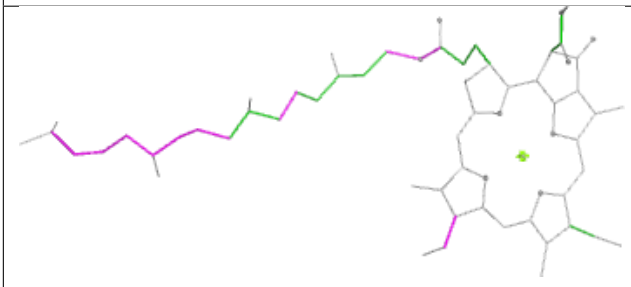
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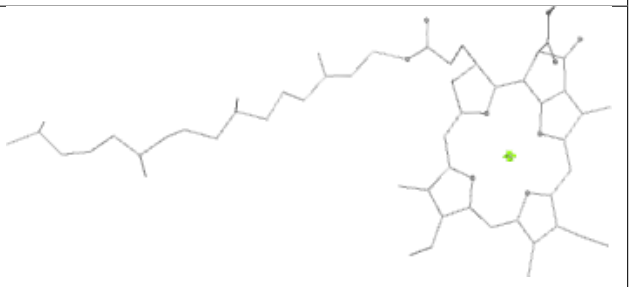
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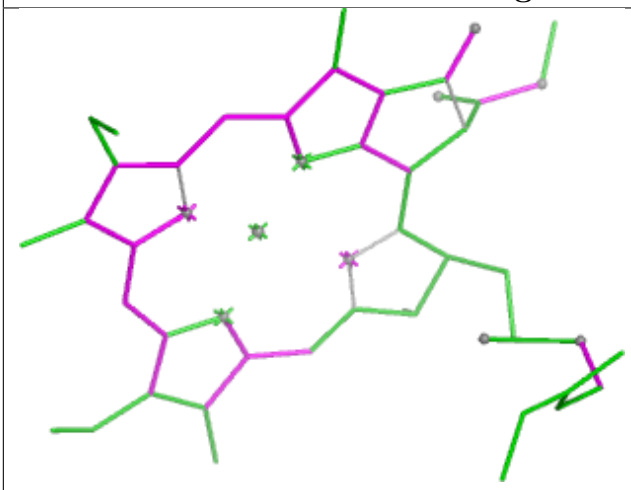


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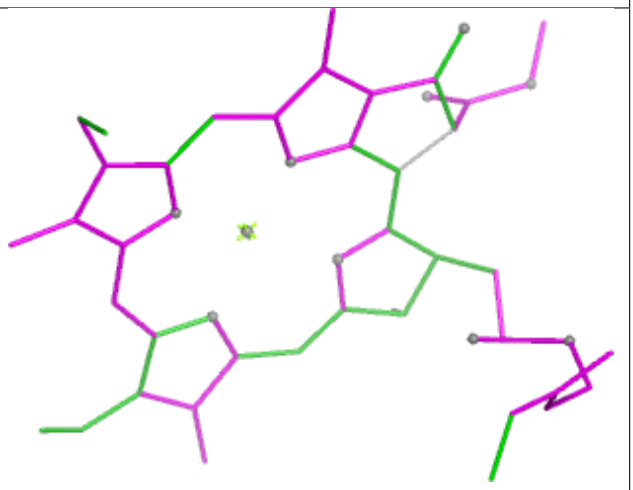


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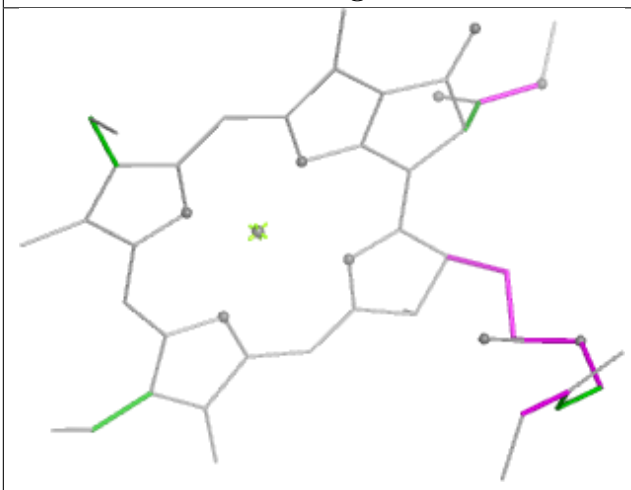
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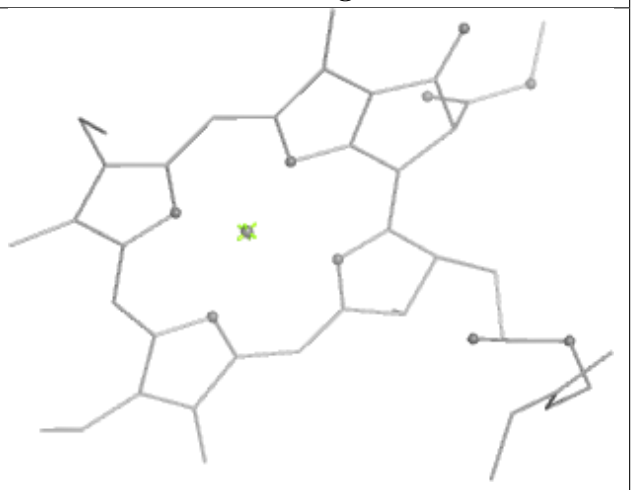
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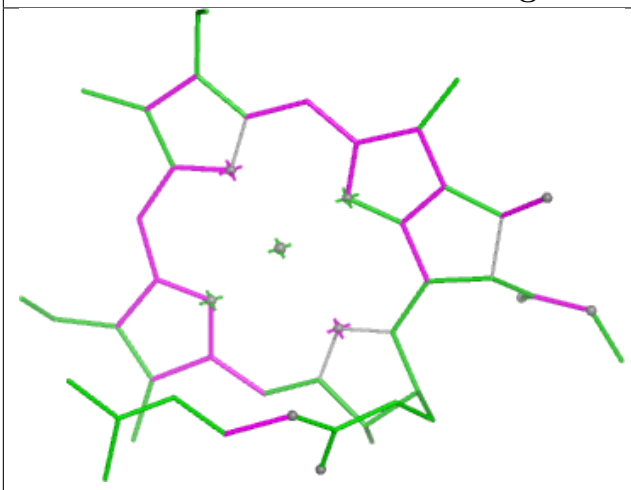


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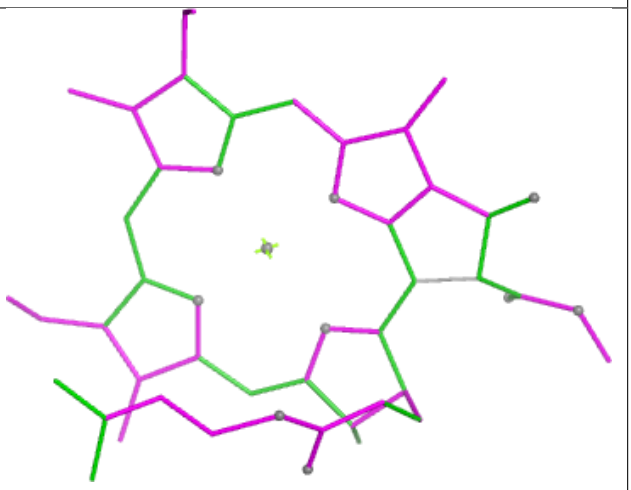


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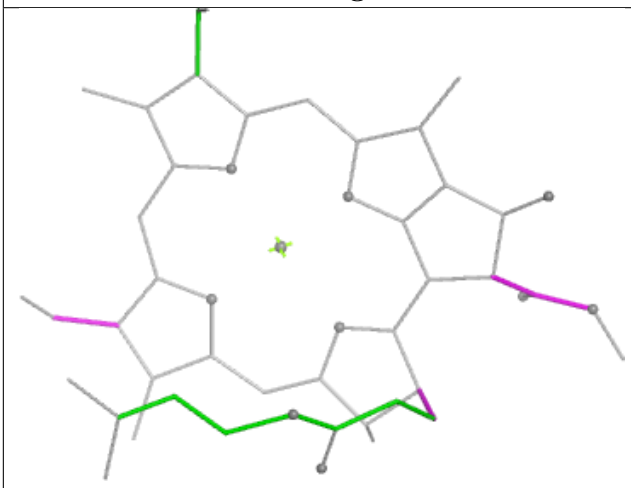
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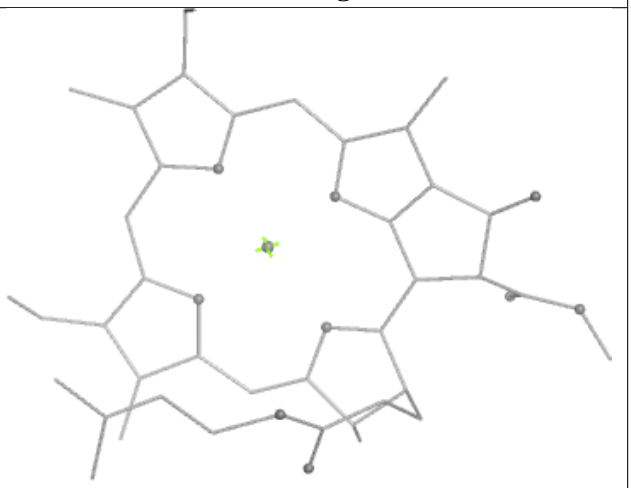
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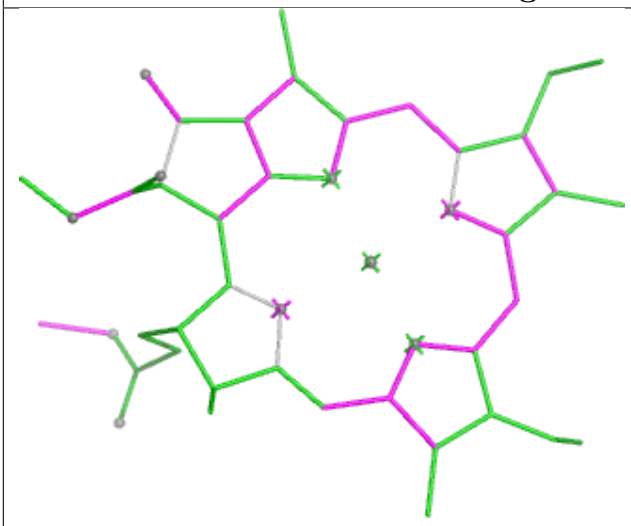


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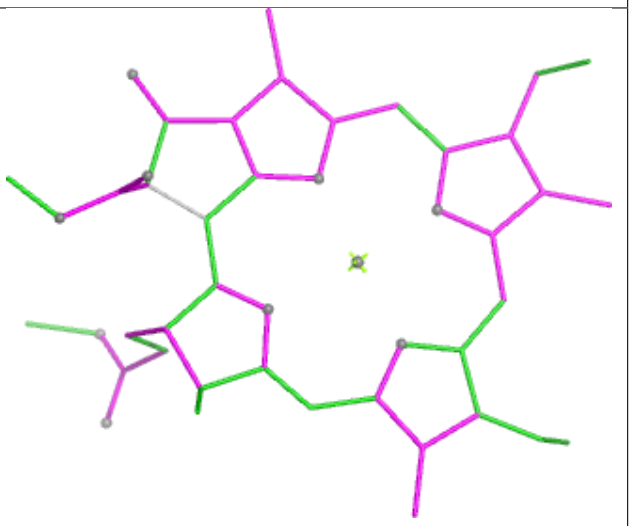


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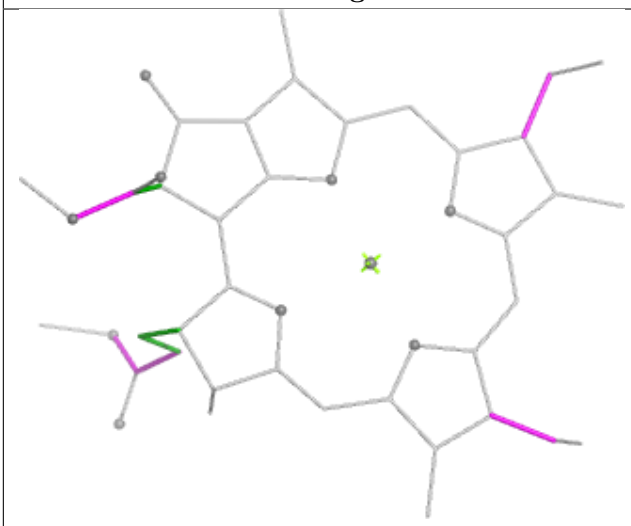
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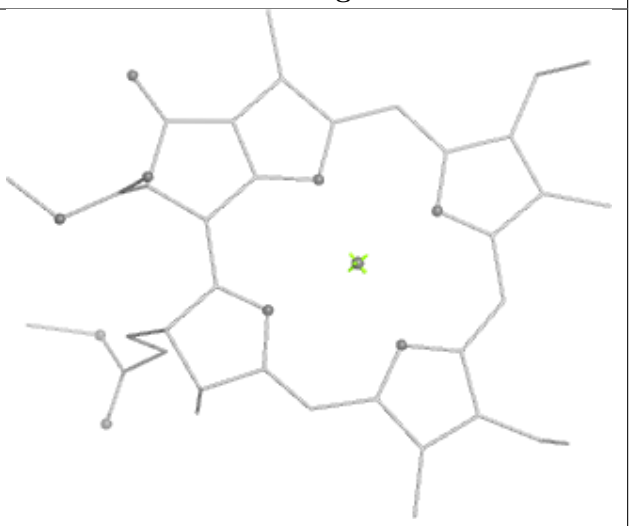
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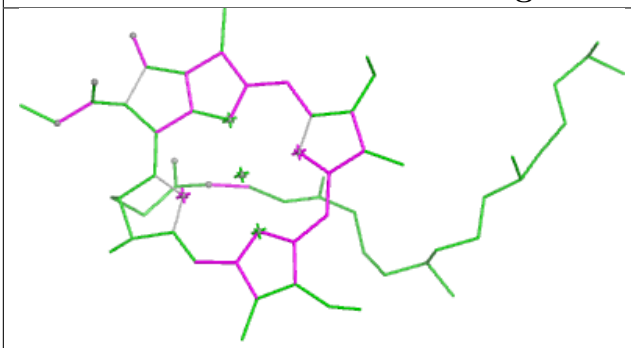


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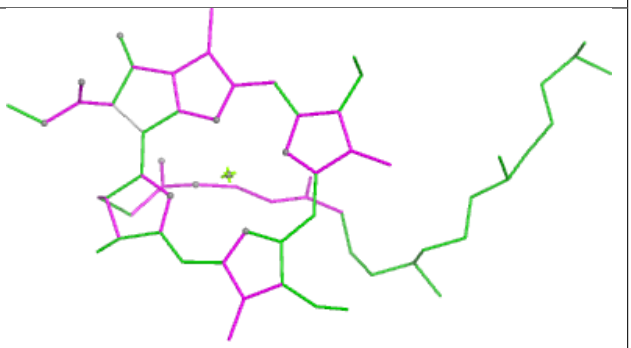


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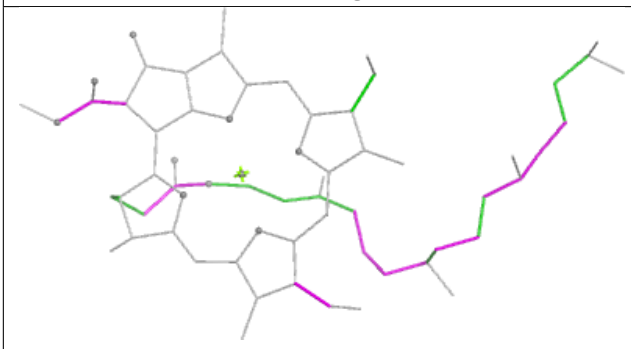
Ligand CLA B 1235



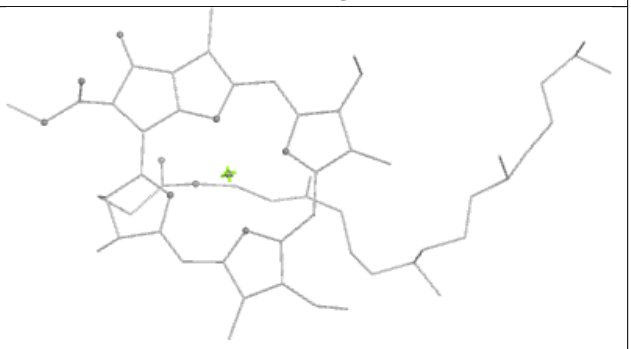
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Bond angles

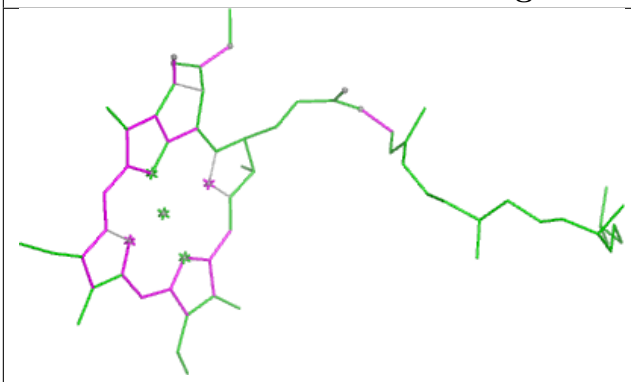


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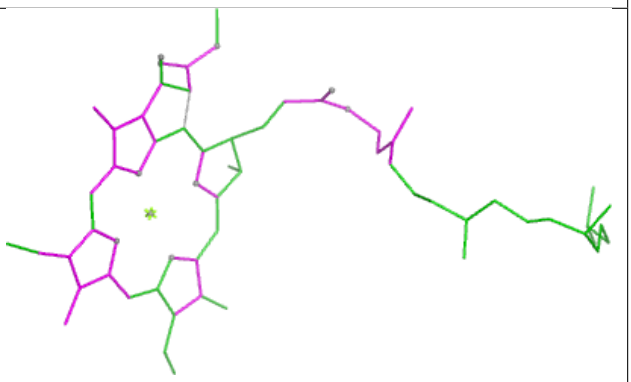


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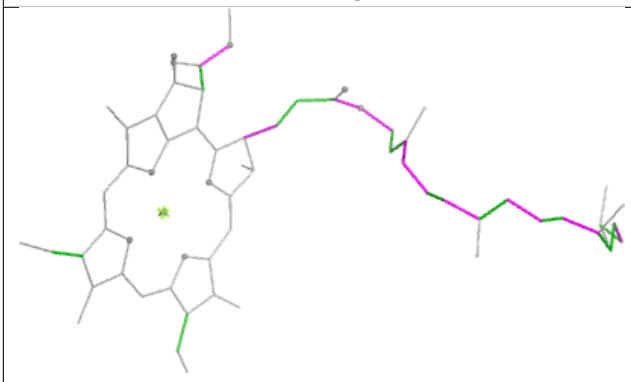
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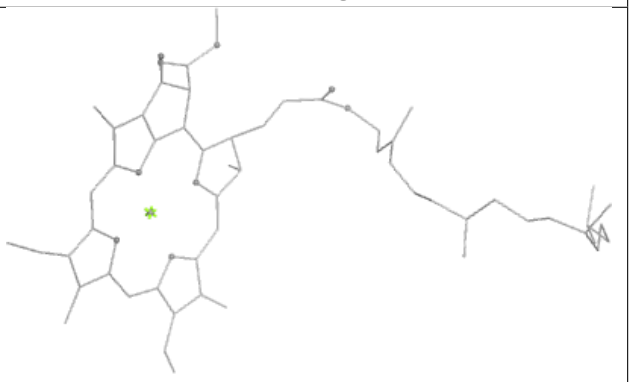
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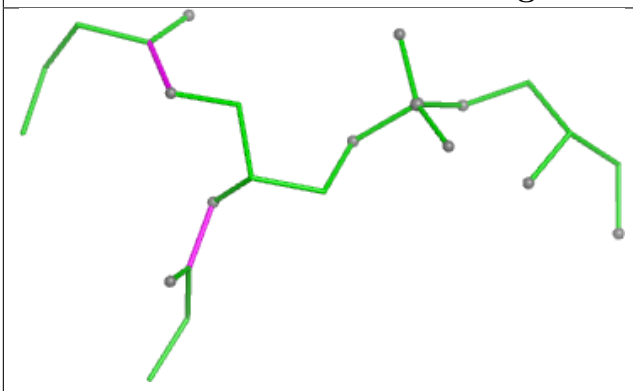


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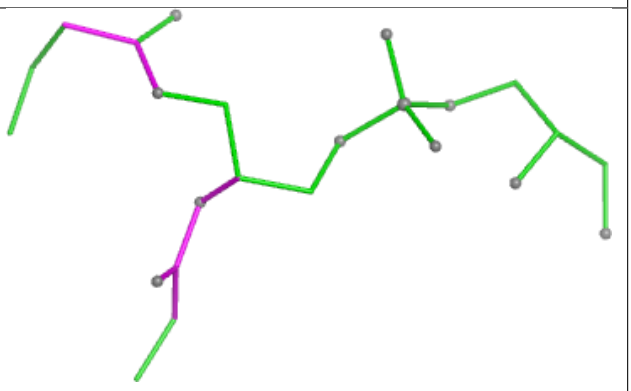


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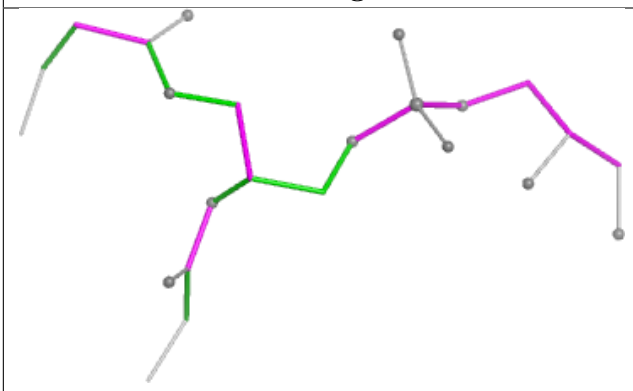
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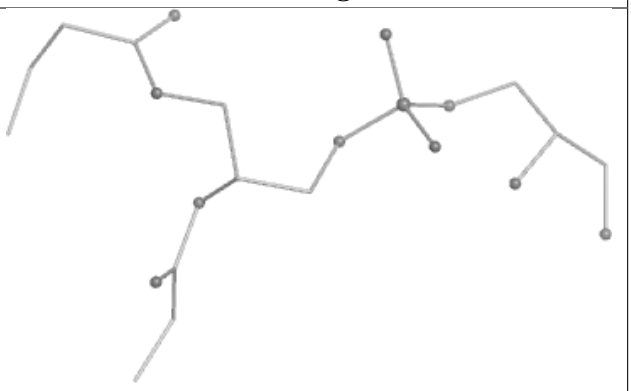
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Bond angles

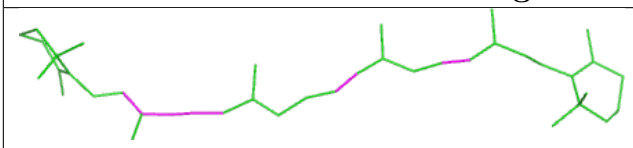


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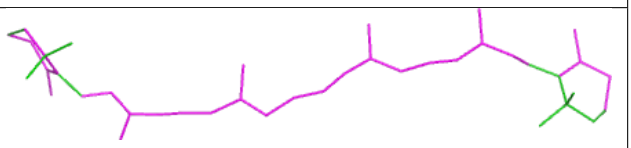


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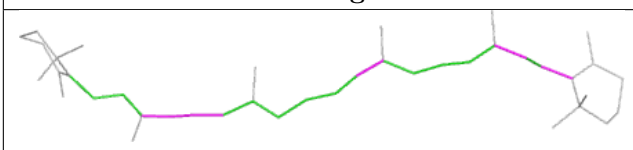
Ligand BCR A 6017



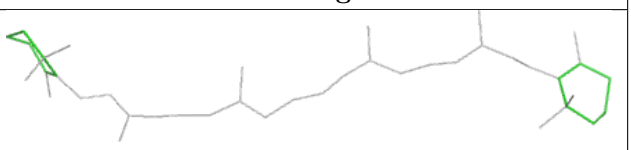
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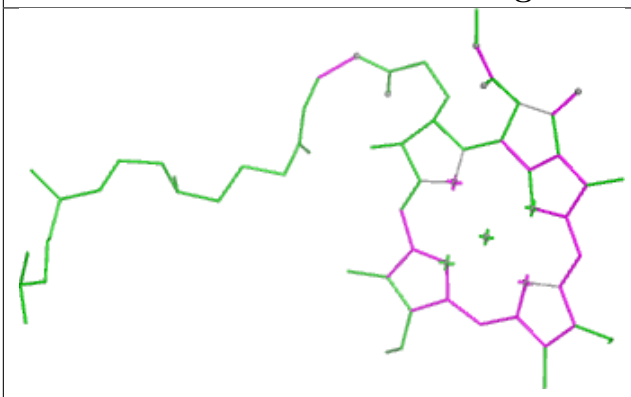


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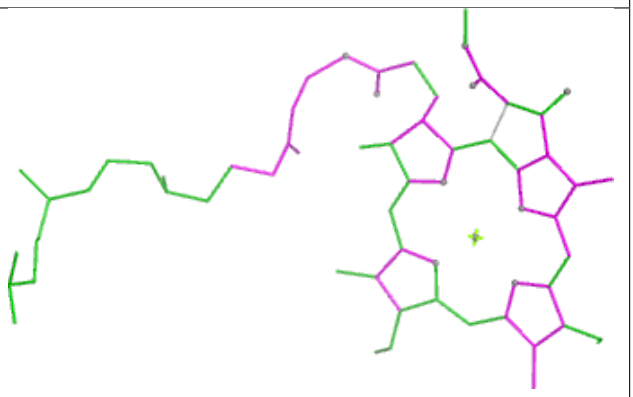


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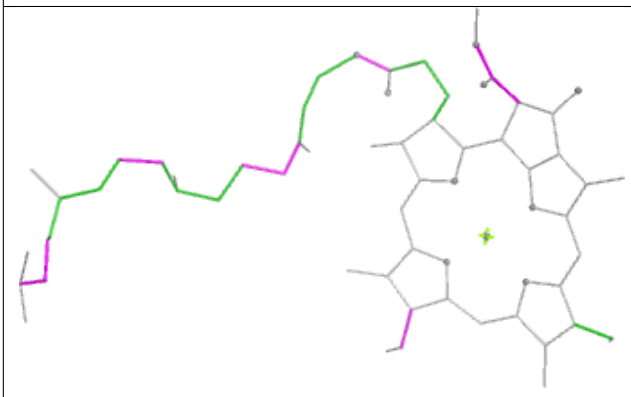
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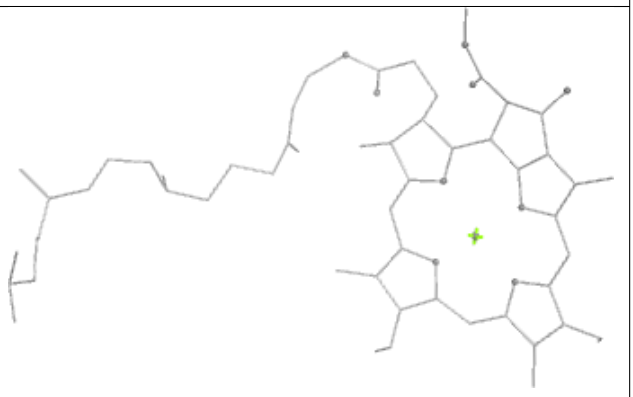
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Bond angles

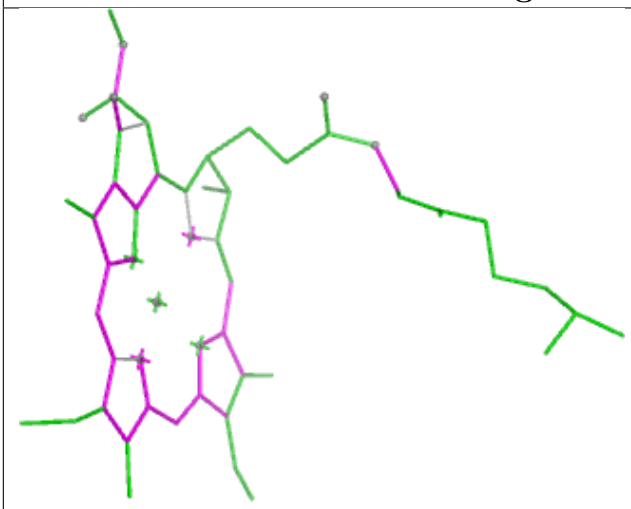


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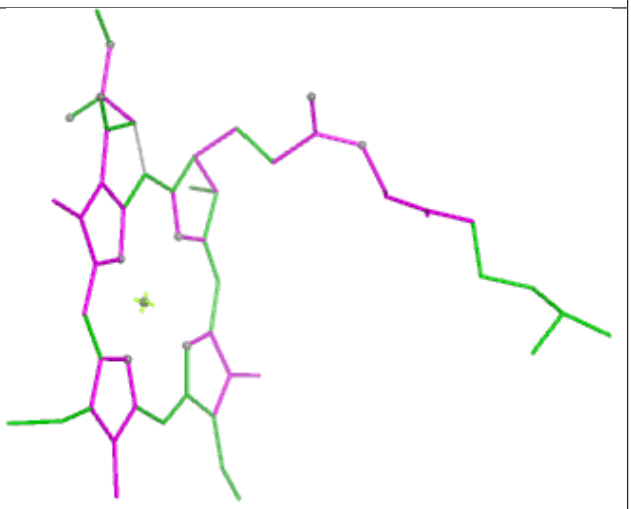


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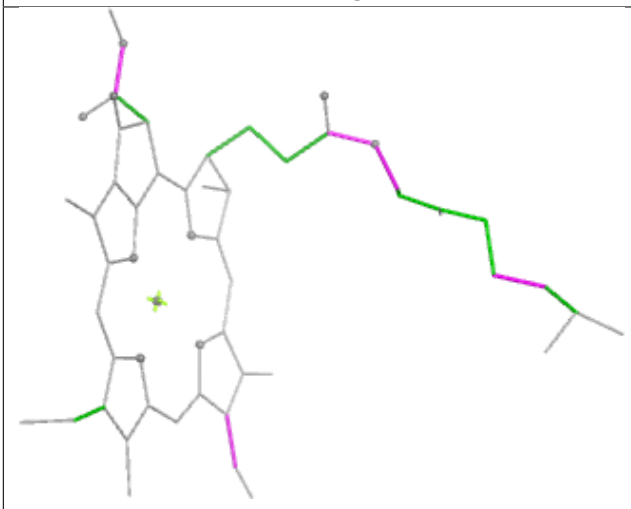
Ligand CLA B 1232



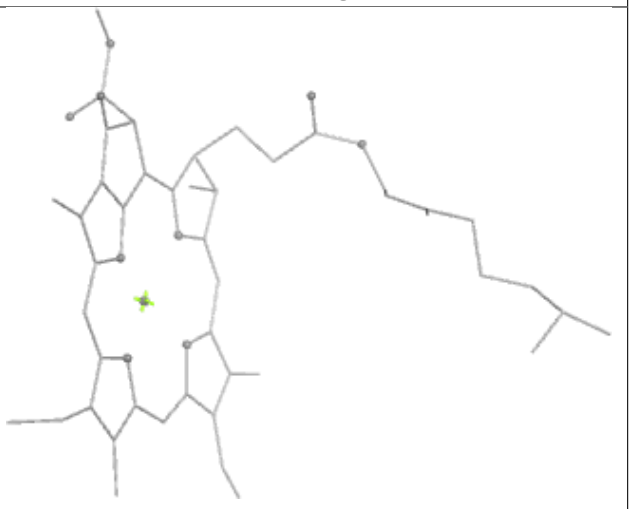
Bond lengths



Bond angles

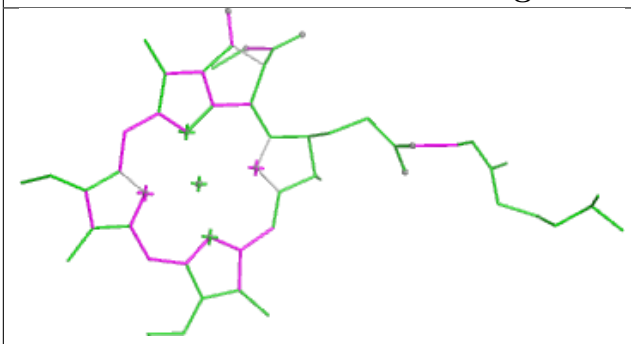


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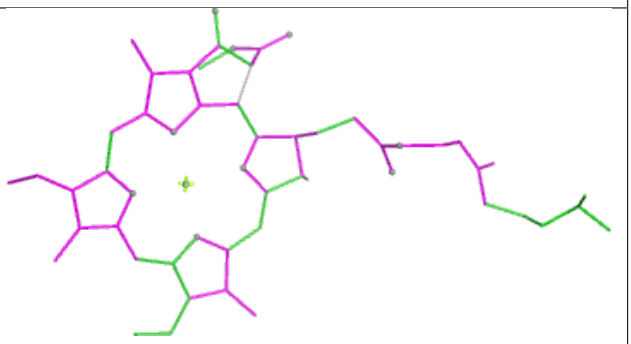


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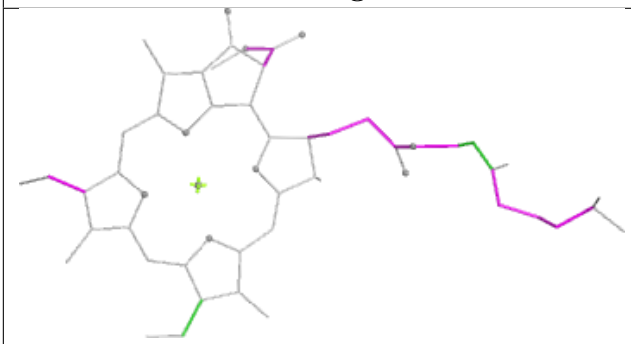
Ligand CLA G 1001



Bond lengths



Bond angles

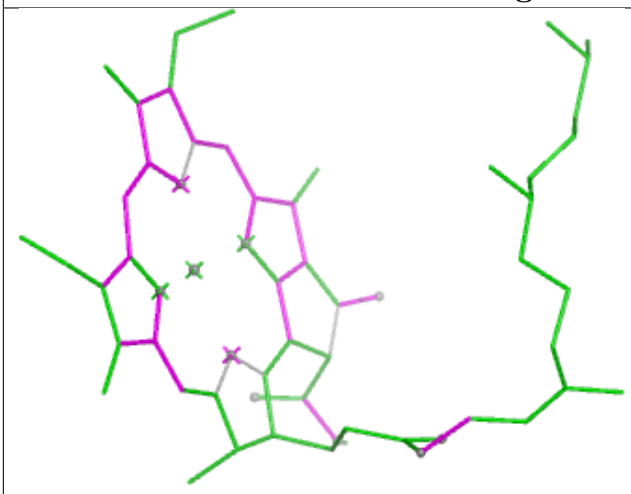


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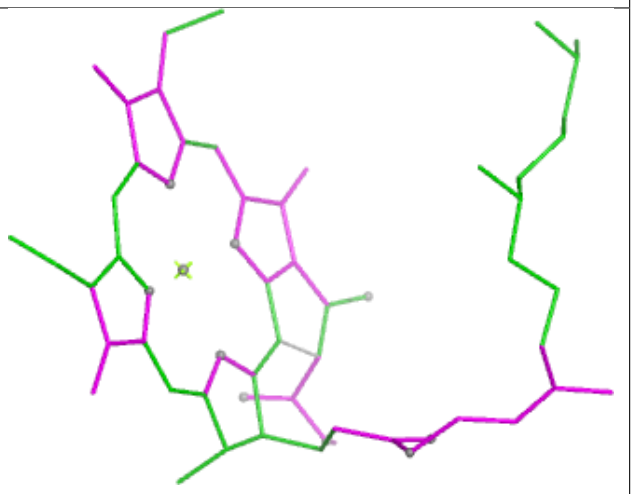


Rings

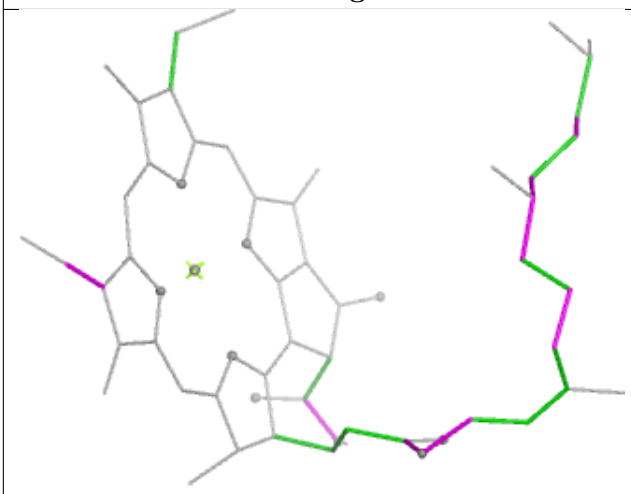
Ligand CLA B 1231



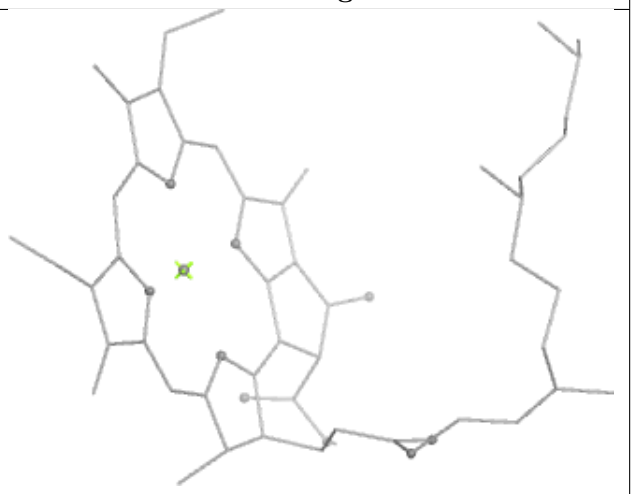
Bond lengths



Bond angles

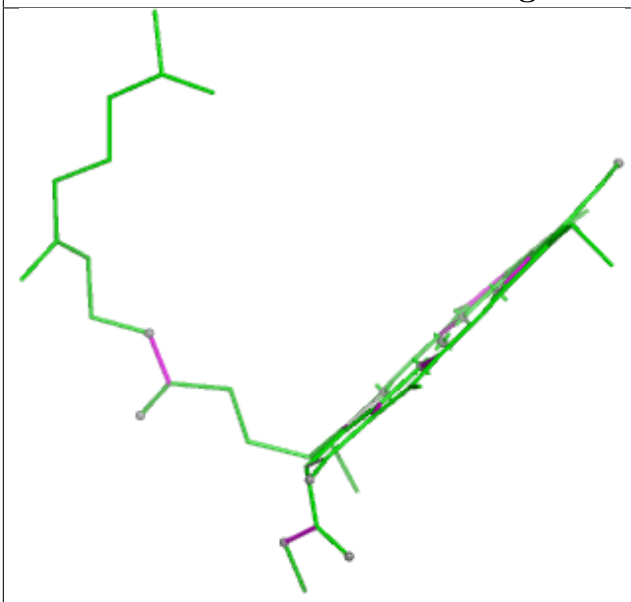


Torsions

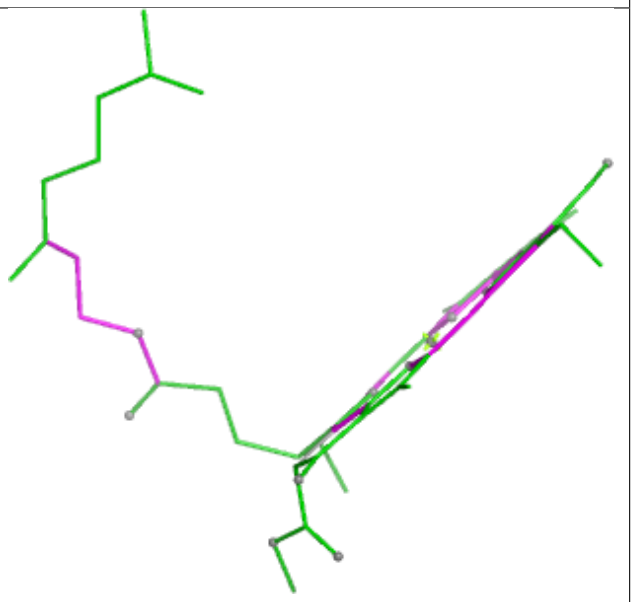


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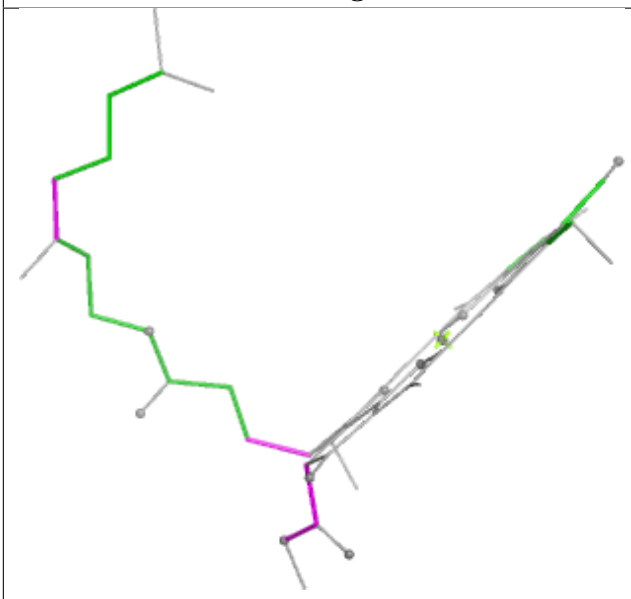
Ligand CHL 1 1009



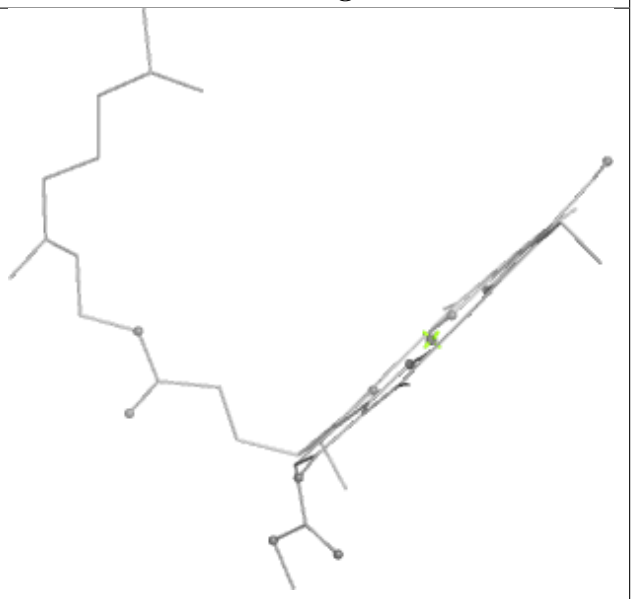
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Bond angles

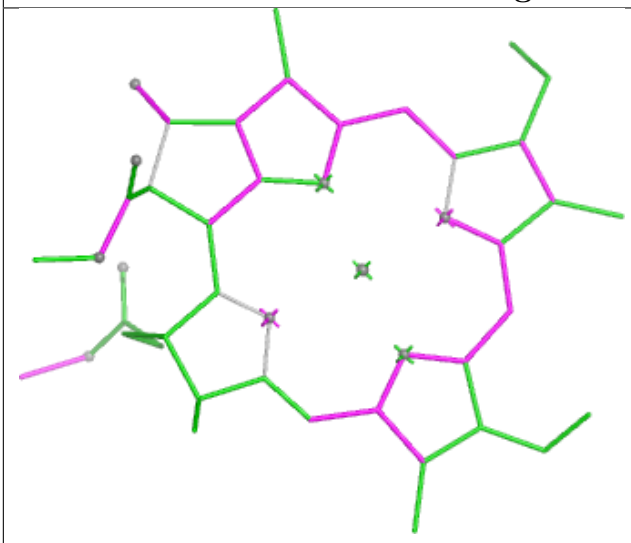


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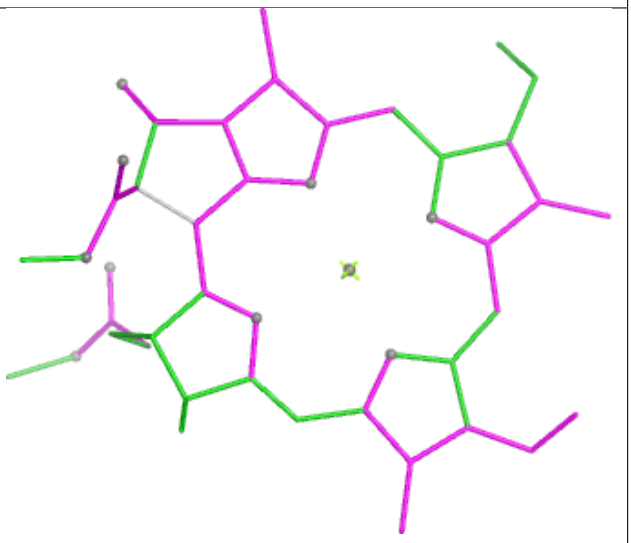


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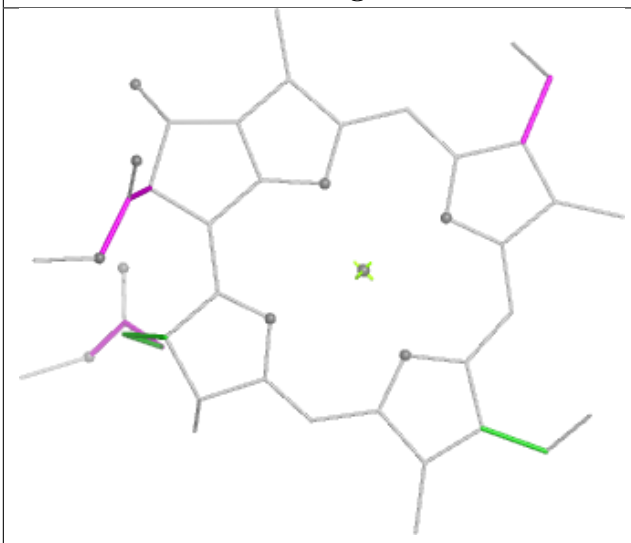
Ligand CLA K 1001



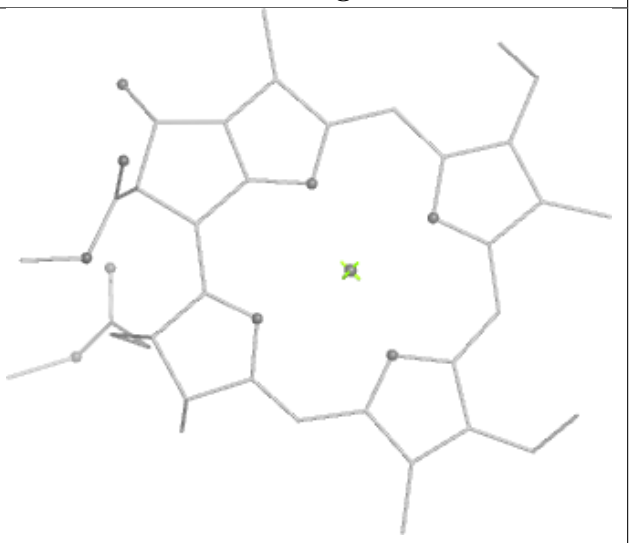
Bond lengths



Bond angles

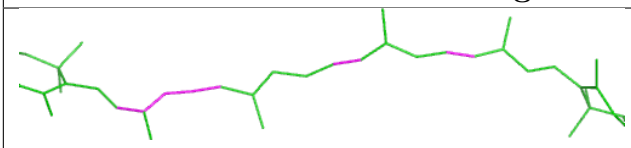


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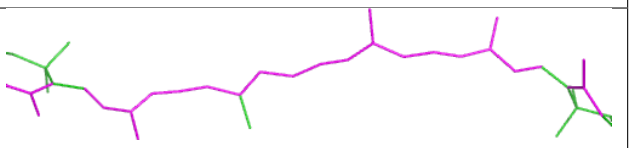


Rings

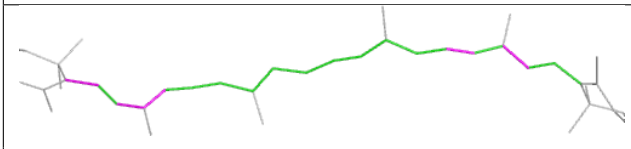
Ligand BCR B 6009



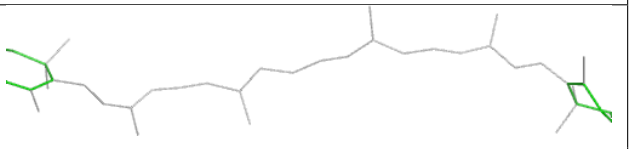
Bond lengths



Bond angles

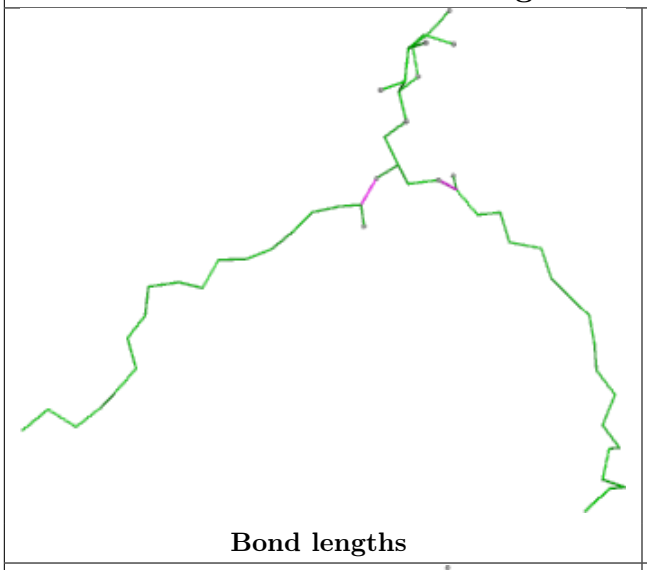


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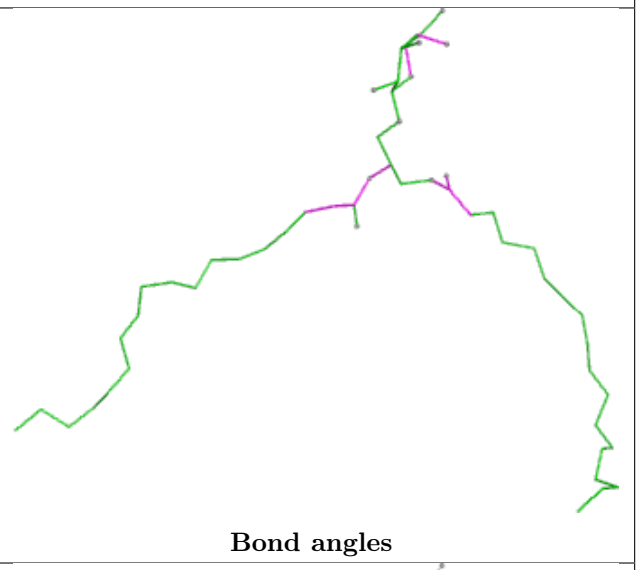


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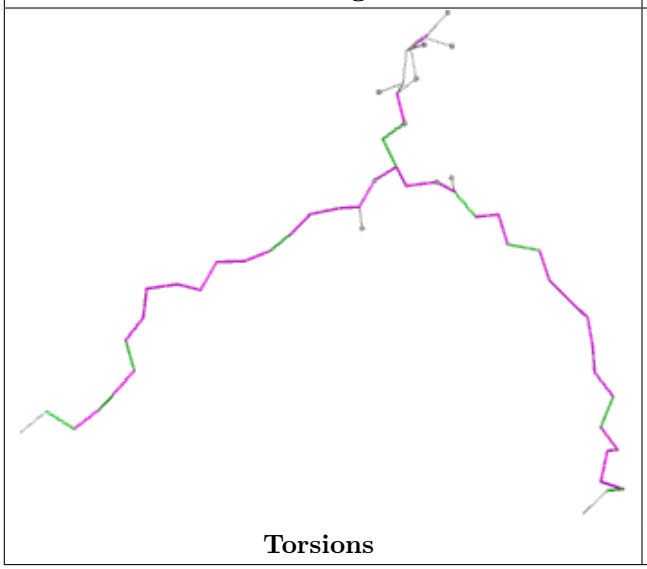
Ligand LMG J 5001



Bond lengths



Bond angles

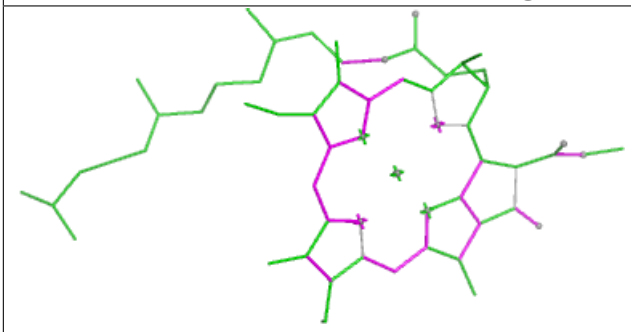


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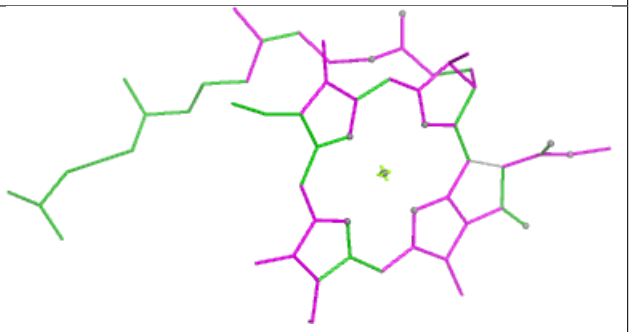


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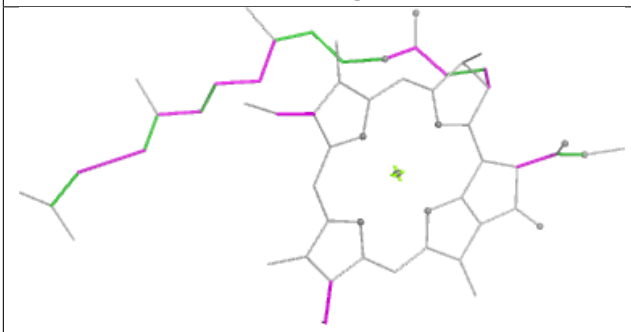
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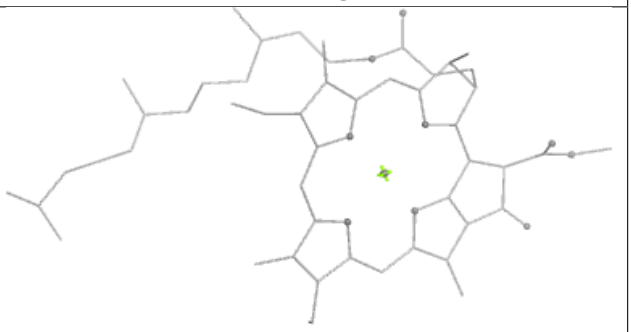
Bond lengths



Bond angles



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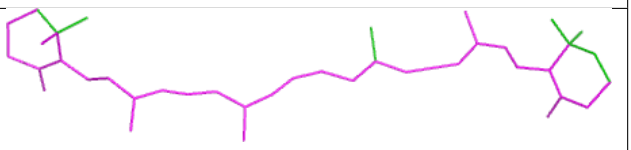


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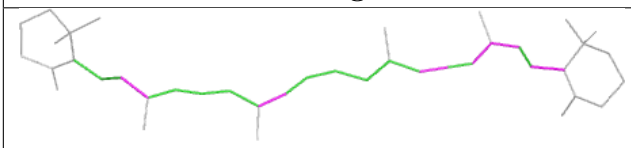
Ligand BCR G 2011



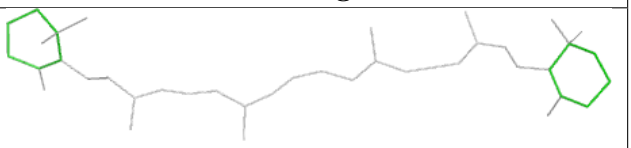
Bond lengths



Bond angles

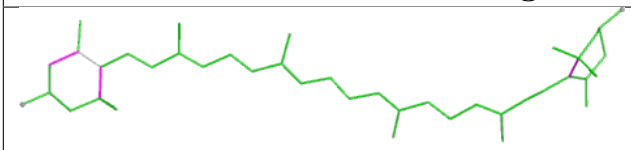


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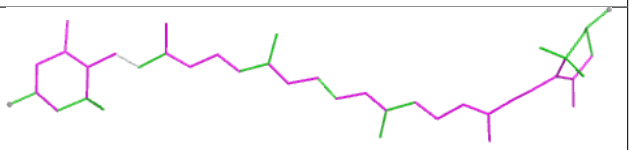


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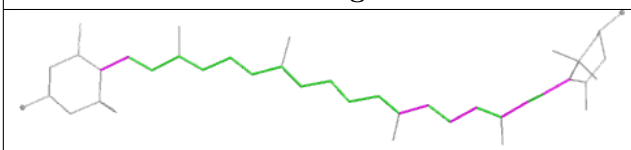
Ligand LUT 3 3502



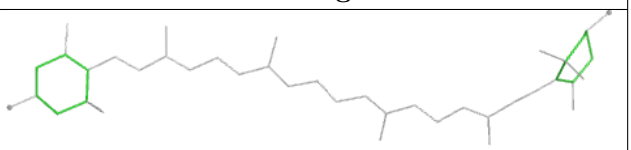
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Bond angles

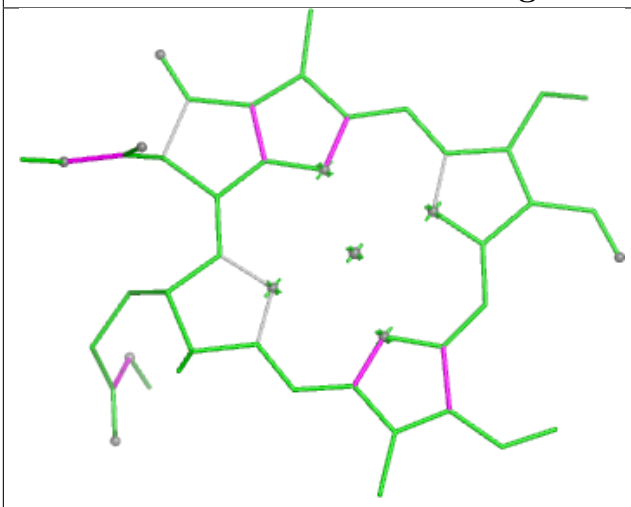


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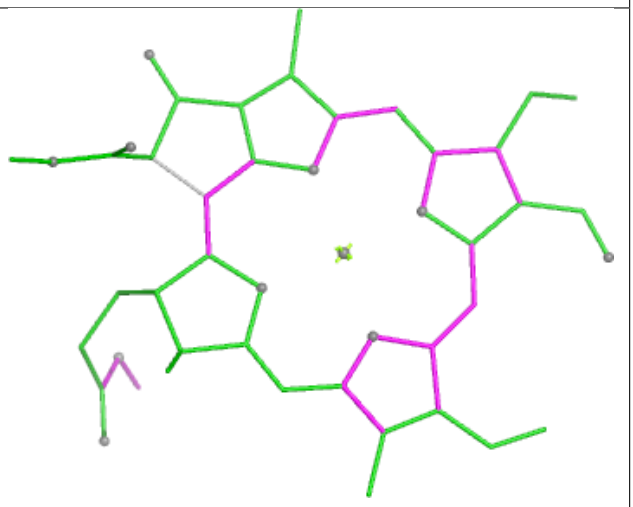


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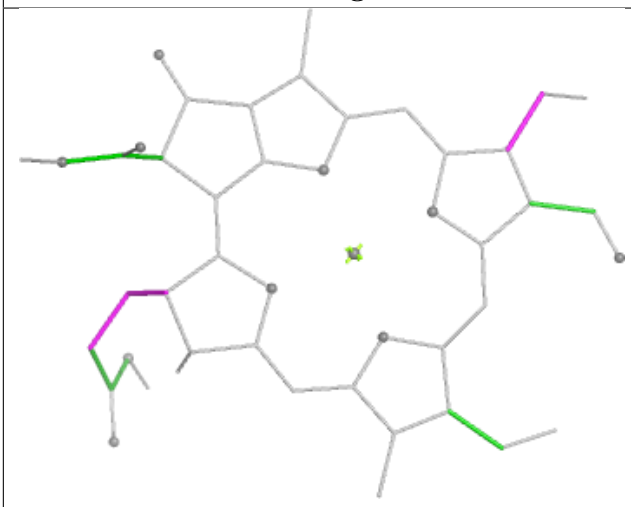
Ligand CHL 1 1010



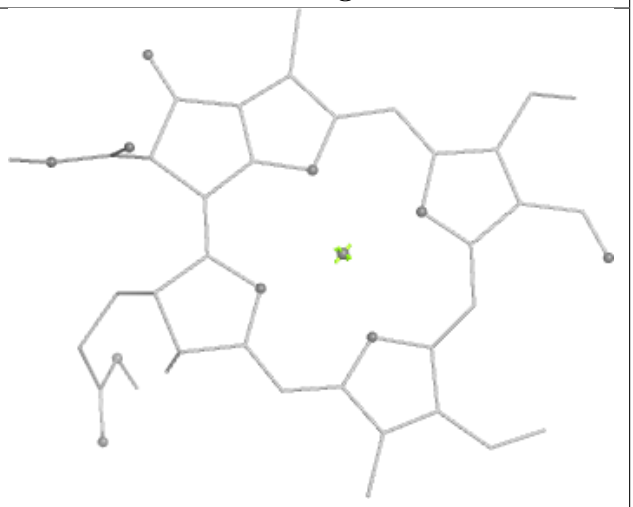
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Bond angles

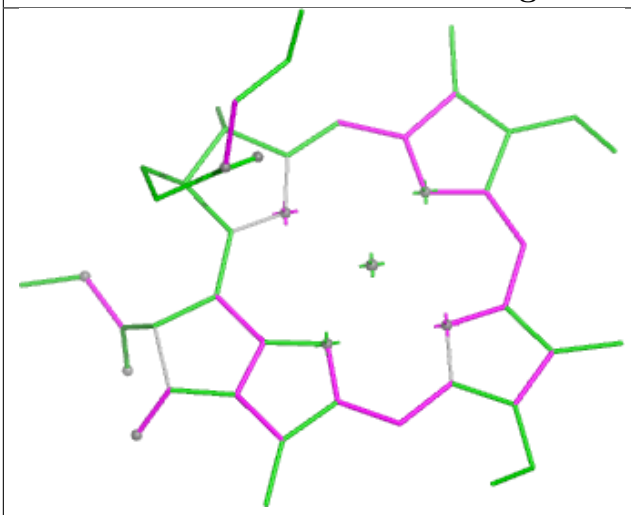


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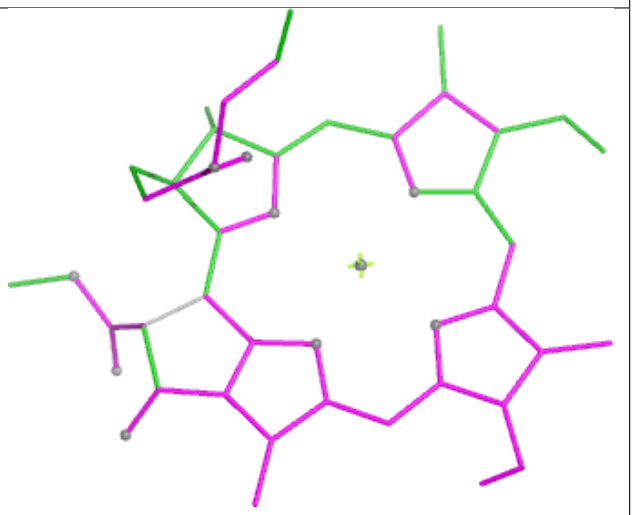


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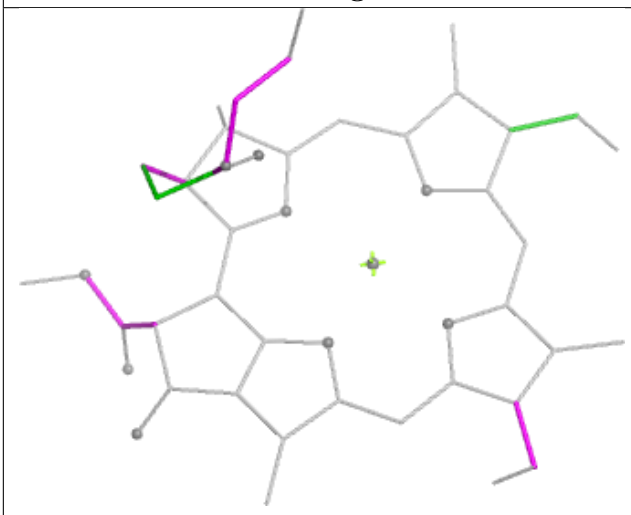
Ligand CLA 3 3008



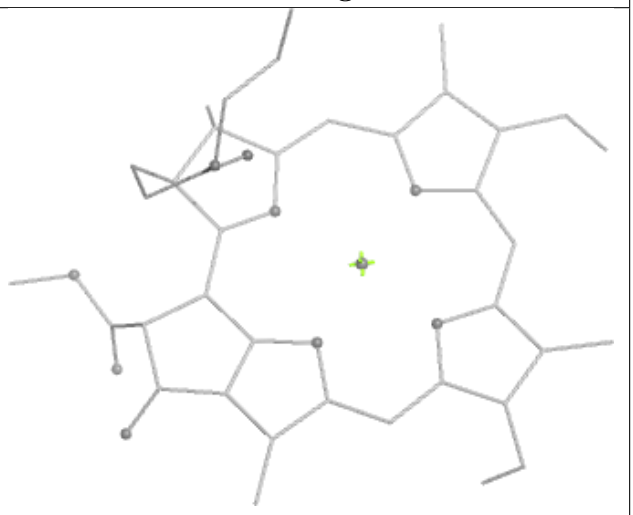
Bond lengths



Bond angles

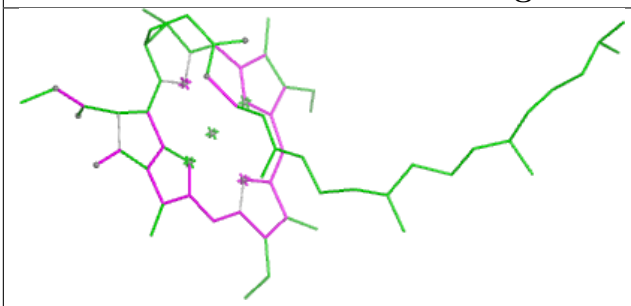


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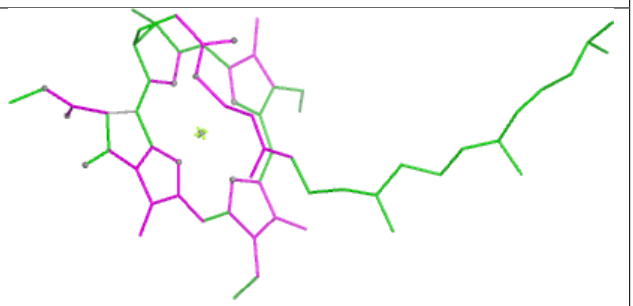


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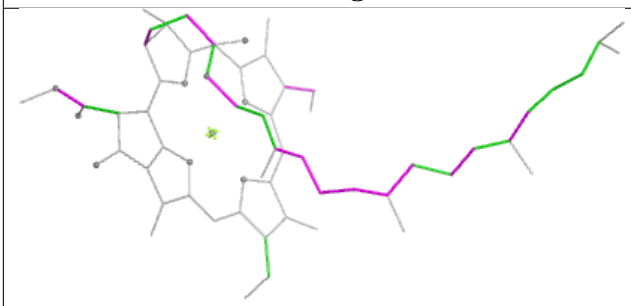
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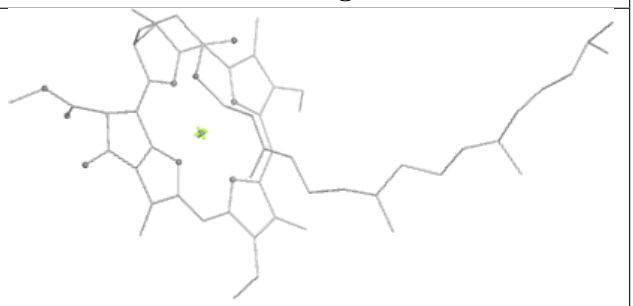
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Bond angles

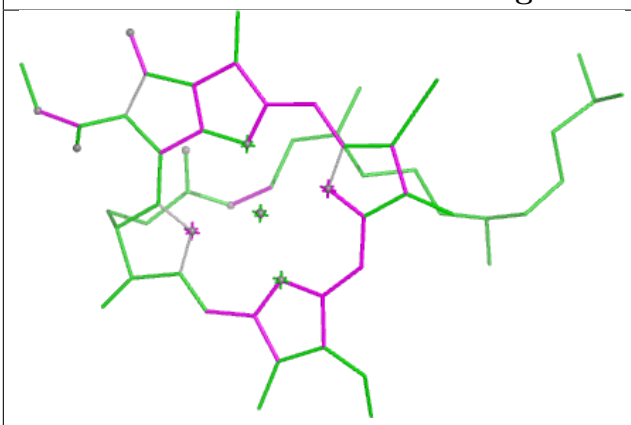


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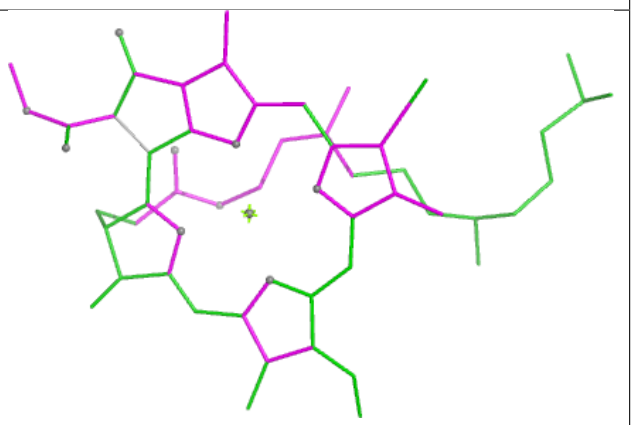


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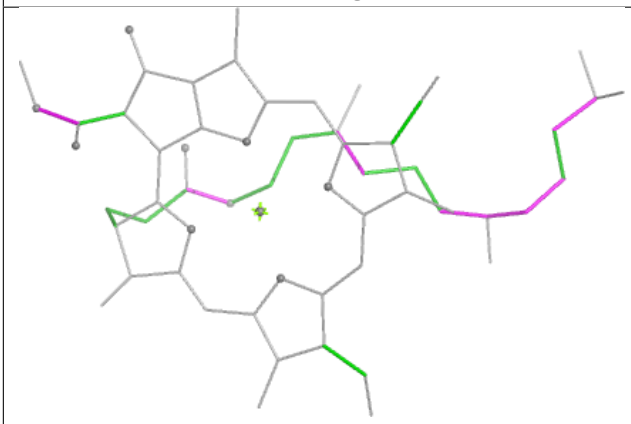
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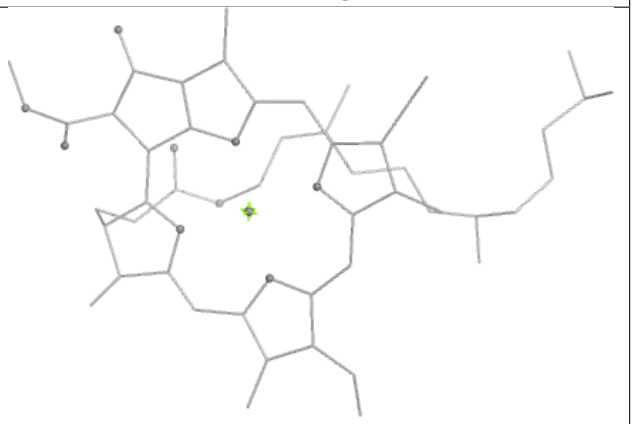
Bond lengths



Bond angles

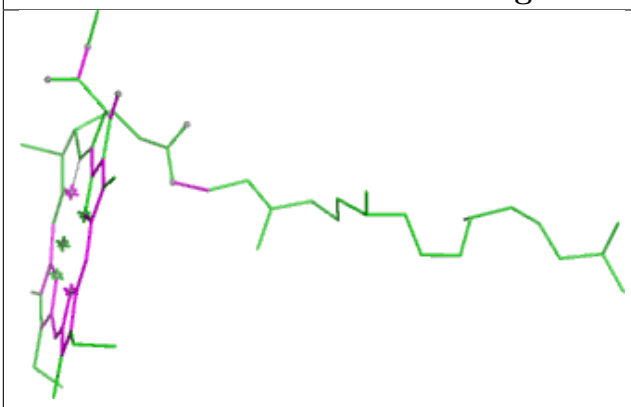


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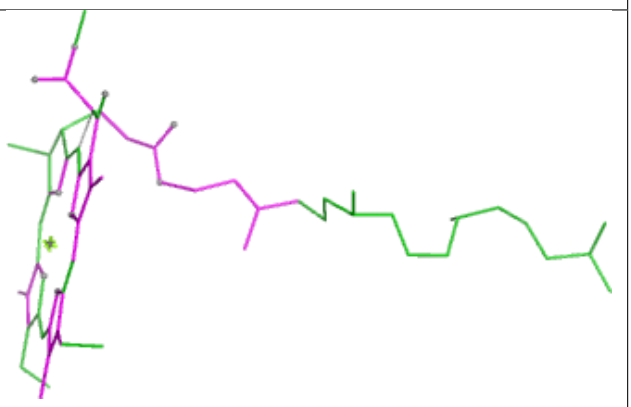


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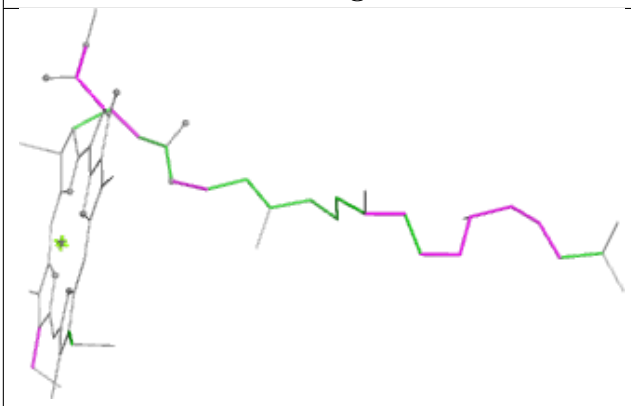
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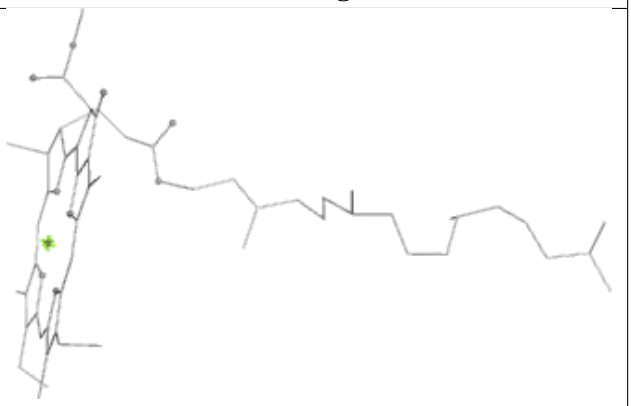
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Bond angles

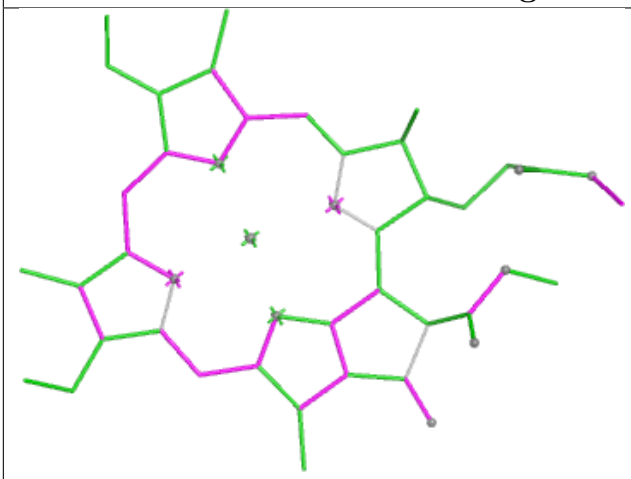


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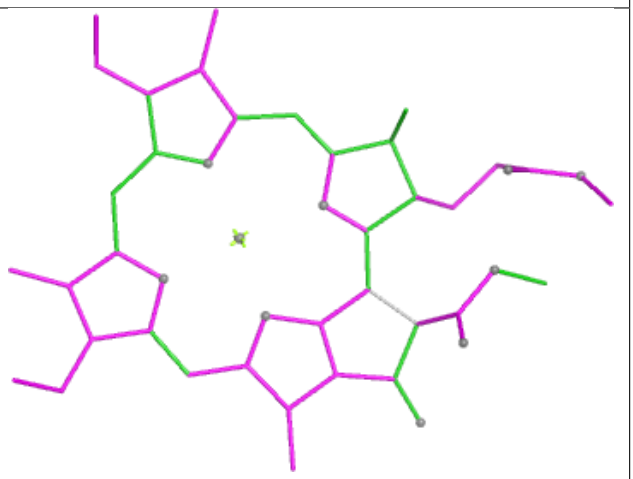


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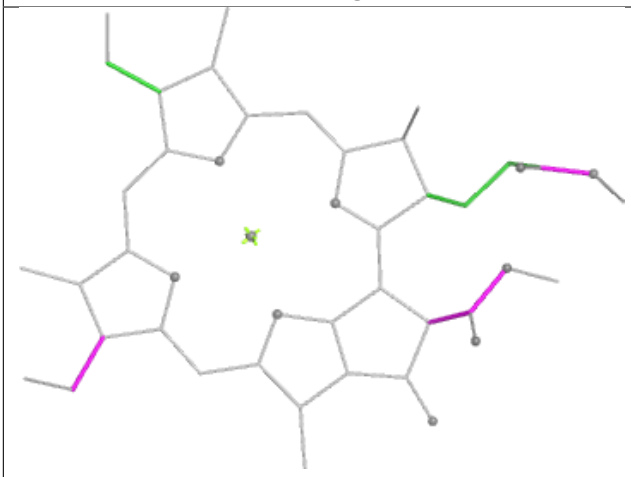
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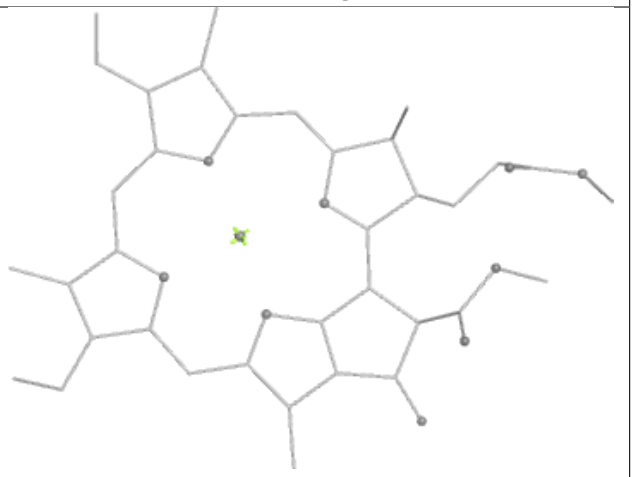
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Bond angles

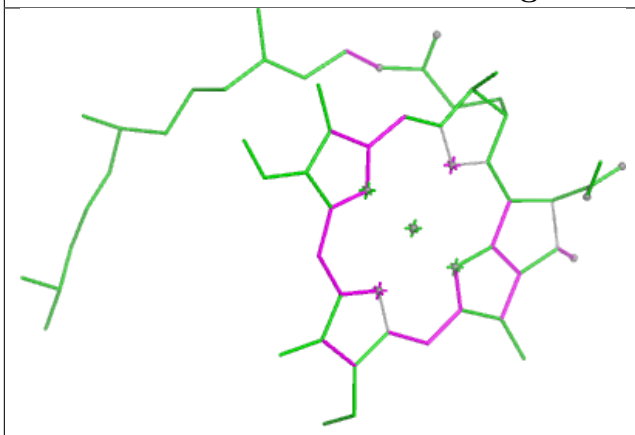


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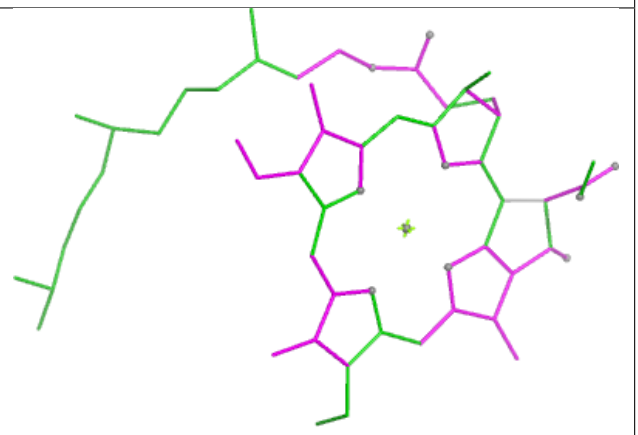


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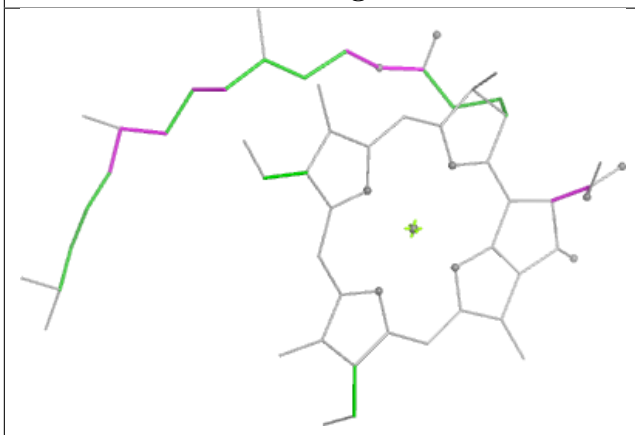
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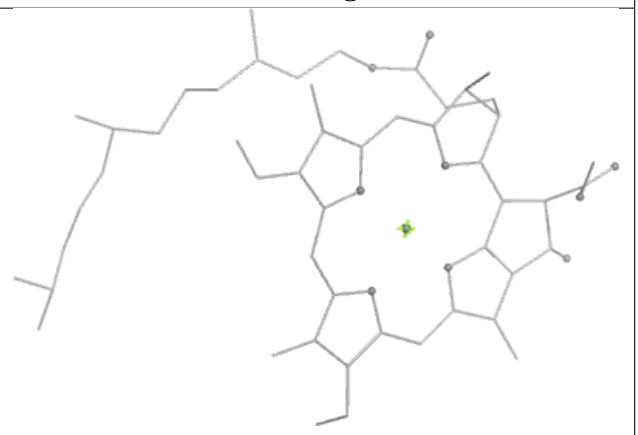
Bond lengths



Bond angles

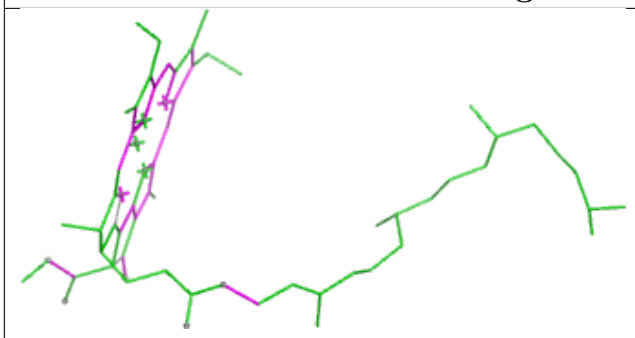


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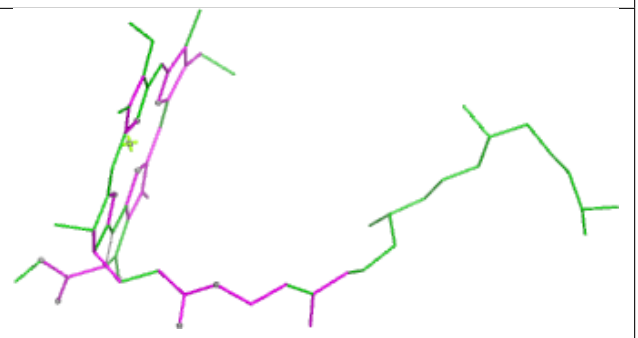


Rings

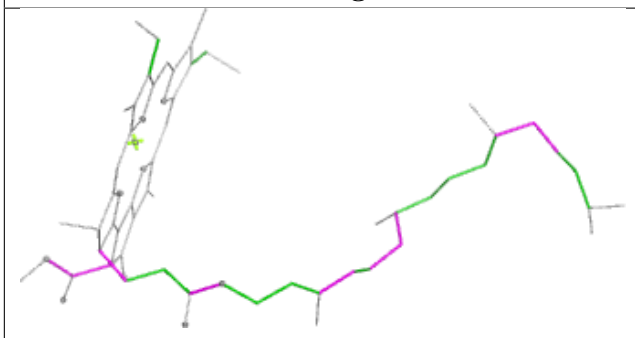
Ligand CLA A 1128



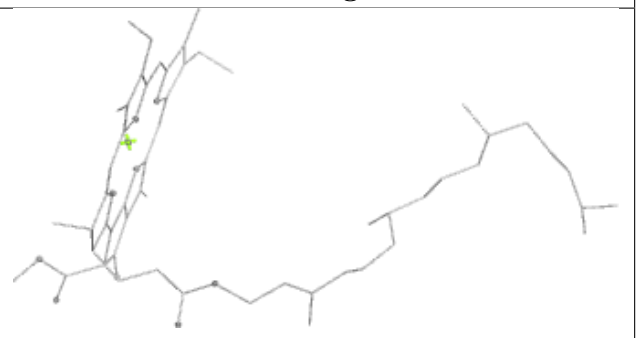
Bond lengths



Bond angles

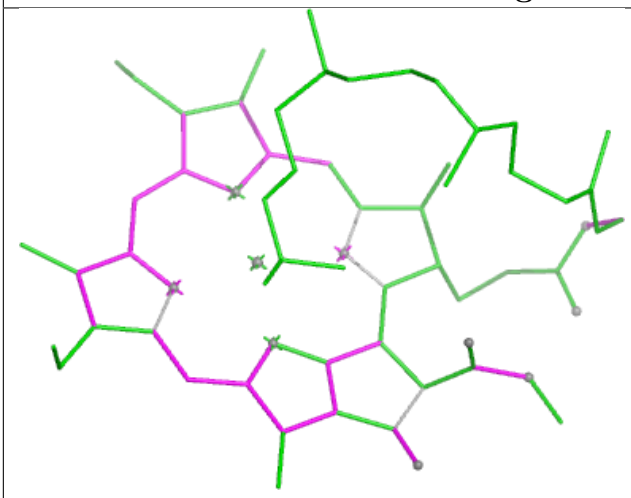


Torsions

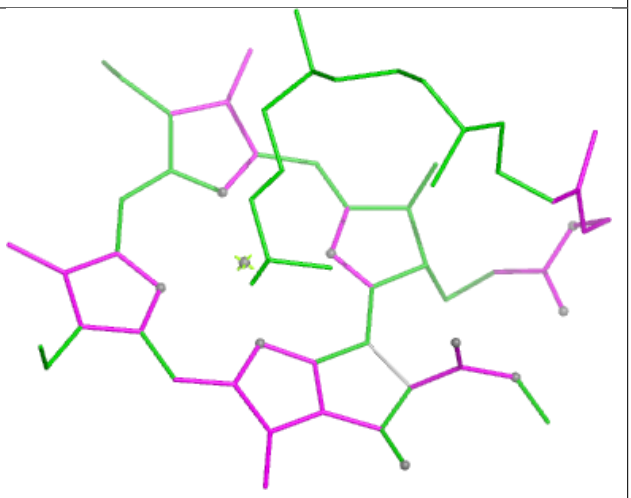


Rings

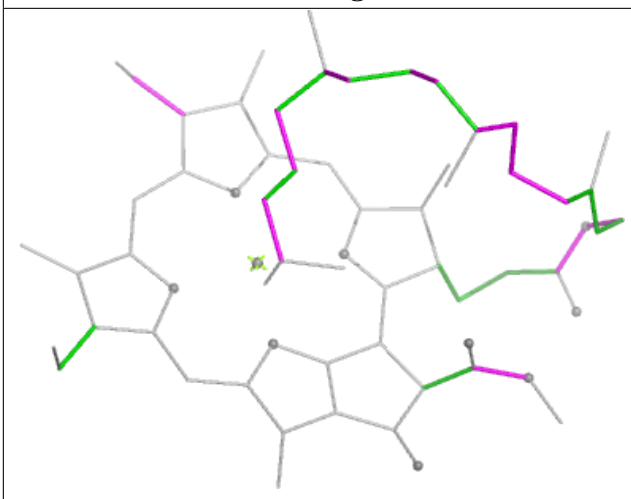
Ligand CLA B 1203



Bond lengths



Bond angles

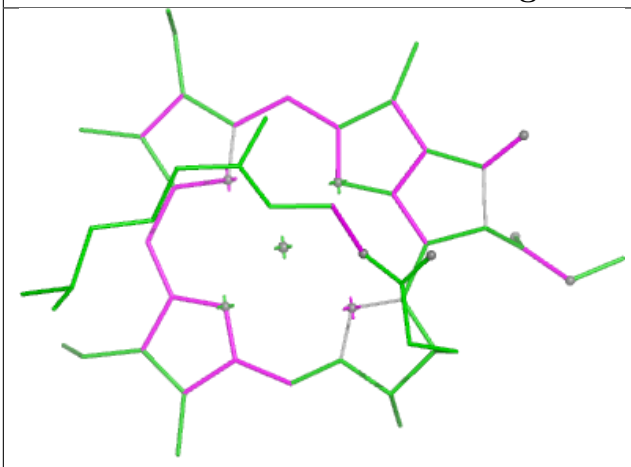


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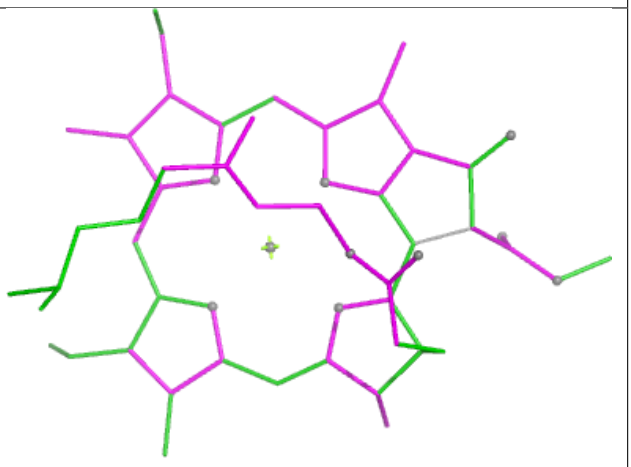


Rings

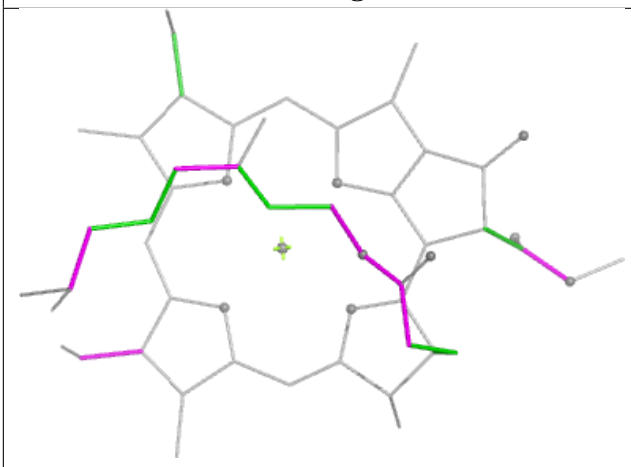
Ligand CLA 2 2003



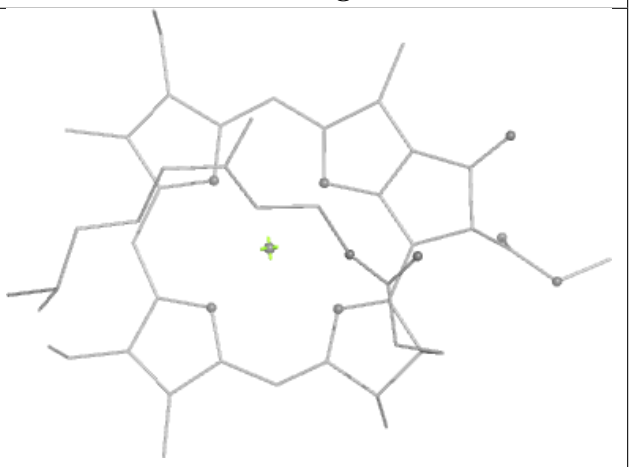
Bond lengths



Bond angles

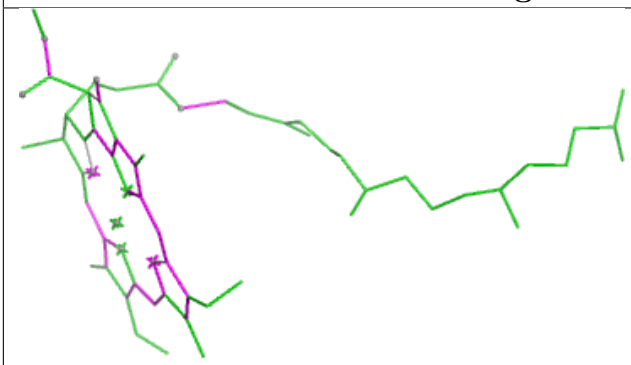


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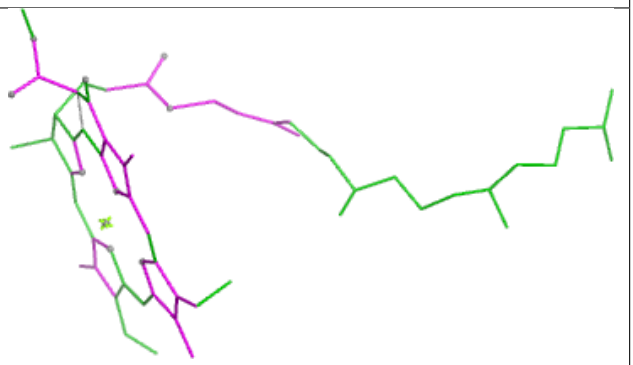


Rings

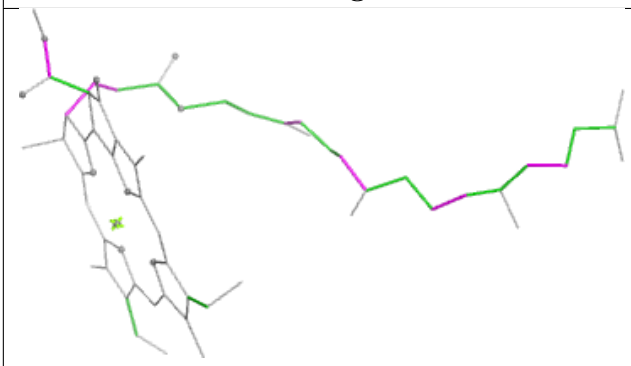
Ligand CLA A 1109



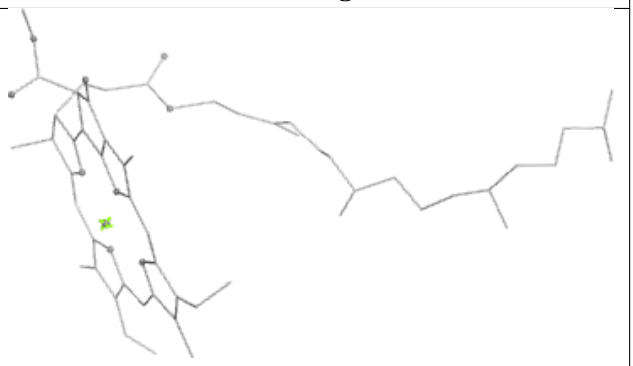
Bond lengths



Bond angles

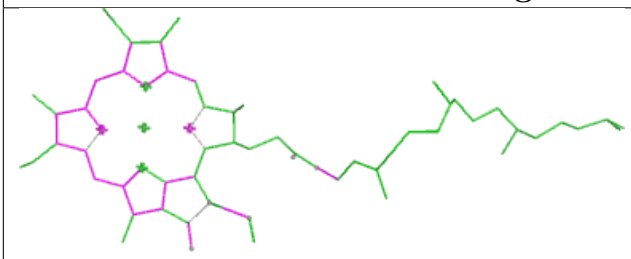


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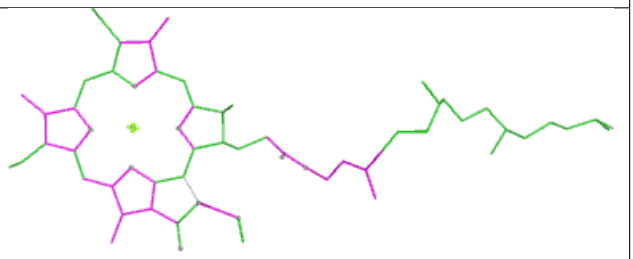


Rings

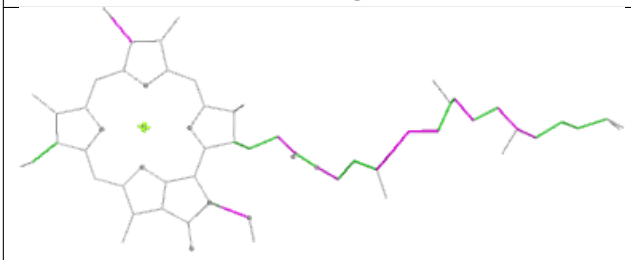
Ligand CLA A 1131



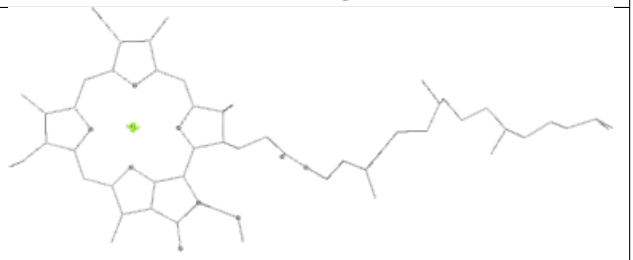
Bond lengths



Bond angles

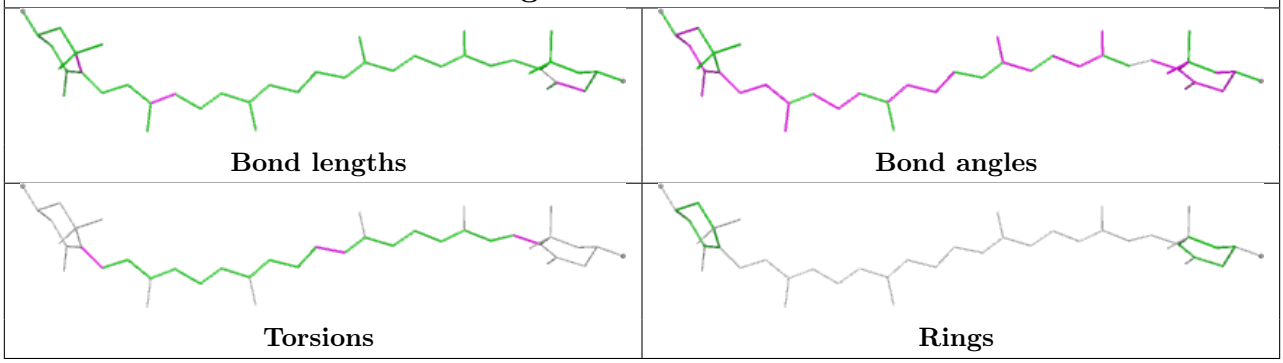


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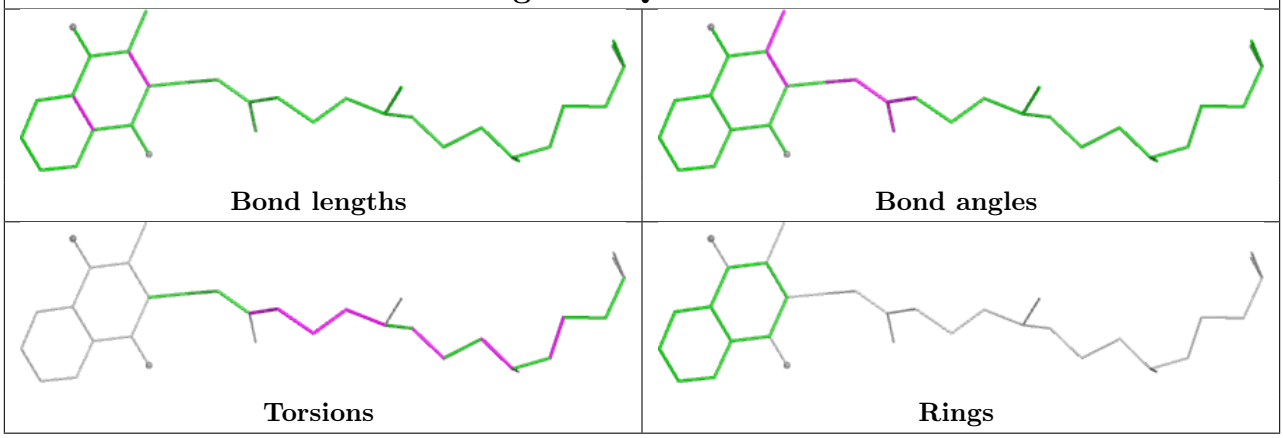


Rings

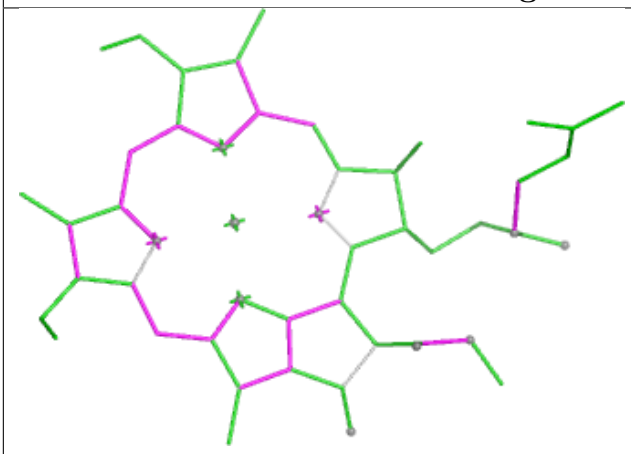
Ligand LUT 4 4501



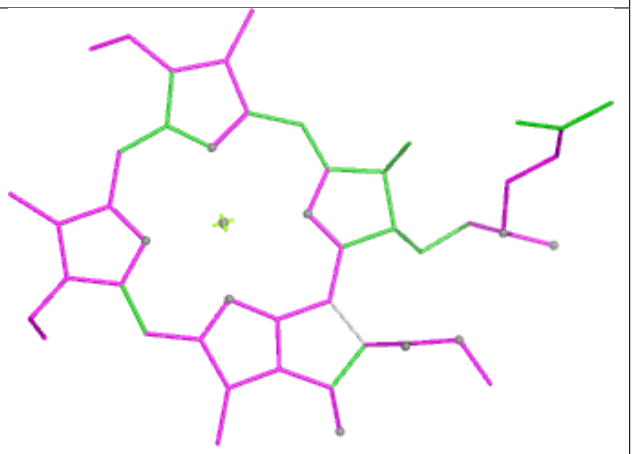
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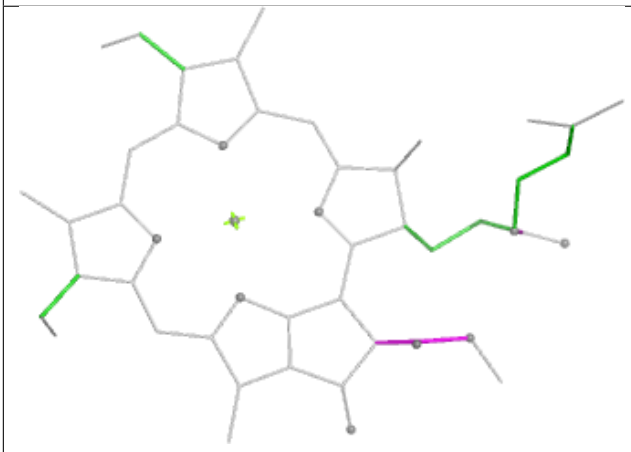
Ligand CLA 4 4002



Bond lengths



Bond angles

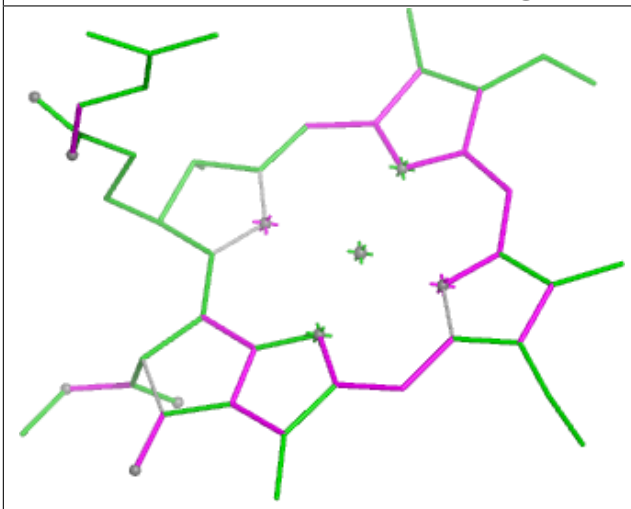


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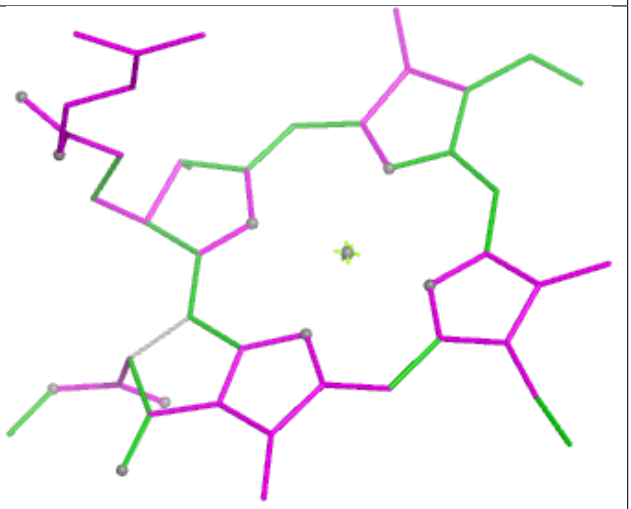


Rings

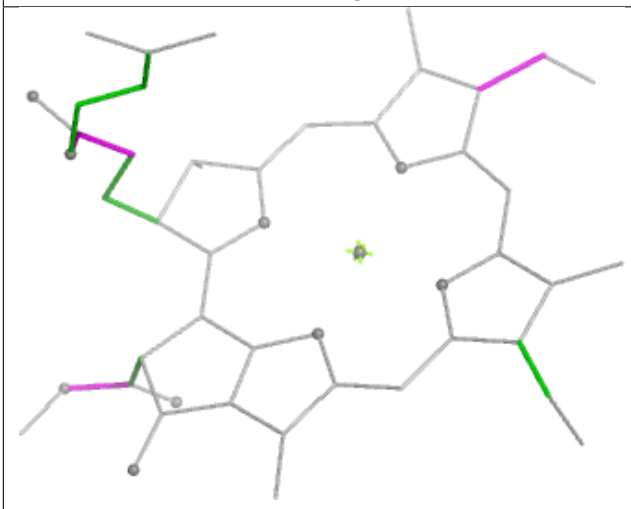
Ligand CLA L 1503



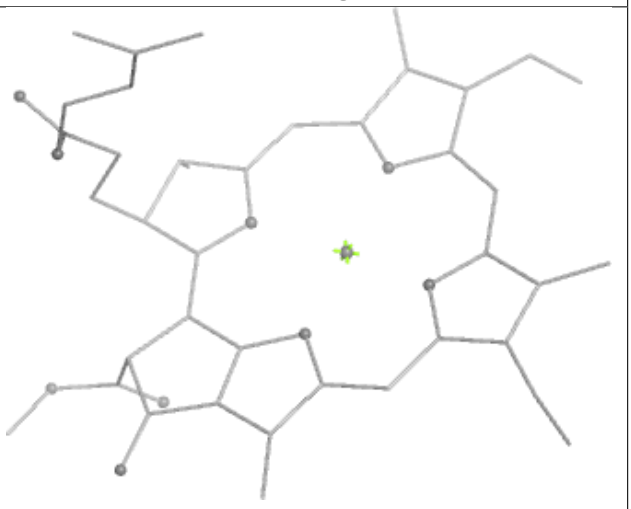
Bond lengths



Bond angles

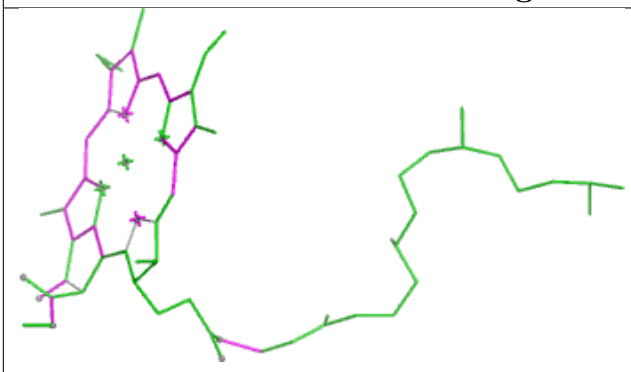


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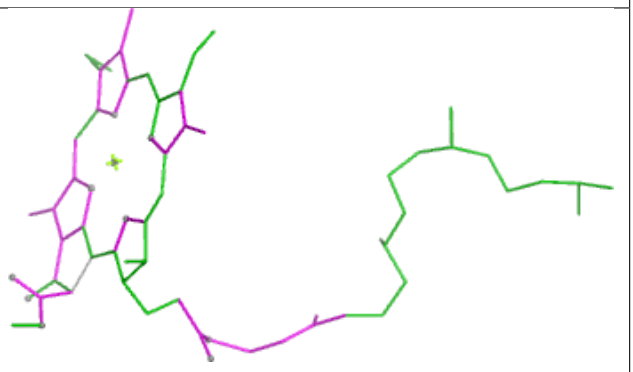


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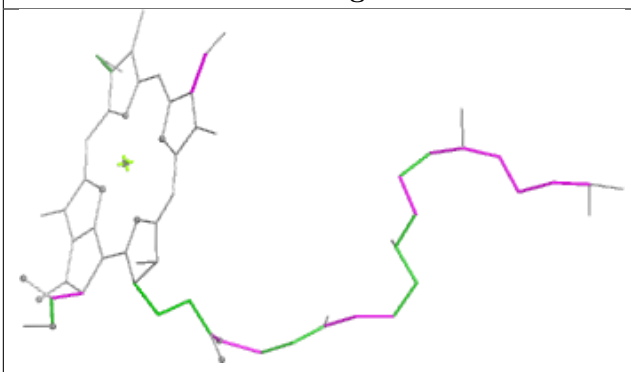
Ligand CLA B 1218



Bond lengths



Bond angles

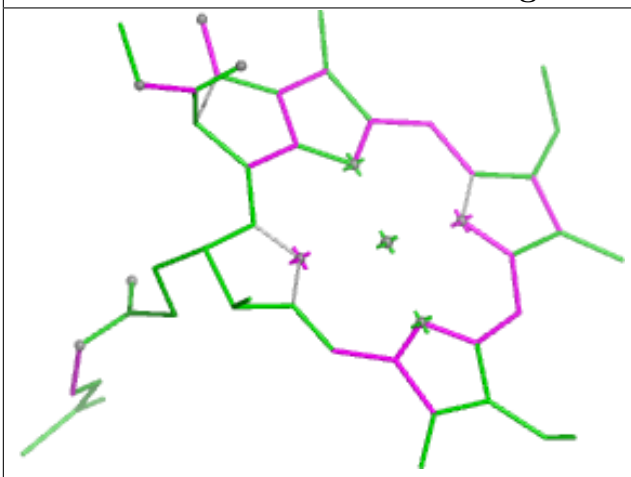


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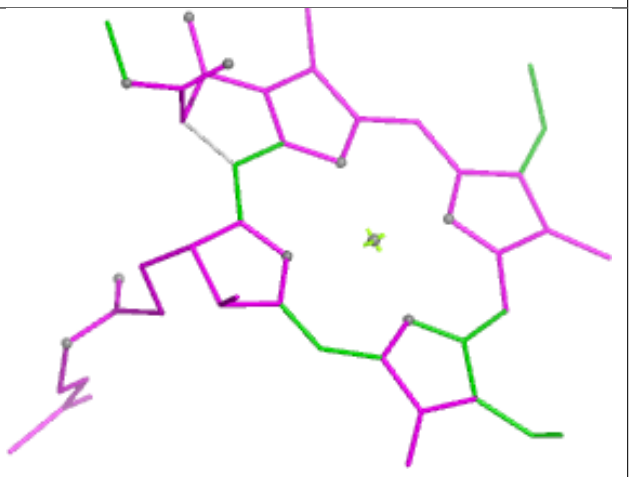


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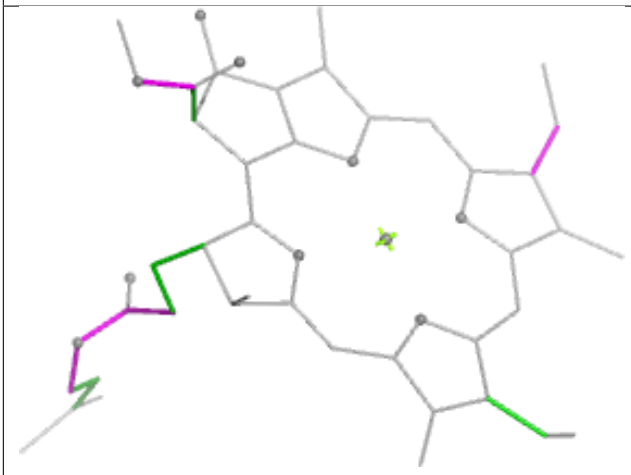
Ligand CLA 2 2008



Bond lengths



Bond angles

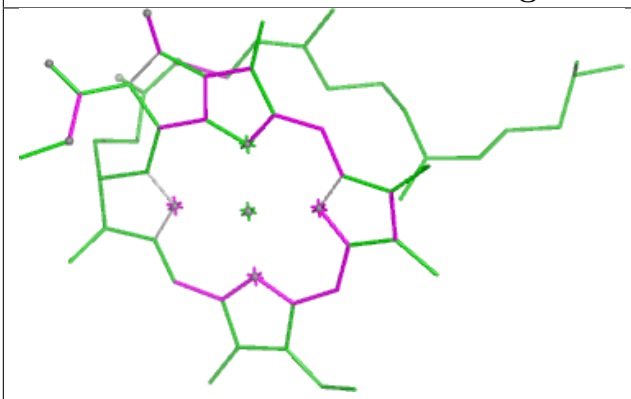


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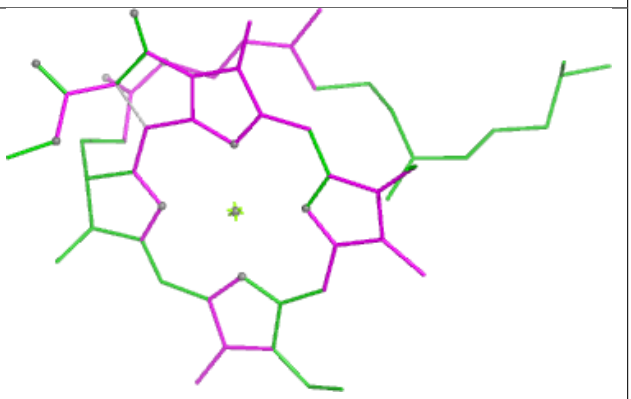


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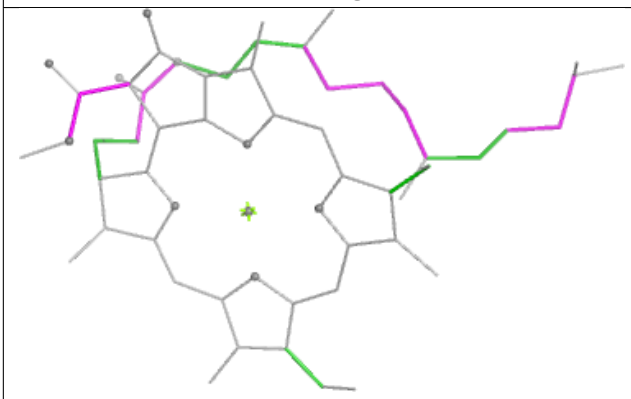
Ligand CLA 3 3010



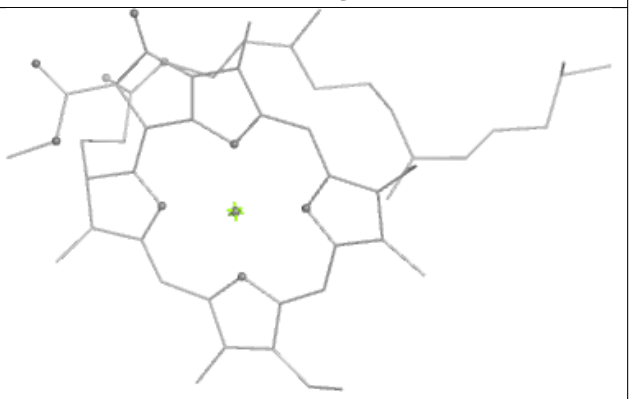
Bond lengths



Bond angles

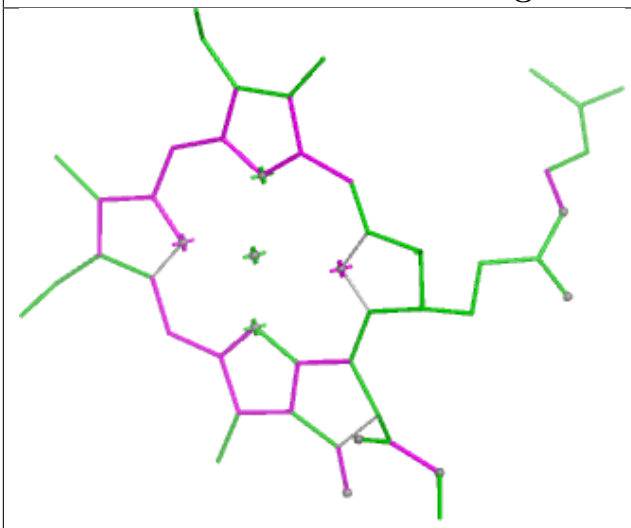


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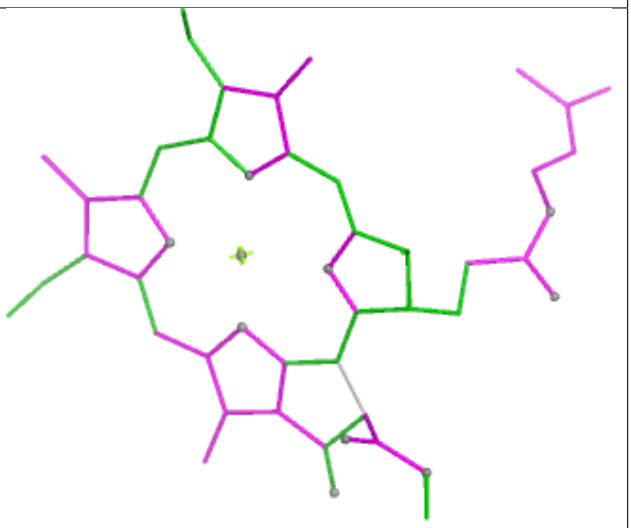


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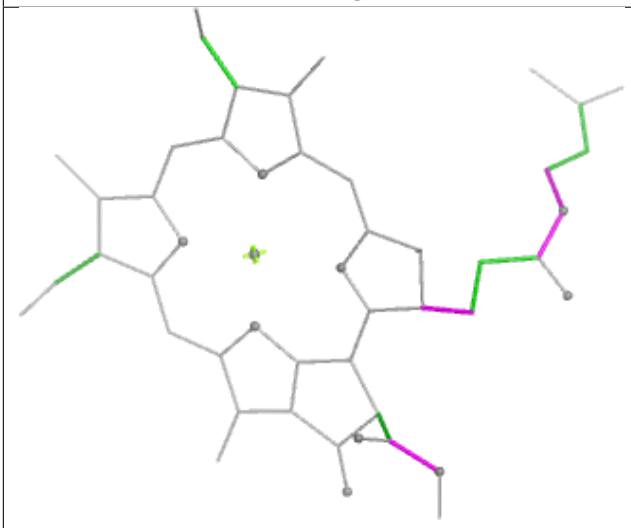
Ligand CLA A 1102



Bond lengths



Bond angles

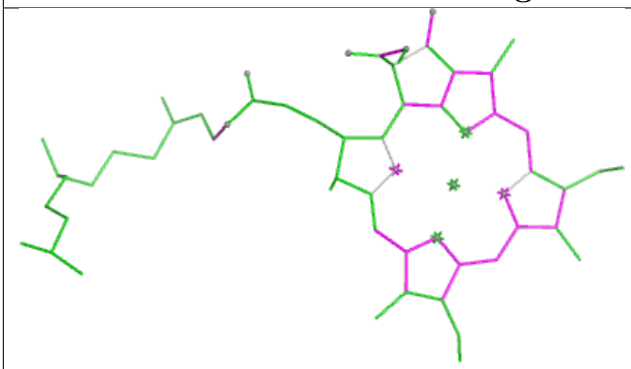


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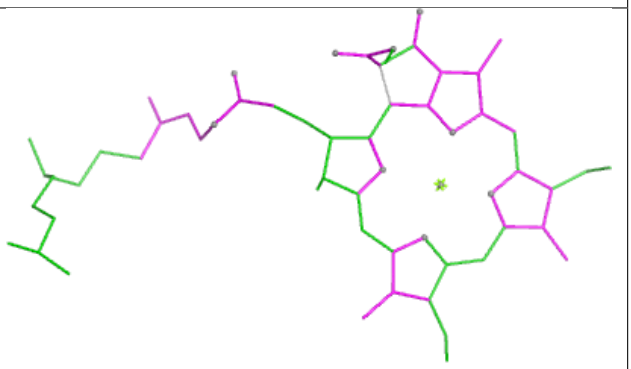


Rings

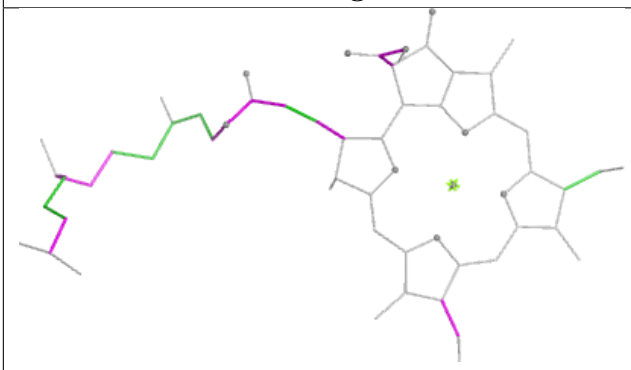
Ligand CLA A 1125



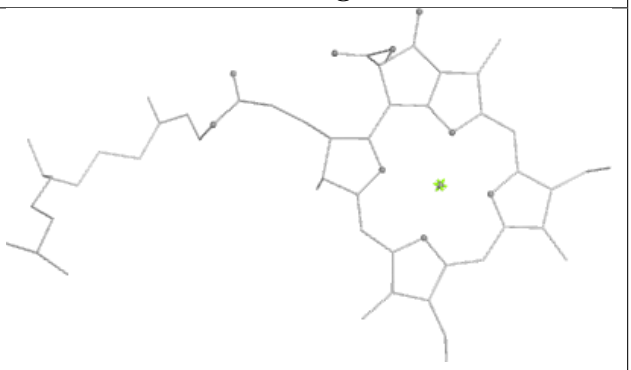
Bond lengths



Bond angles

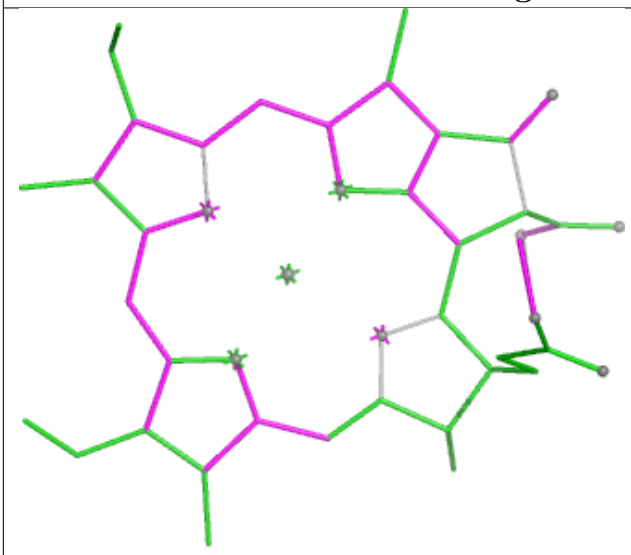


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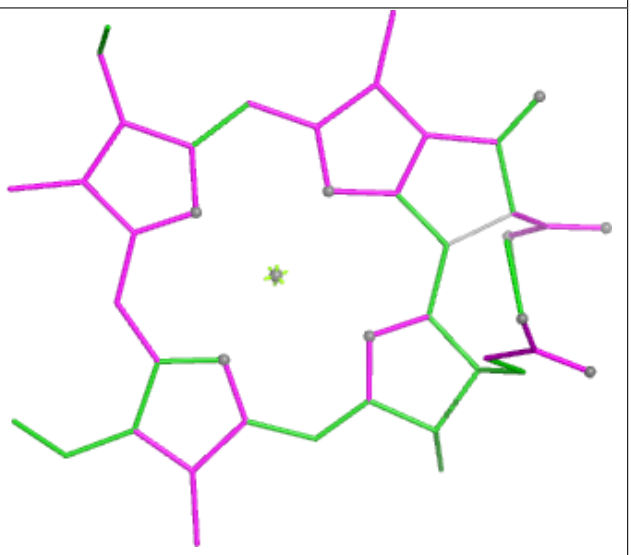


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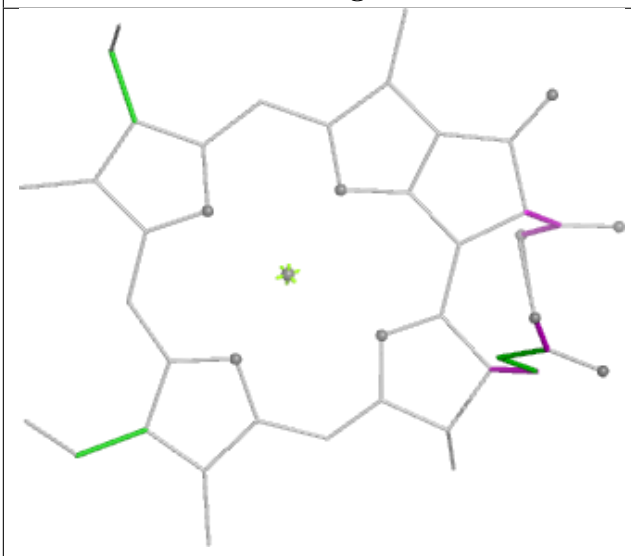
Ligand CLA A 1114



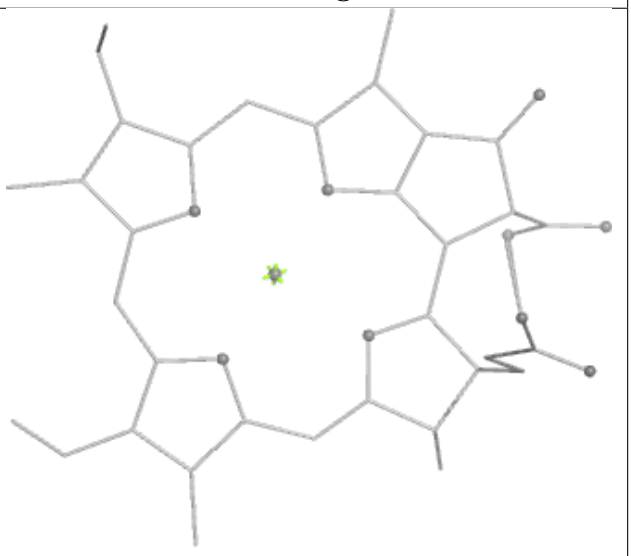
Bond lengths



Bond angles

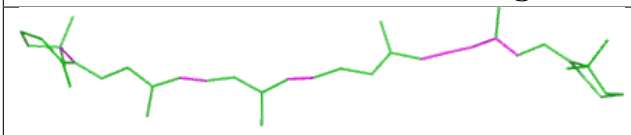


Torsions

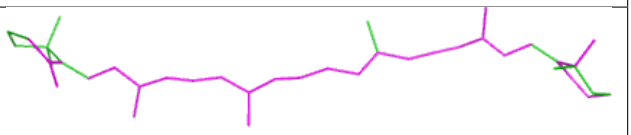


Rings

Ligand BCR A 6007



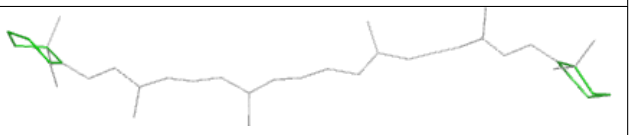
Bond lengths



Bond angles

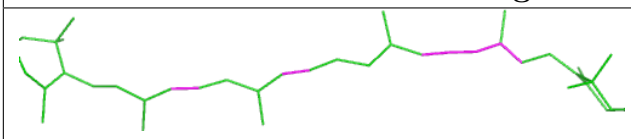


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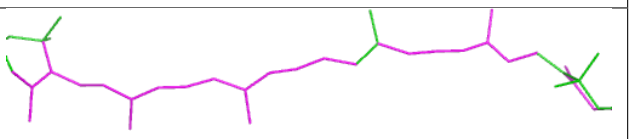


Rings

Ligand BCR A 6002



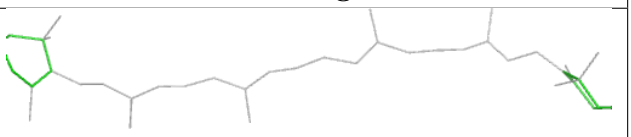
Bond lengths



Bond angles

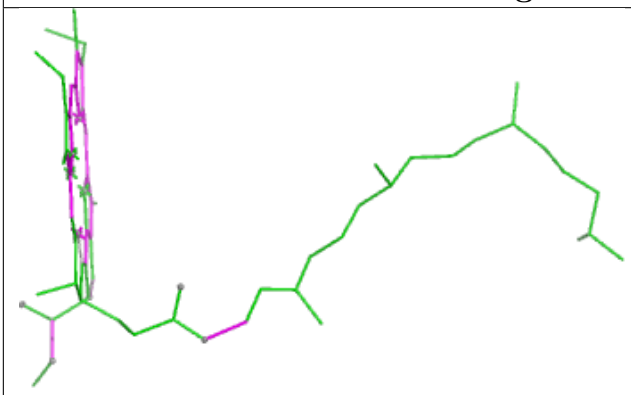


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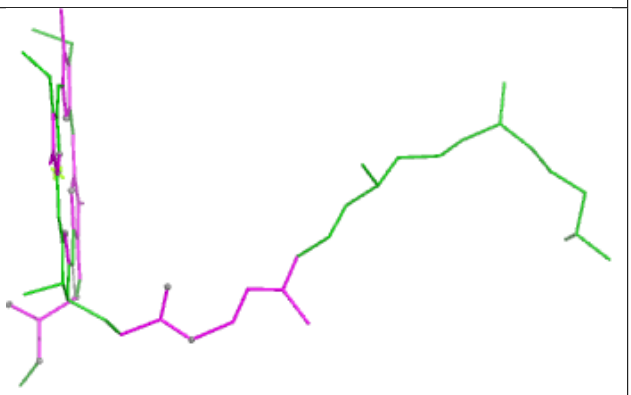


Rings

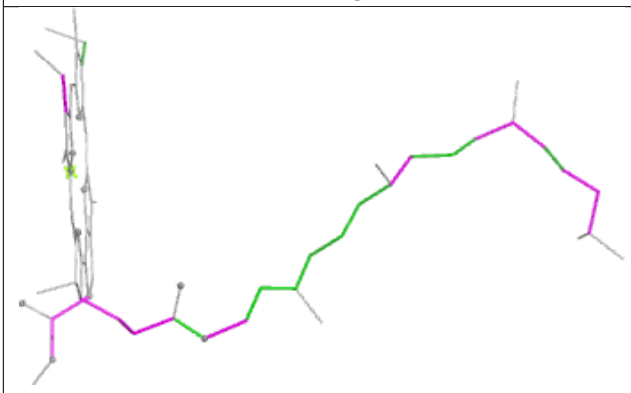
Ligand CLA B 1239



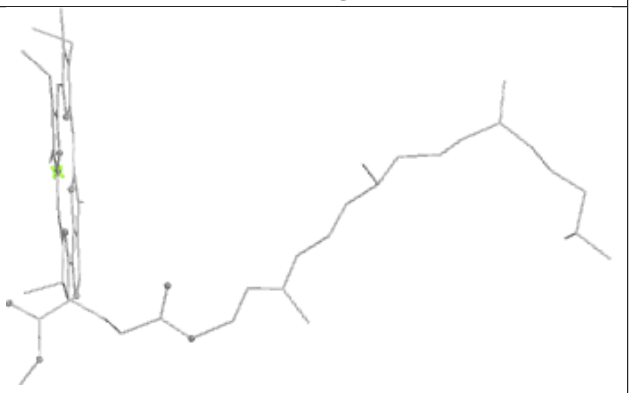
Bond lengths



Bond angles

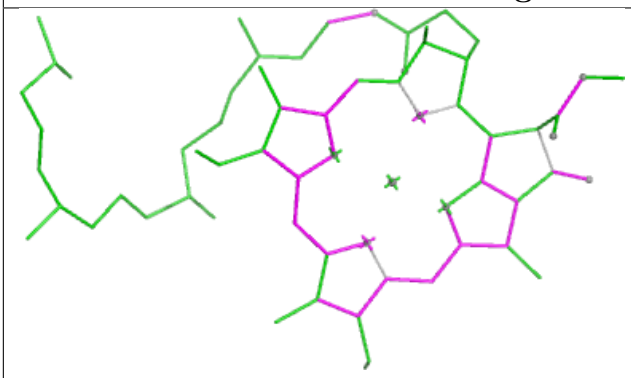


Torsions

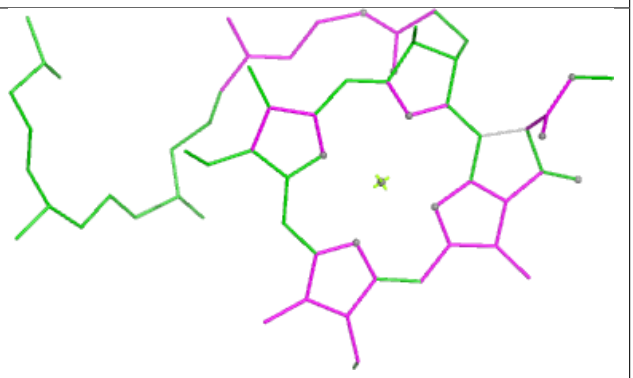


Rings

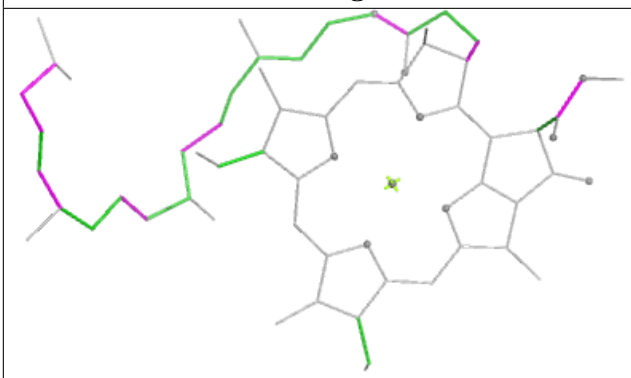
Ligand CLA A 1117



Bond lengths



Bond angles

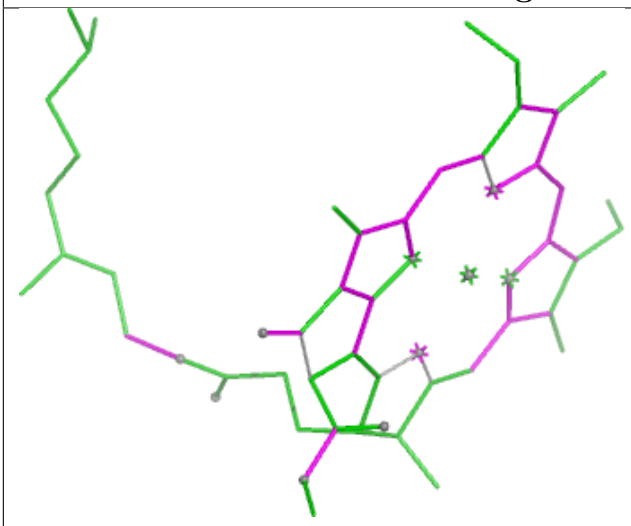


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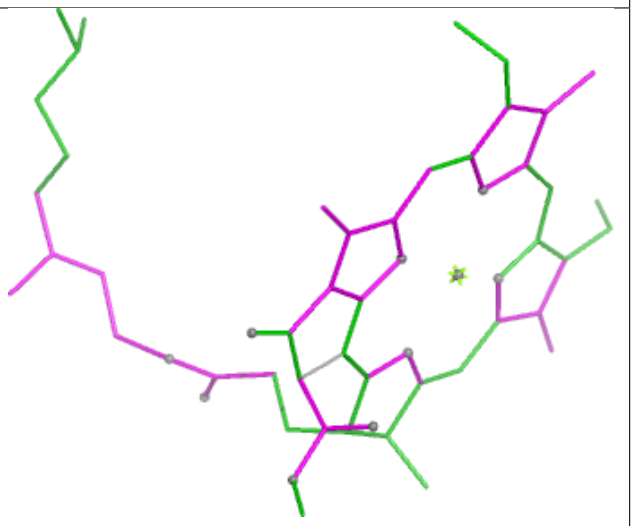


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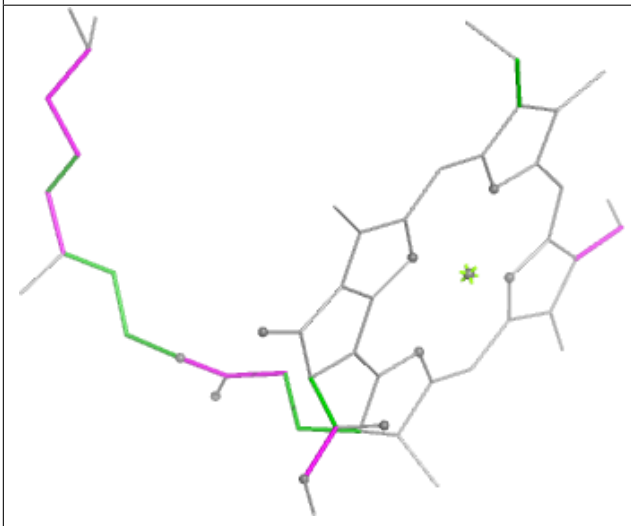
Ligand CLA B 1236



Bond lengths



Bond angles



Torsions

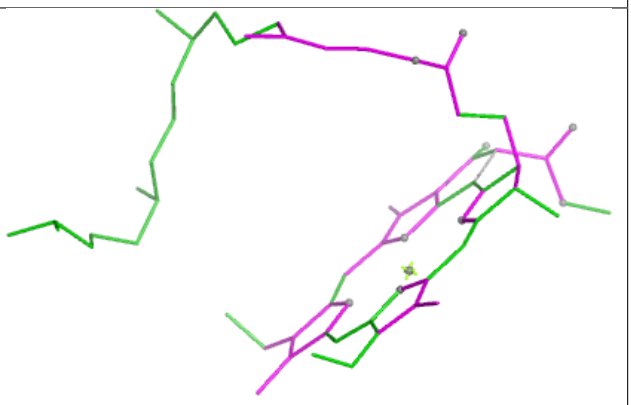


Rings

Ligand CLA B 1227



Bond lengths



Bond angles

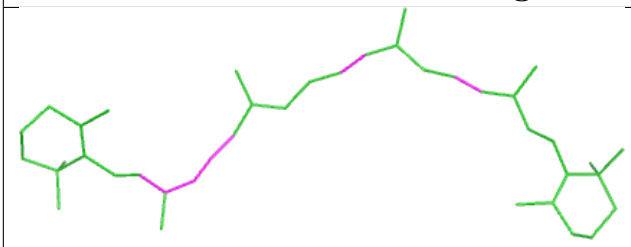


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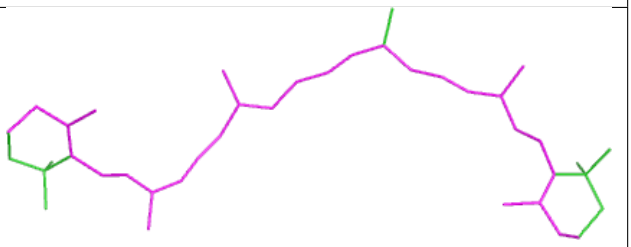


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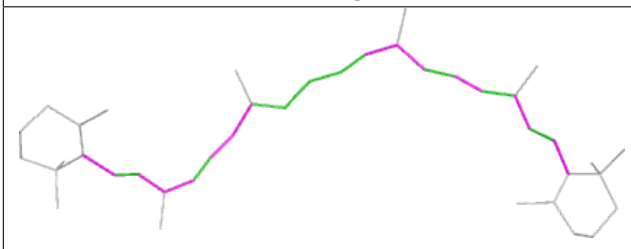
Ligand BCR A 6011



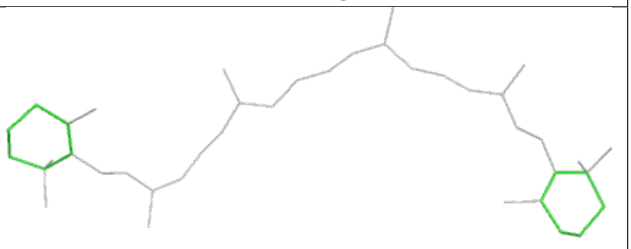
Bond lengths



Bond angles

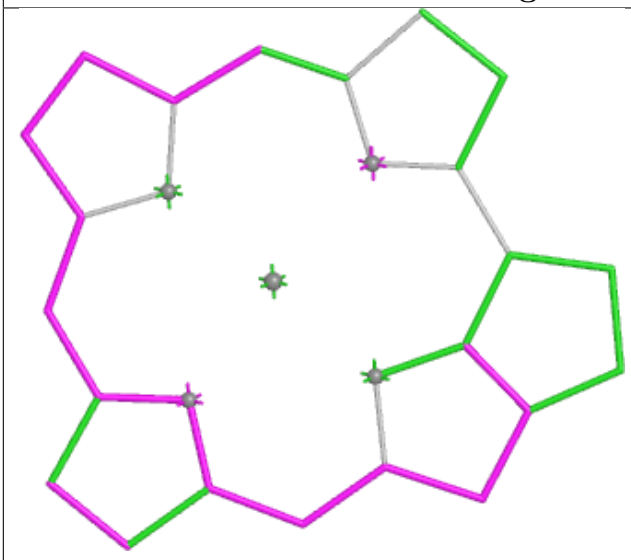


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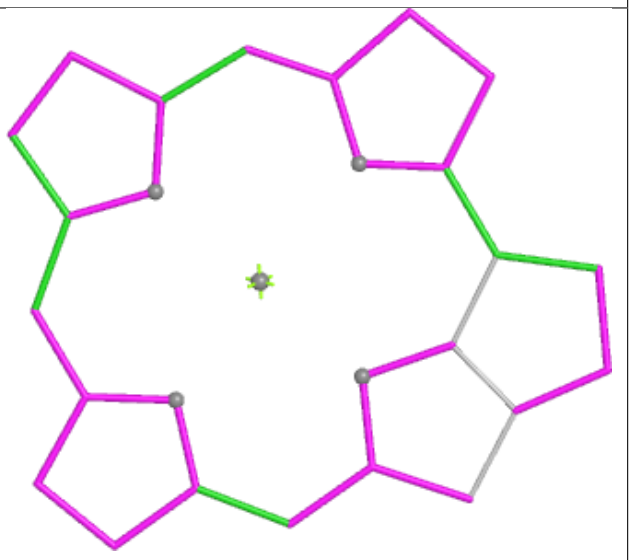


Rings

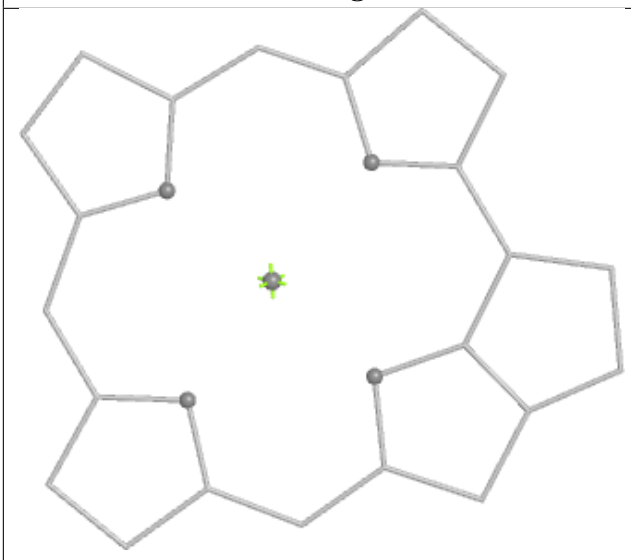
Ligand CLA 2 2019



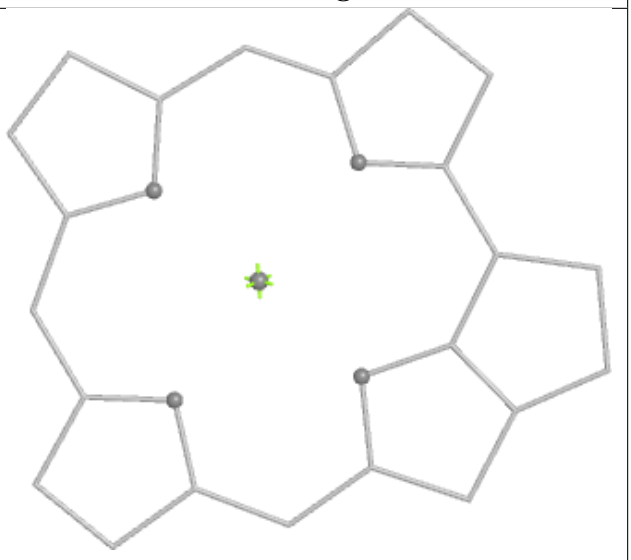
Bond lengths



Bond angles

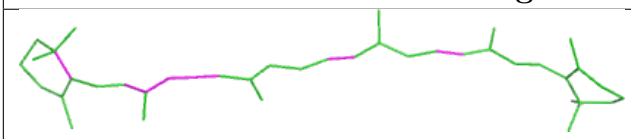


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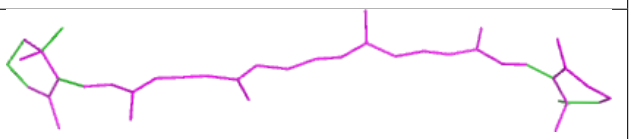


Rings

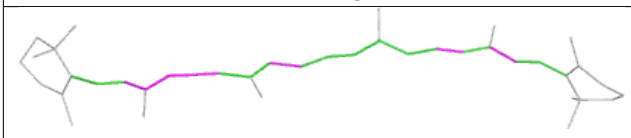
Ligand BCR L 6020



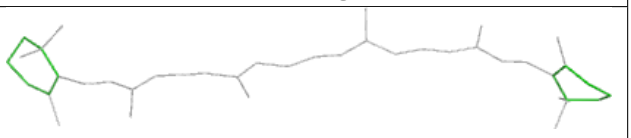
Bond lengths



Bond angles

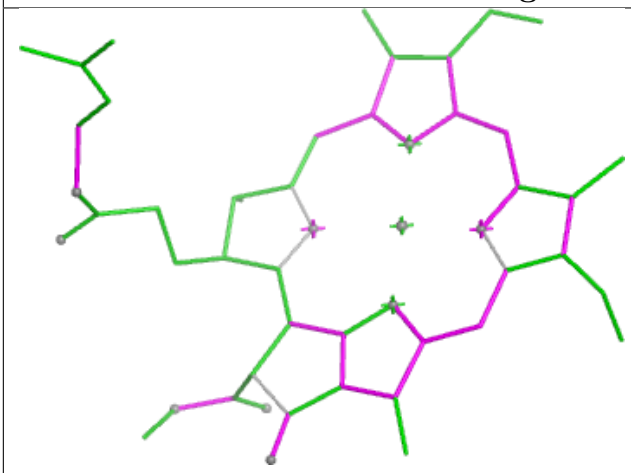


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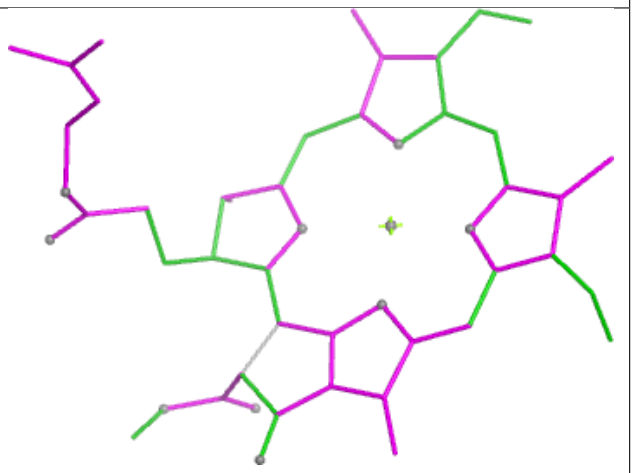


Rings

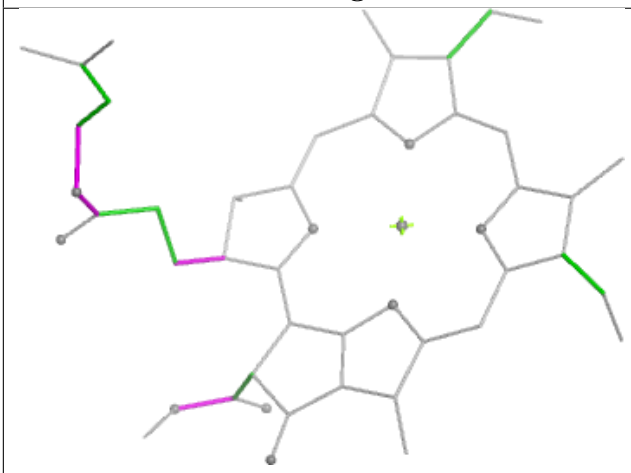
Ligand CLA 2 2009



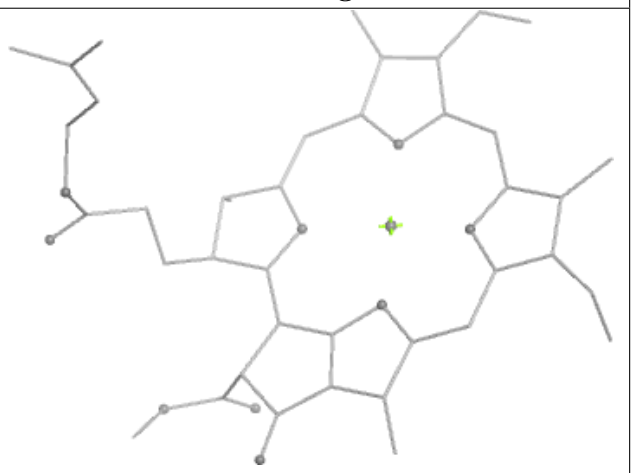
Bond lengths



Bond angles

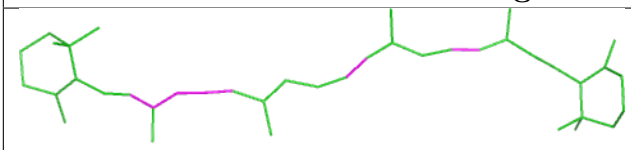


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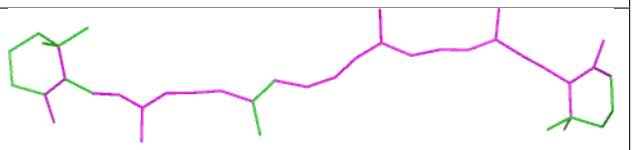


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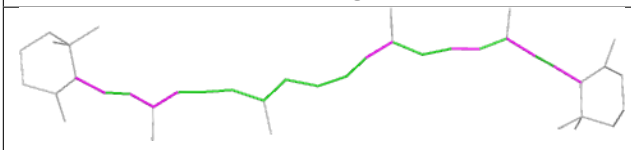
Ligand BCR B 6005



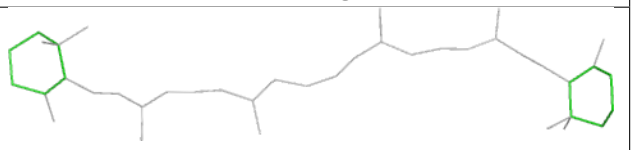
Bond lengths



Bond angles

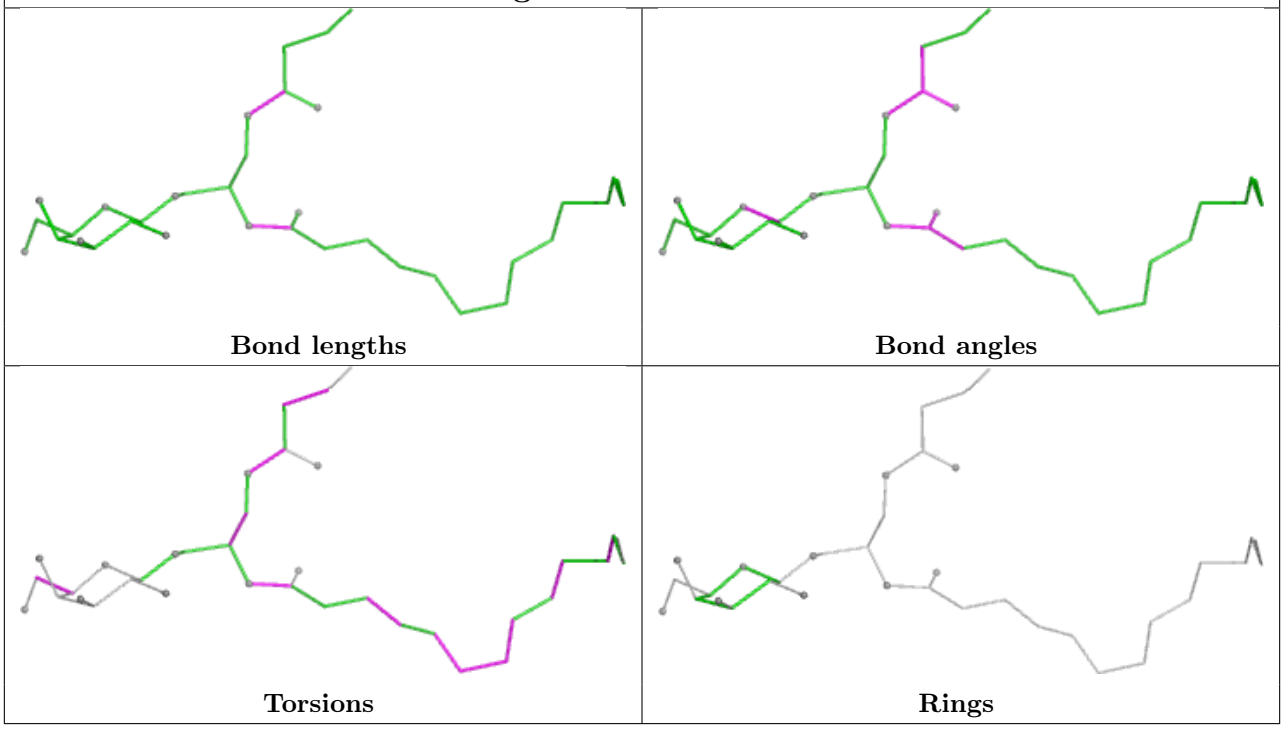


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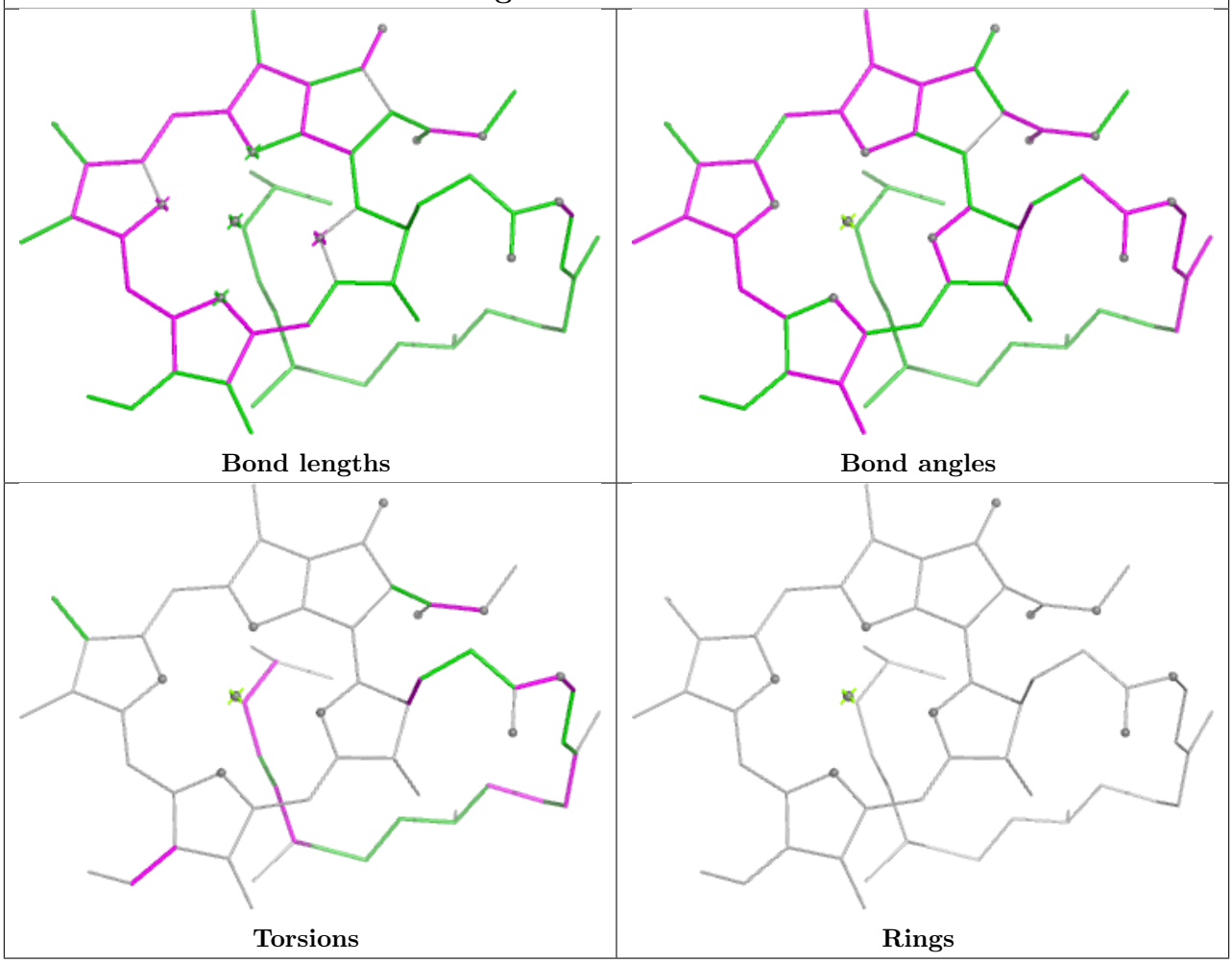


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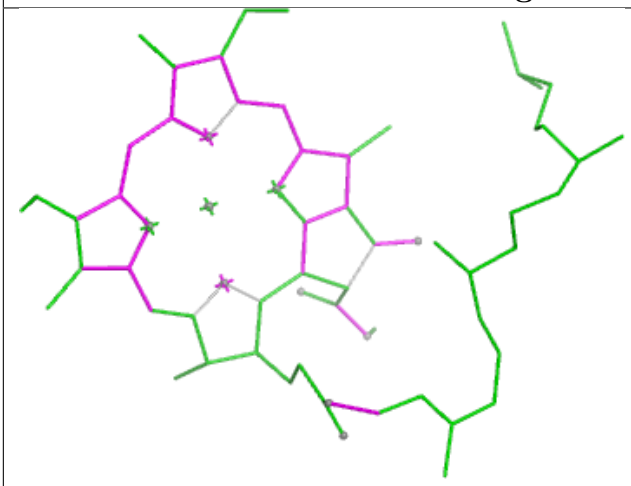
Ligand LMG F 5002



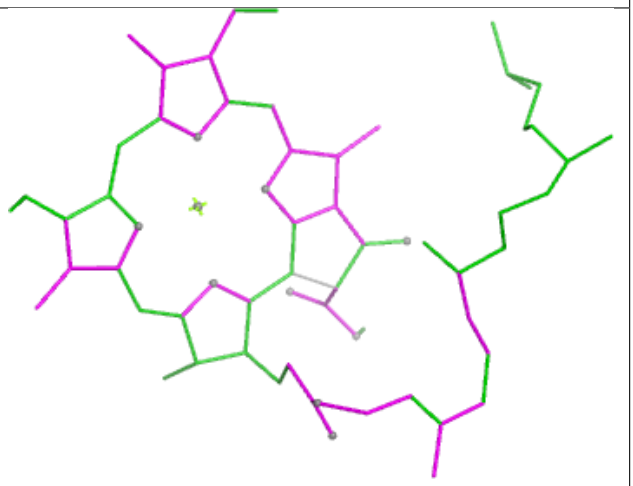
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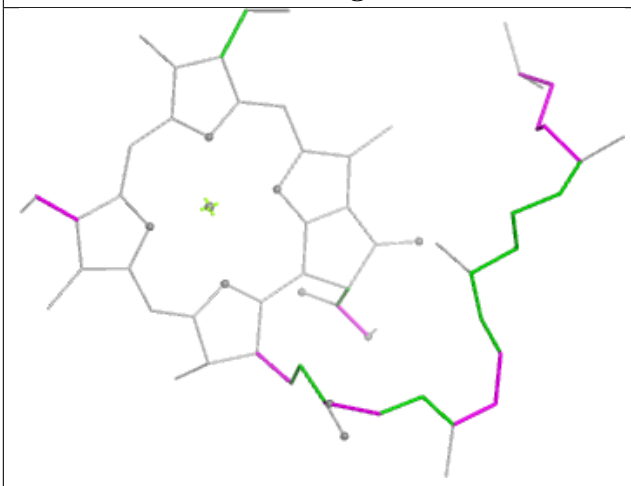
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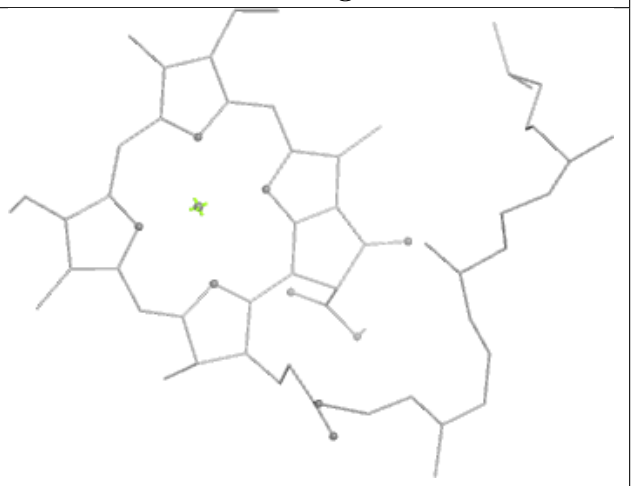
Bond lengths



Bond angles

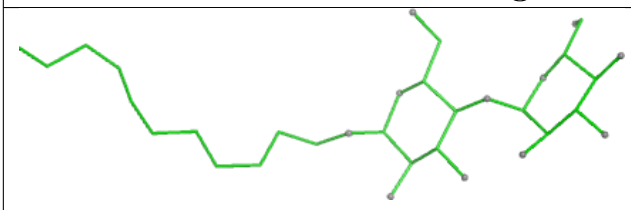


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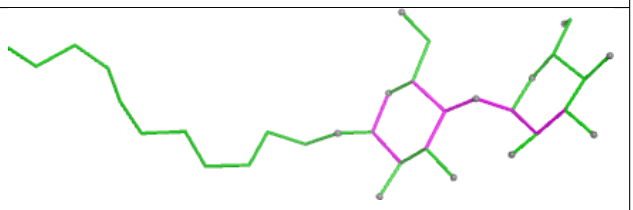


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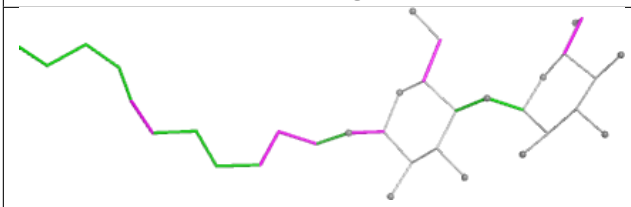
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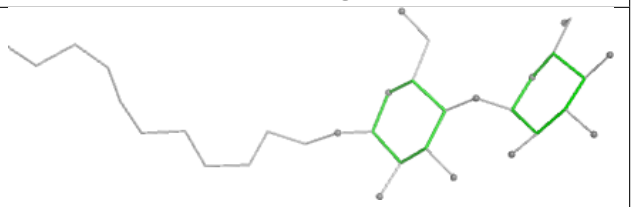
Bond lengths



Bond angles

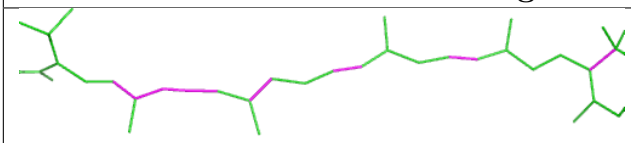


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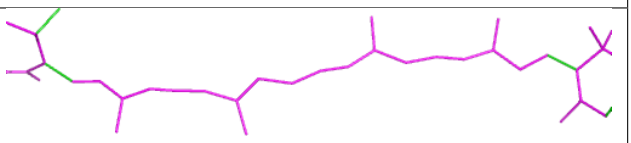


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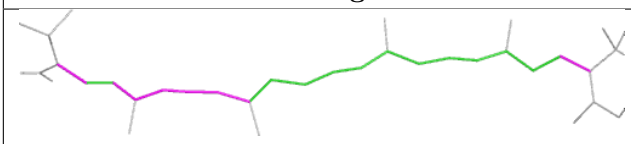
Ligand BCR J 6012



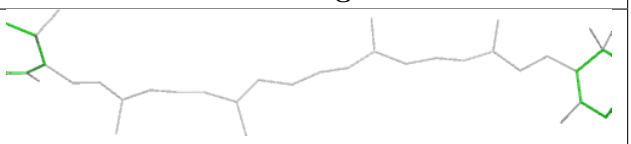
Bond lengths



Bond angles

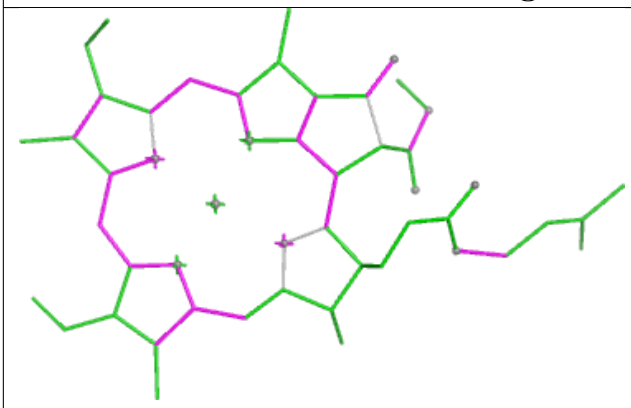


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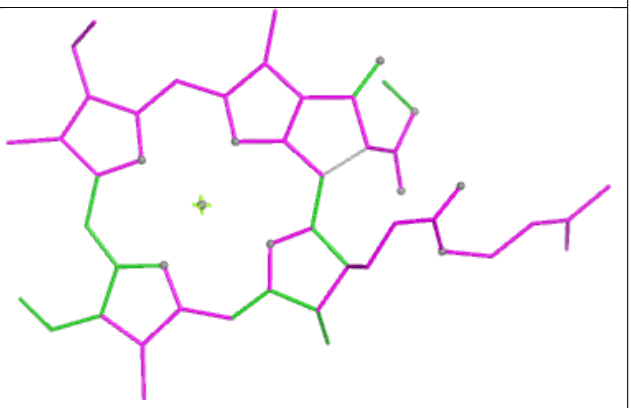


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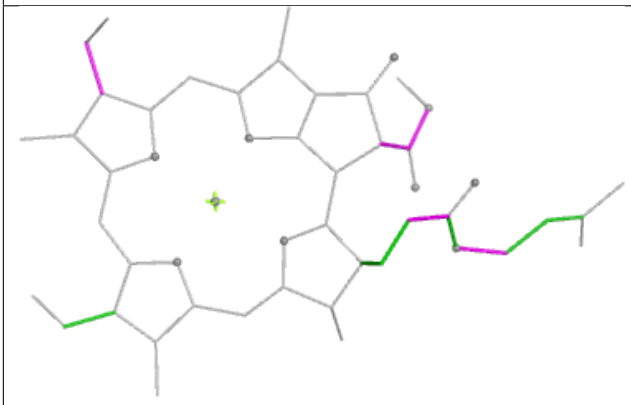
Ligand CLA 2 2016



Bond lengths



Bond angles

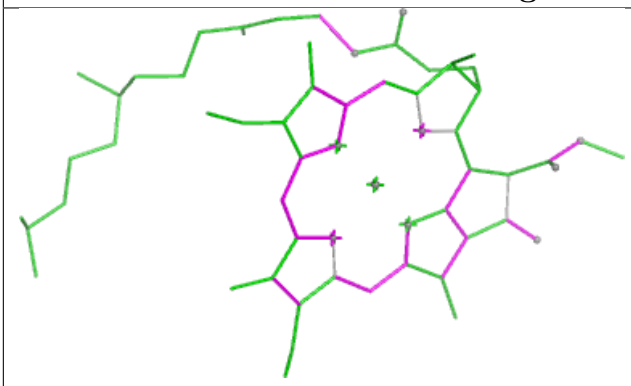


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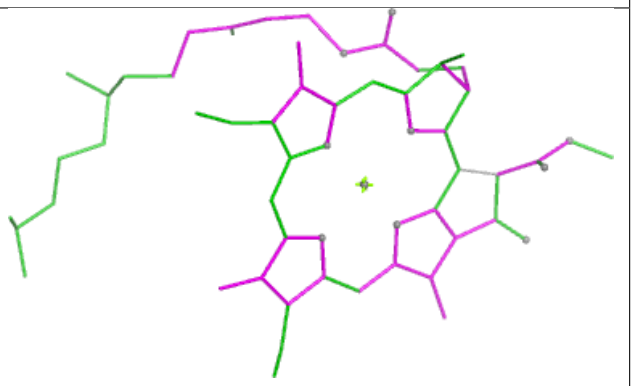


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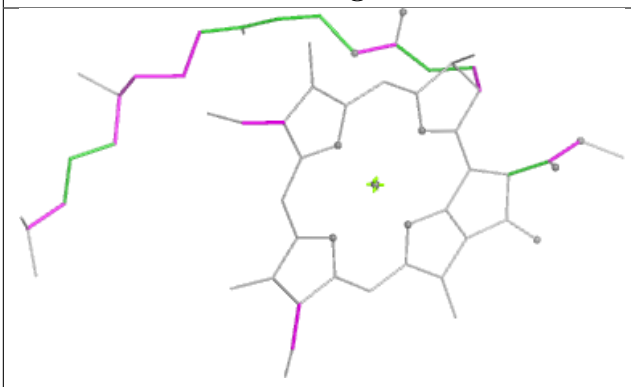
Ligand CLA 1 1001



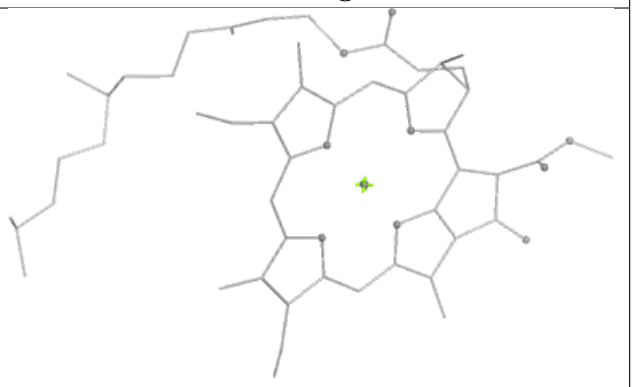
Bond lengths



Bond angles

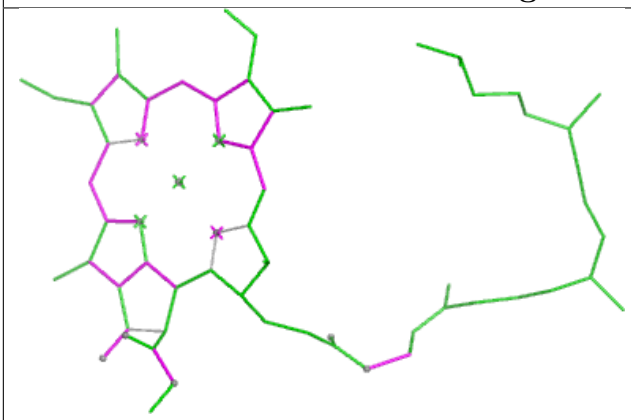


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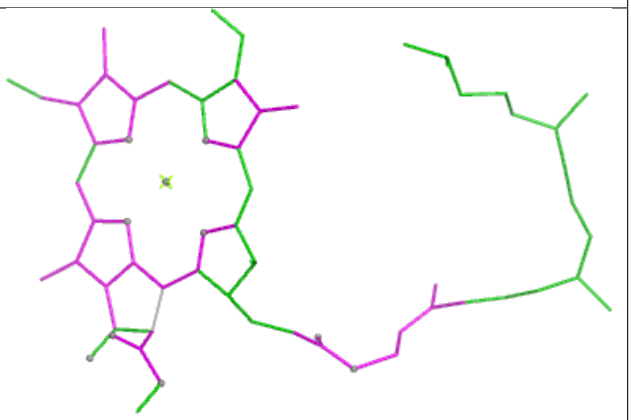


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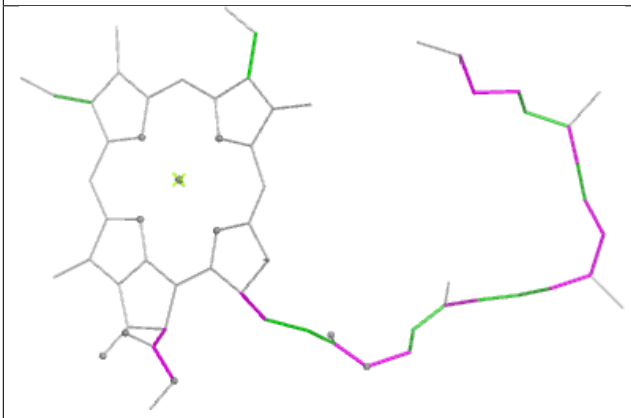
Ligand CLA 4 4017



Bond lengths



Bond angles

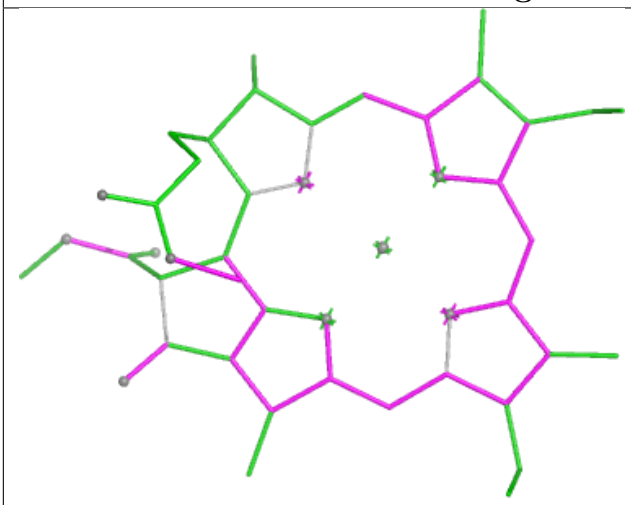


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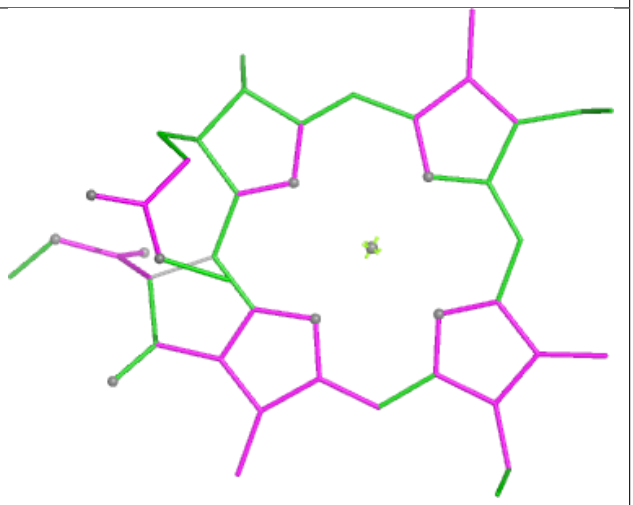


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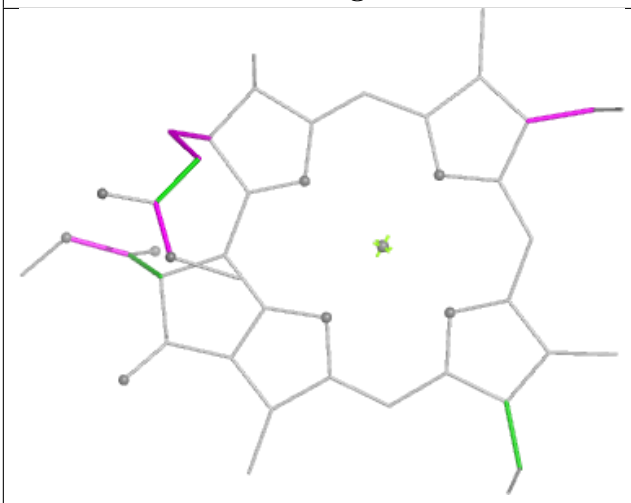
Ligand CLA A 1115



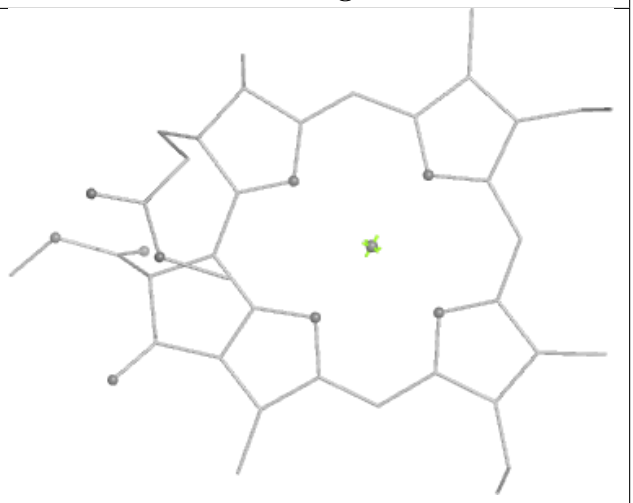
Bond lengths



Bond angles

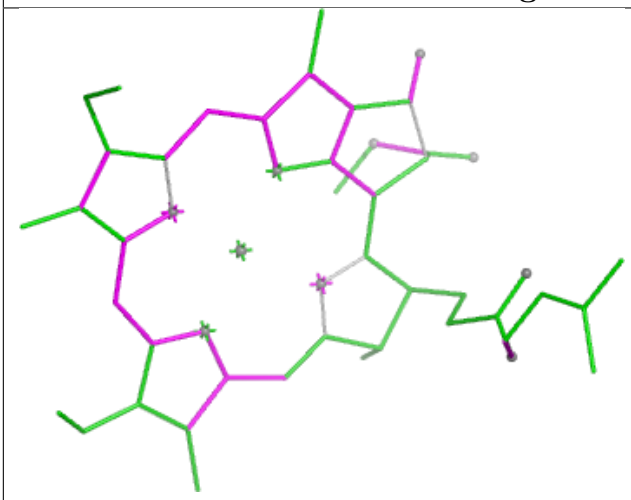


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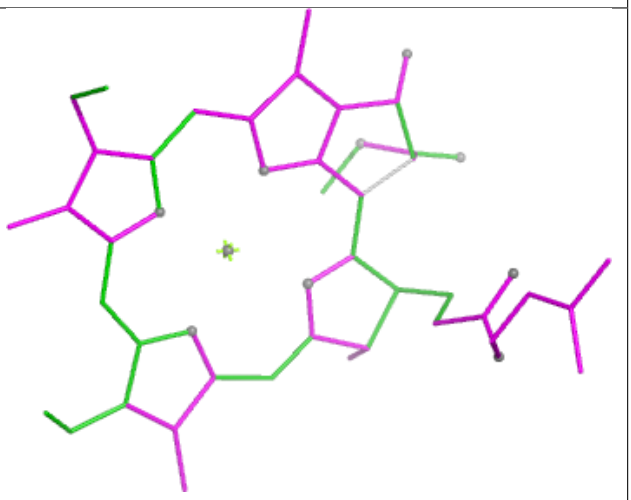


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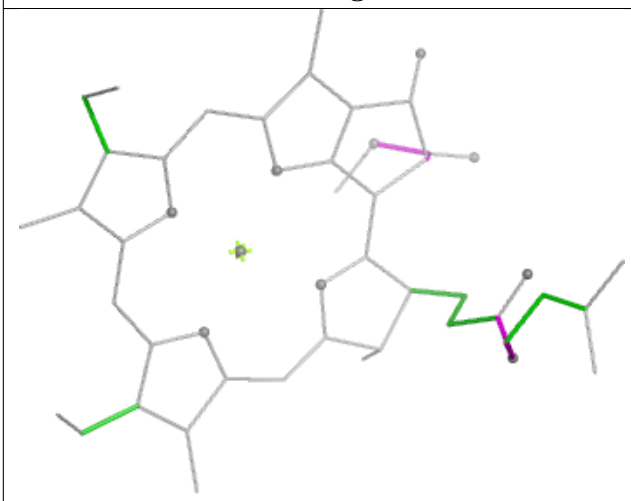
Ligand CLA 3 3006



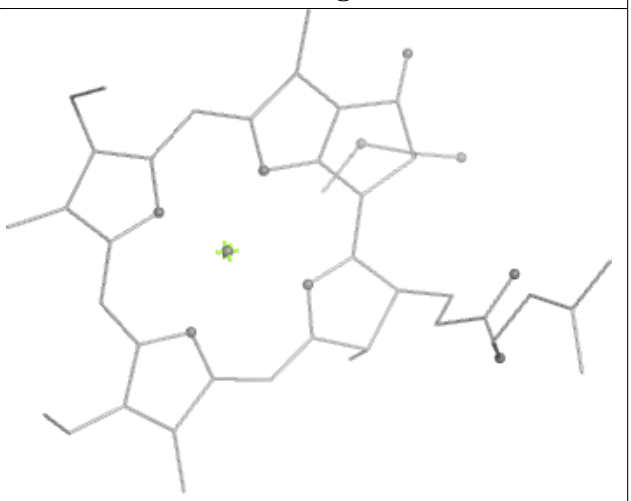
Bond lengths



Bond angles

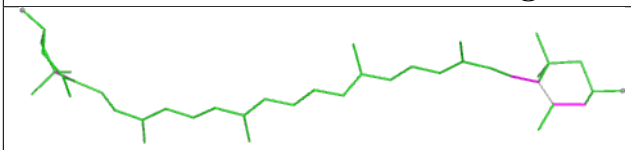


Torsions

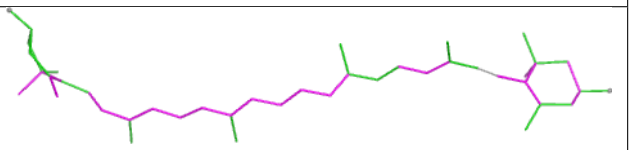


Rings

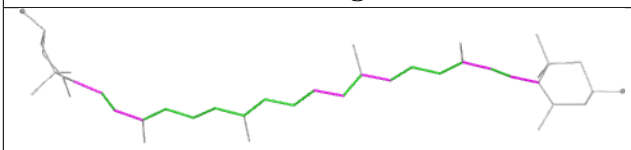
Ligand LUT 4 4503



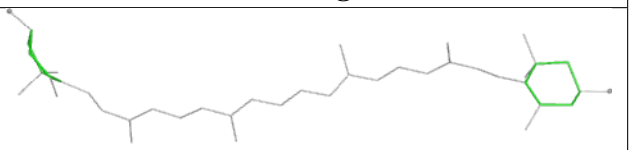
Bond lengths



Bond angles



Torsions

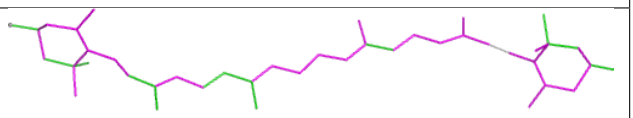


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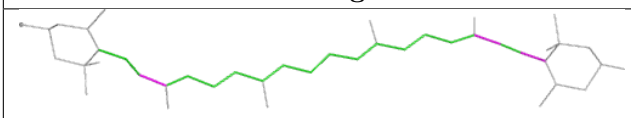
Ligand LUT 3 3501



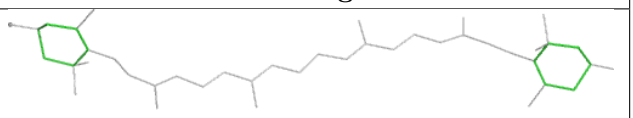
Bond lengths



Bond angles

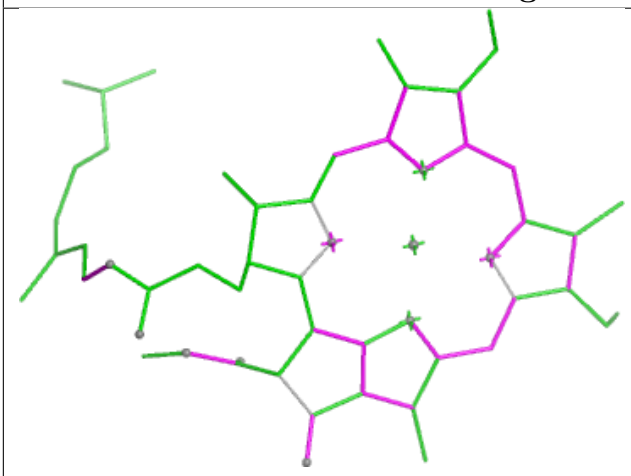


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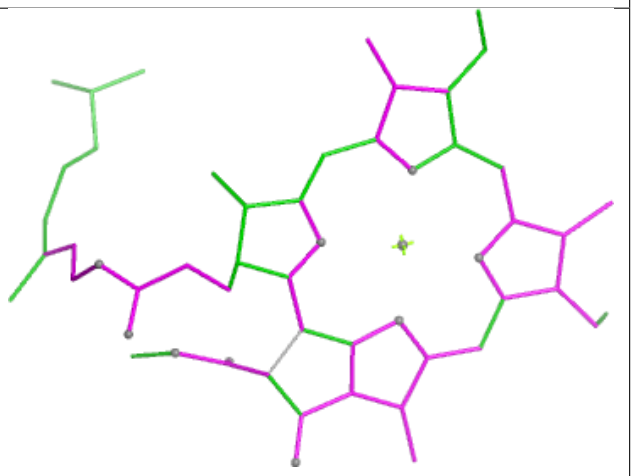


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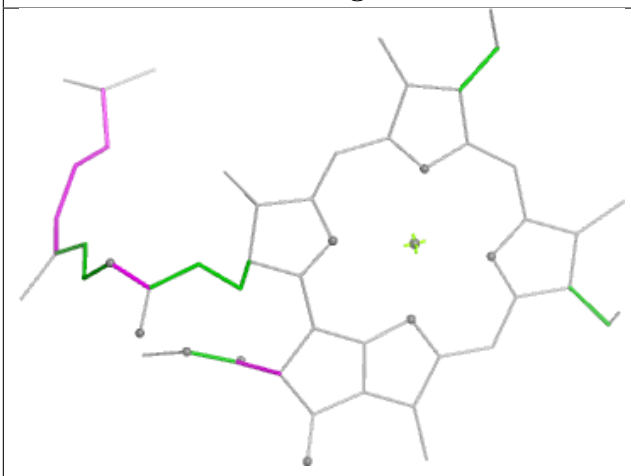
Ligand CLA 1 1005



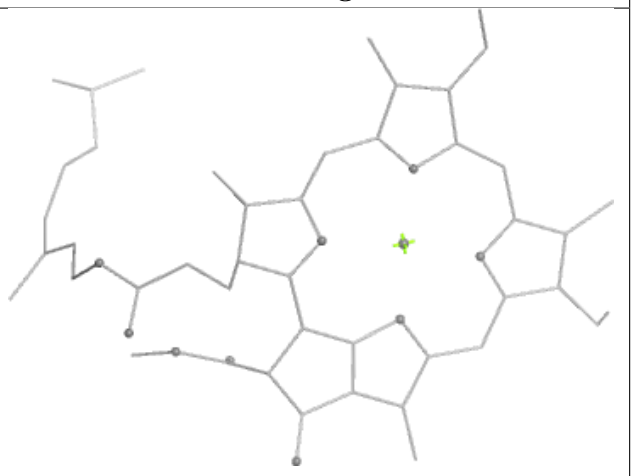
Bond lengths



Bond angles

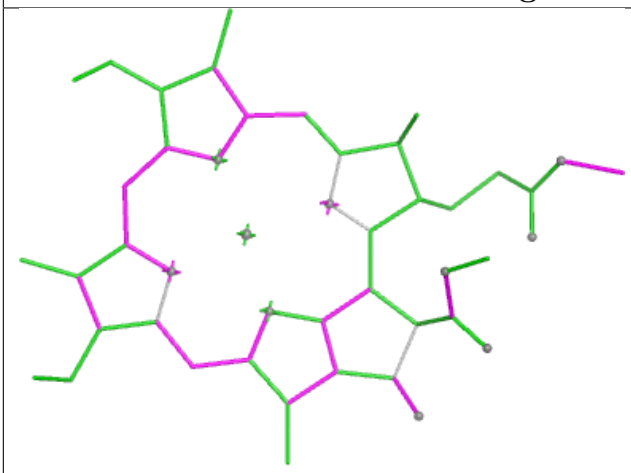


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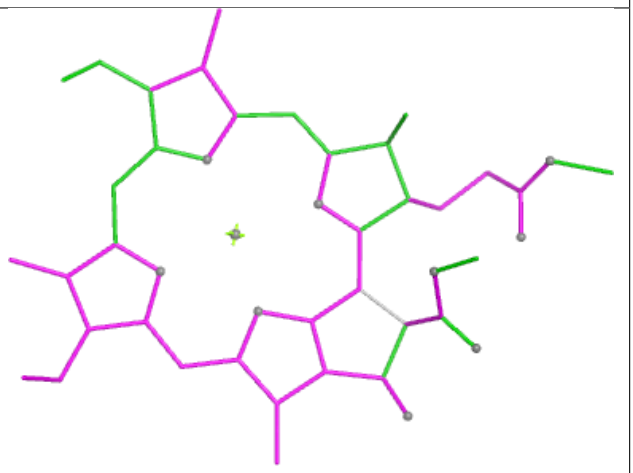


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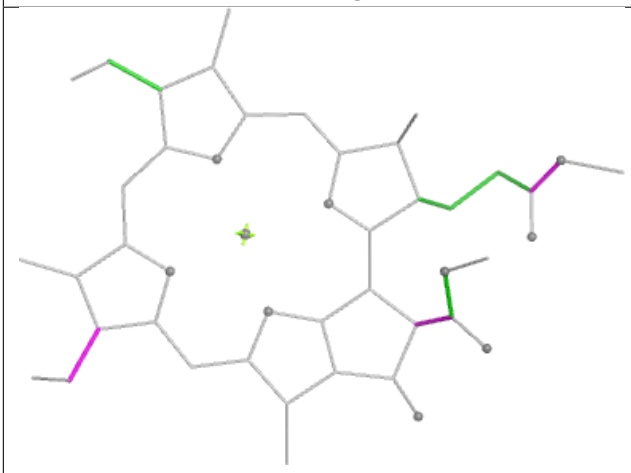
Ligand CLA 1 1002



Bond lengths



Bond angles

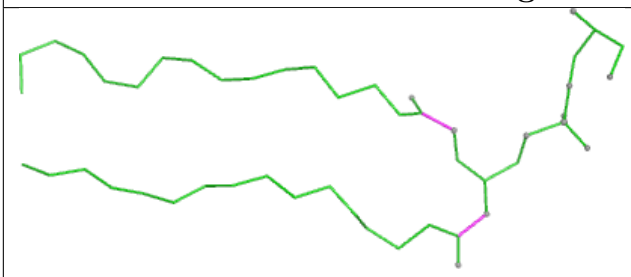


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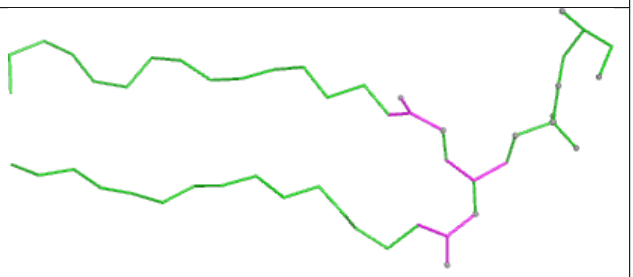


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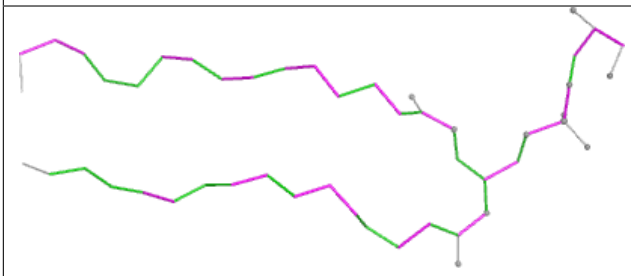
Ligand LHG 1 1801



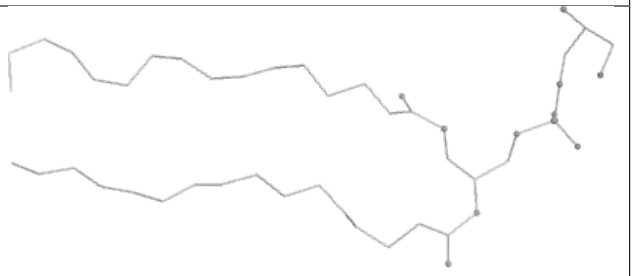
Bond lengths



Bond angles

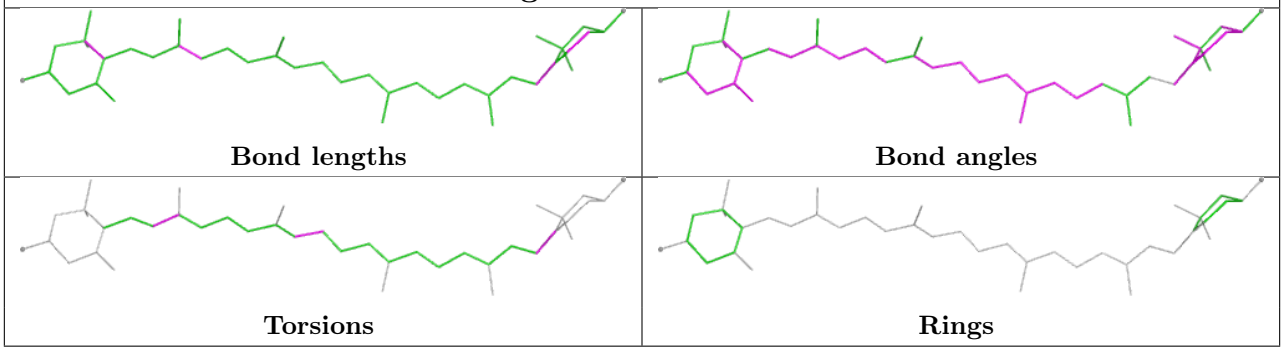


Torsions



Rings

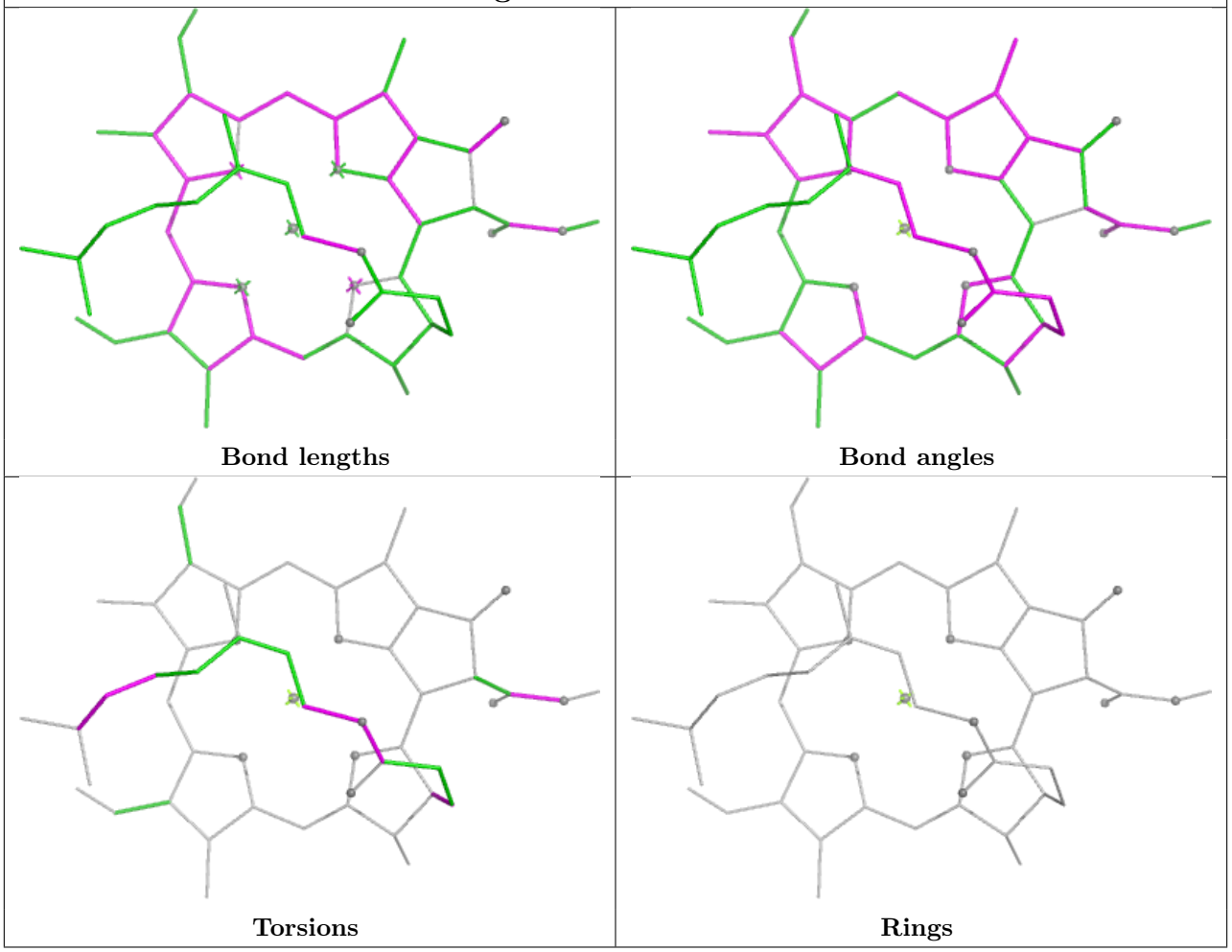
Ligand LUT 1 1502



Bond lengths | Bond angles

Torsions | Rings

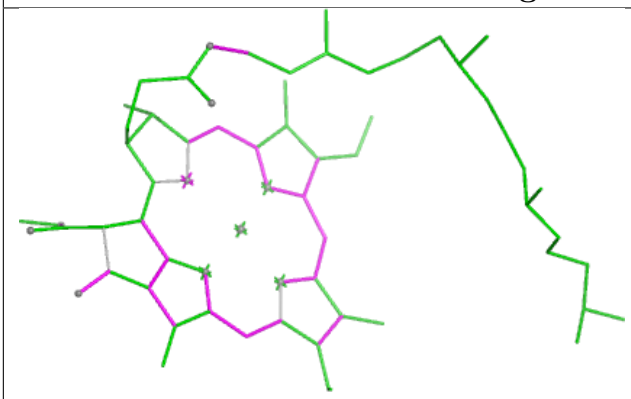
Ligand CLA A 1110



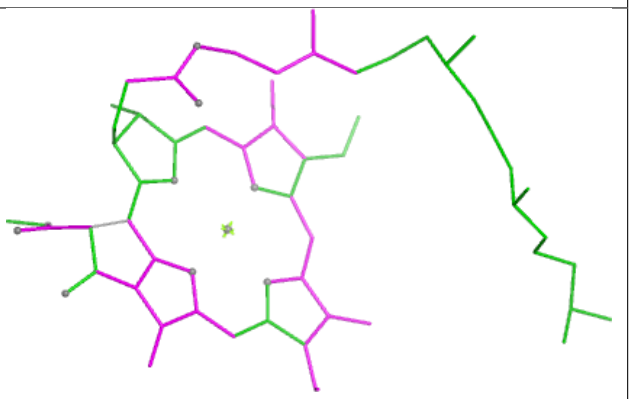
Bond lengths | Bond angles

Torsions | Rings

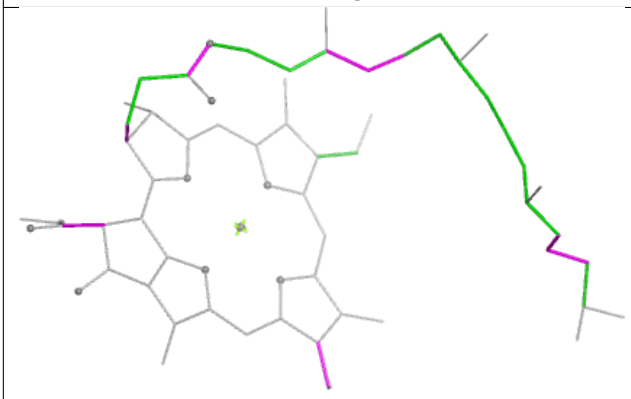
Ligand CLA 2 2004



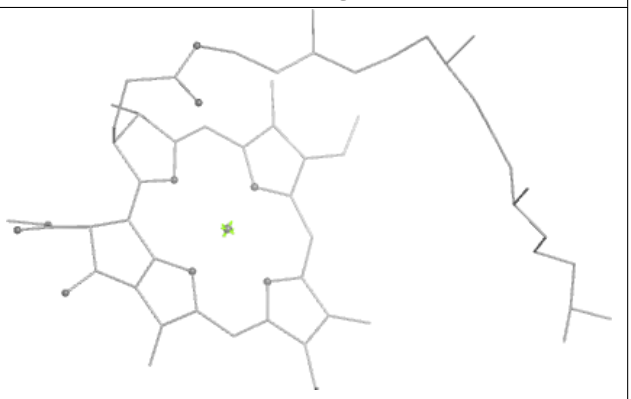
Bond lengths



Bond angles

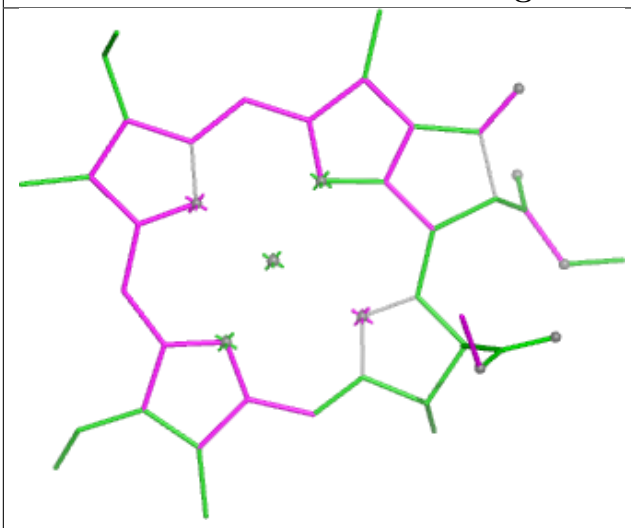


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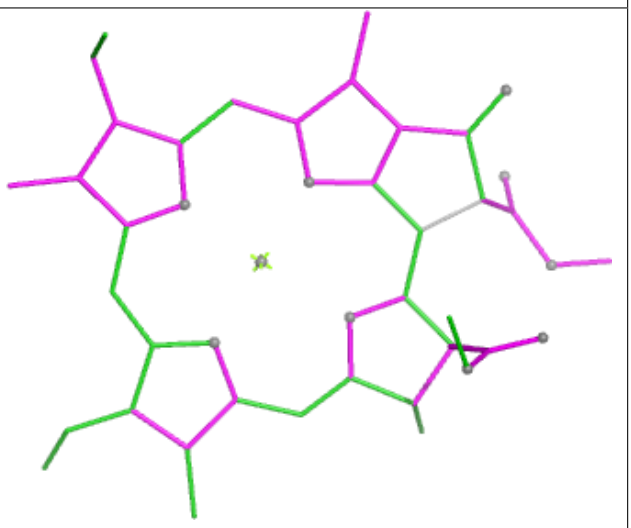


Rings

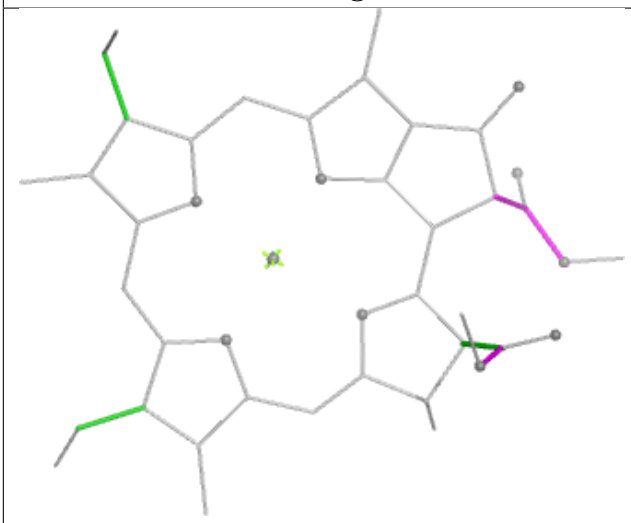
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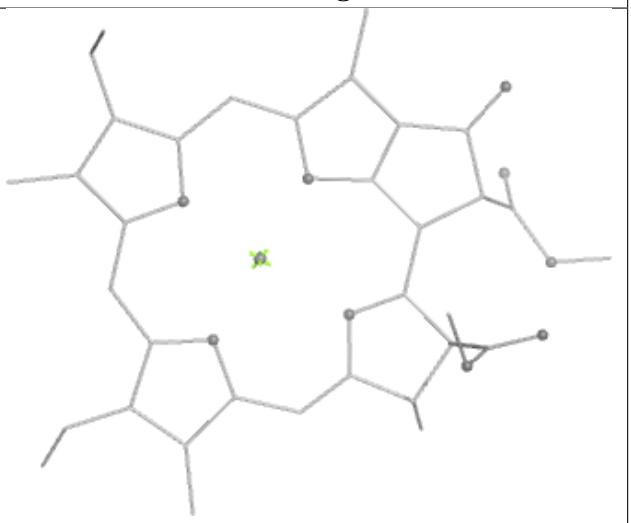
Bond lengths



Bond angles

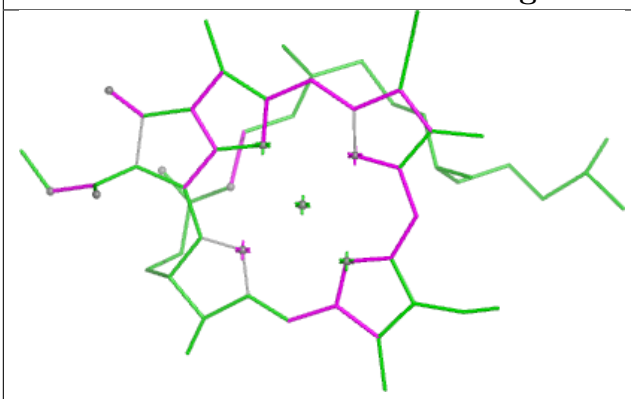


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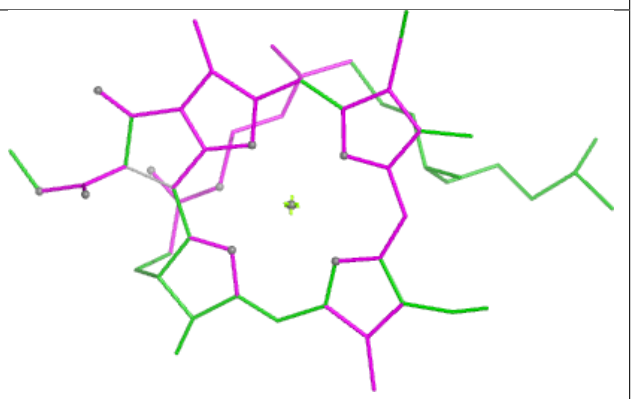


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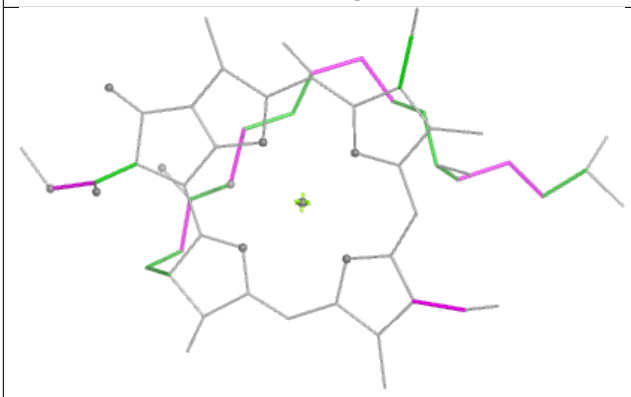
Ligand CLA 3 3003



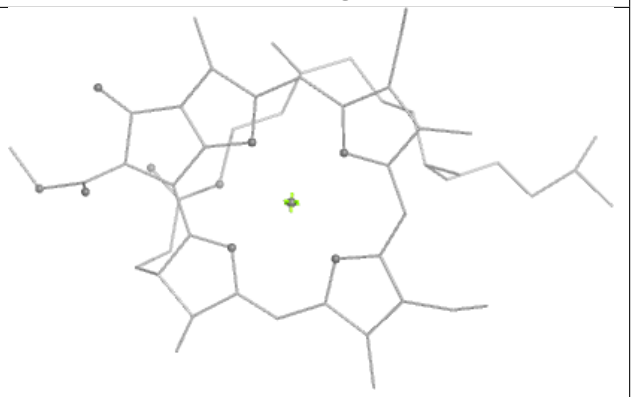
Bond lengths



Bond angles

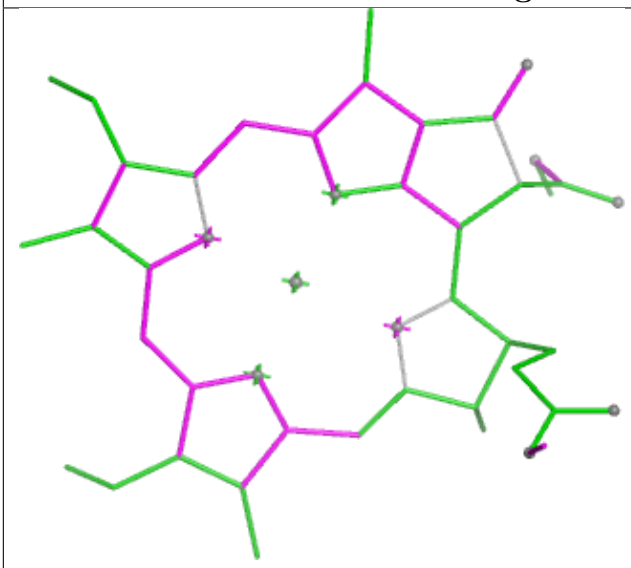


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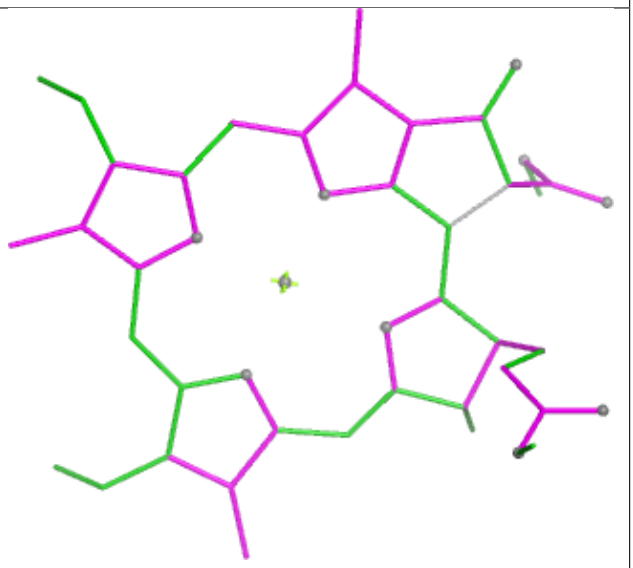


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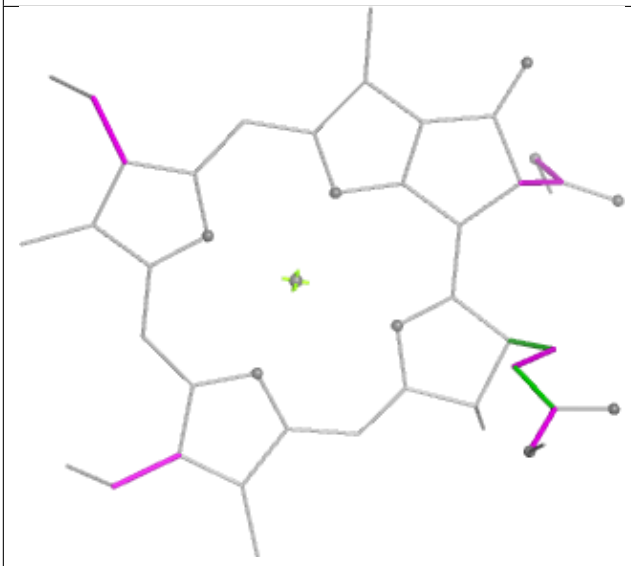
Ligand CLA A 1118



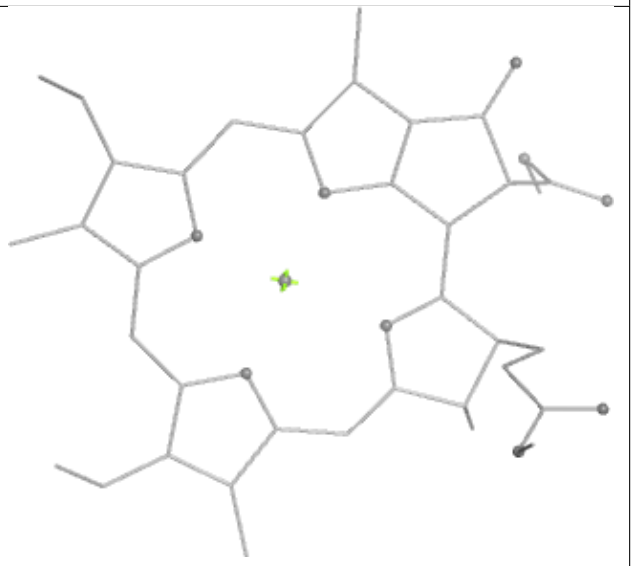
Bond lengths



Bond angles

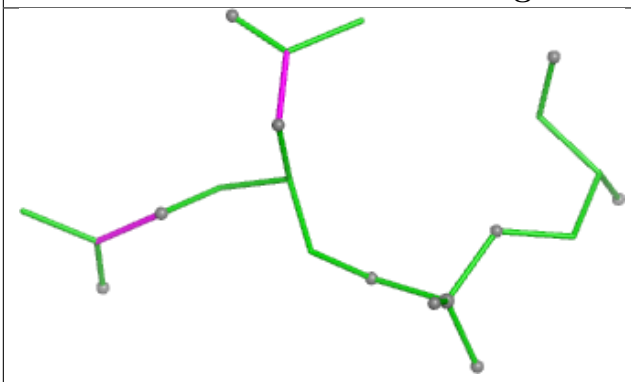


Torsions



Rings

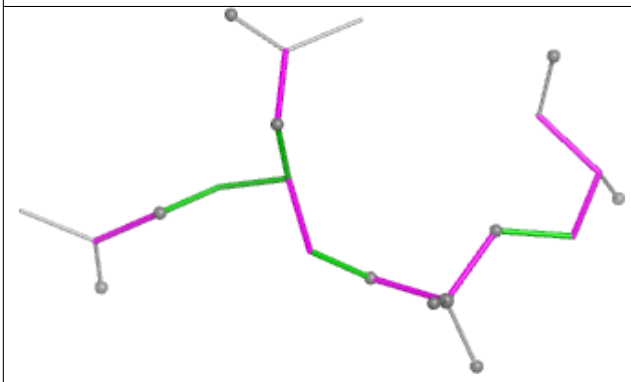
Ligand LHG B 5004



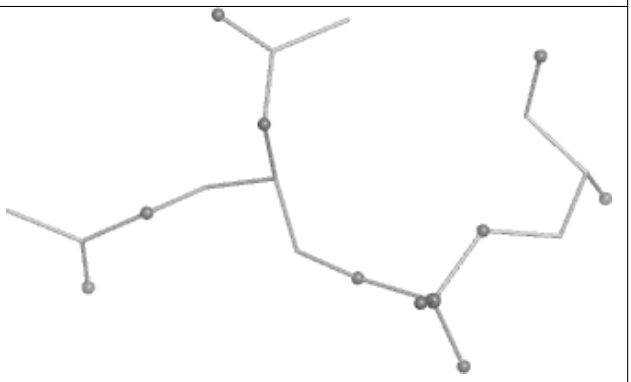
Bond lengths



Bond angles

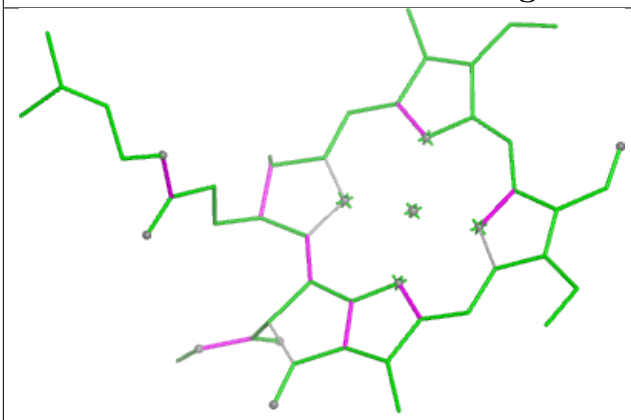


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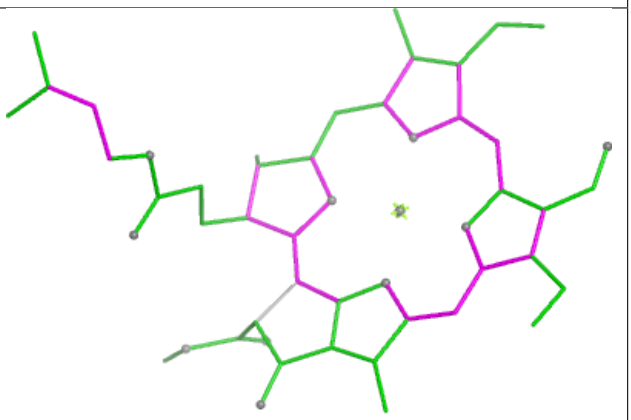


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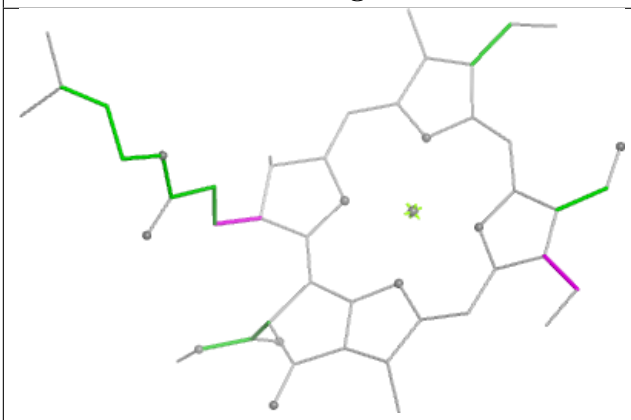
Ligand CHL 4 4011



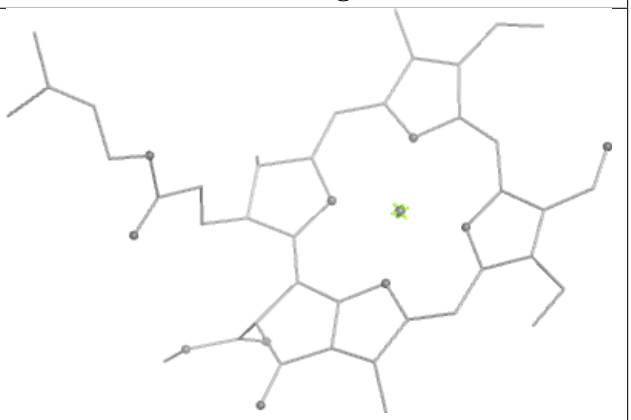
Bond lengths



Bond angles

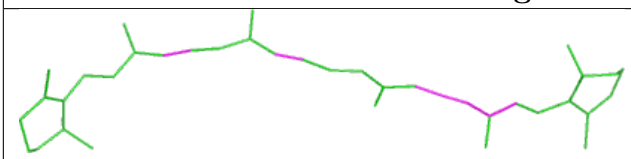


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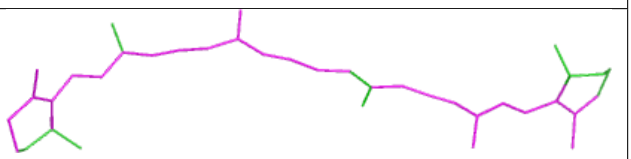


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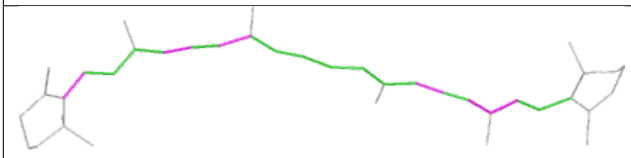
Ligand BCR B 6010



Bond lengths



Bond angles

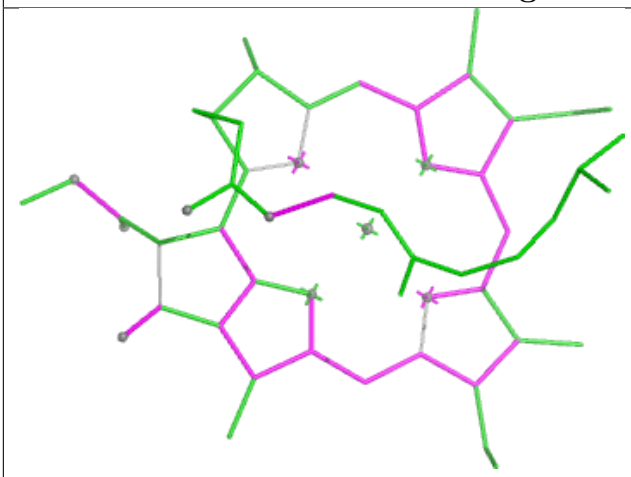


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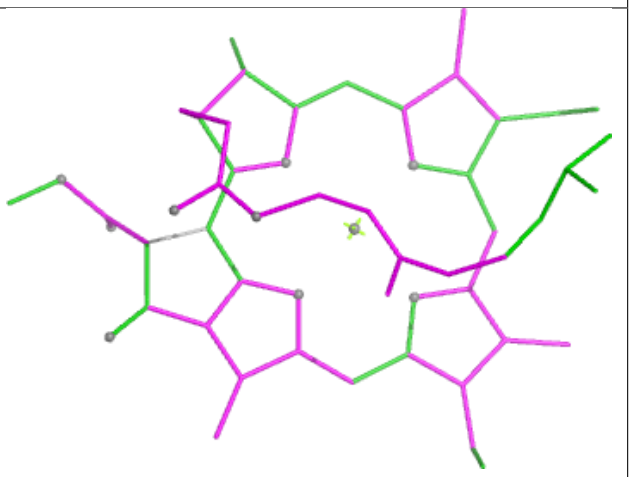


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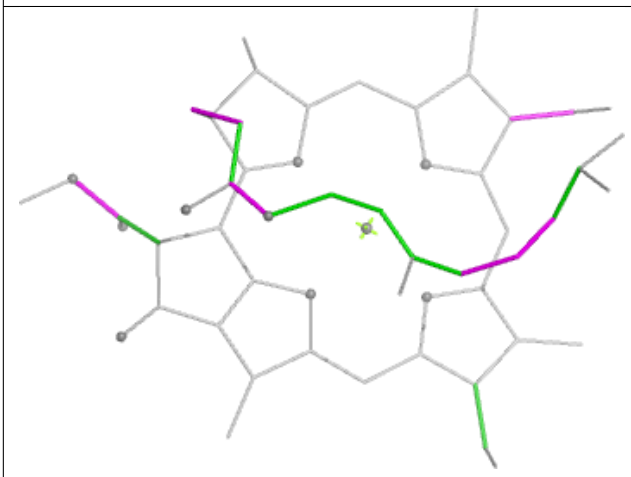
Ligand CLA 1 1003



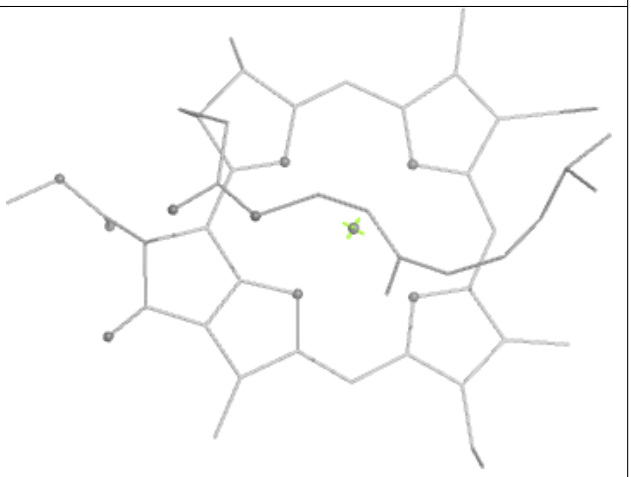
Bond lengths



Bond angles

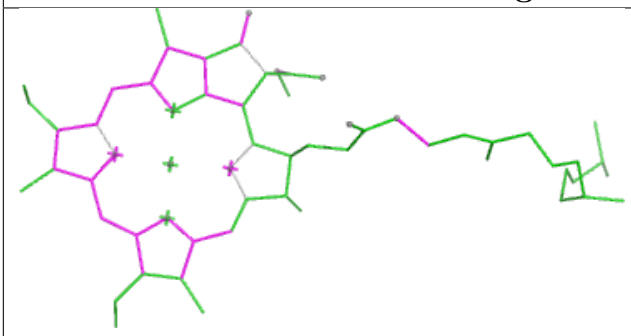


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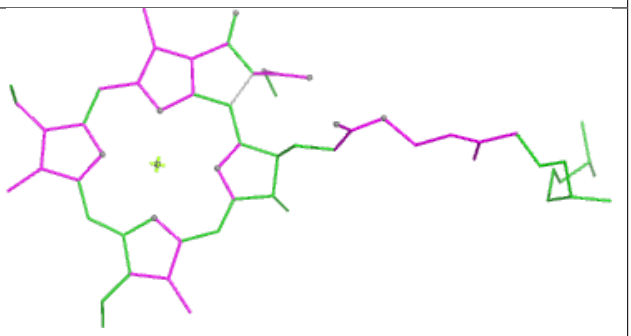


Rings

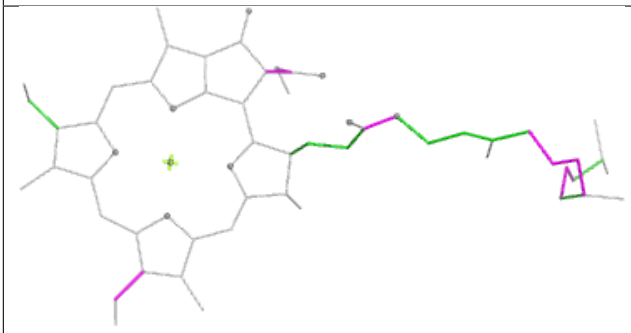
Ligand CLA B 1234



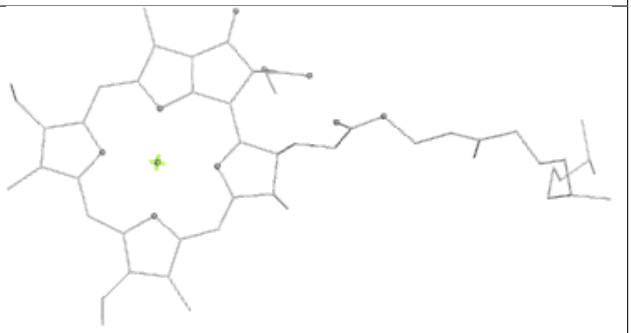
Bond lengths



Bond angles

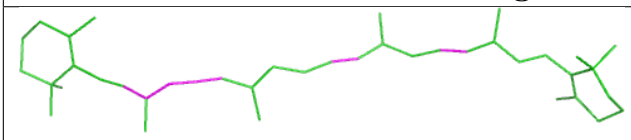


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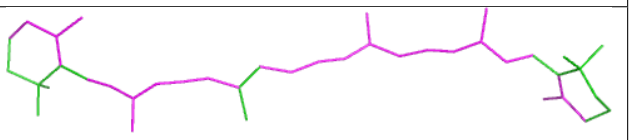


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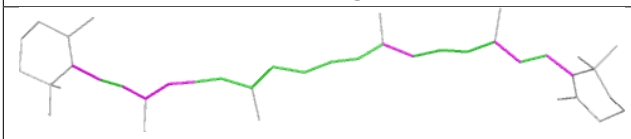
Ligand BCR A 6003



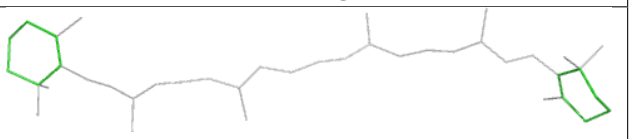
Bond lengths



Bond angles

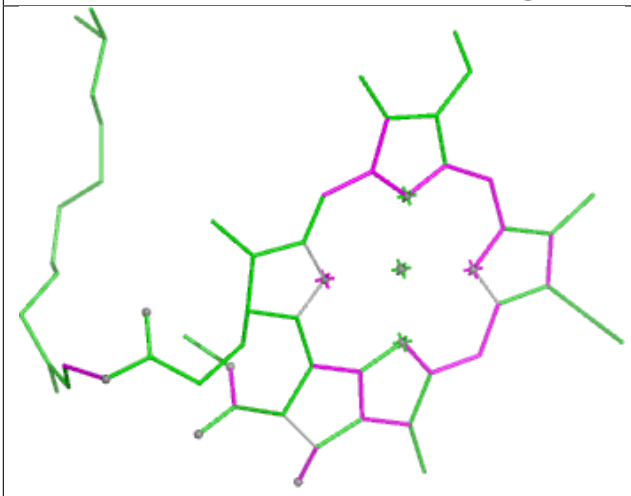


Torsions

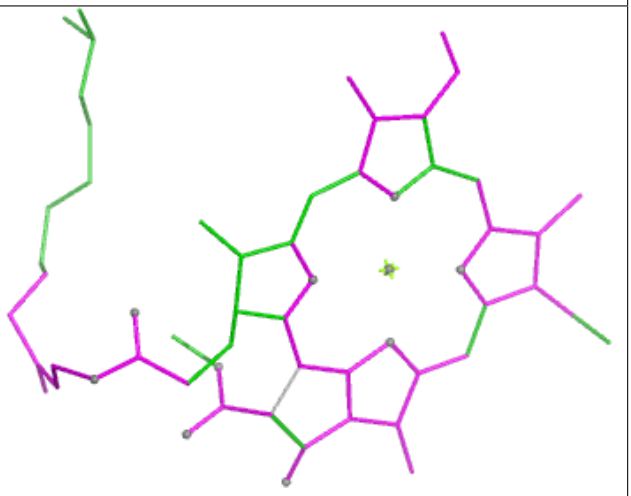


Rings

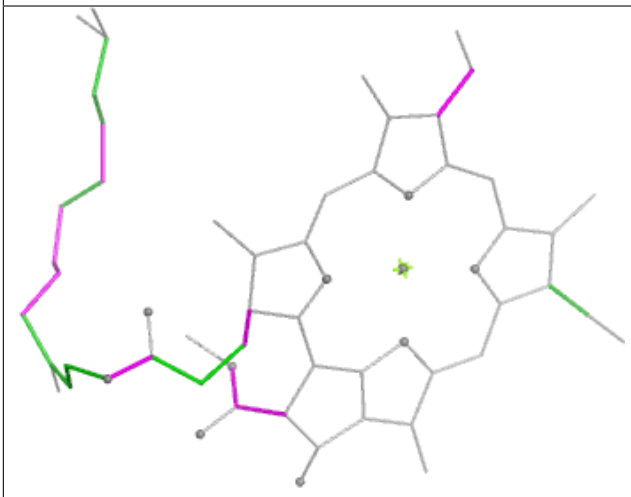
Ligand CLA 4 4005



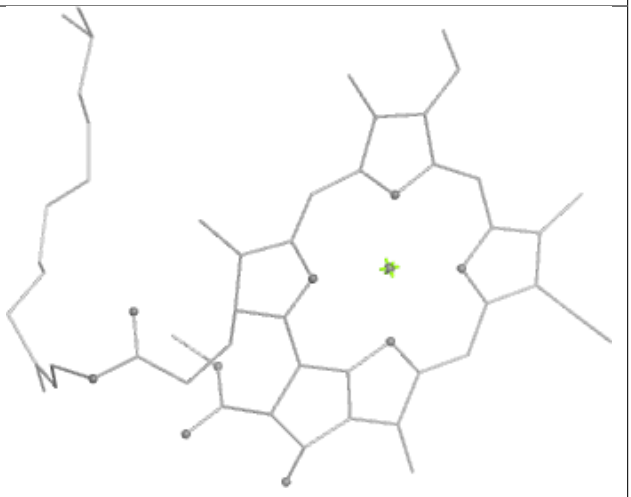
Bond lengths



Bond angles

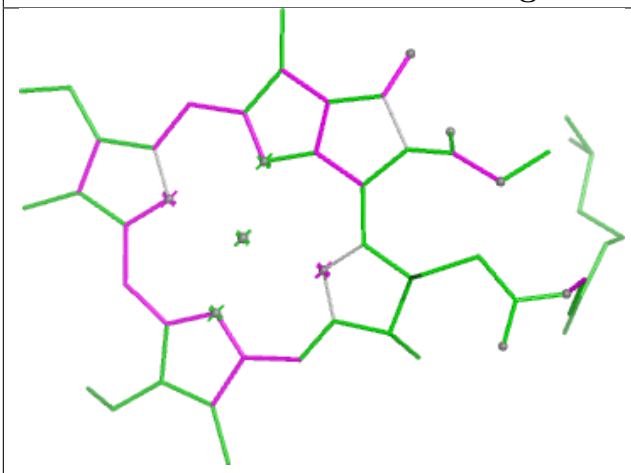


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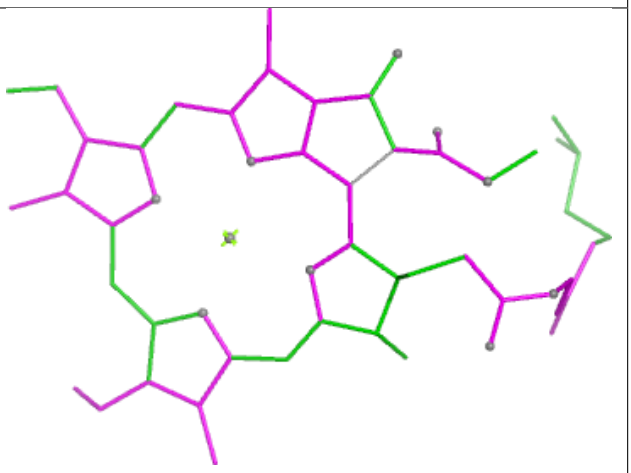


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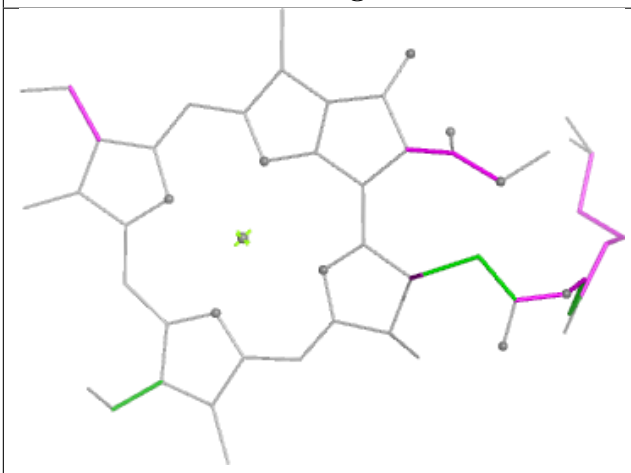
Ligand CLA 3 3005



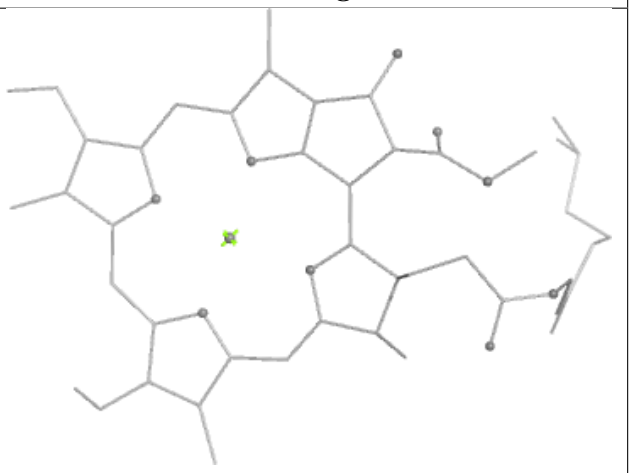
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Bond angles

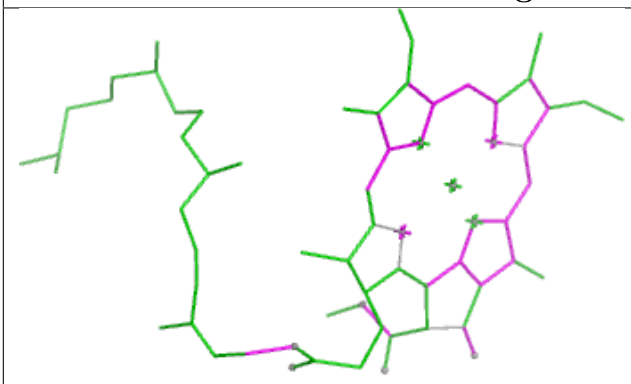


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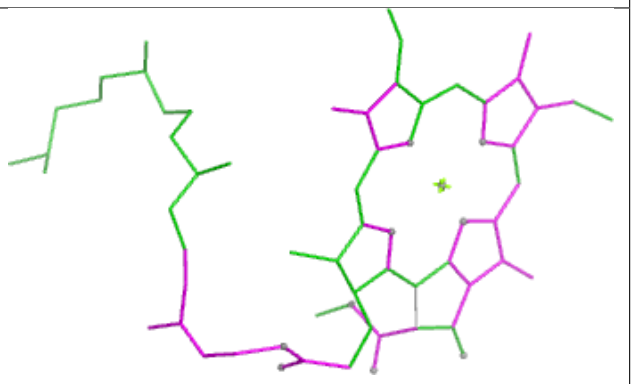


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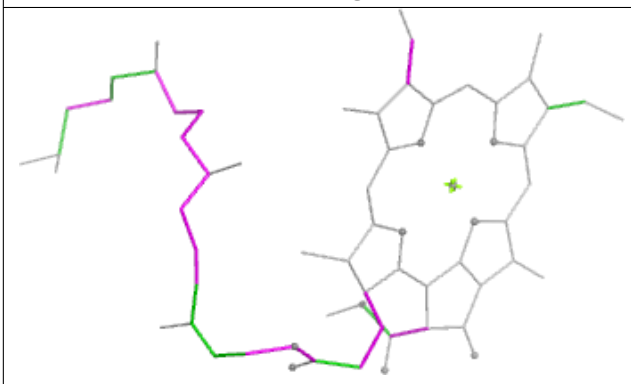
Ligand CLA B 1221



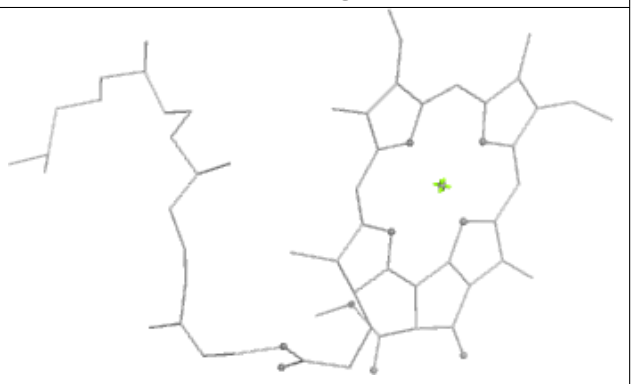
Bond lengths



Bond angles

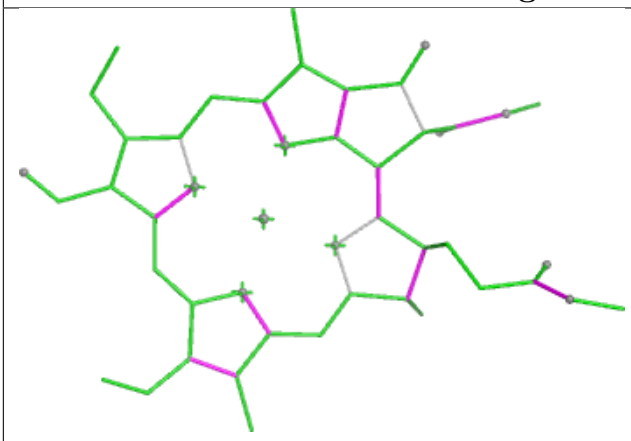


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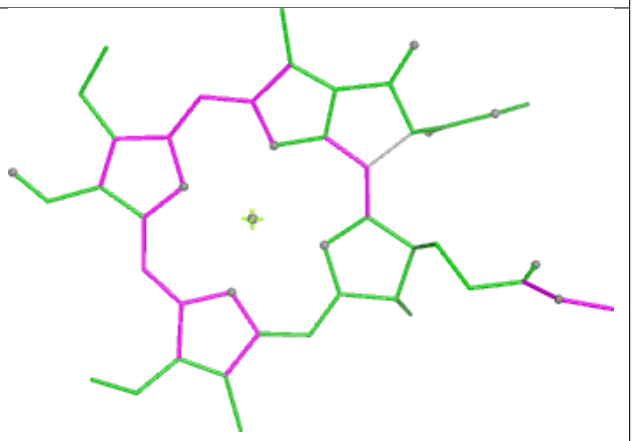


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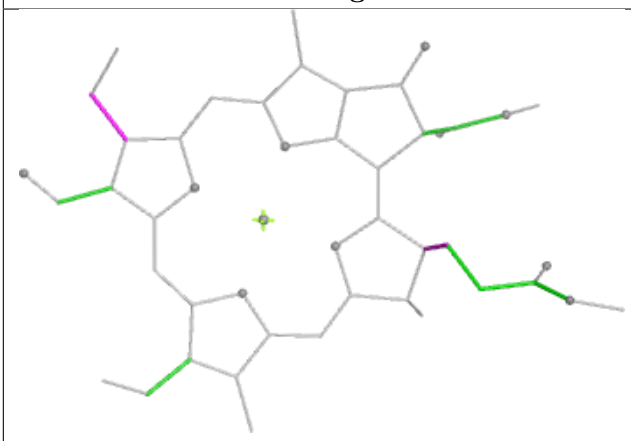
Ligand CHL 4 4013



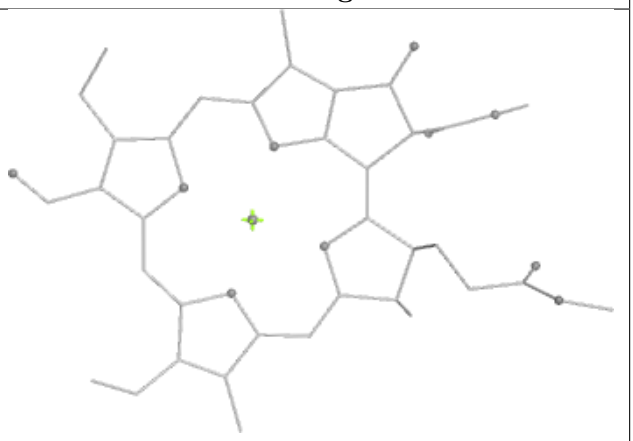
Bond lengths



Bond angles

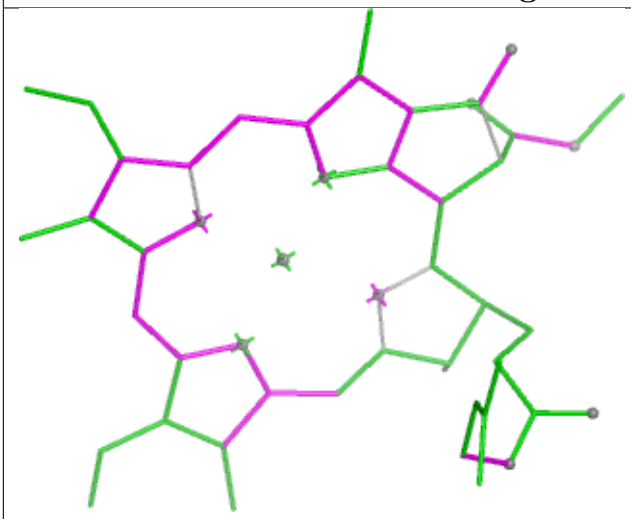


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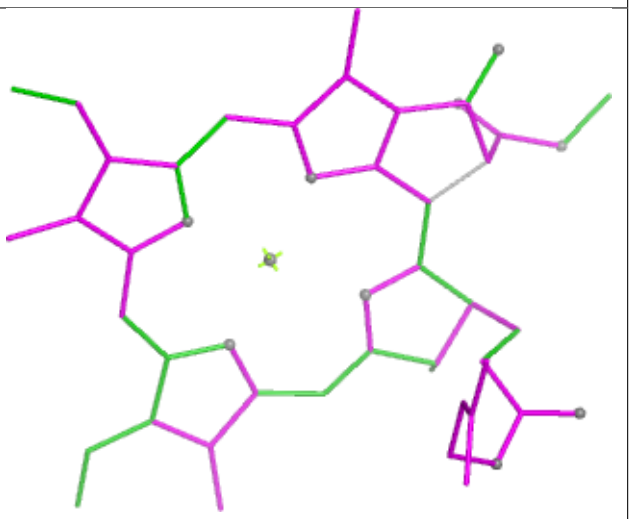


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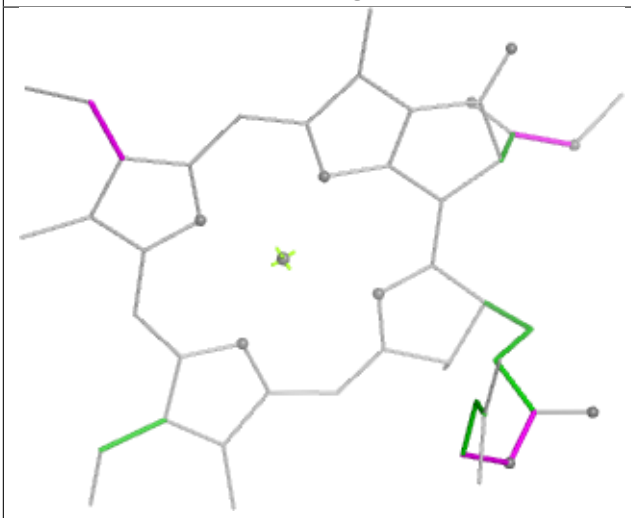
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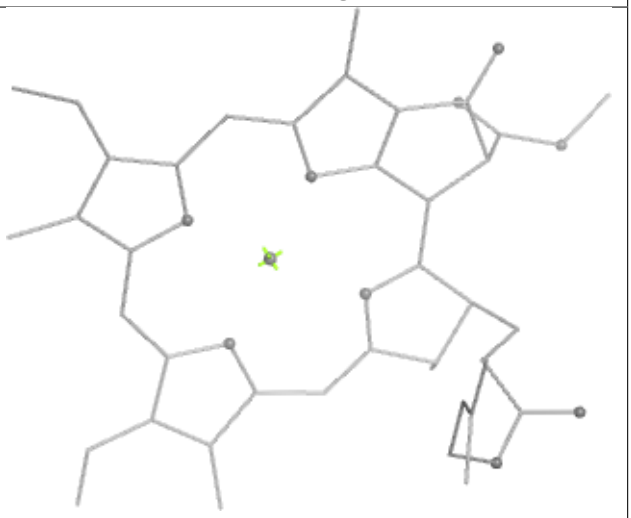
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Bond angles

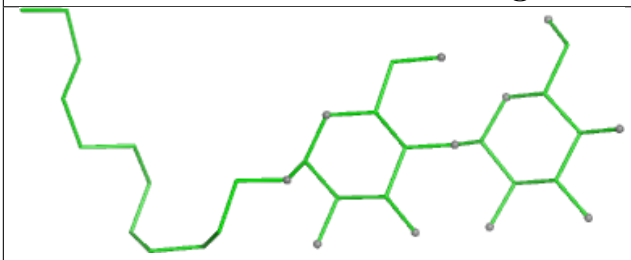


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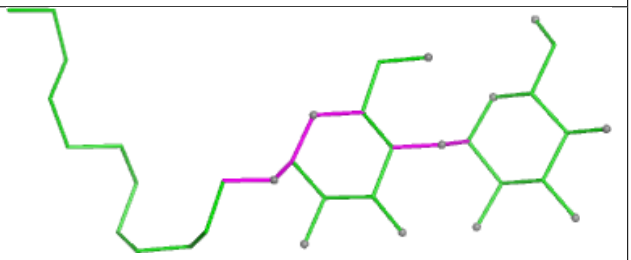


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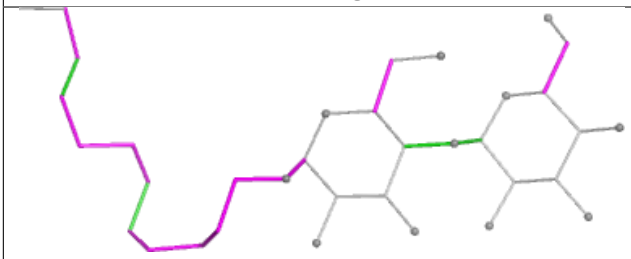
Ligand LMU B 8002



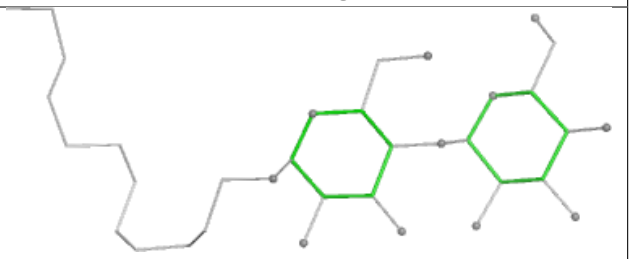
Bond lengths



Bond angles

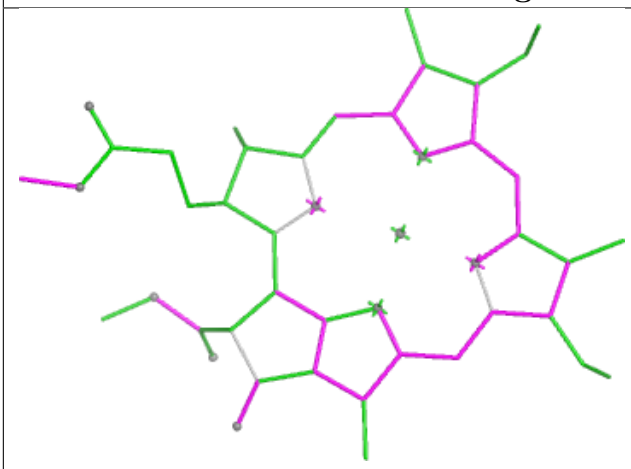


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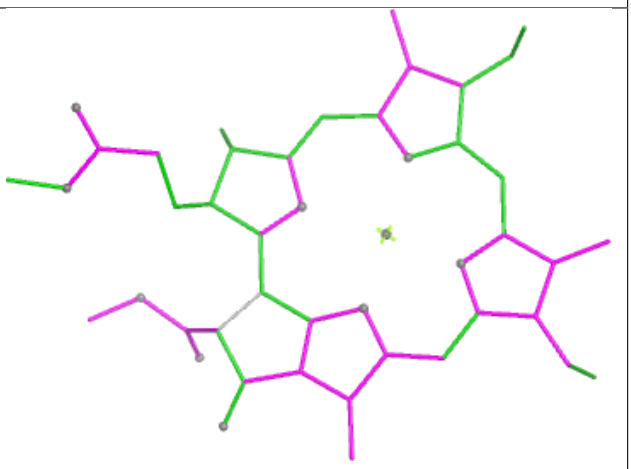


Rings

Ligand CLA H 1000



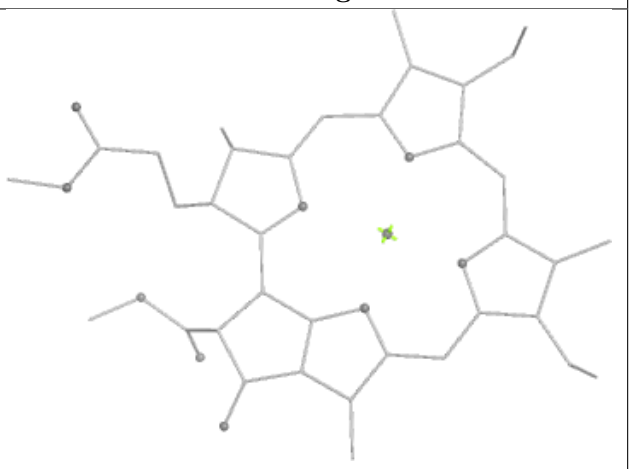
Bond lengths



Bond angles

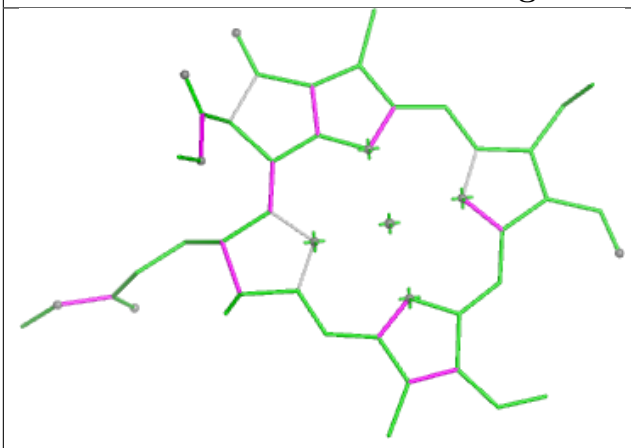


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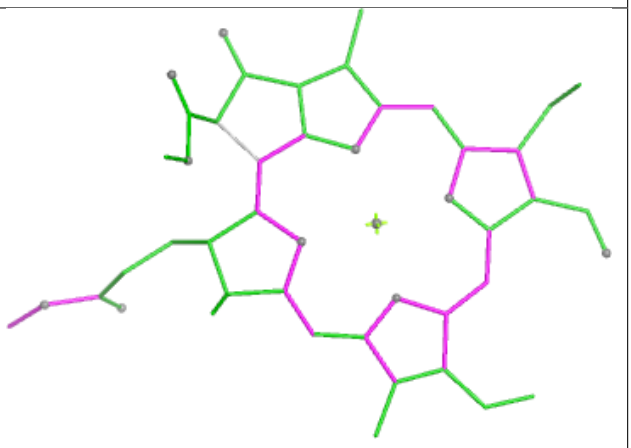


Rings

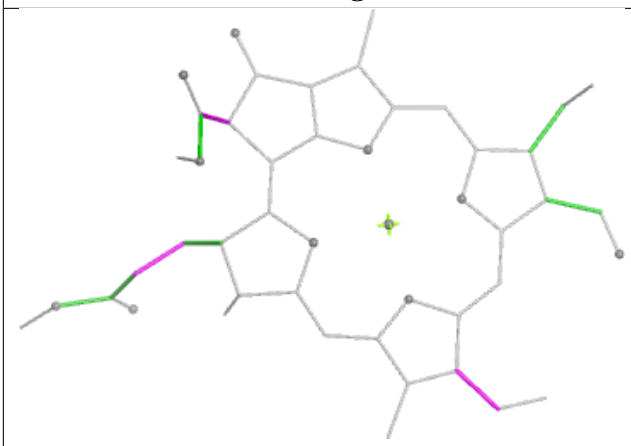
Ligand CHL 2 2010



Bond lengths



Bond angles

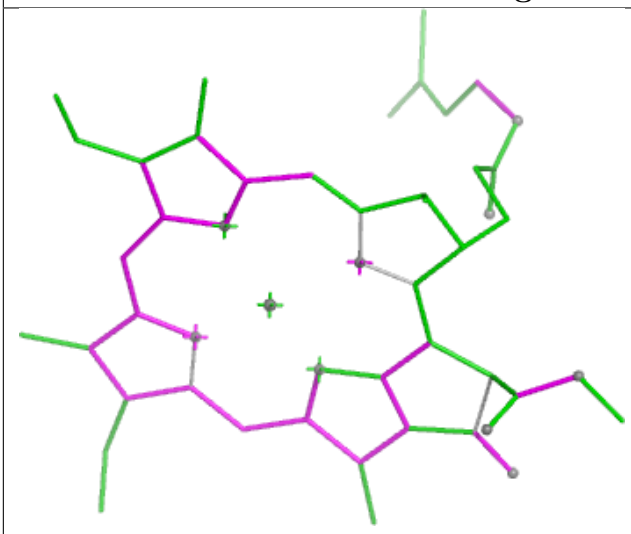


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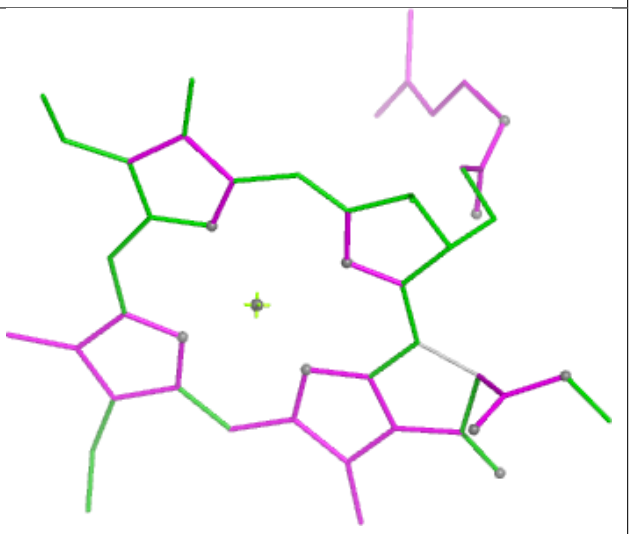


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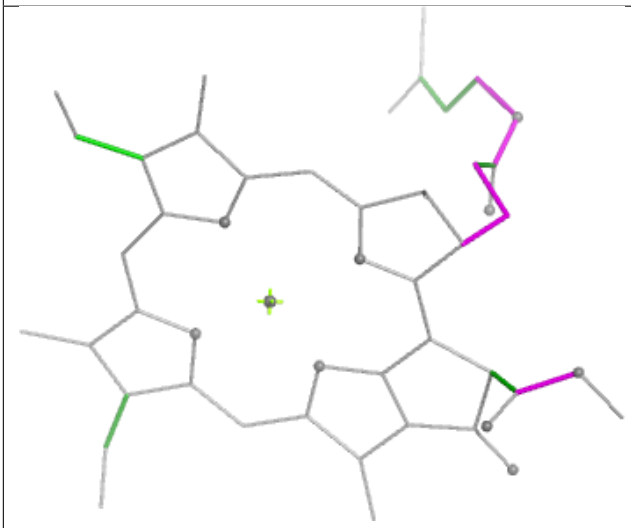
Ligand CLA A 1130



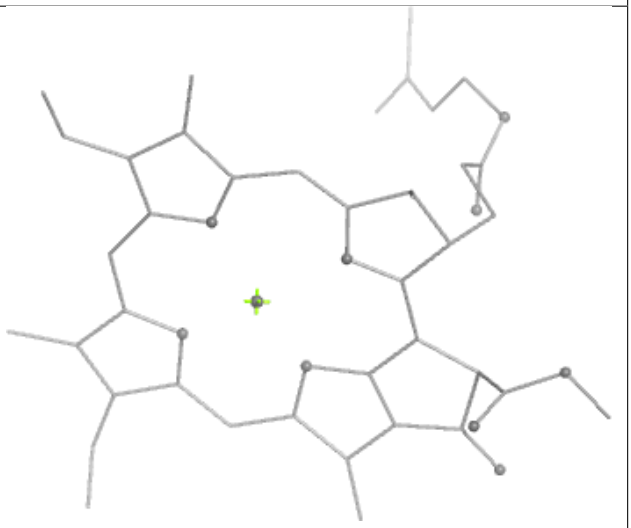
Bond lengths



Bond angles

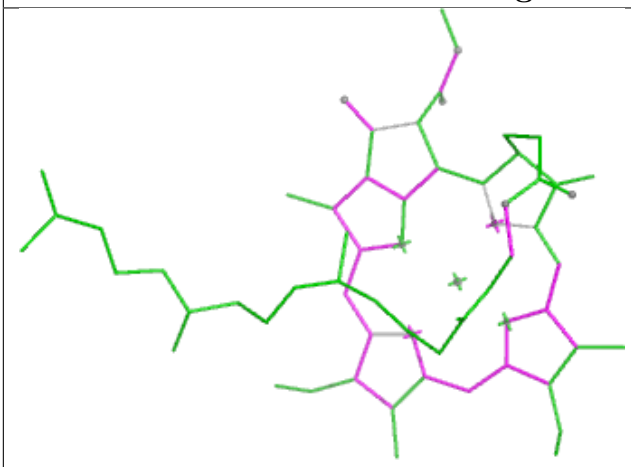


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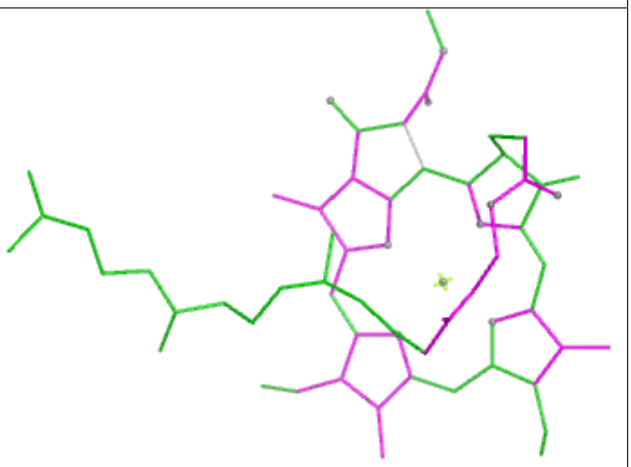


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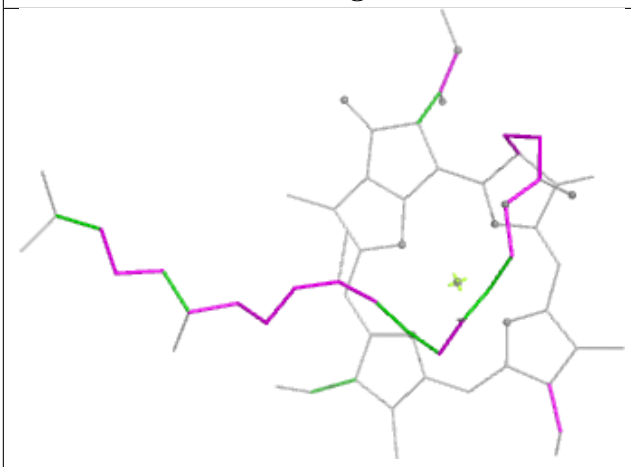
Ligand CLA B 1224



Bond lengths



Bond angles

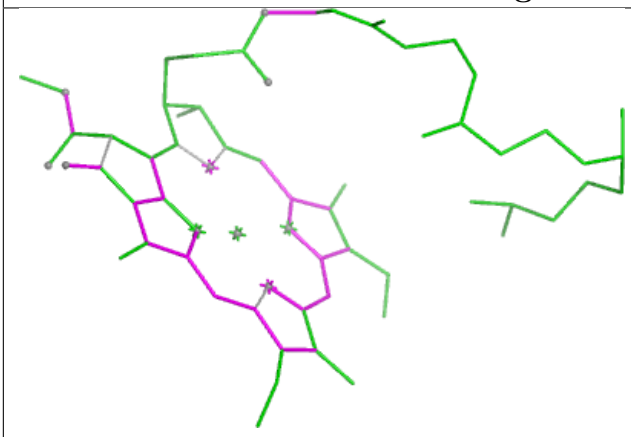


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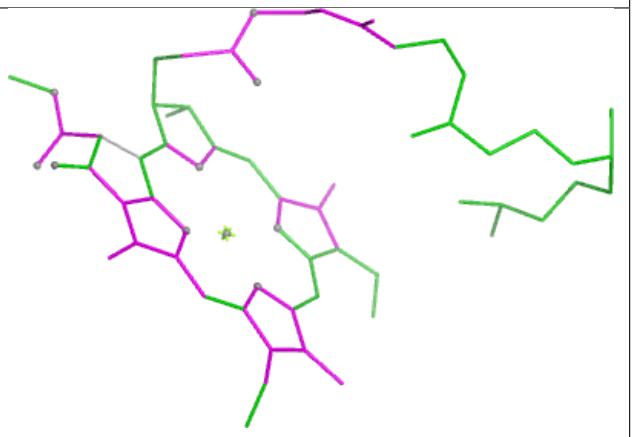


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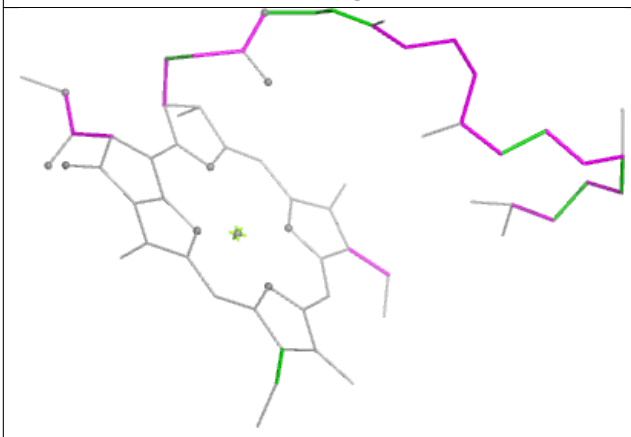
Ligand CLA A 1122



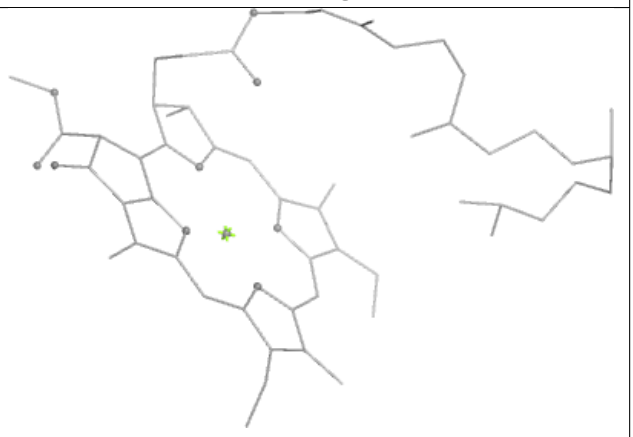
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Bond angles

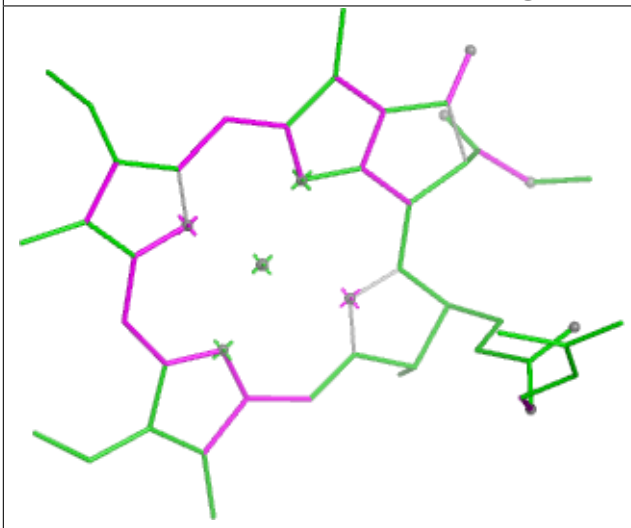


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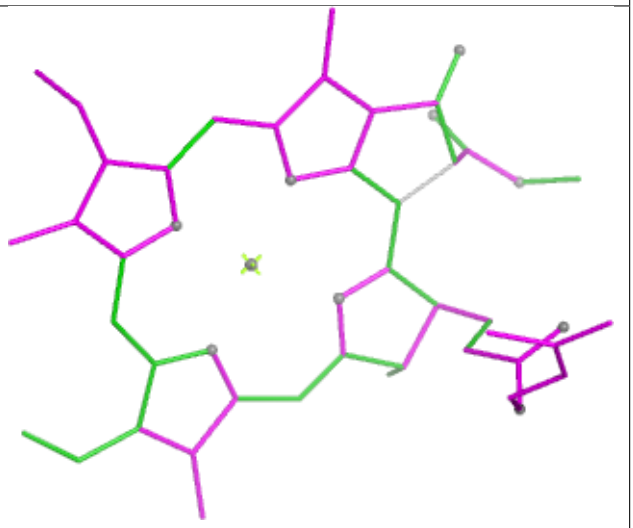


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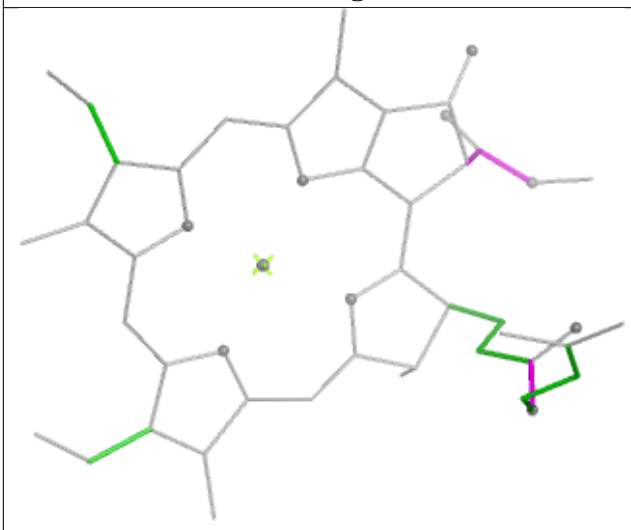
Ligand CLA 4 4006



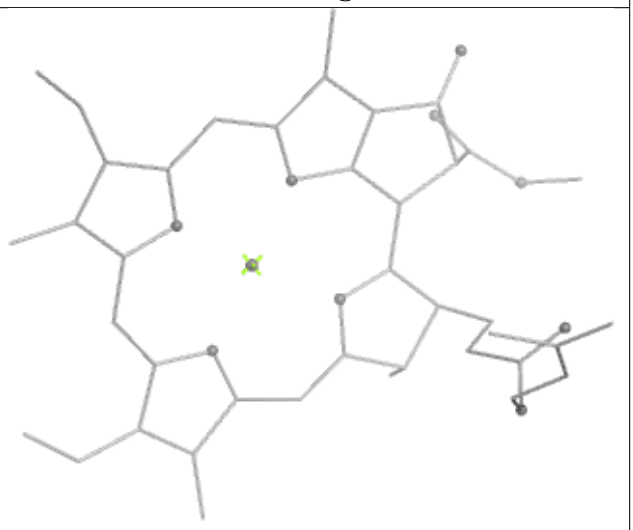
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Bond angles

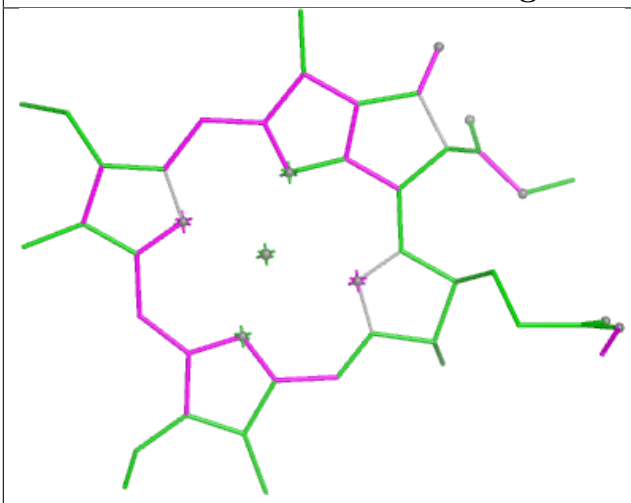


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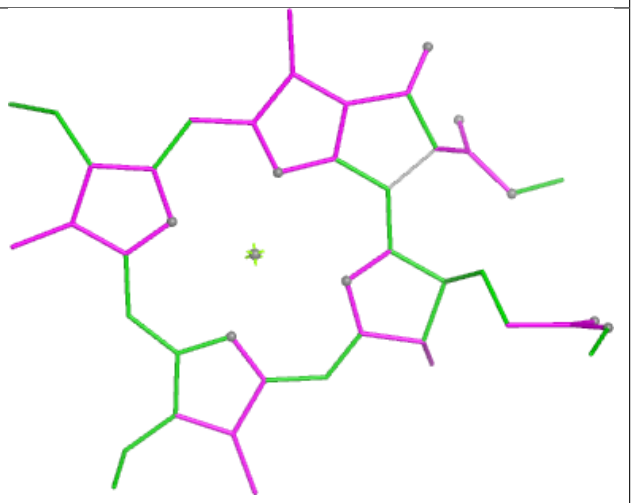


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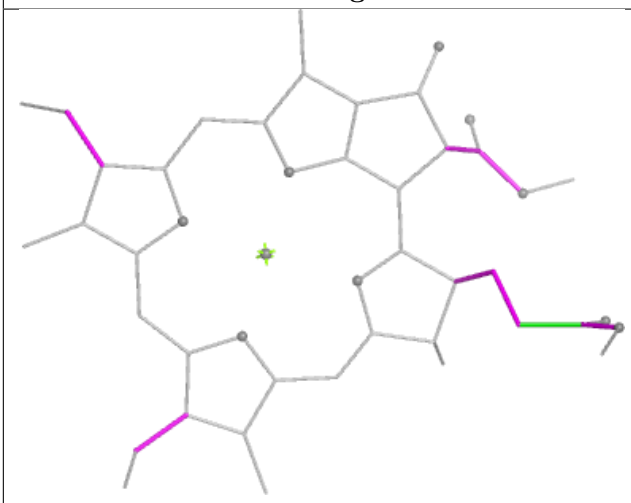
Ligand CLA 3 3013



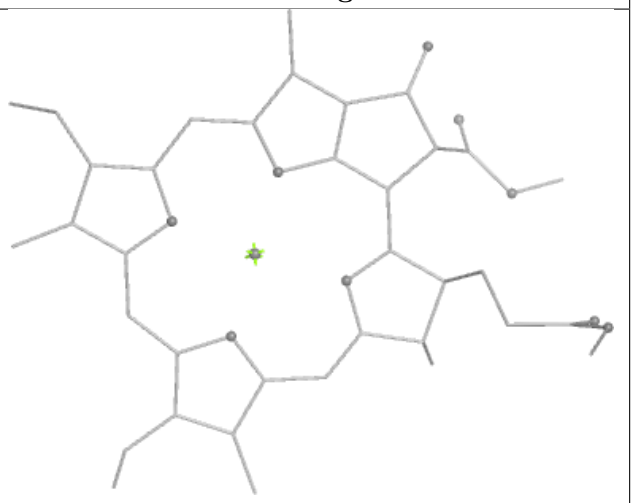
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Bond angles

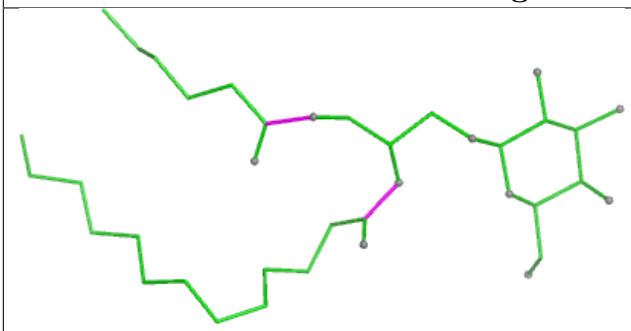


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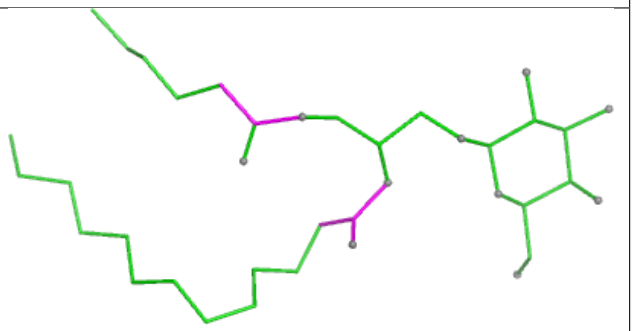


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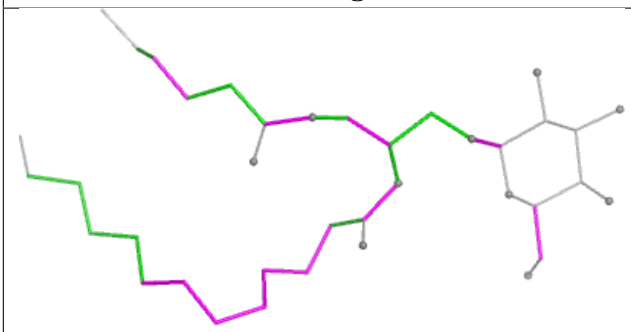
Ligand LMG B 5005



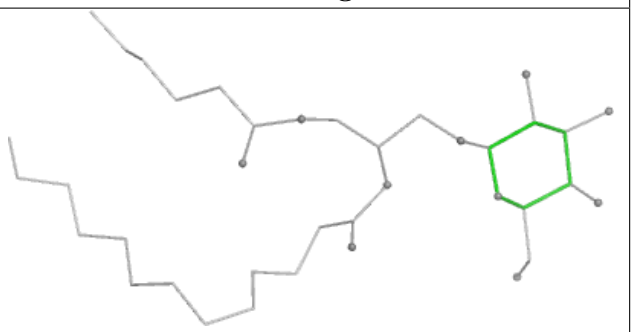
Bond lengths



Bond angles

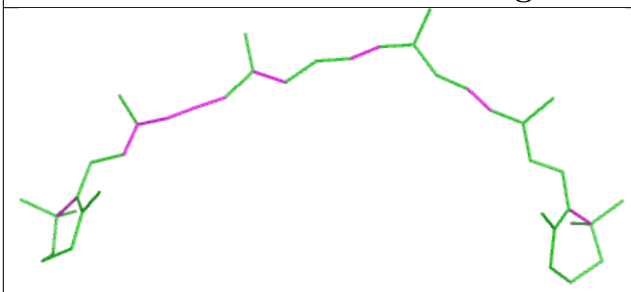


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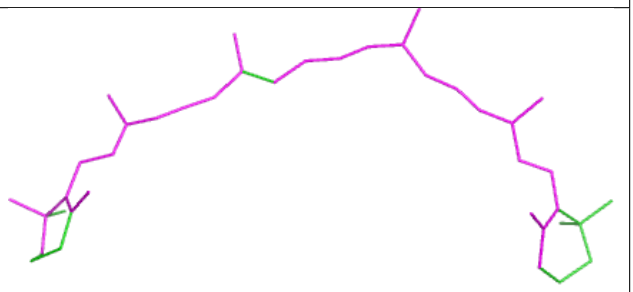


Rings

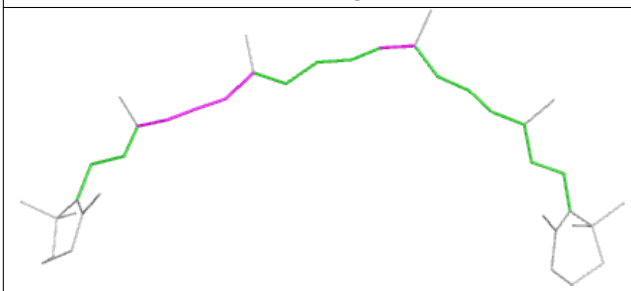
Ligand BCR F 6016



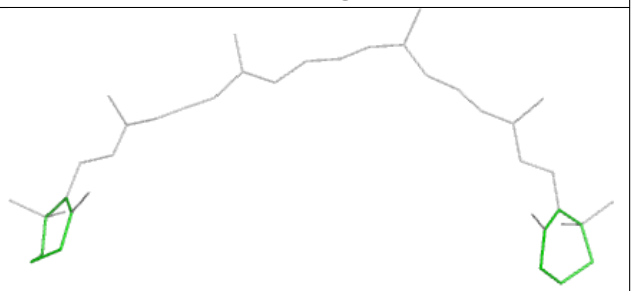
Bond lengths



Bond angles

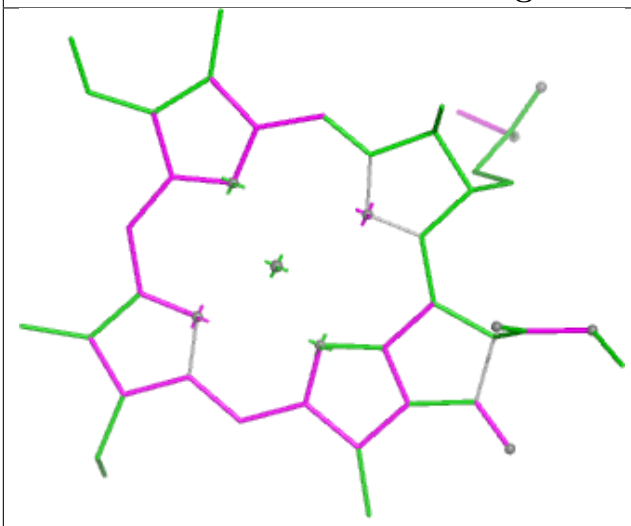


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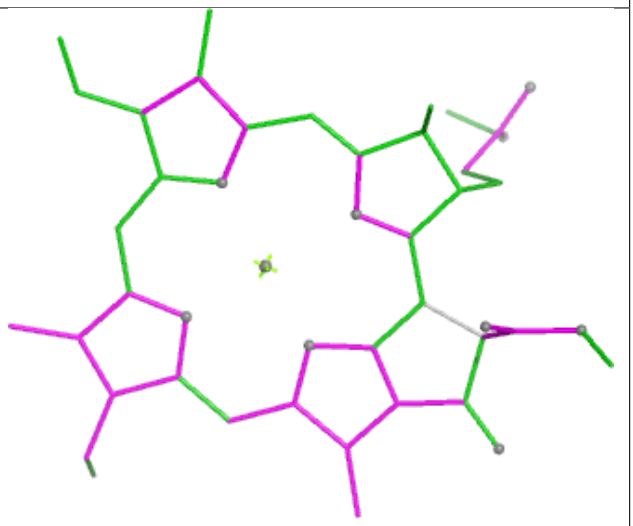


Rings

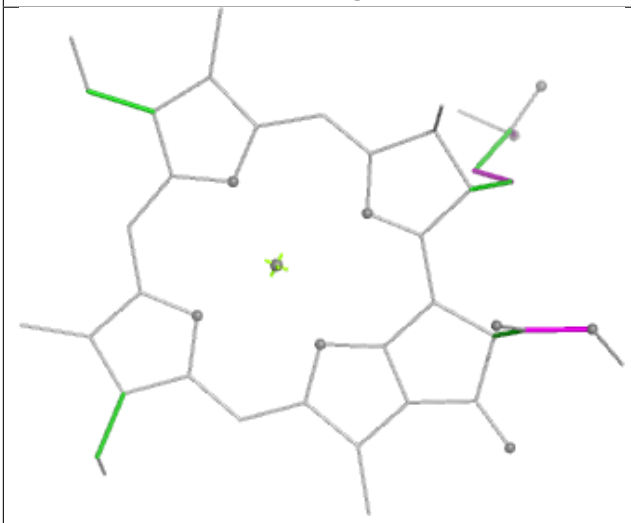
Ligand CLA B 1209



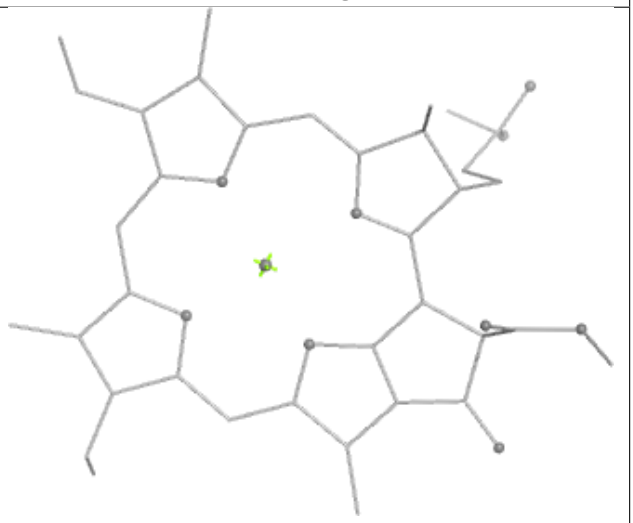
Bond lengths



Bond angles

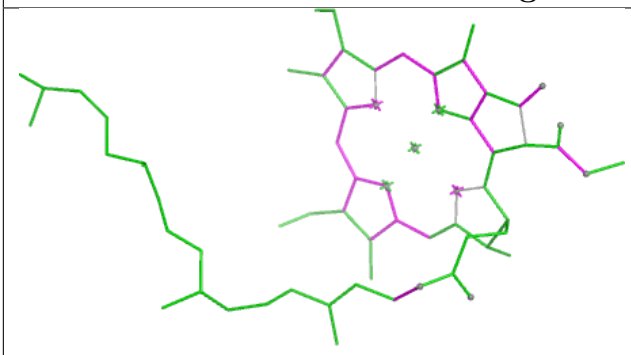


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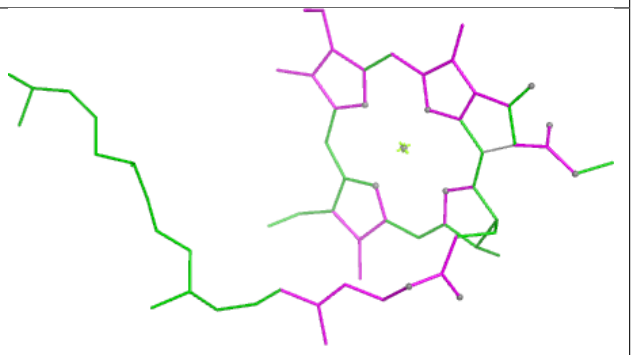


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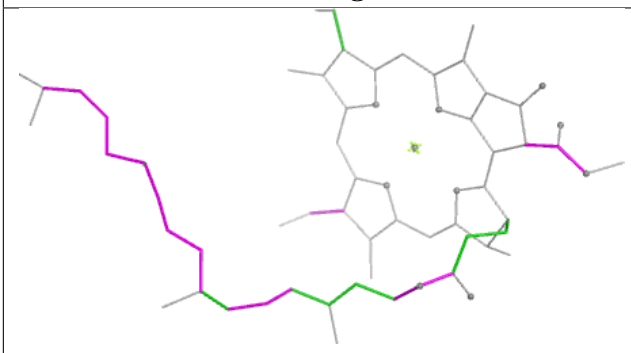
Ligand CLA 1 1004



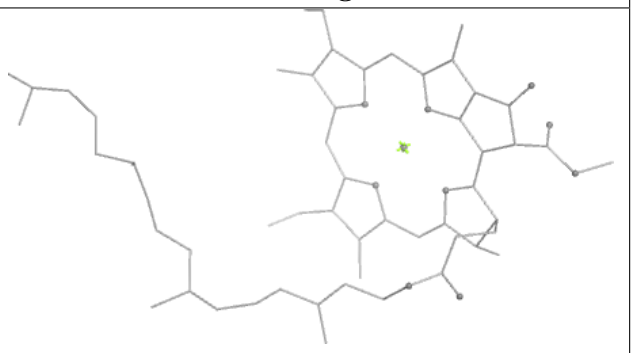
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Bond angles

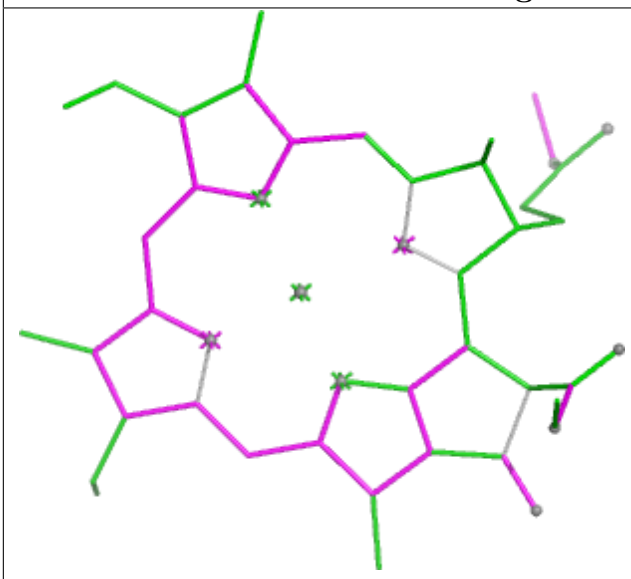


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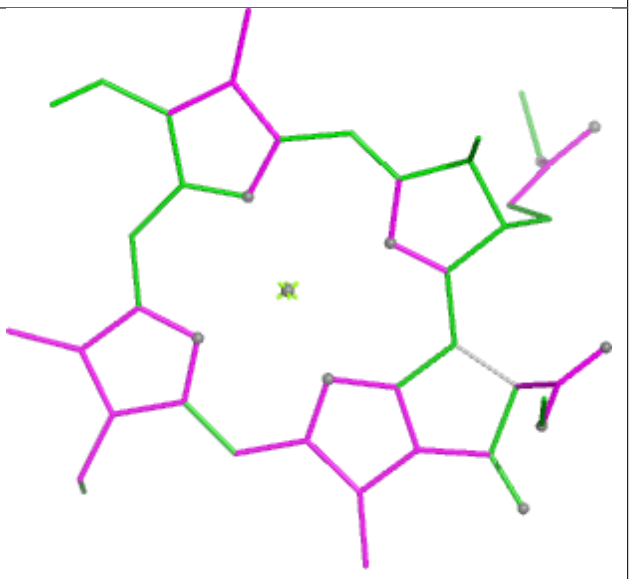


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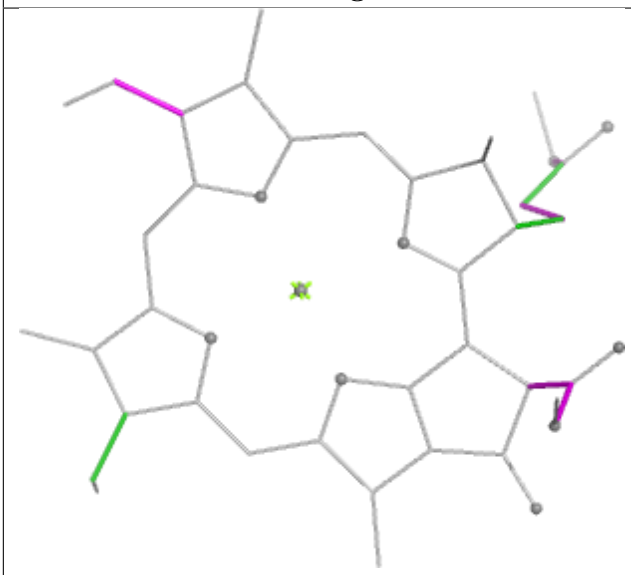
Ligand CLA B 1217



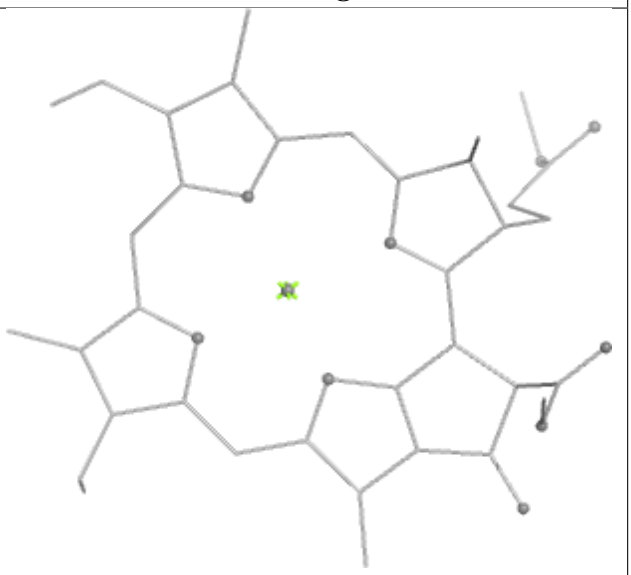
Bond lengths



Bond angles

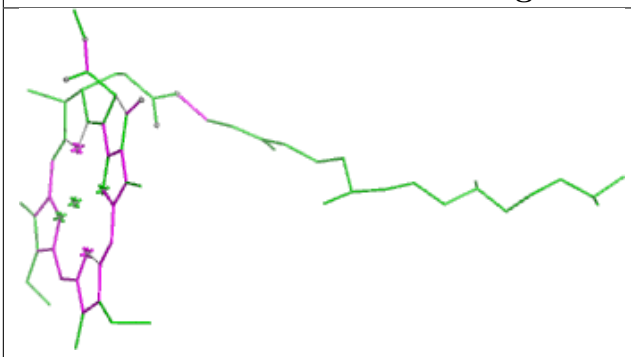


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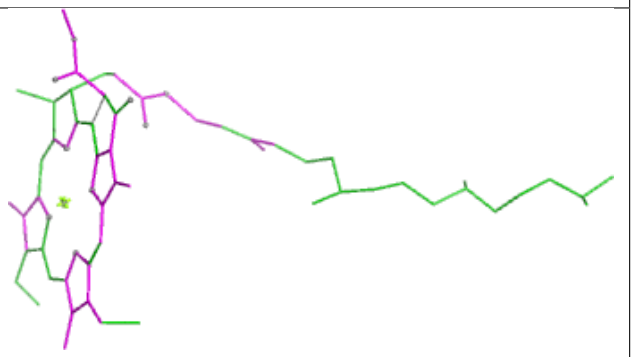


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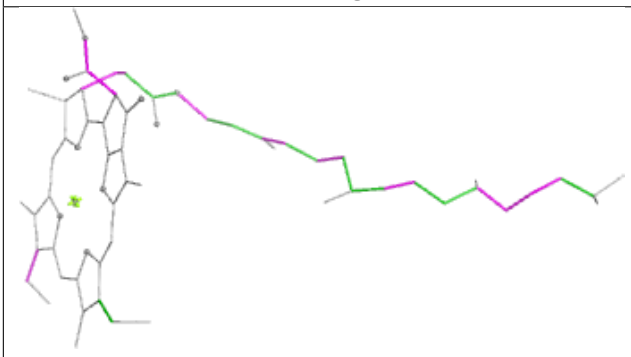
Ligand CLA B 1225



Bond lengths



Bond angles

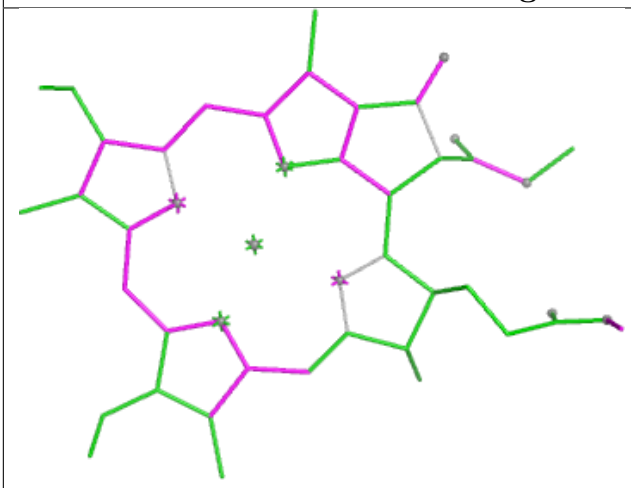


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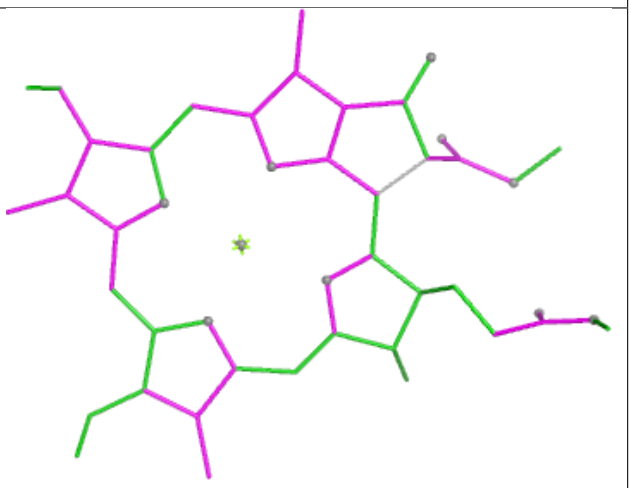


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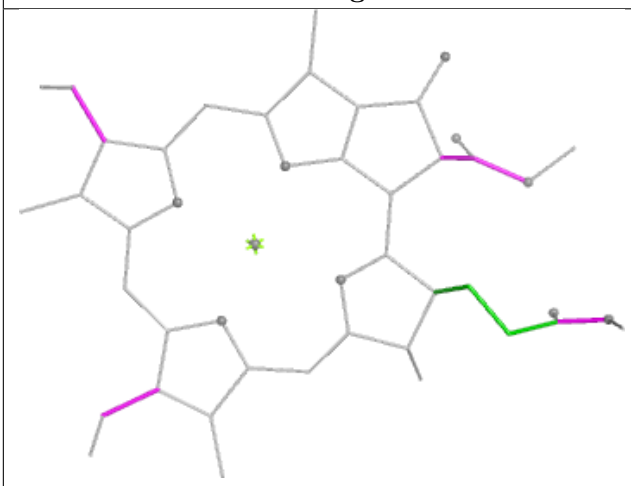
Ligand CLA 1 1013



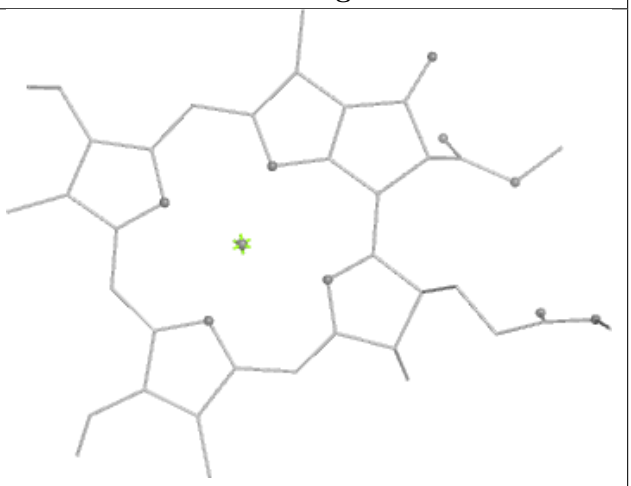
Bond lengths



Bond angles

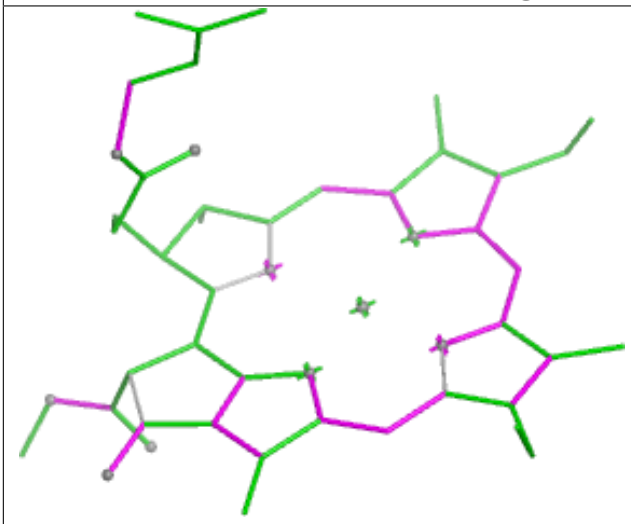


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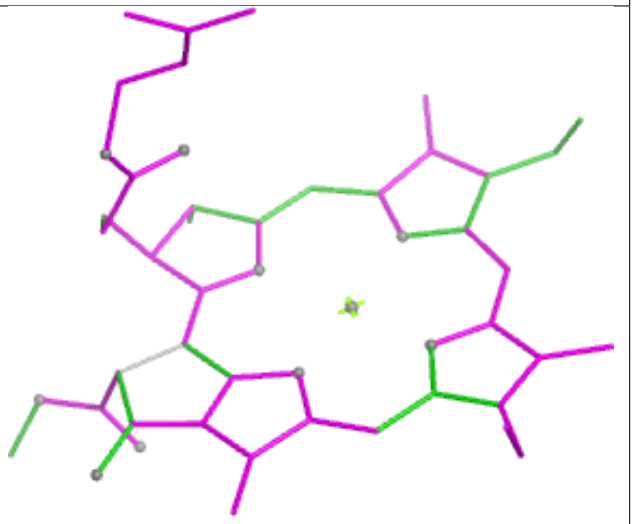


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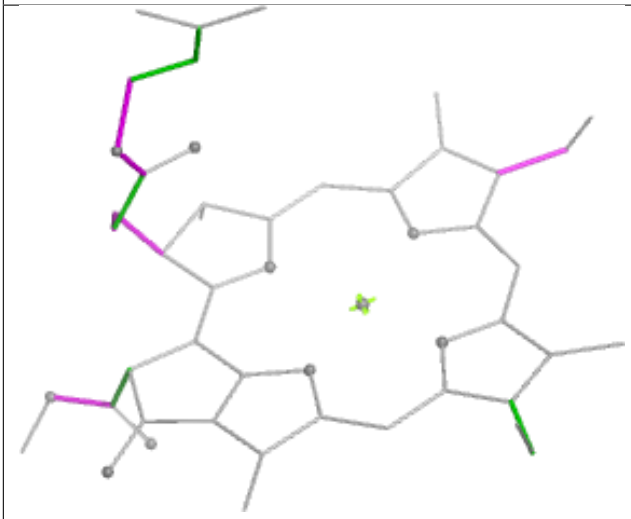
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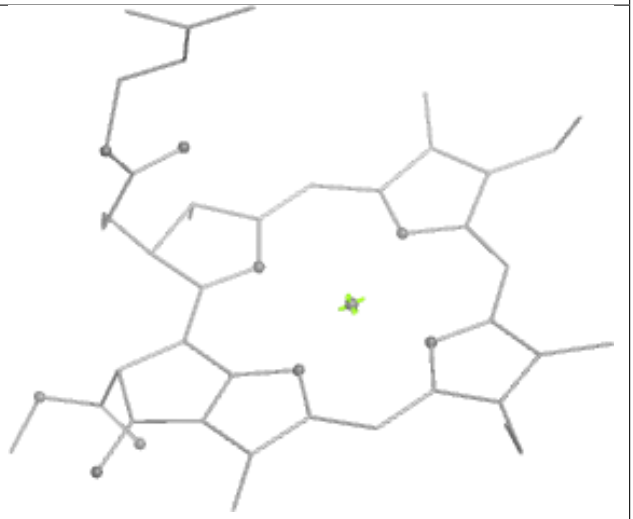
Bond lengths



Bond angles

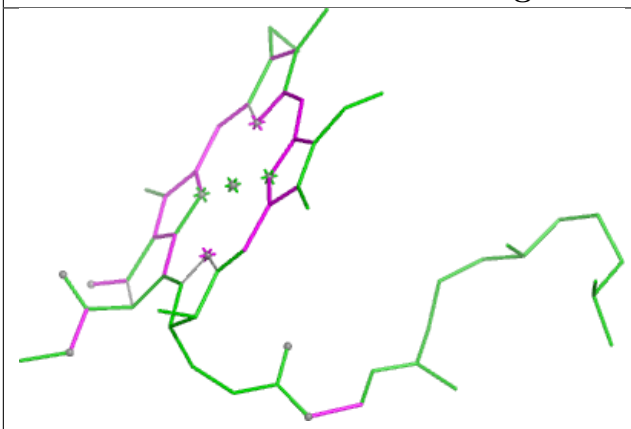


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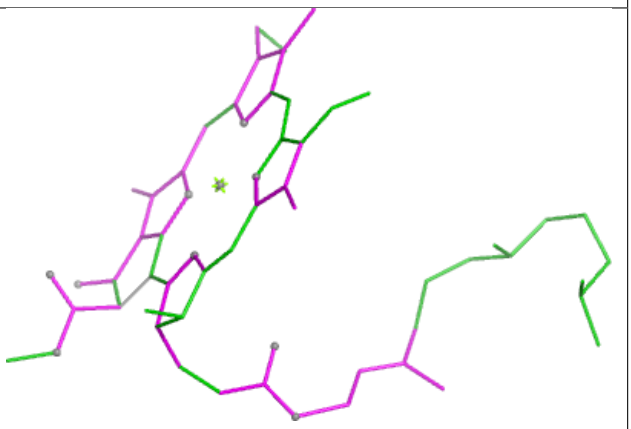


Rings

Ligand CLA G 1003



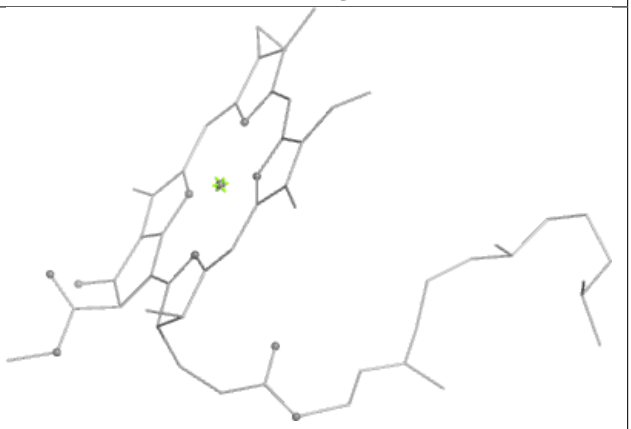
Bond lengths



Bond angles

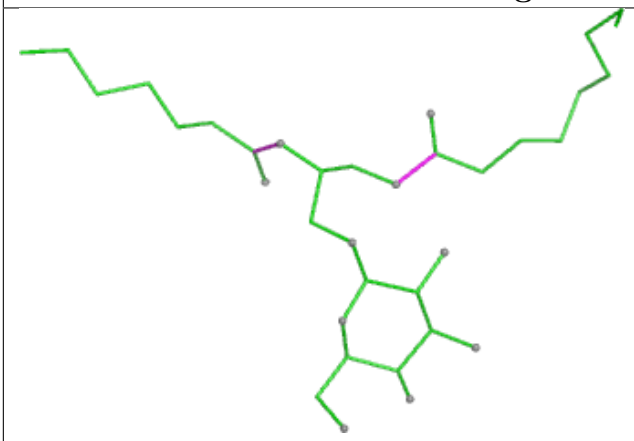


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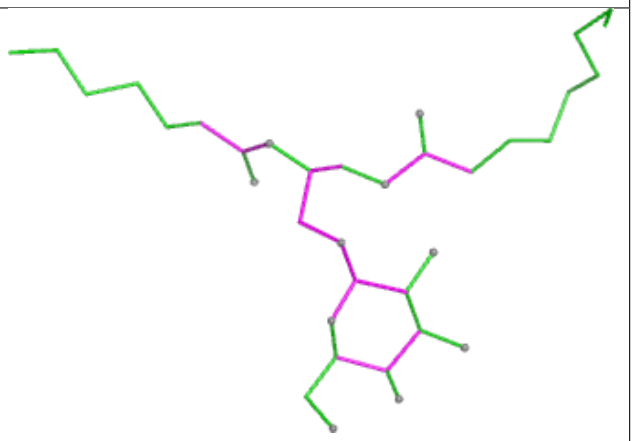


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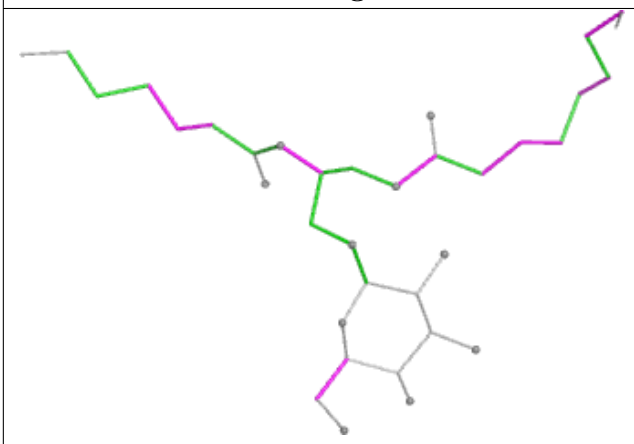
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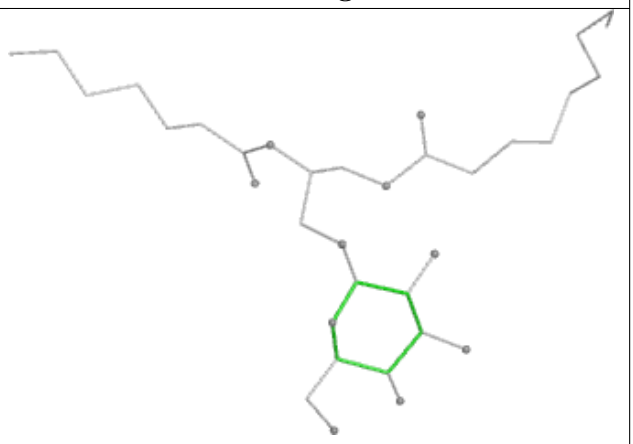
Bond lengths



Bond angles



Torsions

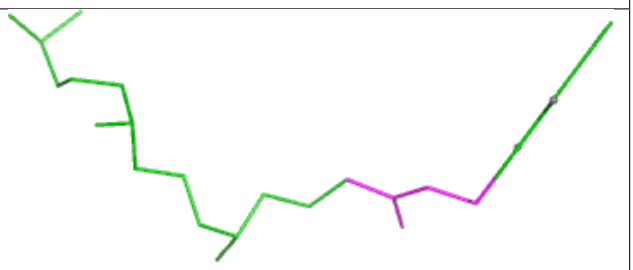


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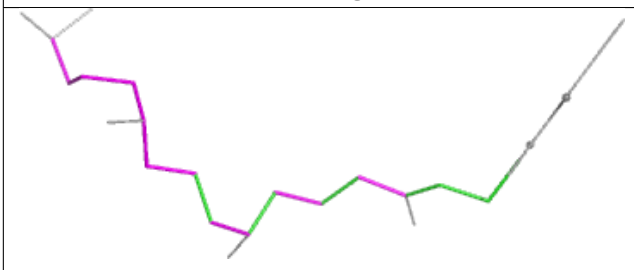
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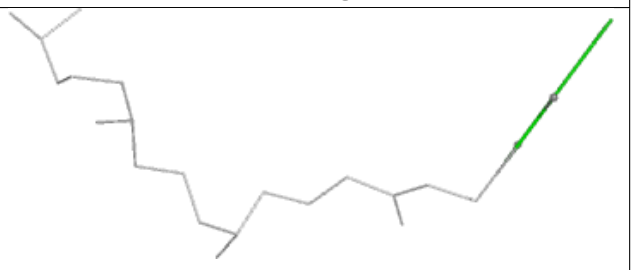
Bond lengths



Bond angles

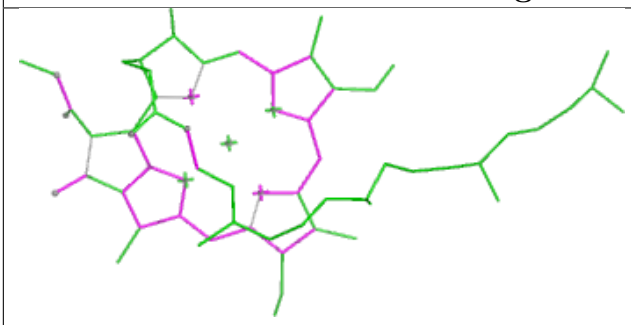


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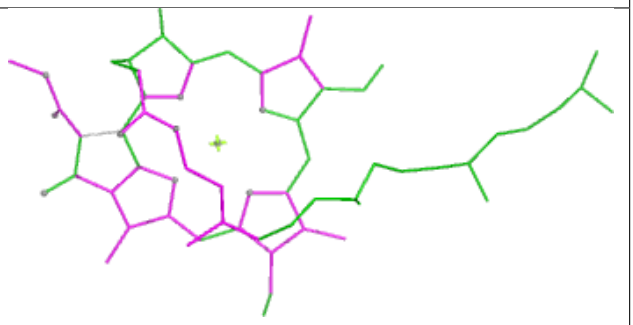


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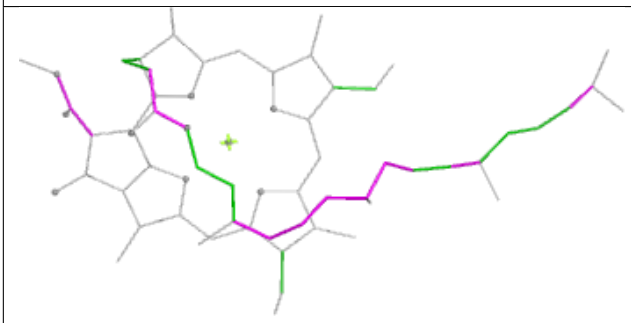
Ligand CLA A 1138



Bond lengths



Bond angles

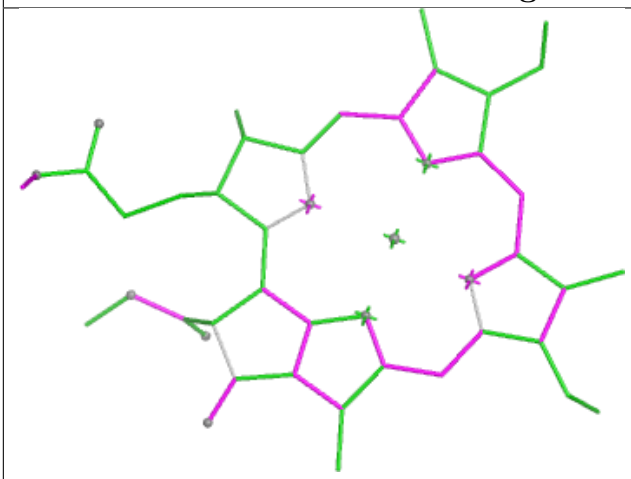


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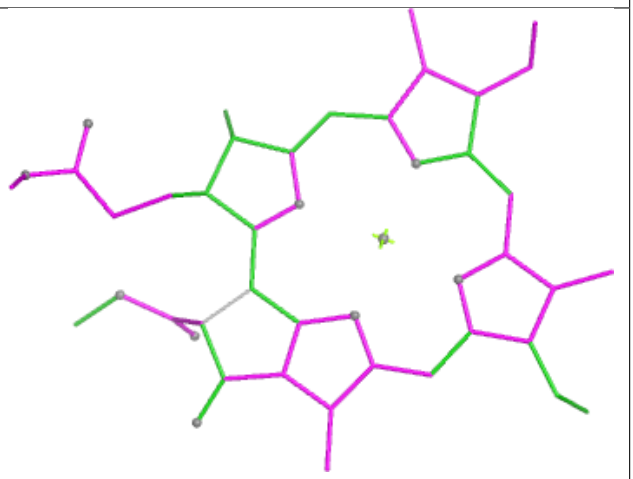


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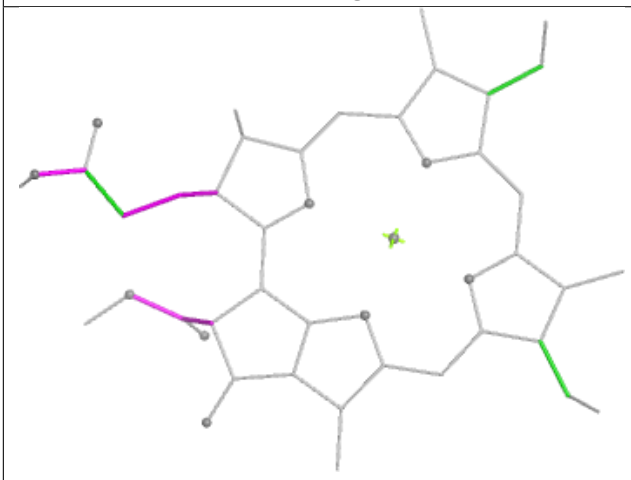
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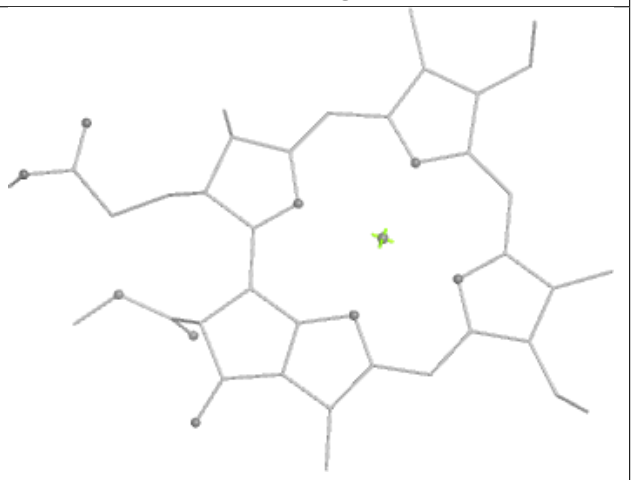
Bond lengths



Bond angles

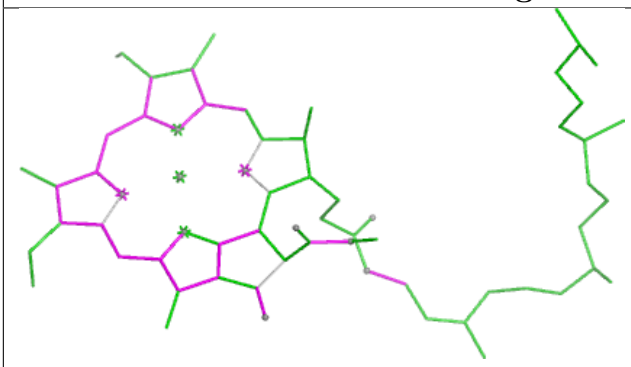


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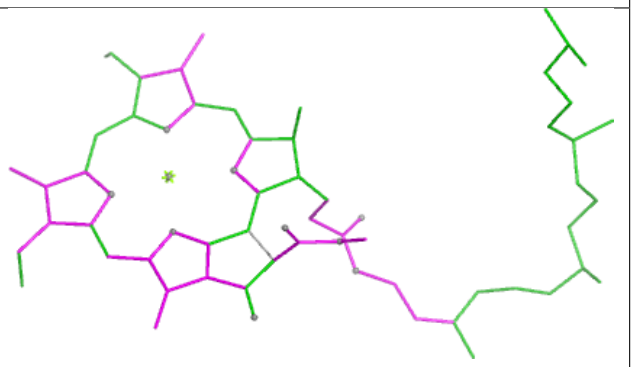


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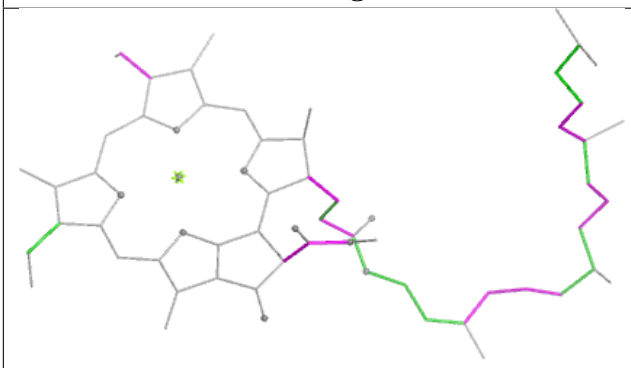
Ligand CLA B 1220



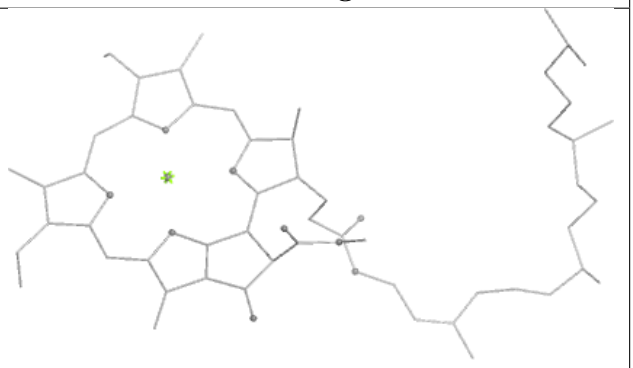
Bond lengths



Bond angles

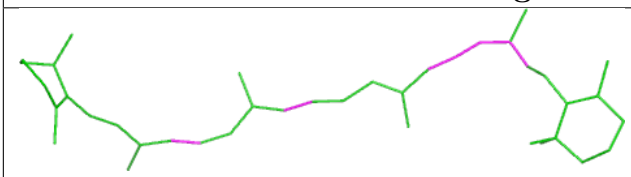


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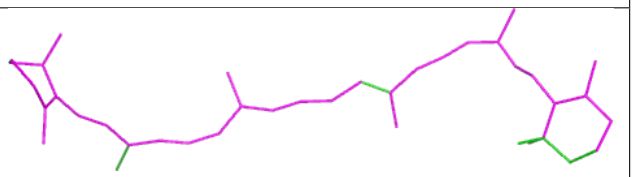


Rings

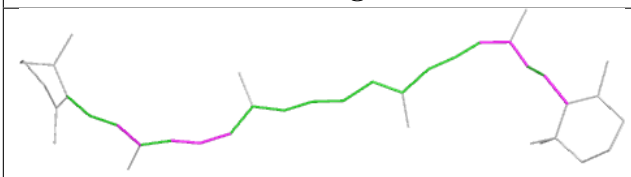
Ligand BCR B 6006



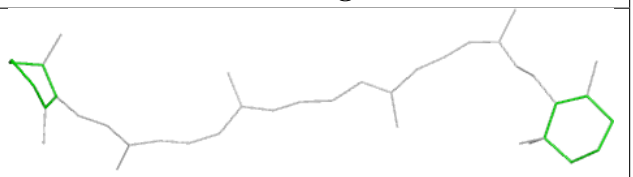
Bond lengths



Bond angles

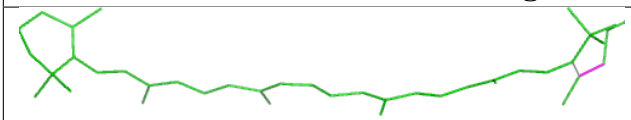


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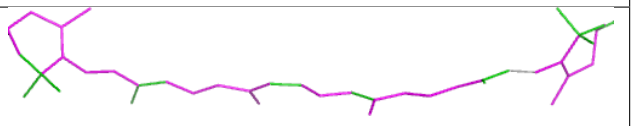


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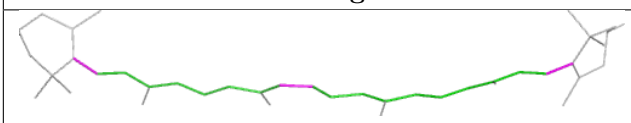
Ligand LUT I 6018



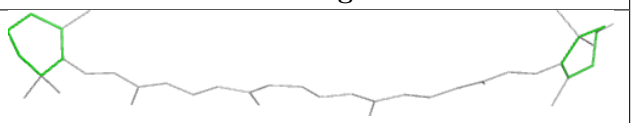
Bond lengths



Bond angles

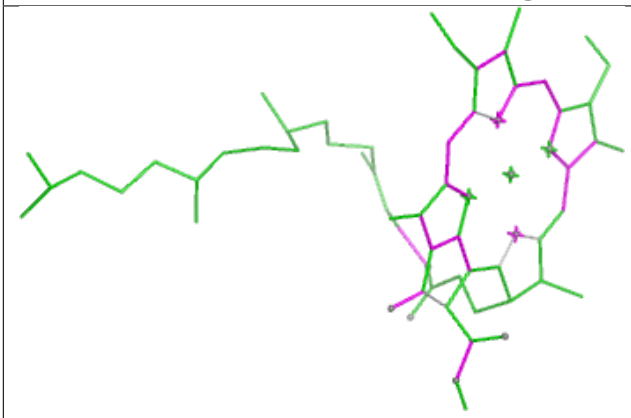


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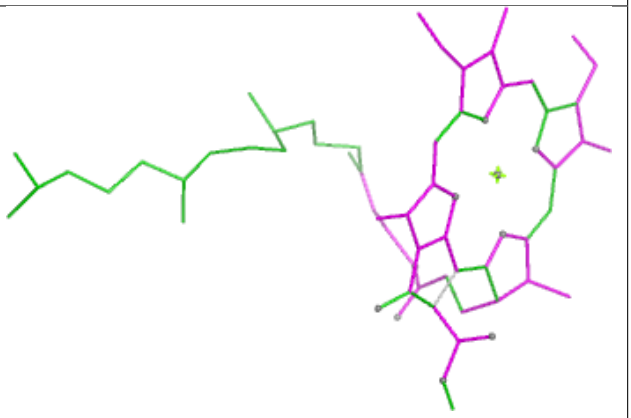


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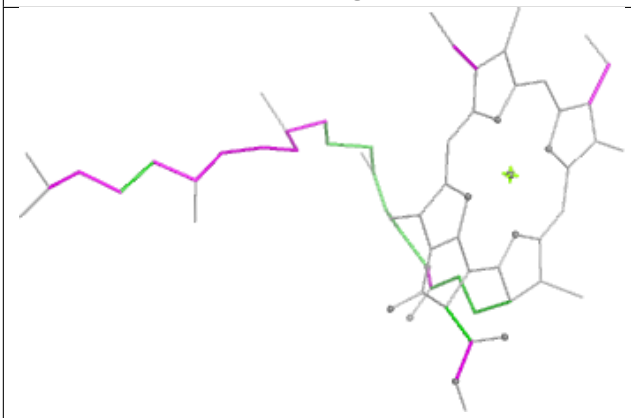
Ligand CLA 4 4012



Bond lengths



Bond angles

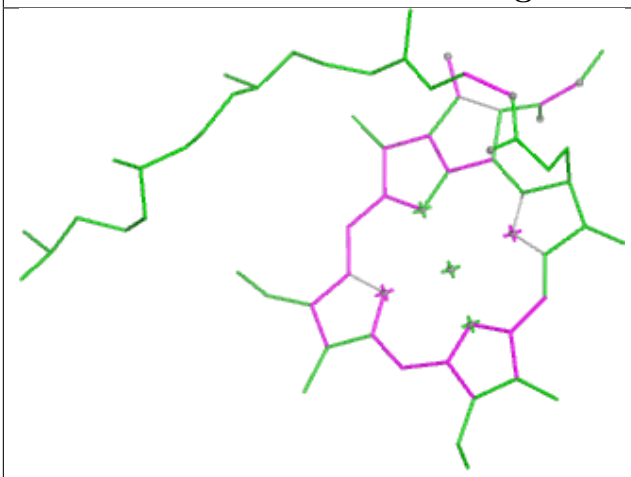


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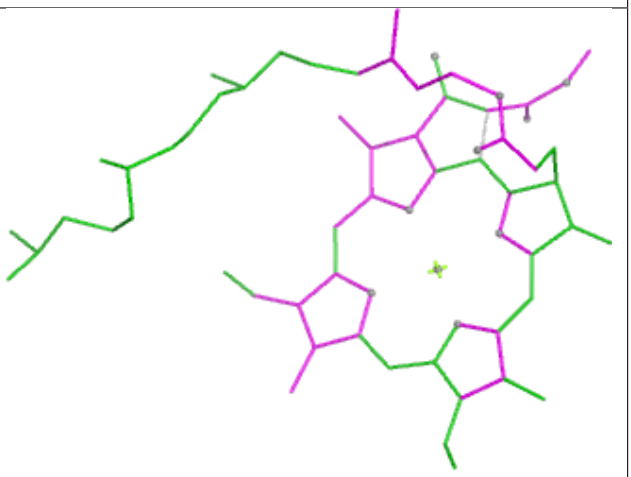


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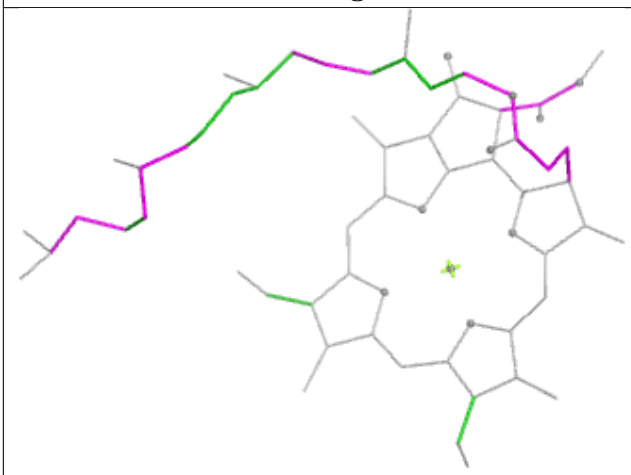
Ligand CLA A 1127



Bond lengths



Bond angles

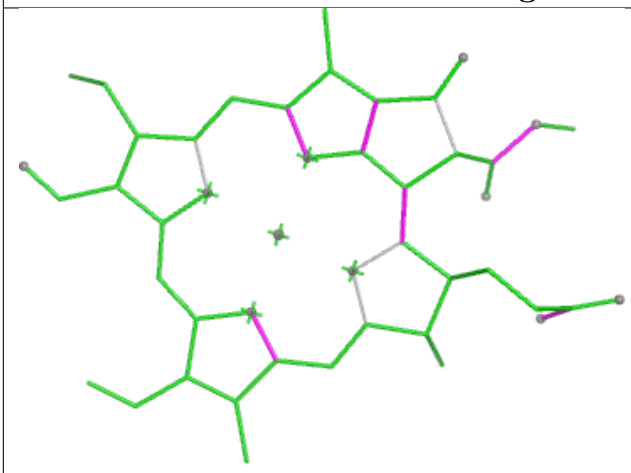


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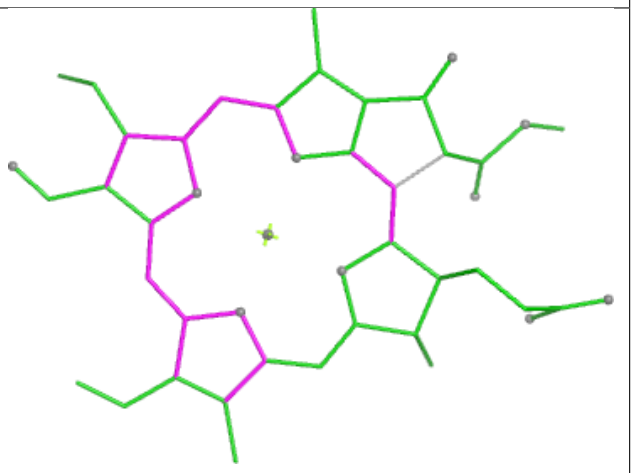


Rings

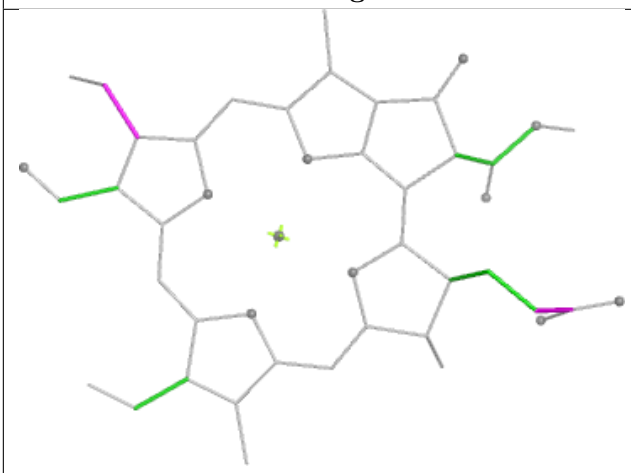
Ligand CHL 2 2013



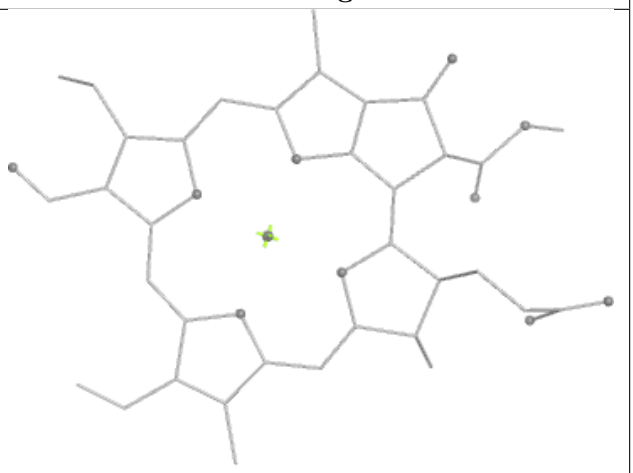
Bond lengths



Bond angles

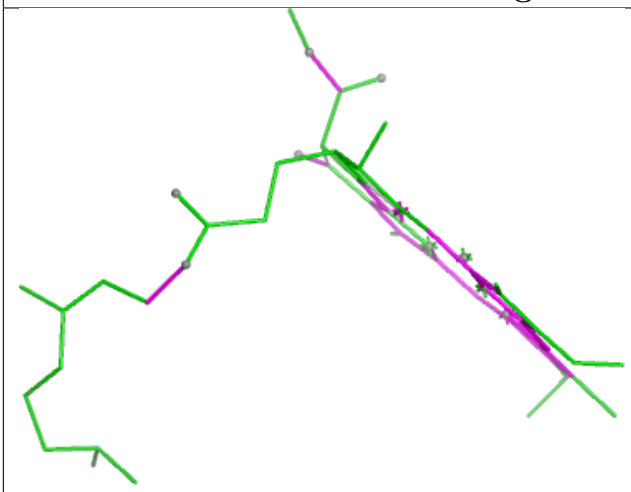


Torsions

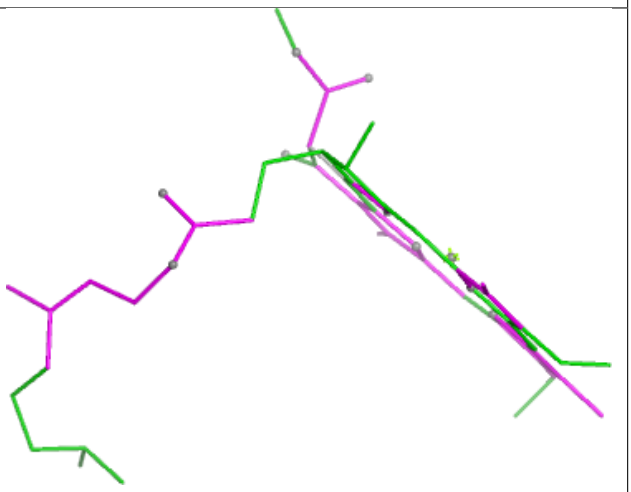


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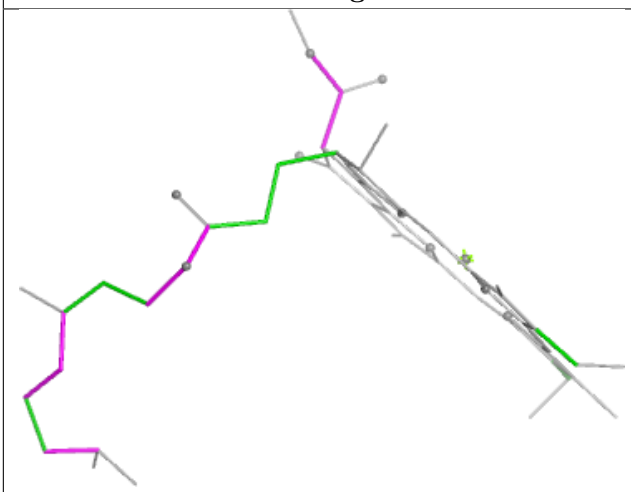
Ligand CLA A 1137



Bond lengths



Bond angles

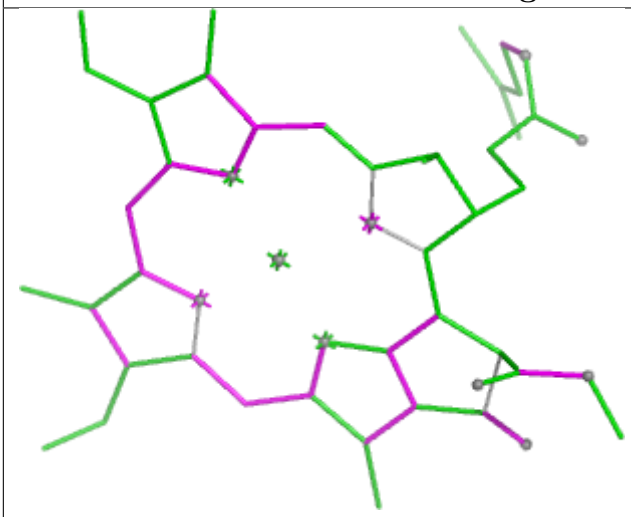


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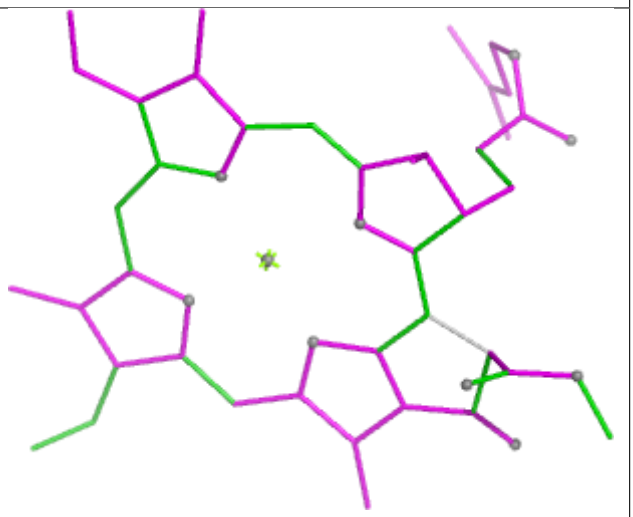


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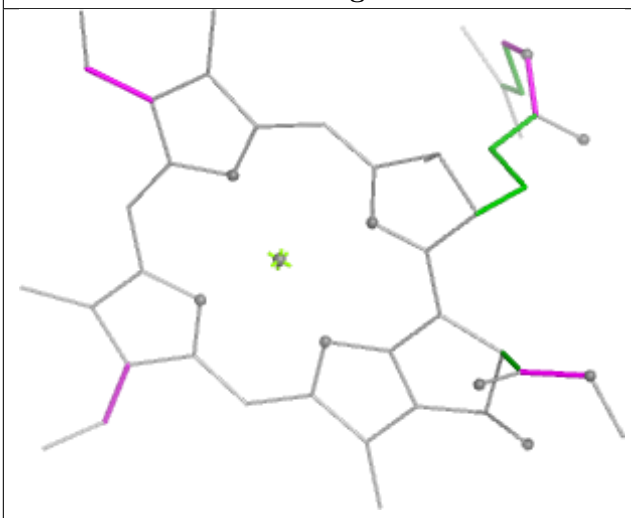
Ligand CLA 3 3012



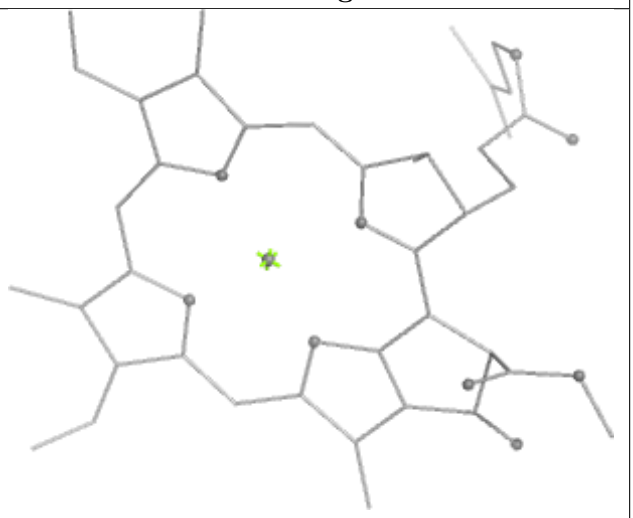
Bond lengths



Bond angles

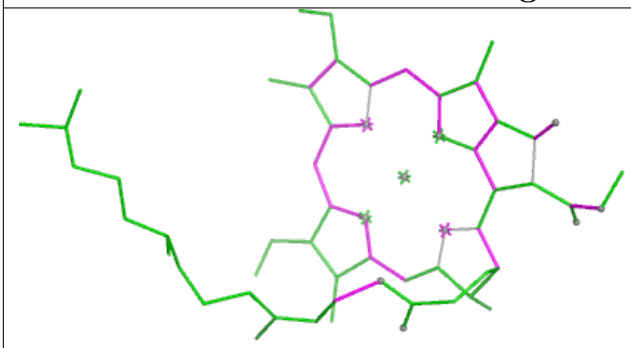


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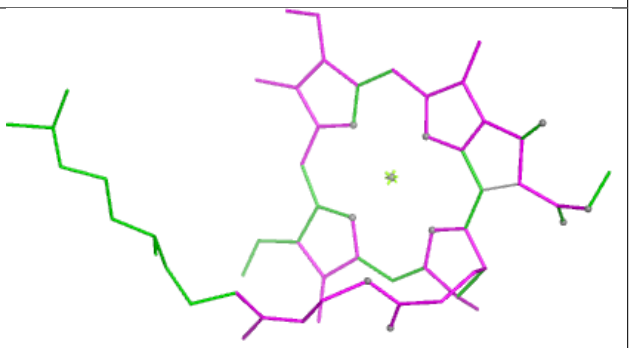


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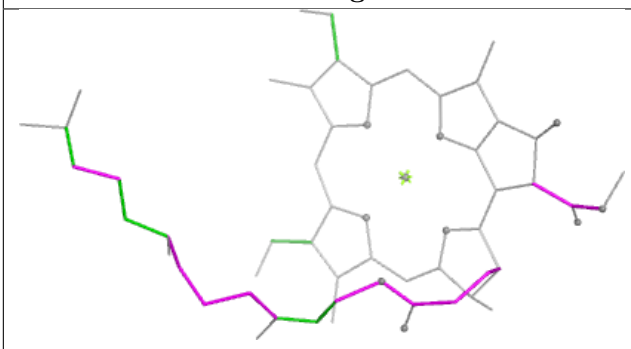
Ligand CLA 2 2001



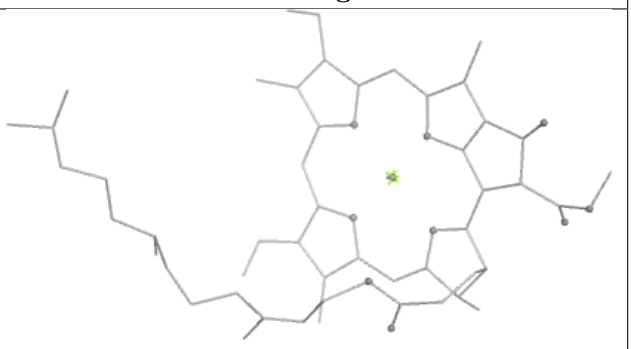
Bond lengths



Bond angles



Torsions



Rings

Ligand LUT 2 2501



Bond lengths



Bond angles

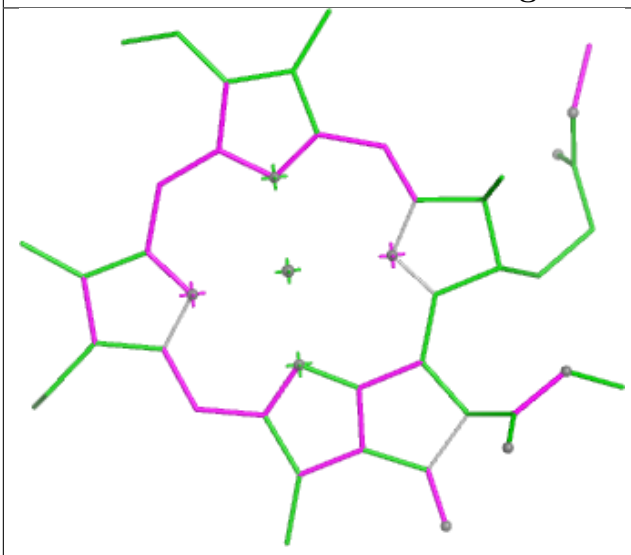


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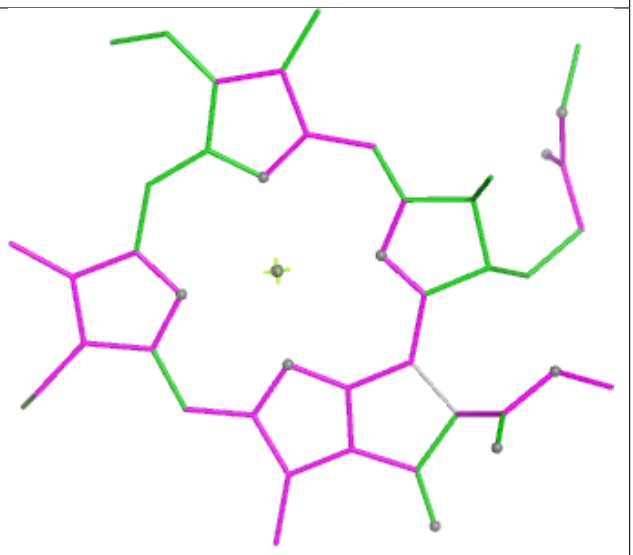


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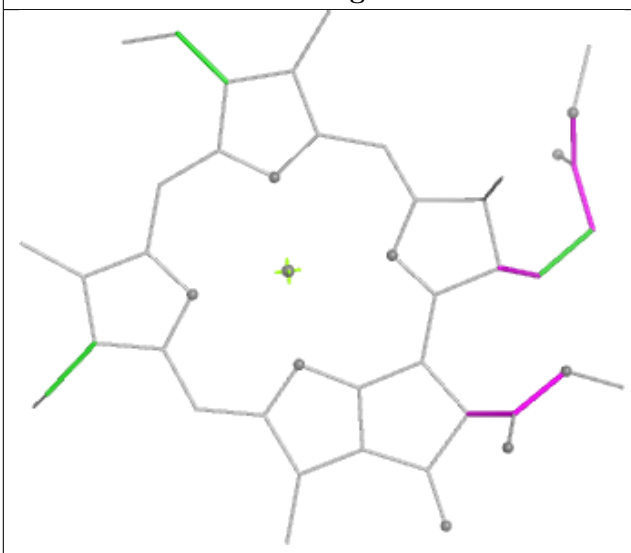
Ligand CLA 3 3017



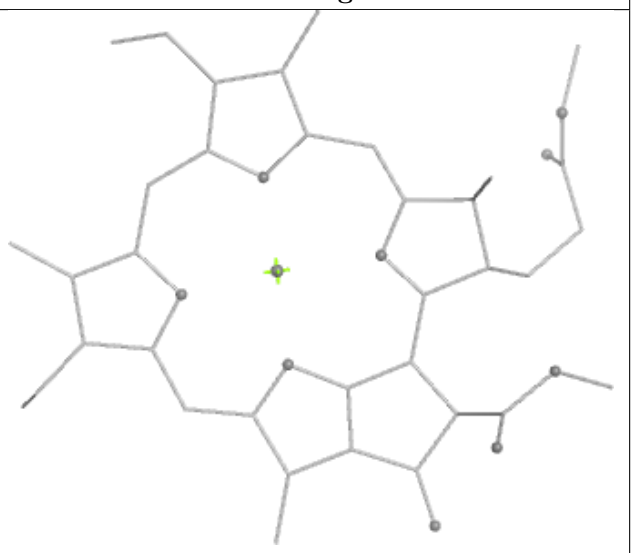
Bond lengths



Bond angles

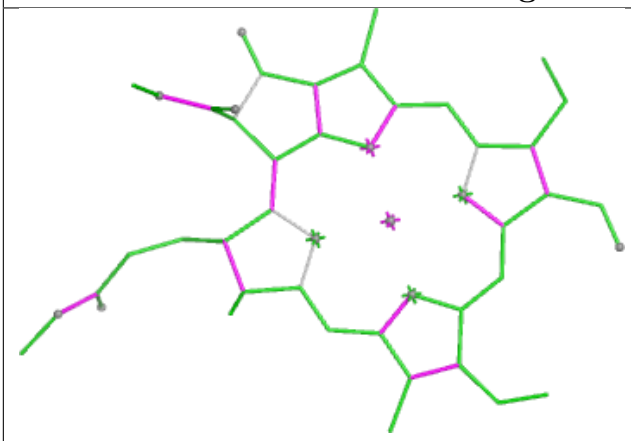


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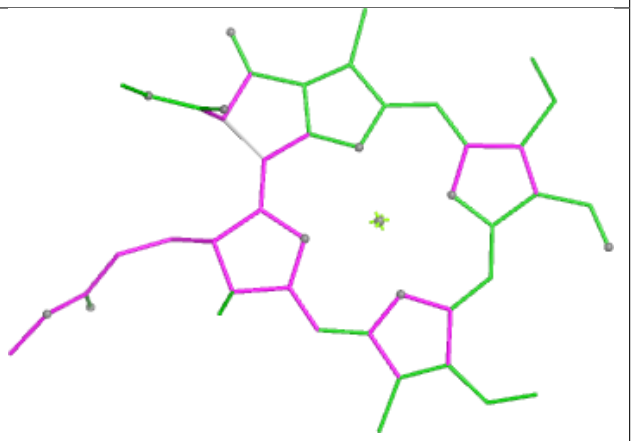


Rings

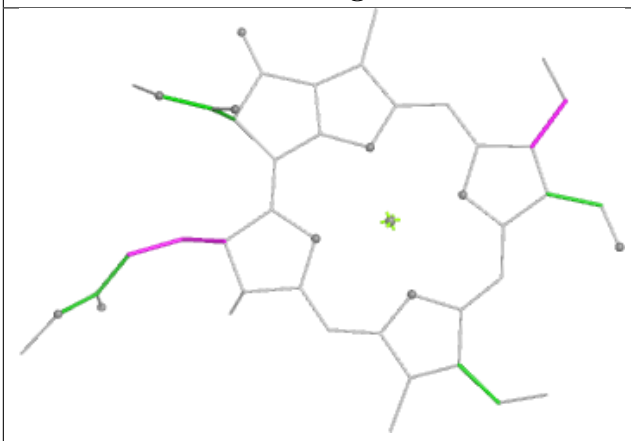
Ligand CHL 4 4010



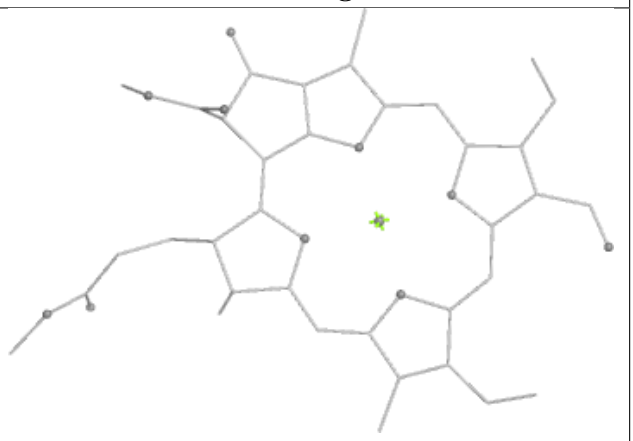
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Bond angles

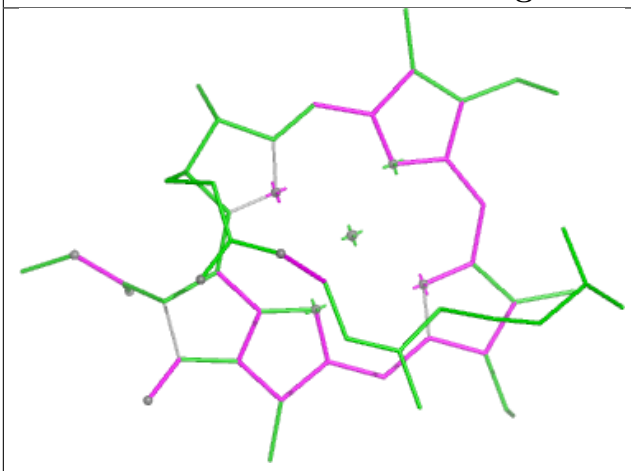


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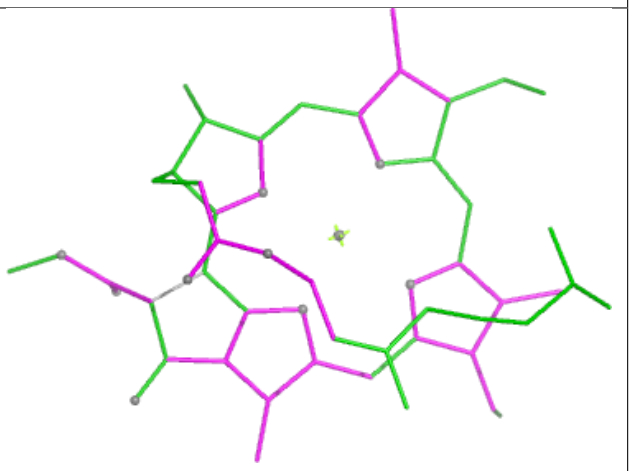


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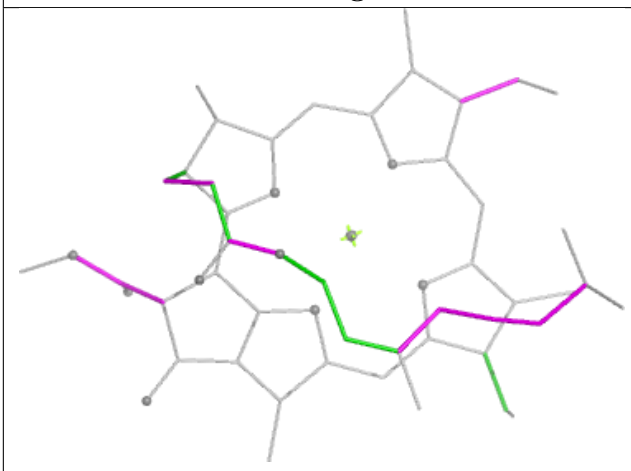
Ligand CLA B 1204



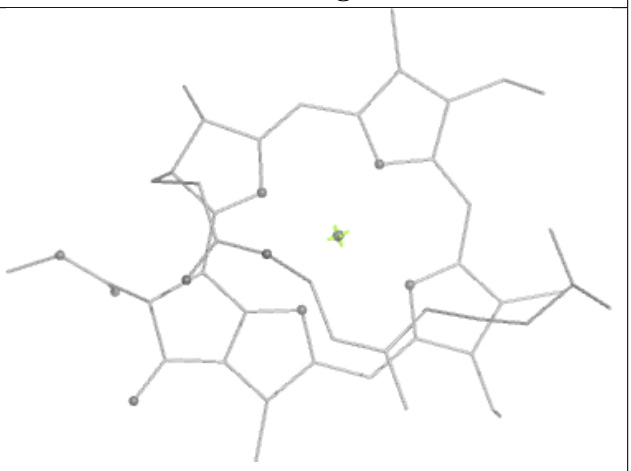
Bond lengths



Bond angles

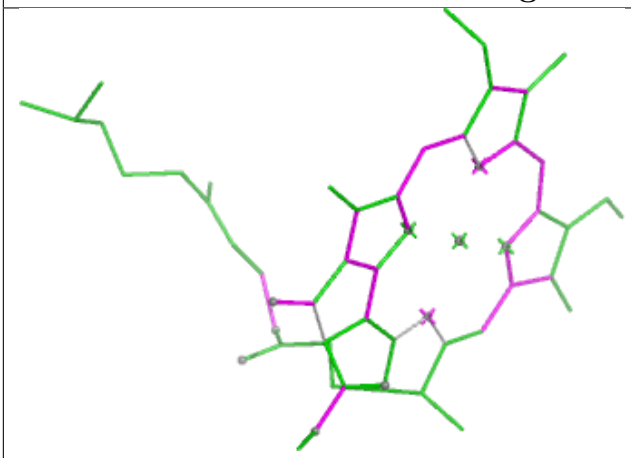


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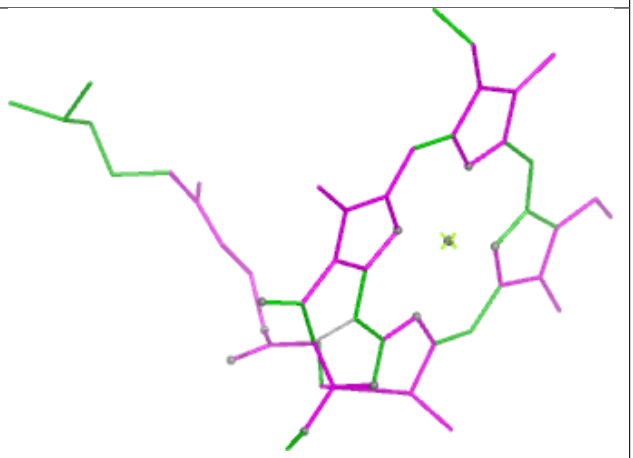


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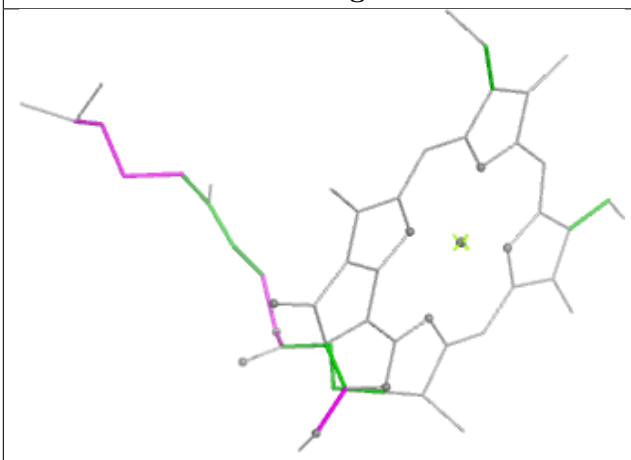
Ligand CLA 2 2012



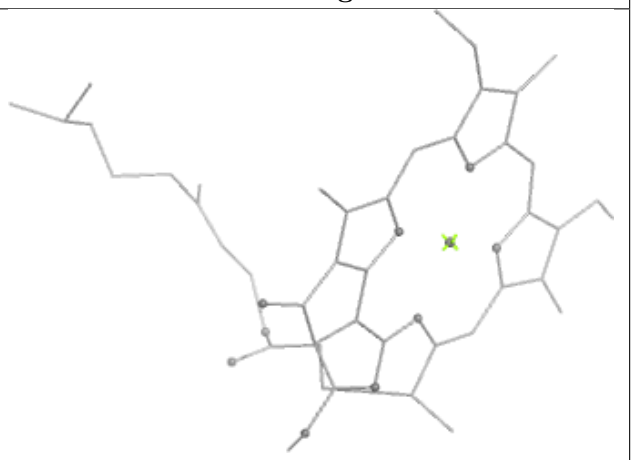
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Bond angles

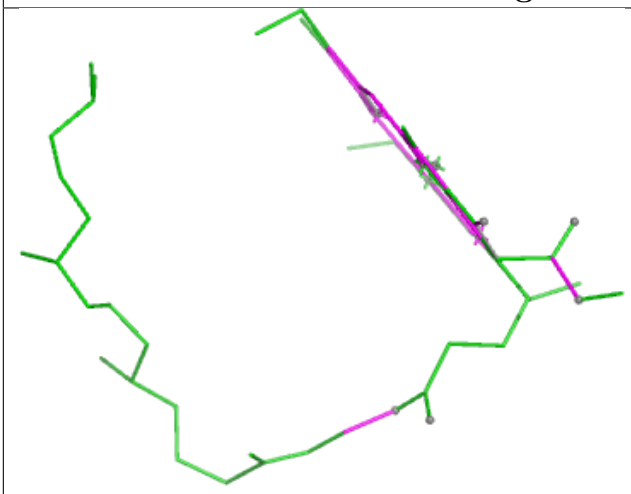


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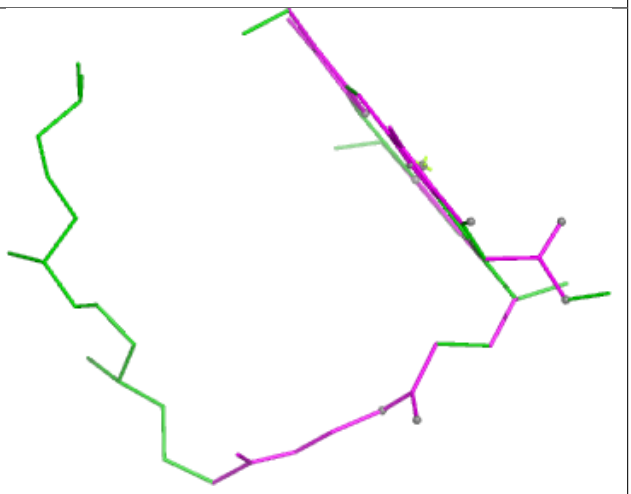


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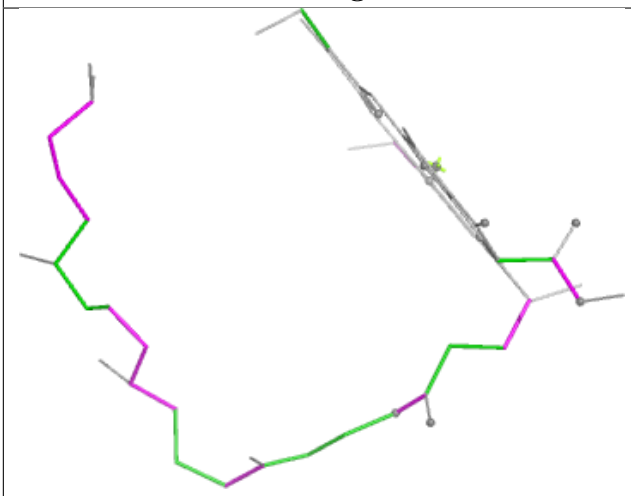
Ligand CLA B 1216



Bond lengths



Bond angles

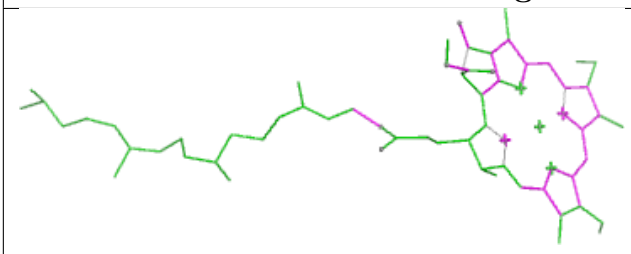


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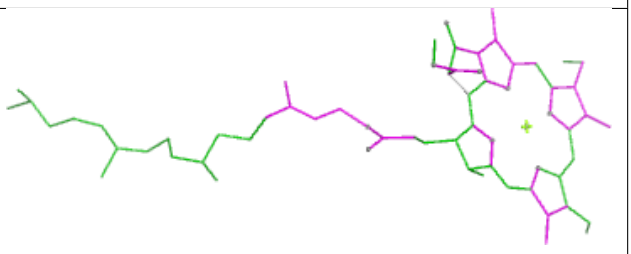


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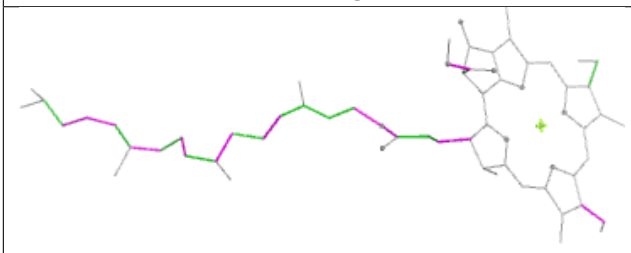
Ligand CLA A 1107



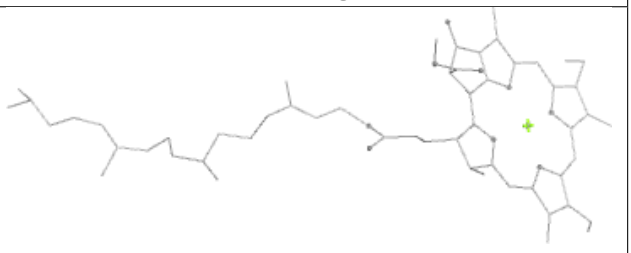
Bond lengths



Bond angles

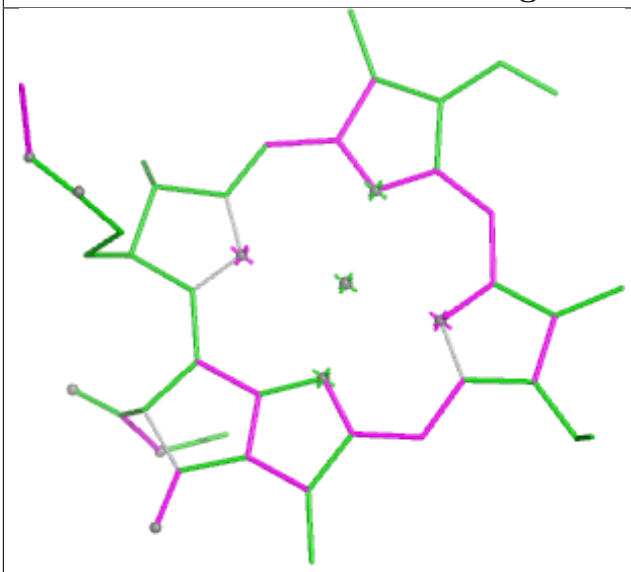


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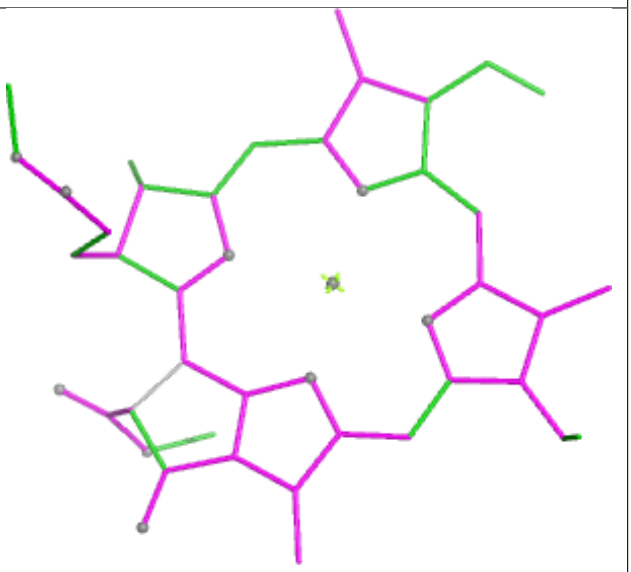


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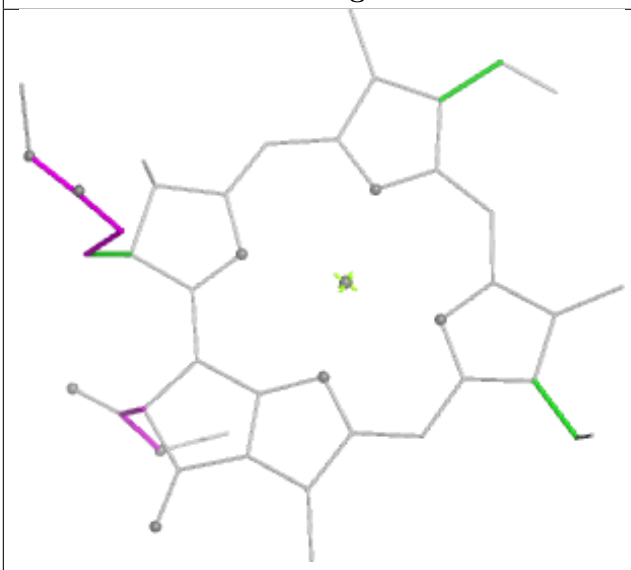
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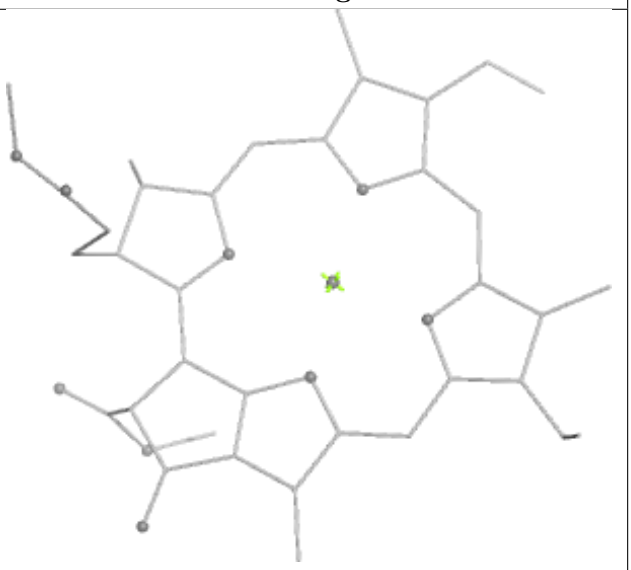
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Bond angles

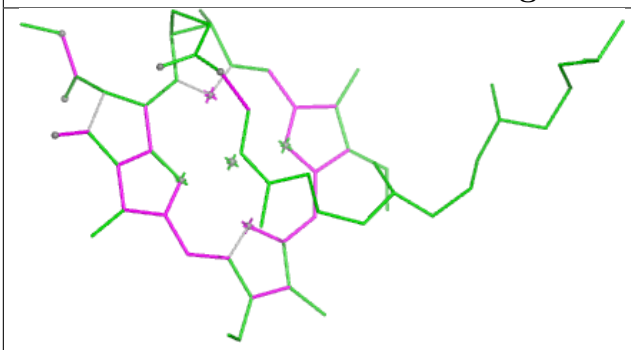


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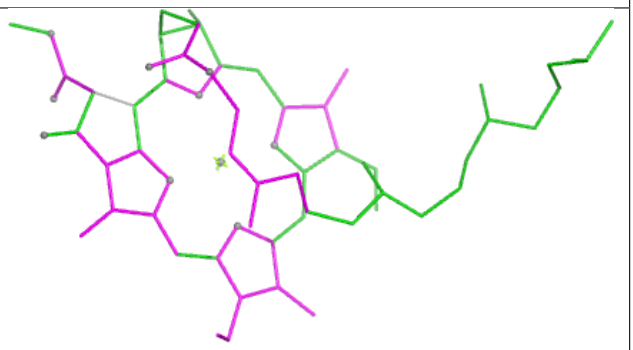


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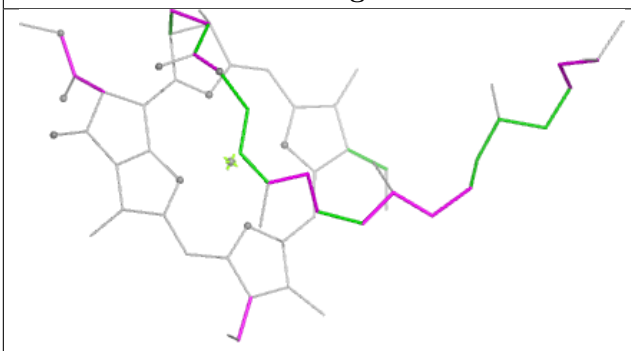
Ligand CLA 4 4003



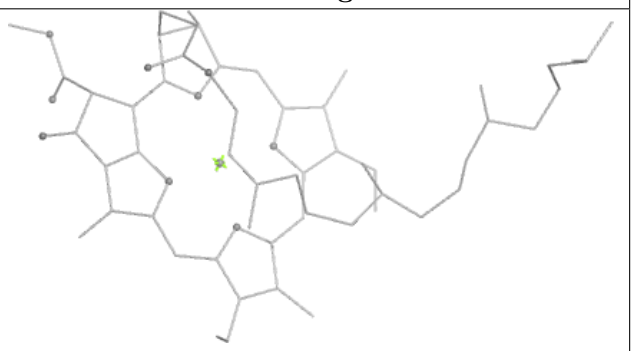
Bond lengths



Bond angles

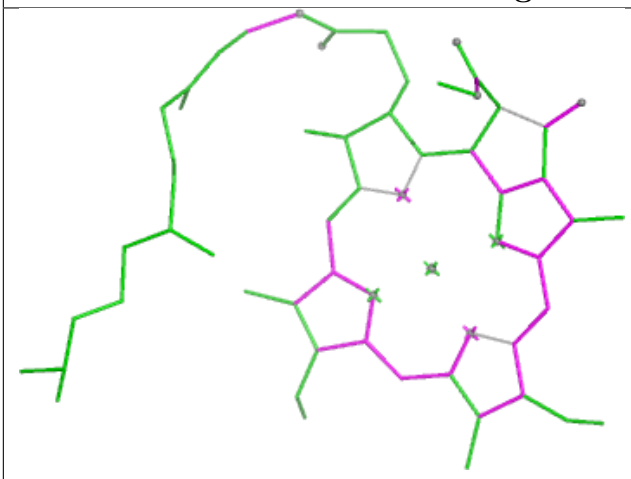


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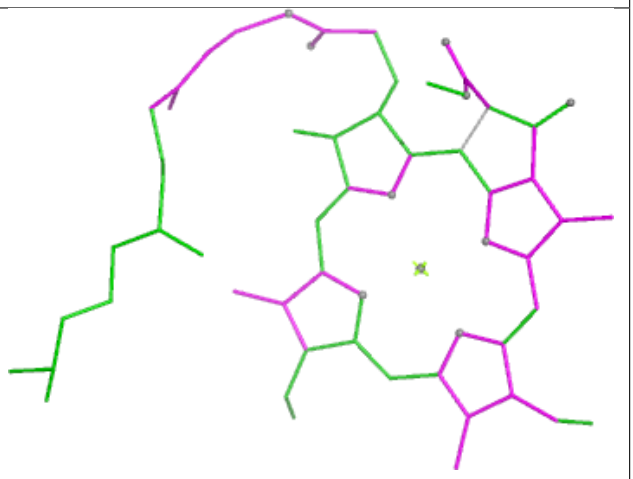


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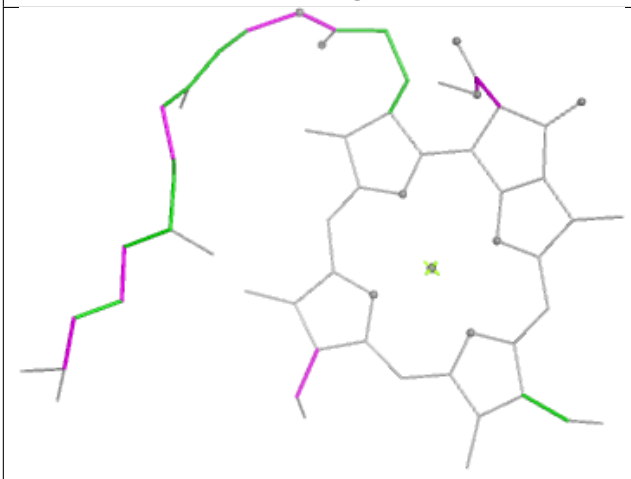
Ligand CLA A 1111



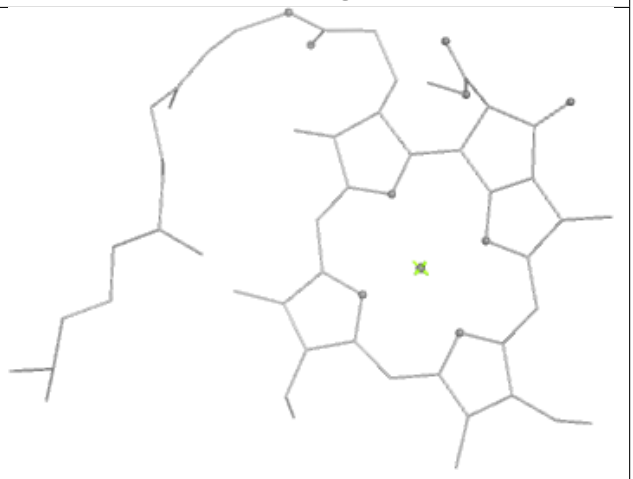
Bond lengths



Bond angles



Torsions



Rings

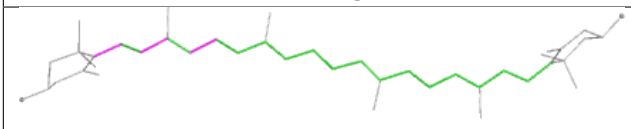
Ligand LUT 2 2502



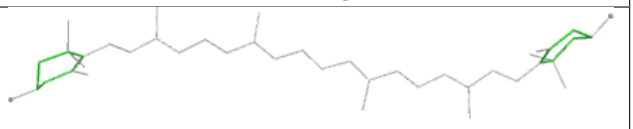
Bond lengths



Bond angles

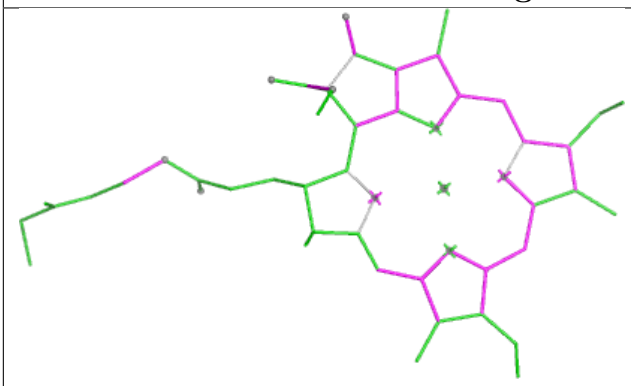


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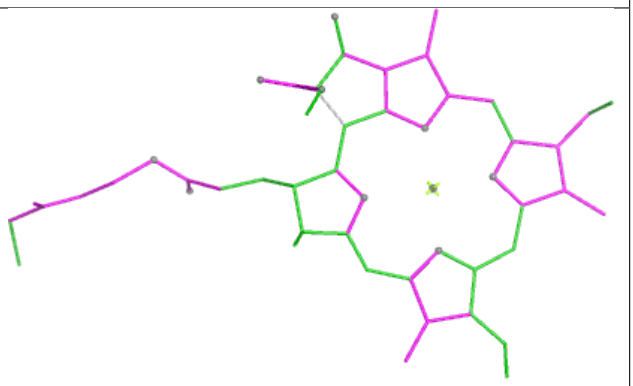


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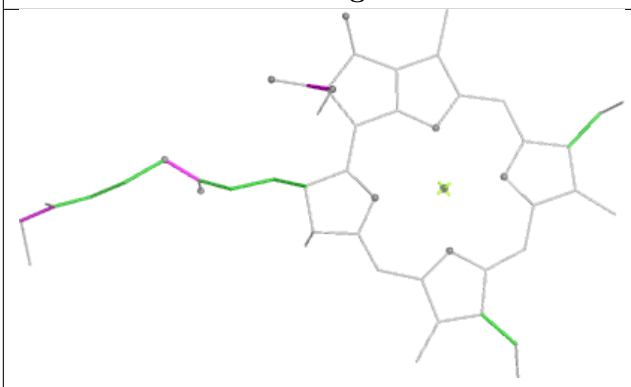
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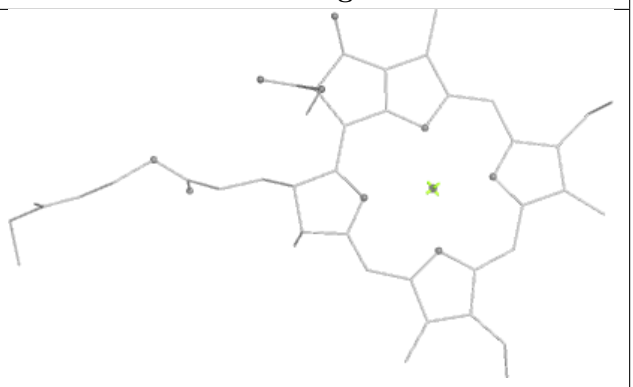
Bond lengths



Bond angles

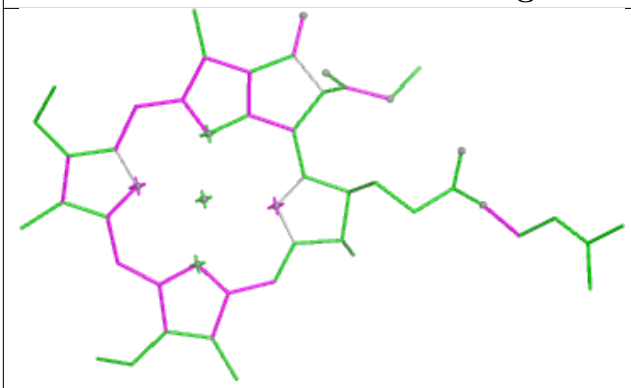


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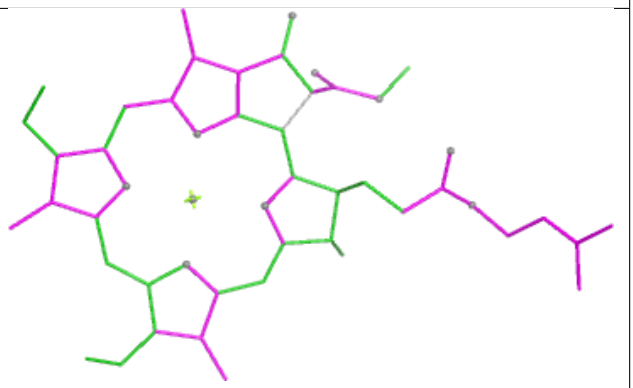


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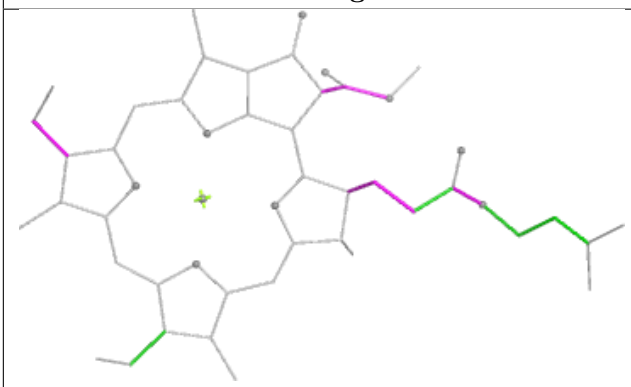
Ligand CLA F 1302



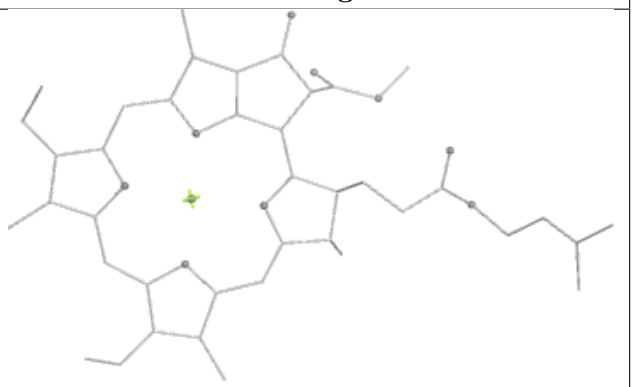
Bond lengths



Bond angles

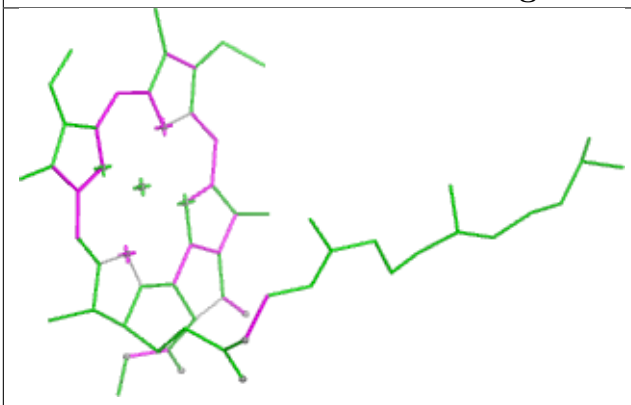


Torsions

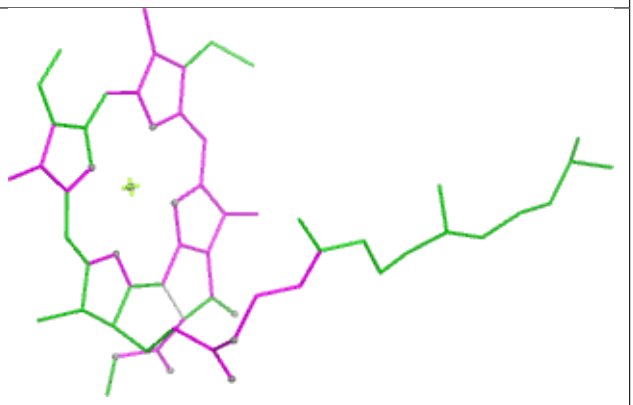


Rings

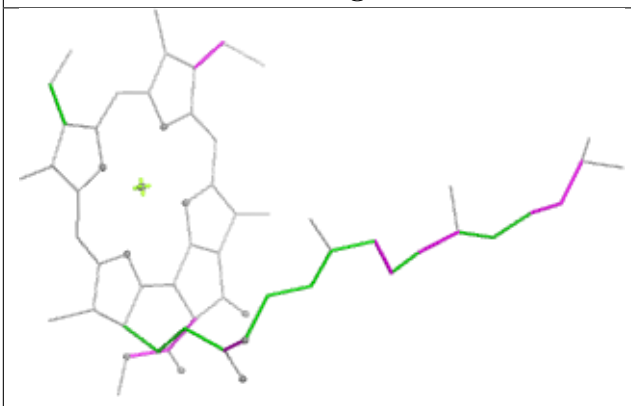
Ligand CLA 4 4007



Bond lengths



Bond angles

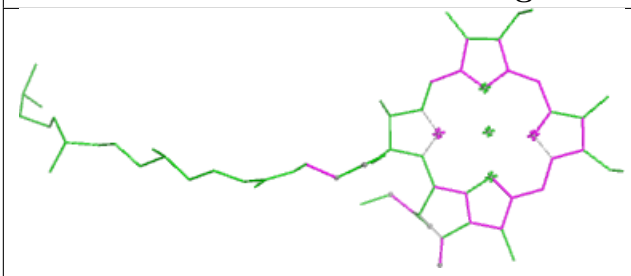


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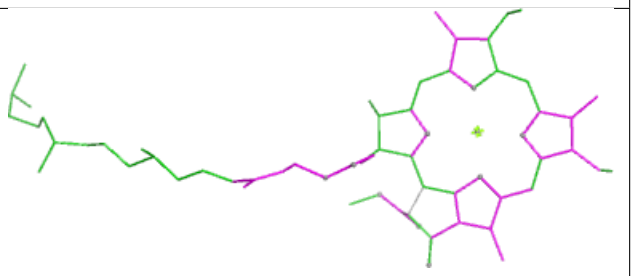


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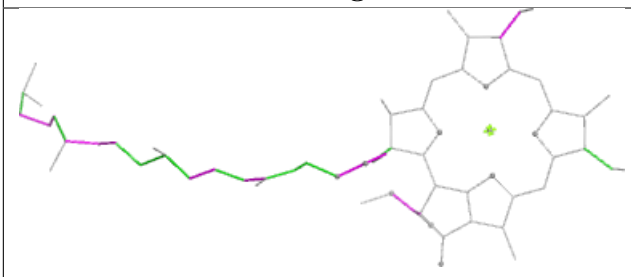
Ligand CLA B 1240



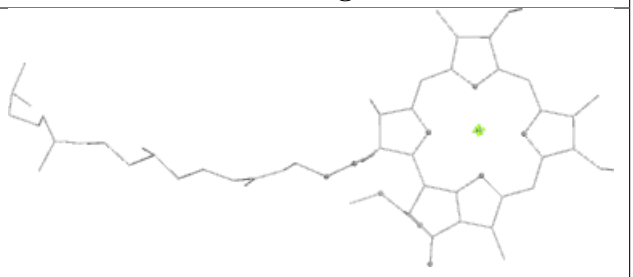
Bond lengths



Bond angles

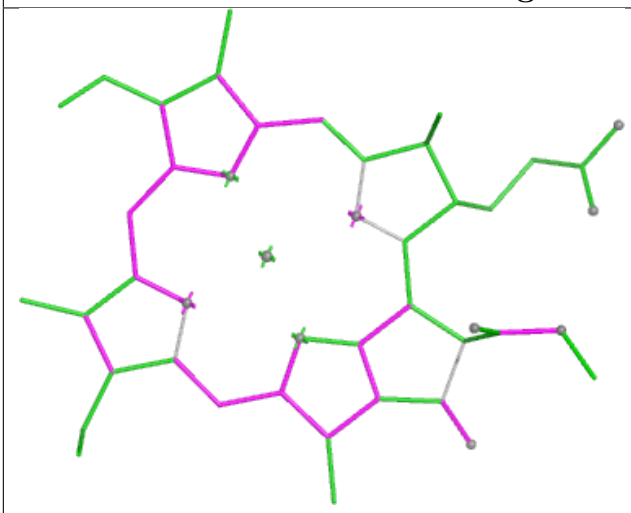


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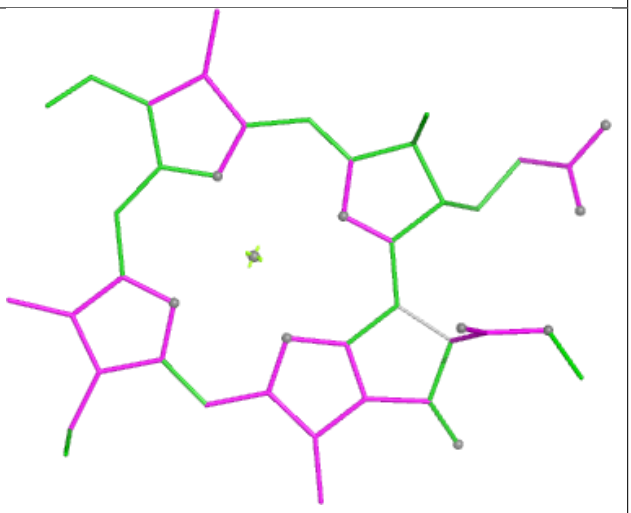


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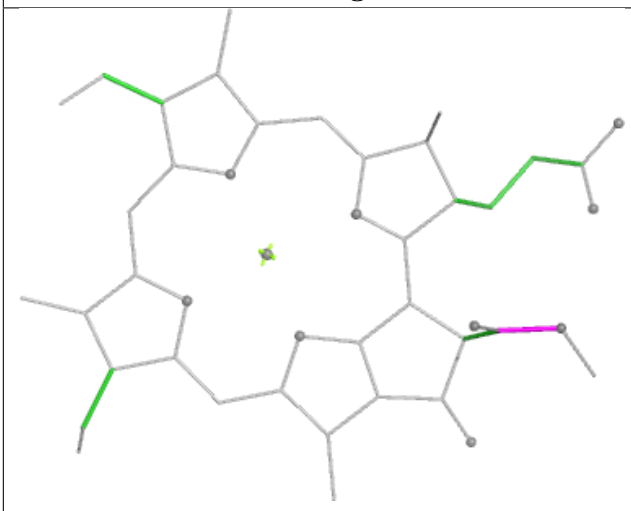
Ligand CLA F 1301



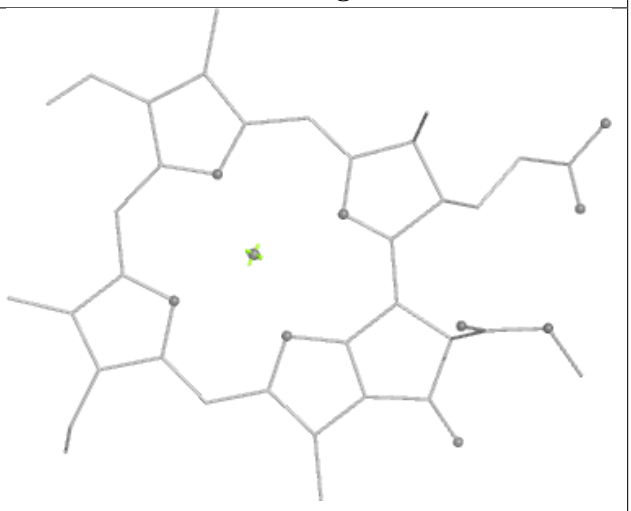
Bond lengths



Bond angles

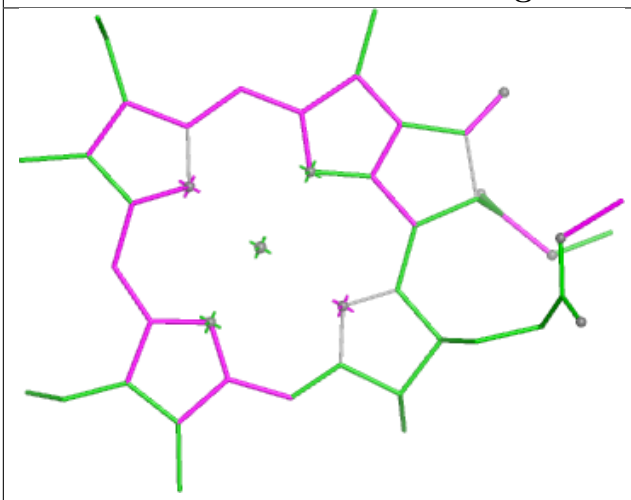


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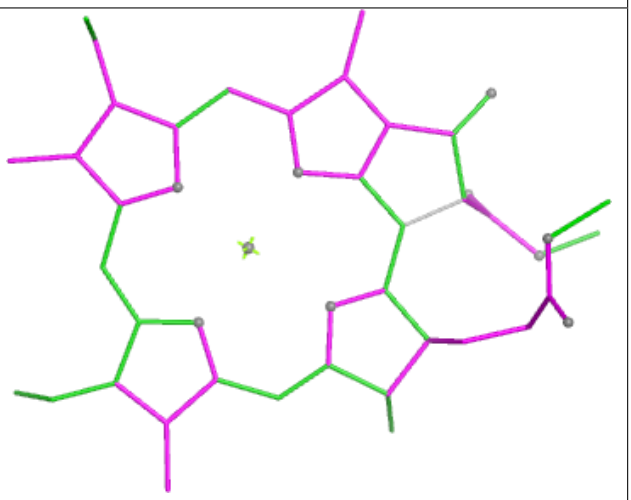


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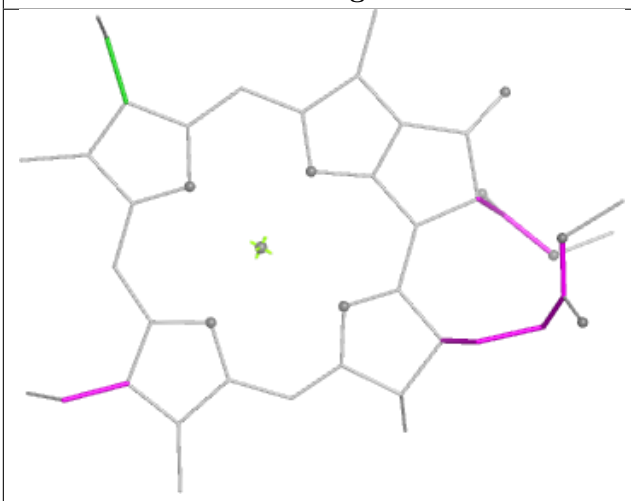
Ligand CLA A 1113



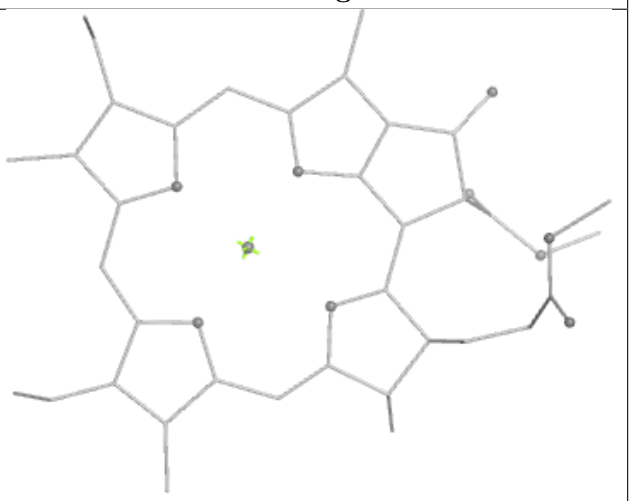
Bond lengths



Bond angles

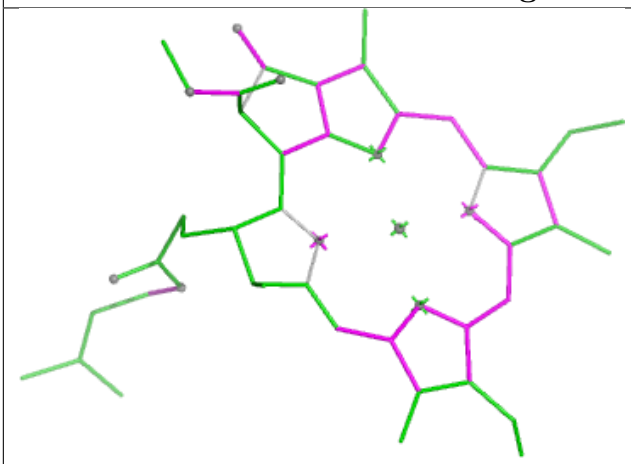


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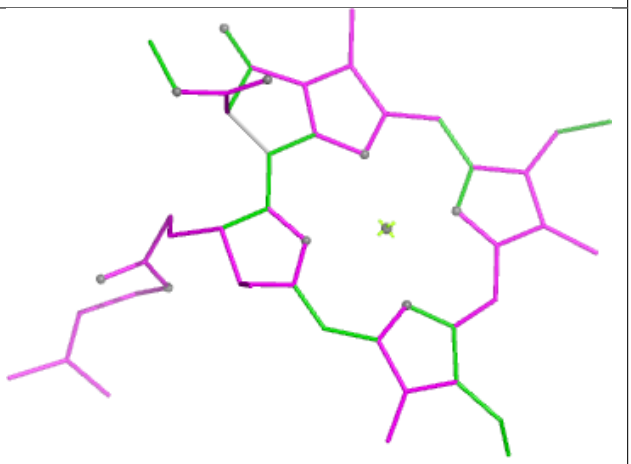


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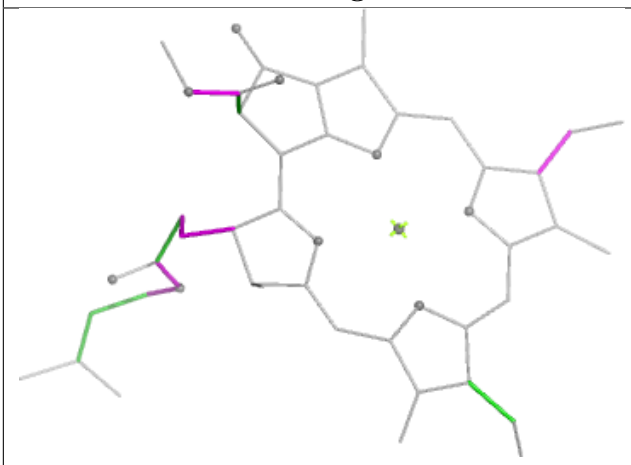
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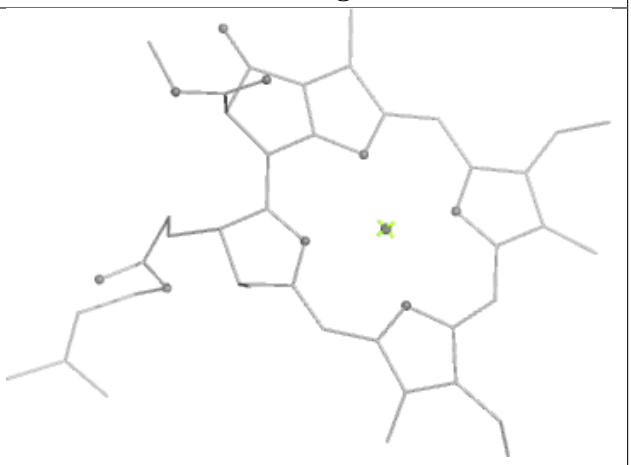
Bond lengths



Bond angles

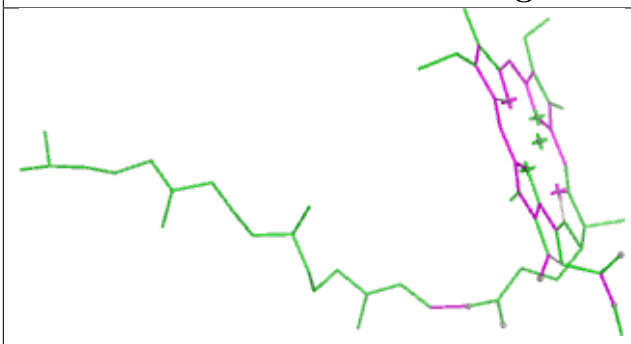


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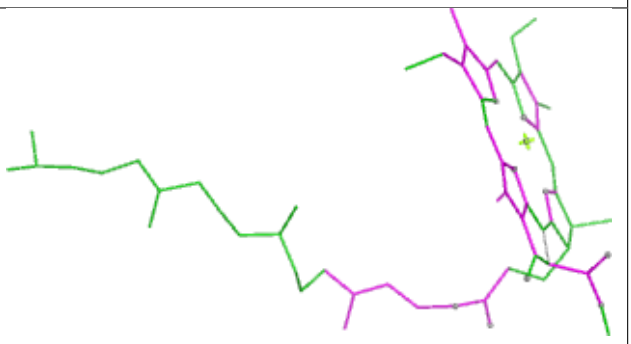


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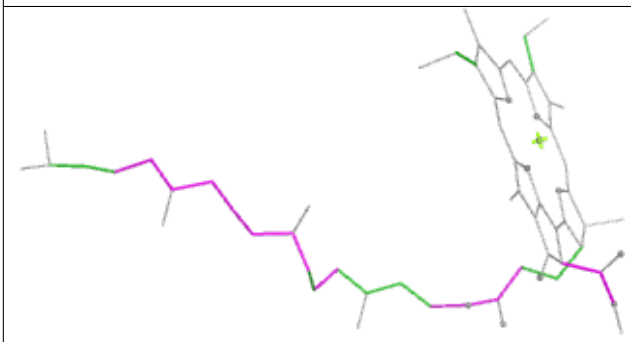
Ligand CLA B 1226



Bond lengths



Bond angles

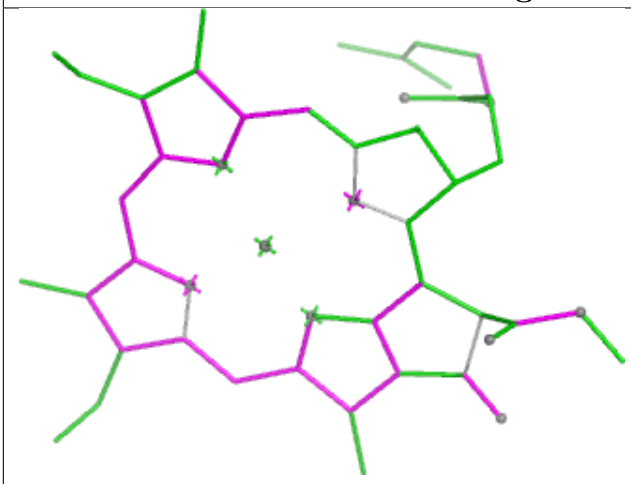


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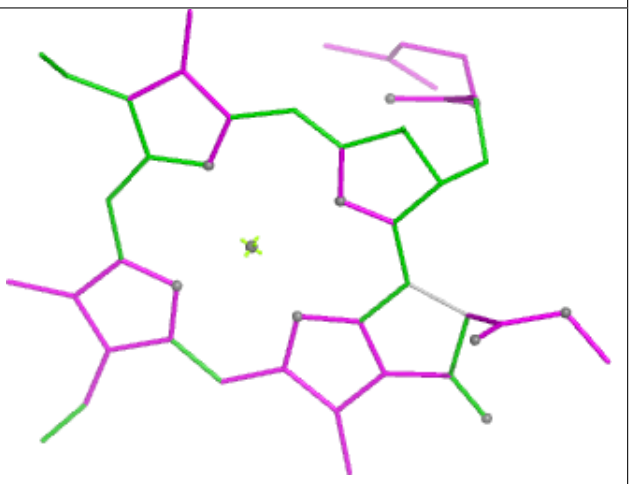


Rings

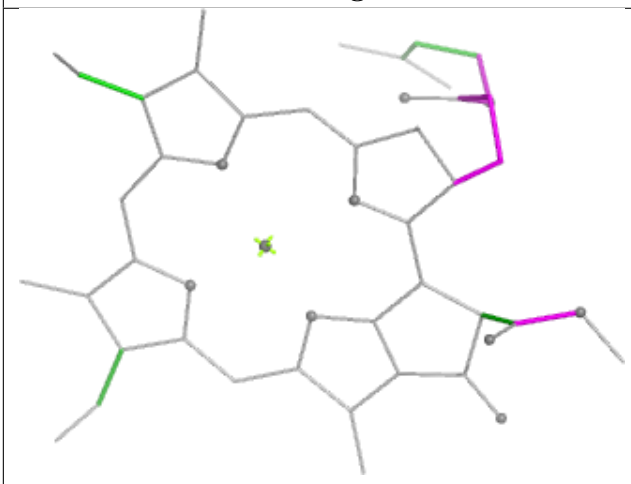
Ligand CLA B 1201



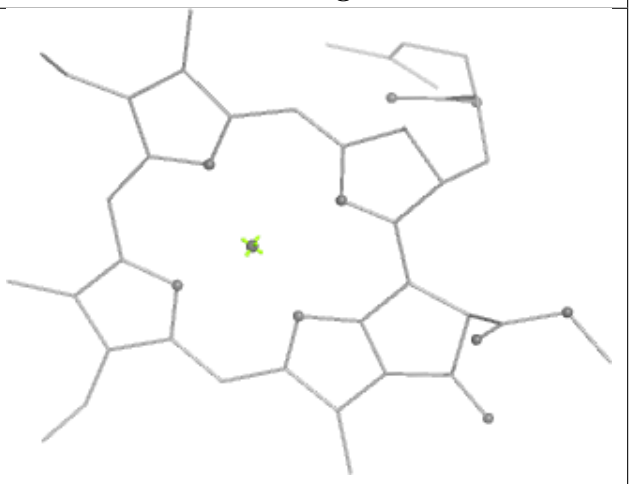
Bond lengths



Bond angles

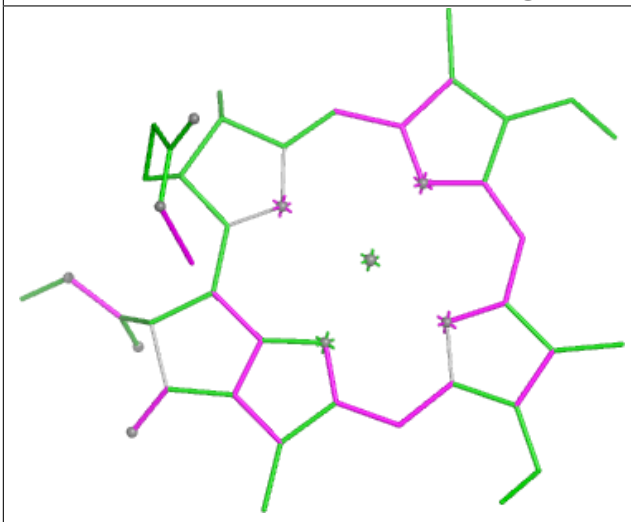


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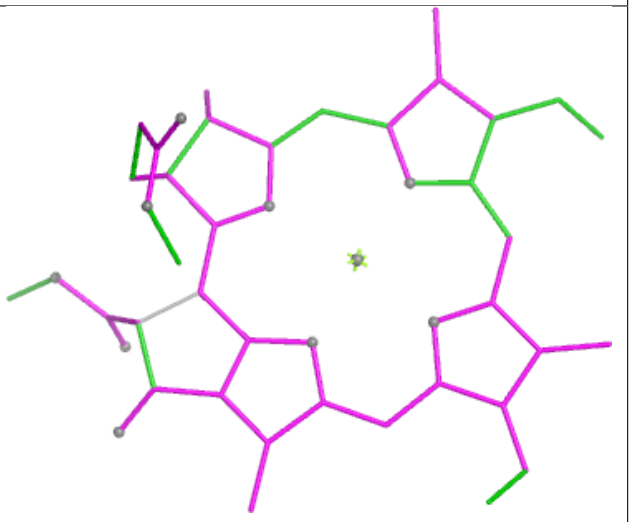


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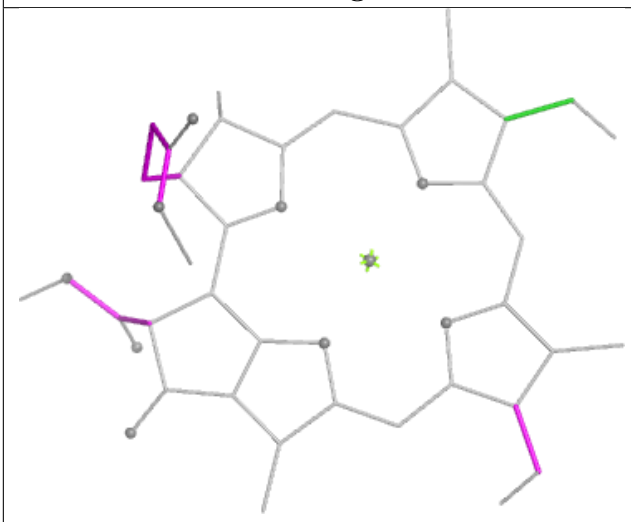
Ligand CLA 4 4008



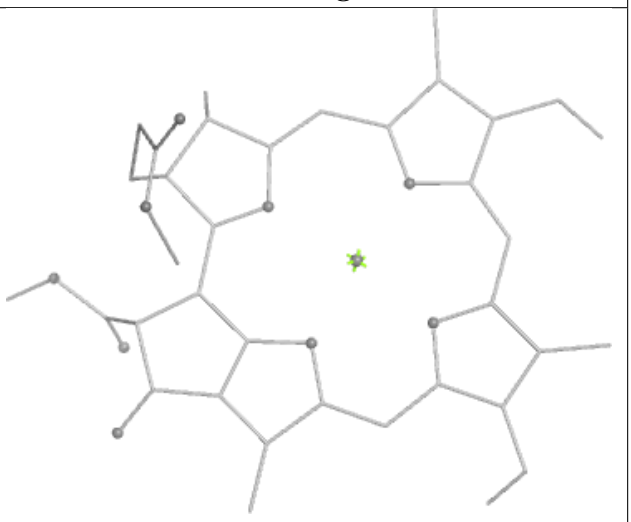
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Bond angles

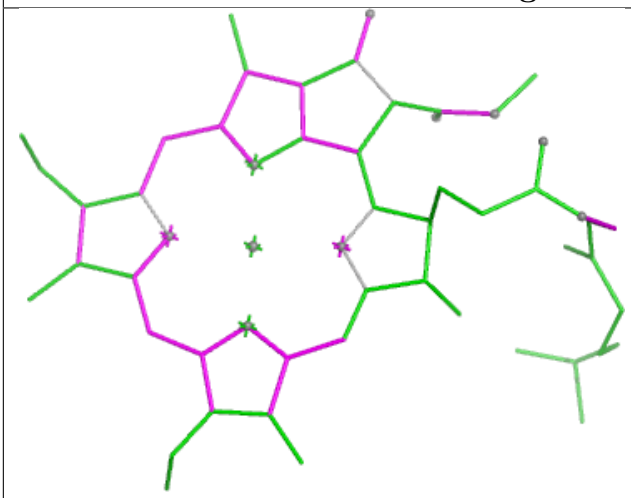


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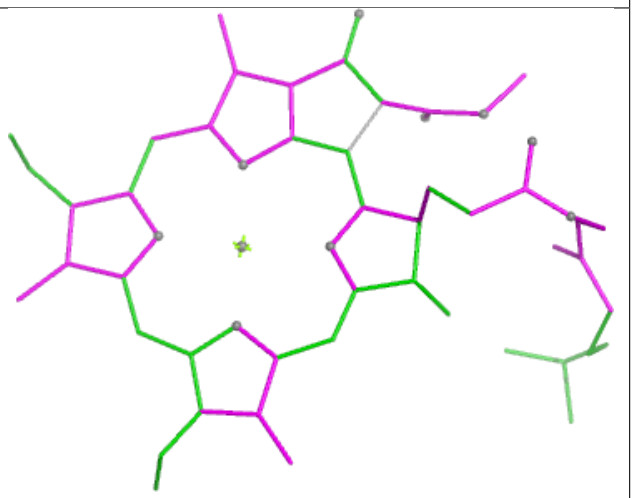


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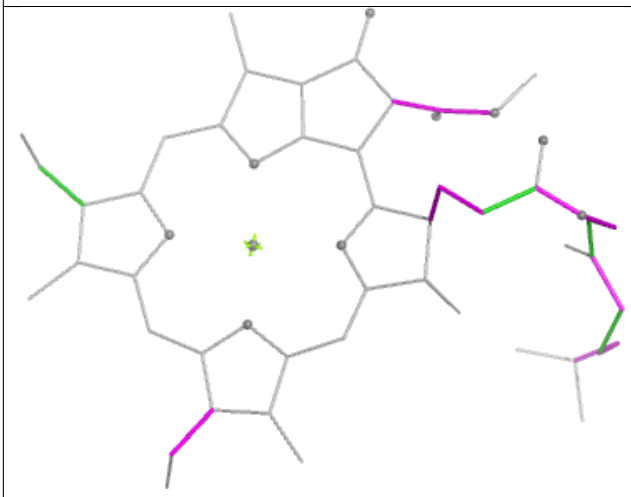
Ligand CLA 2 2005



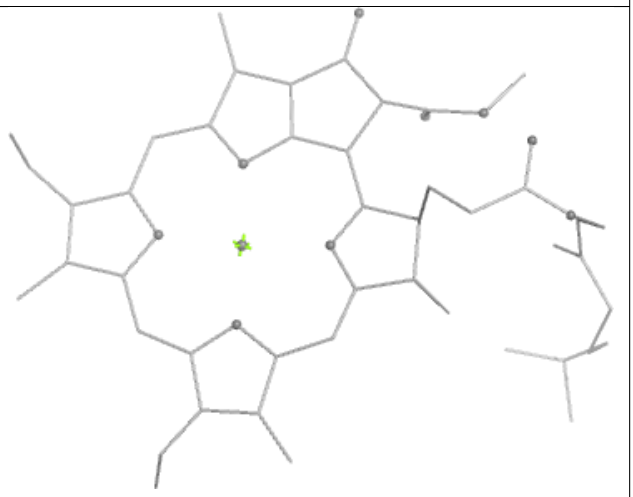
Bond lengths



Bond angles

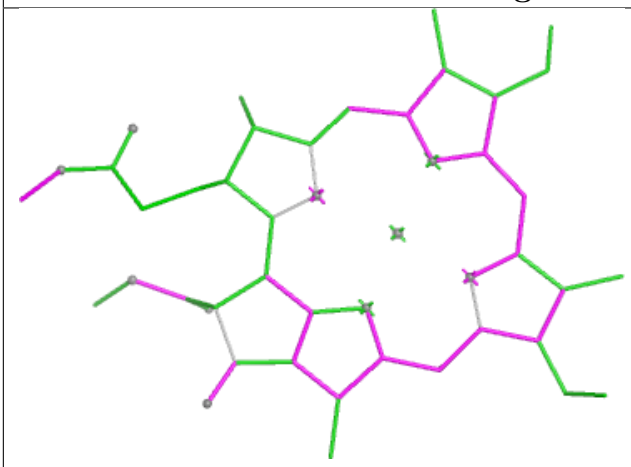


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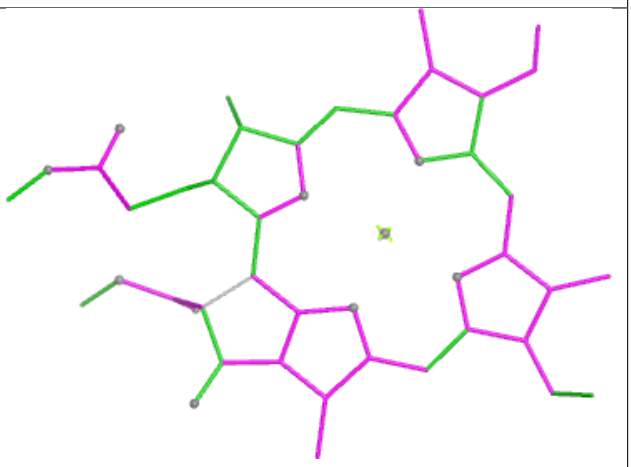


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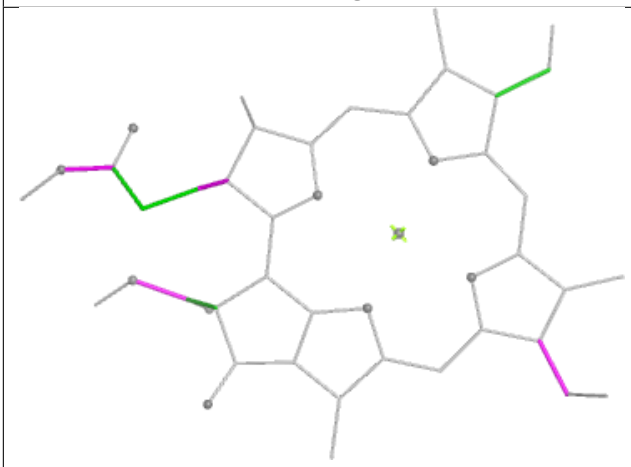
Ligand CLA G 1002



Bond lengths



Bond angles

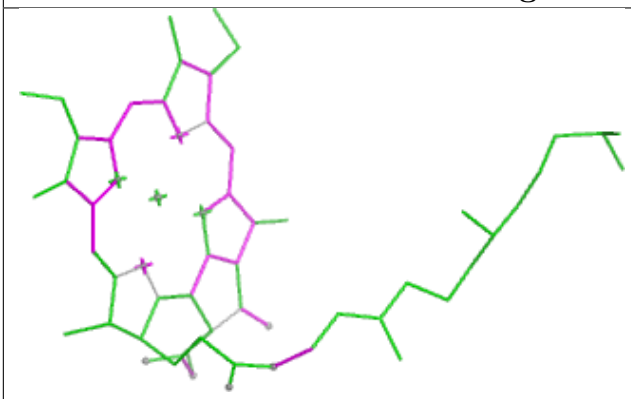


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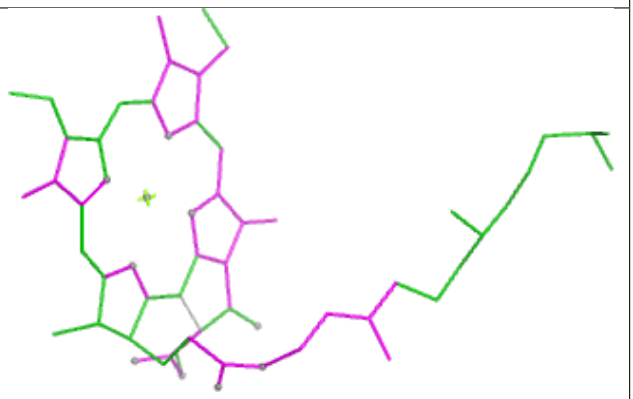


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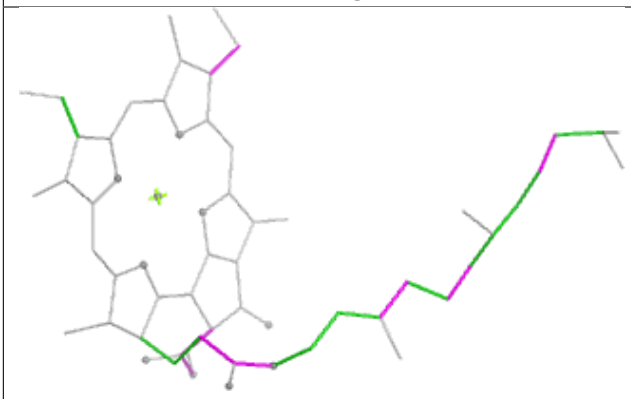
Ligand CLA 2 2007



Bond lengths



Bond angles

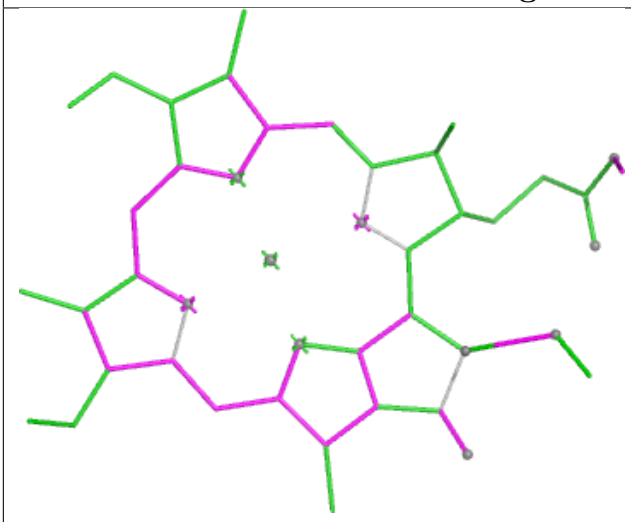


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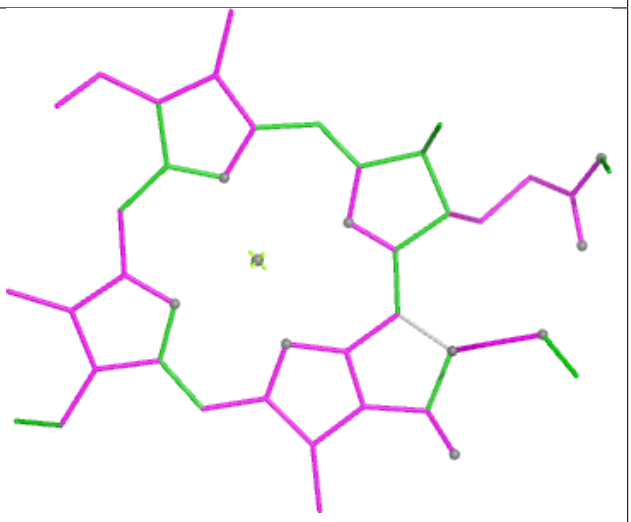


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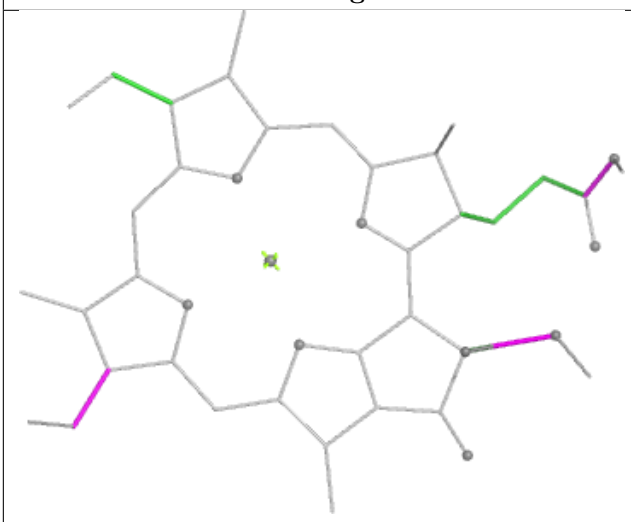
Ligand CLA 3 3002



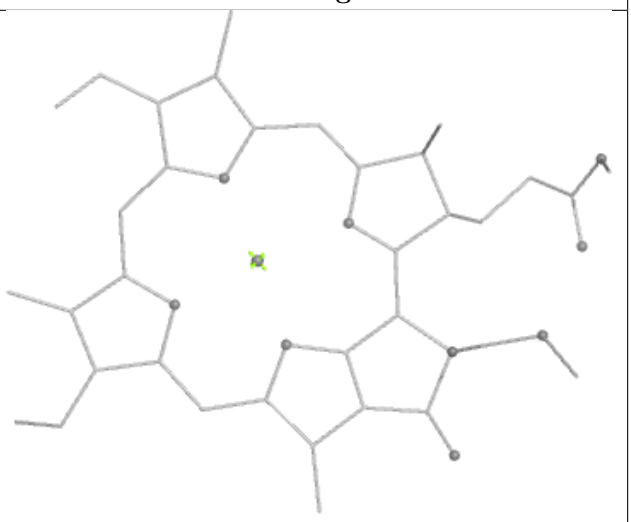
Bond lengths



Bond angles

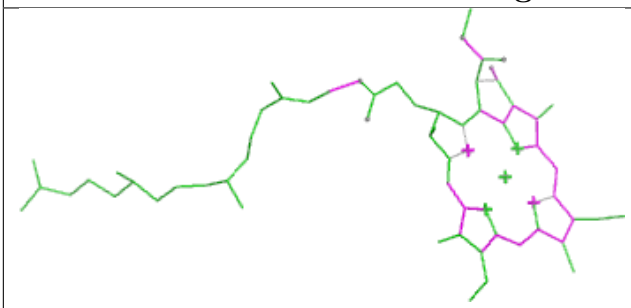


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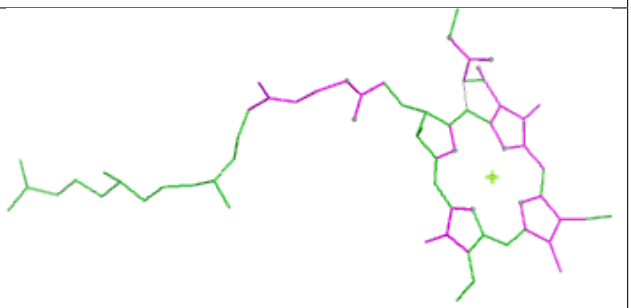


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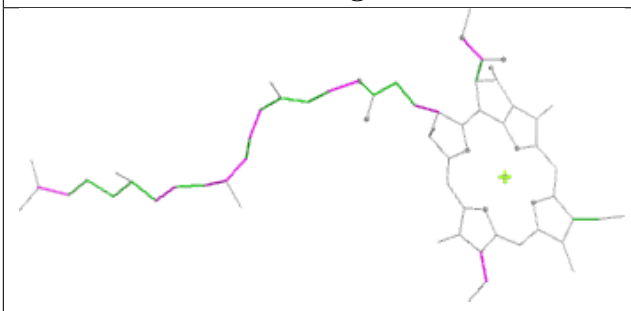
Ligand CLA A 1022



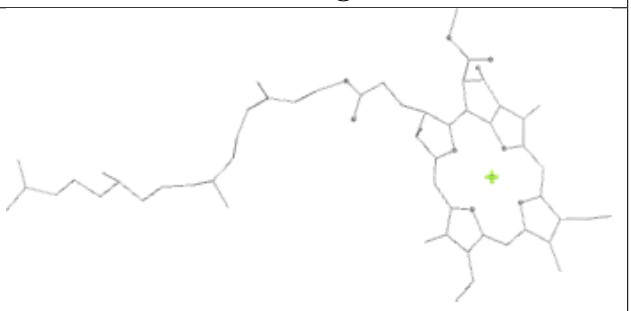
Bond lengths



Bond angles

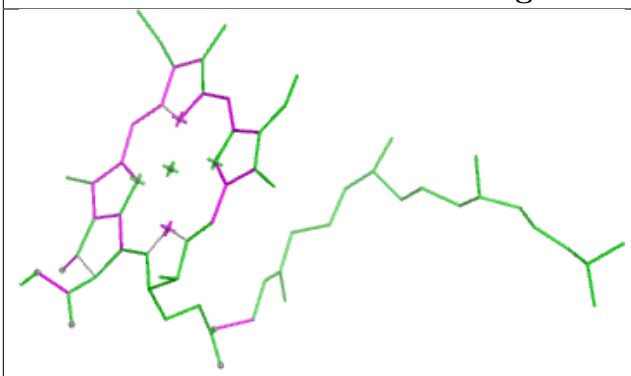


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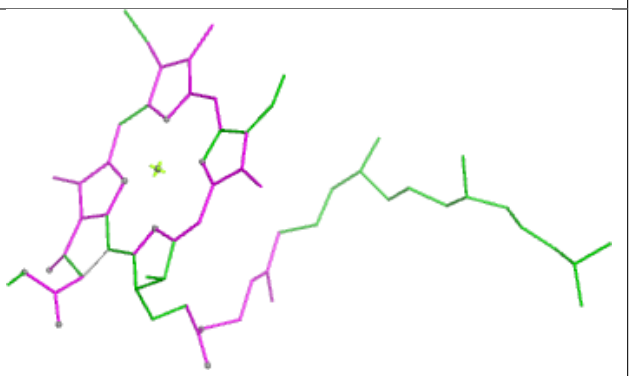


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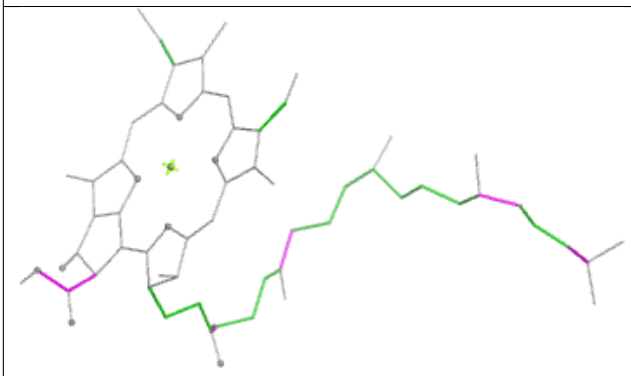
Ligand CLA B 1211



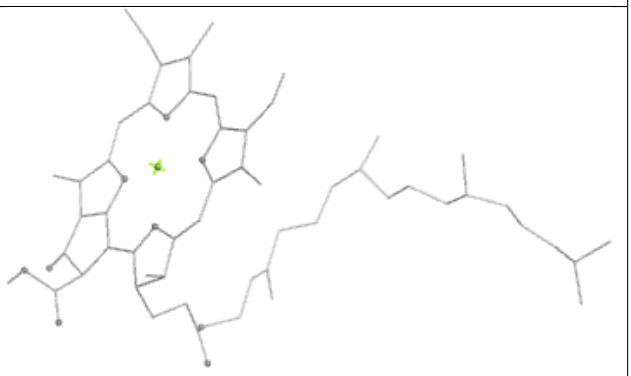
Bond lengths



Bond angles

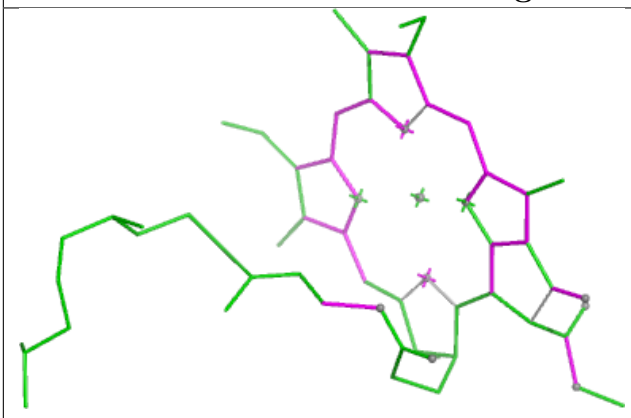


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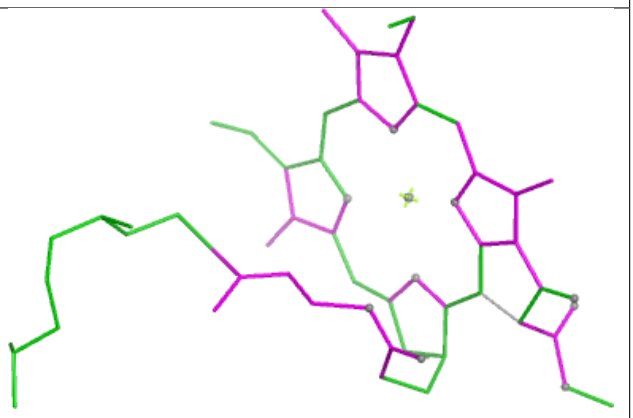


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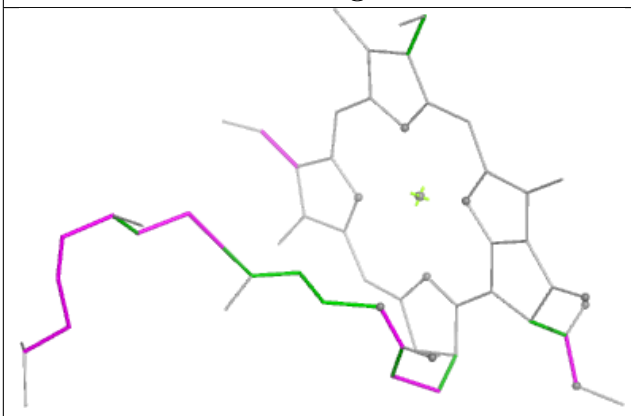
Ligand CLA A 1237



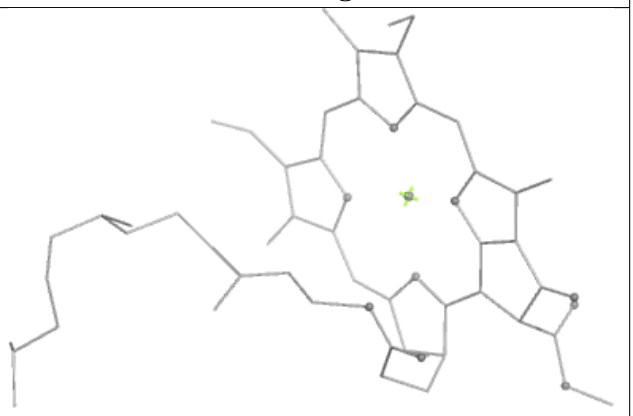
Bond lengths



Bond angles

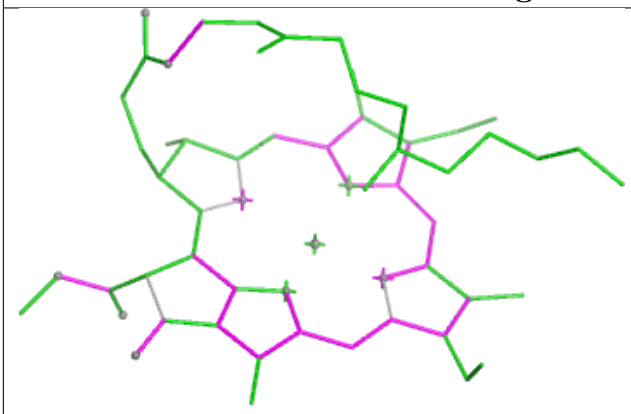


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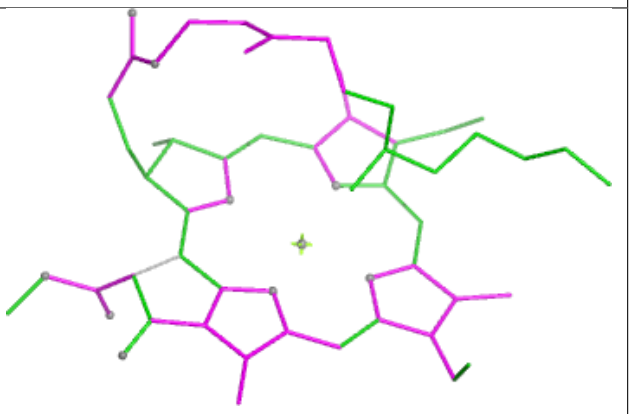


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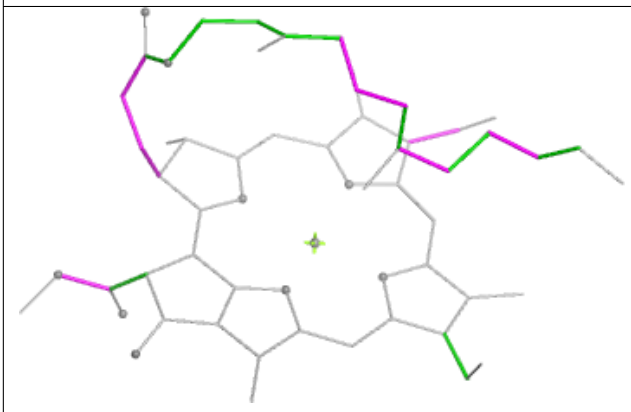
Ligand CLA B 1214



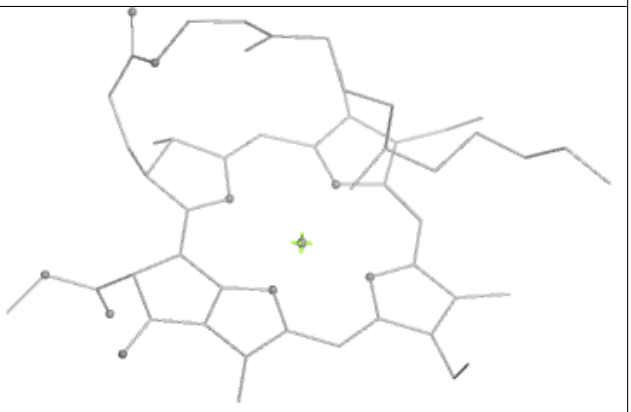
Bond lengths



Bond angles

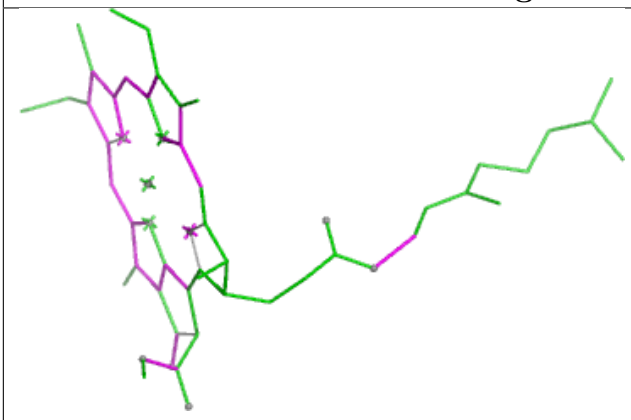


Torsions

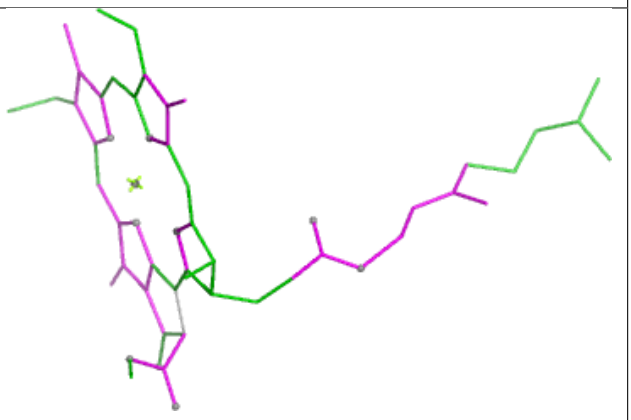


Rings

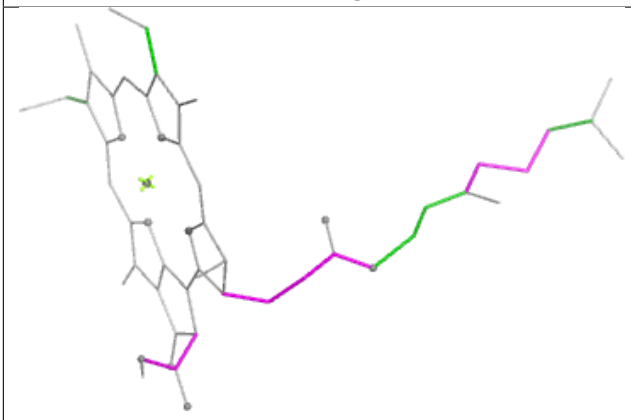
Ligand CLA B 1208



Bond lengths



Bond angles

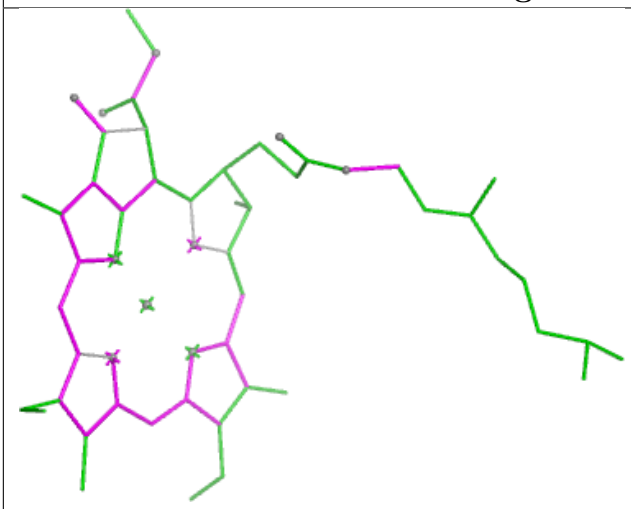


Torsions

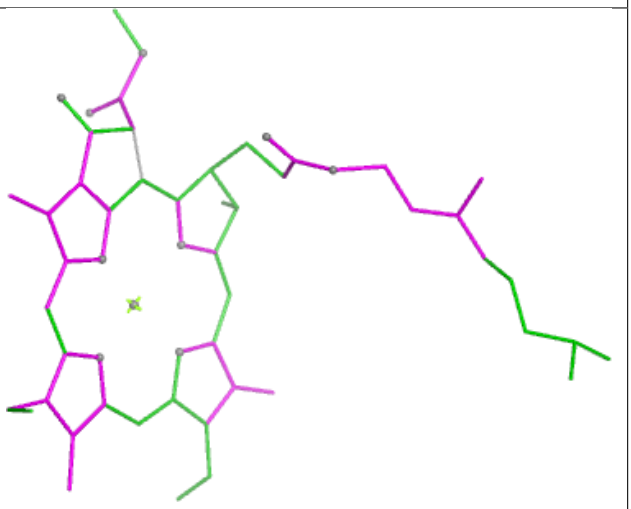


Rings

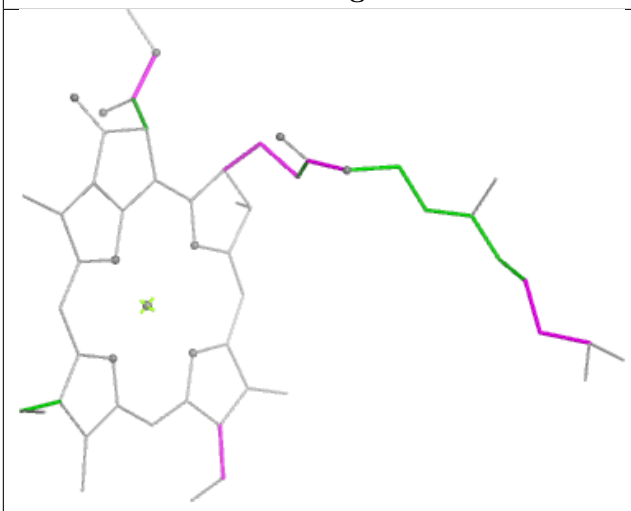
Ligand CLA A 1133



Bond lengths



Bond angles

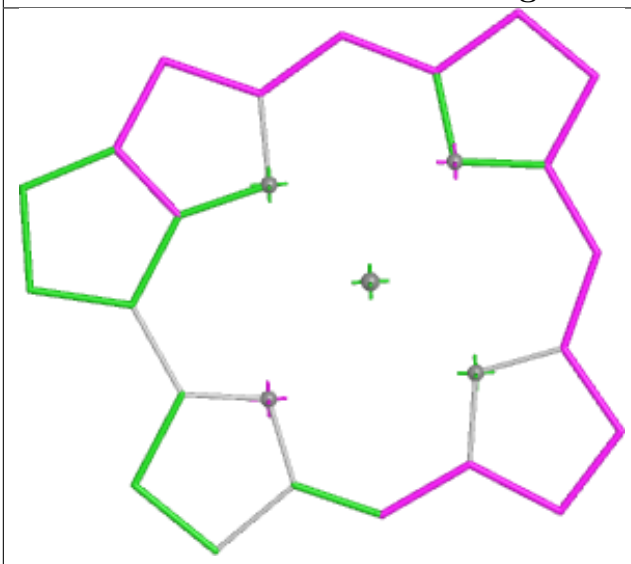


Torsions

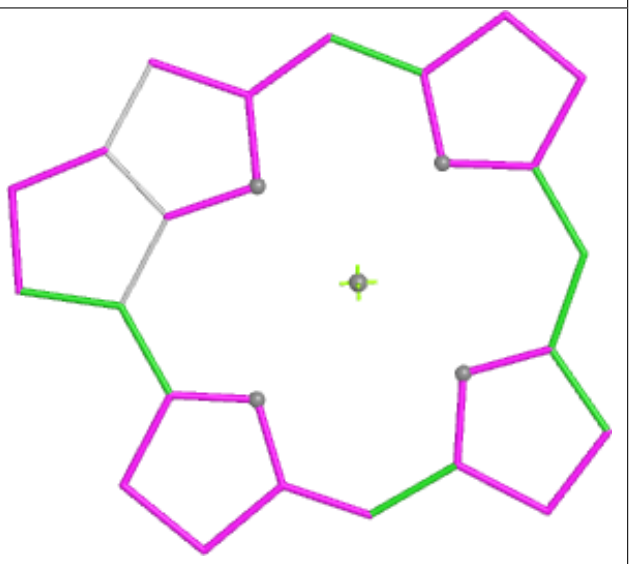


Rings

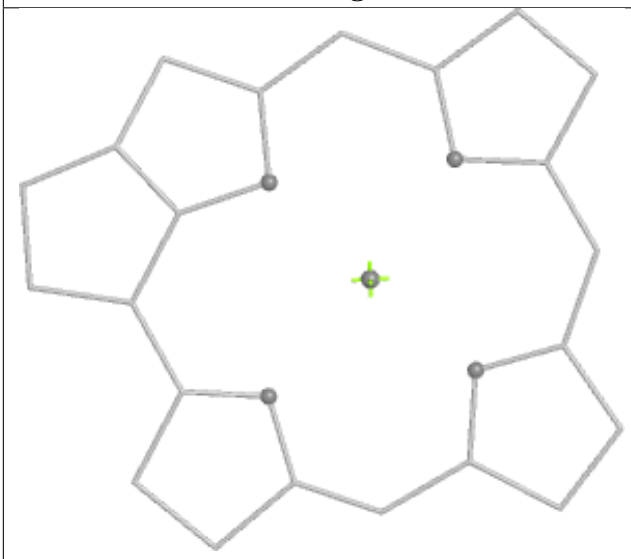
Ligand CLA 3 3019



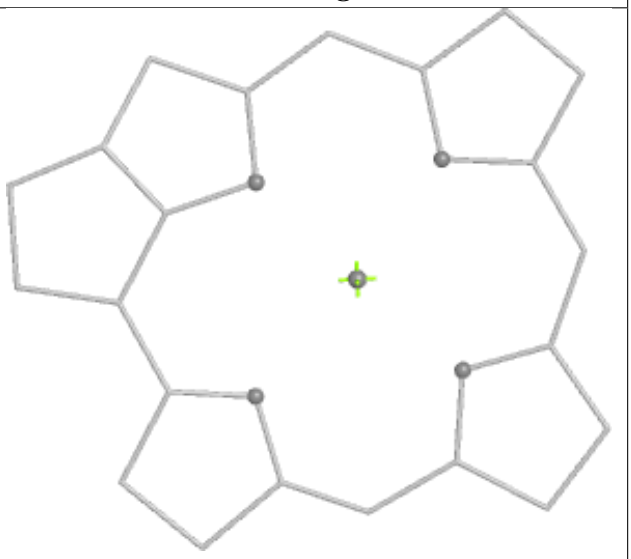
Bond lengths



Bond angles

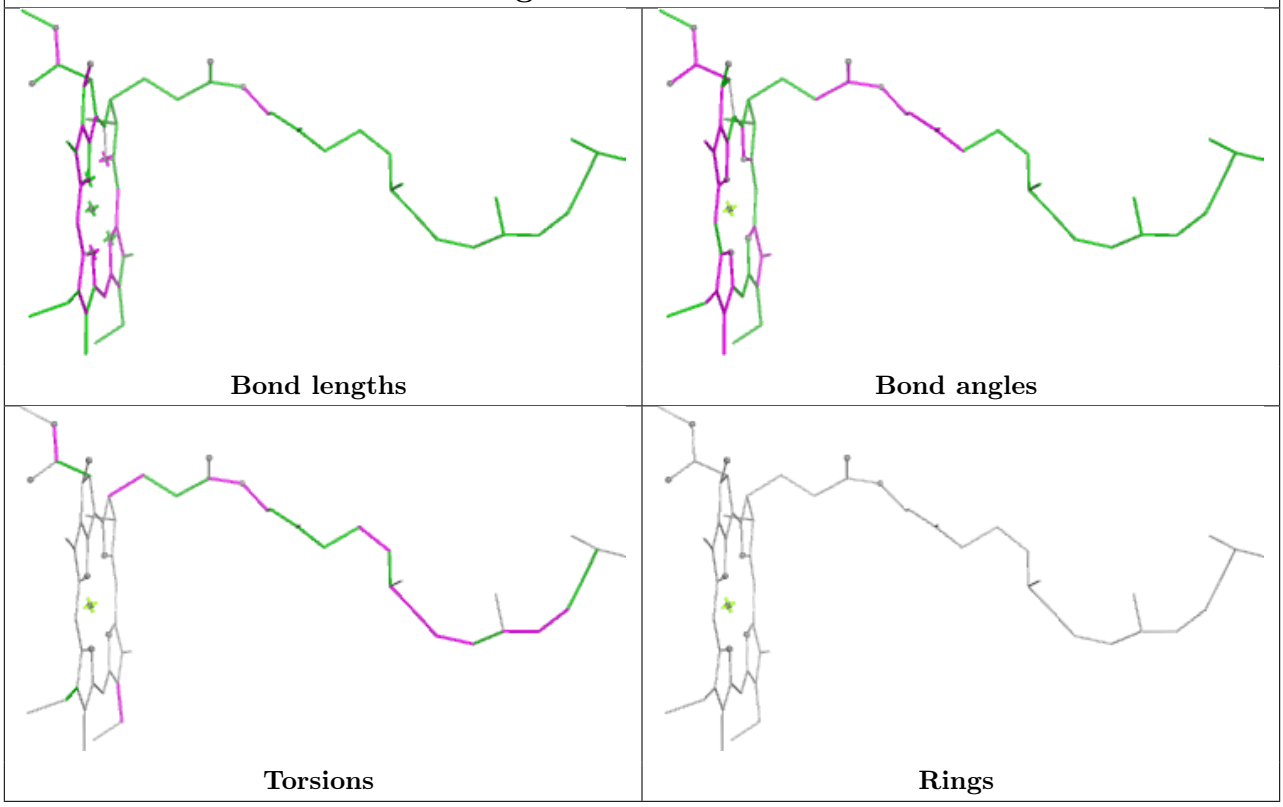


Torsions

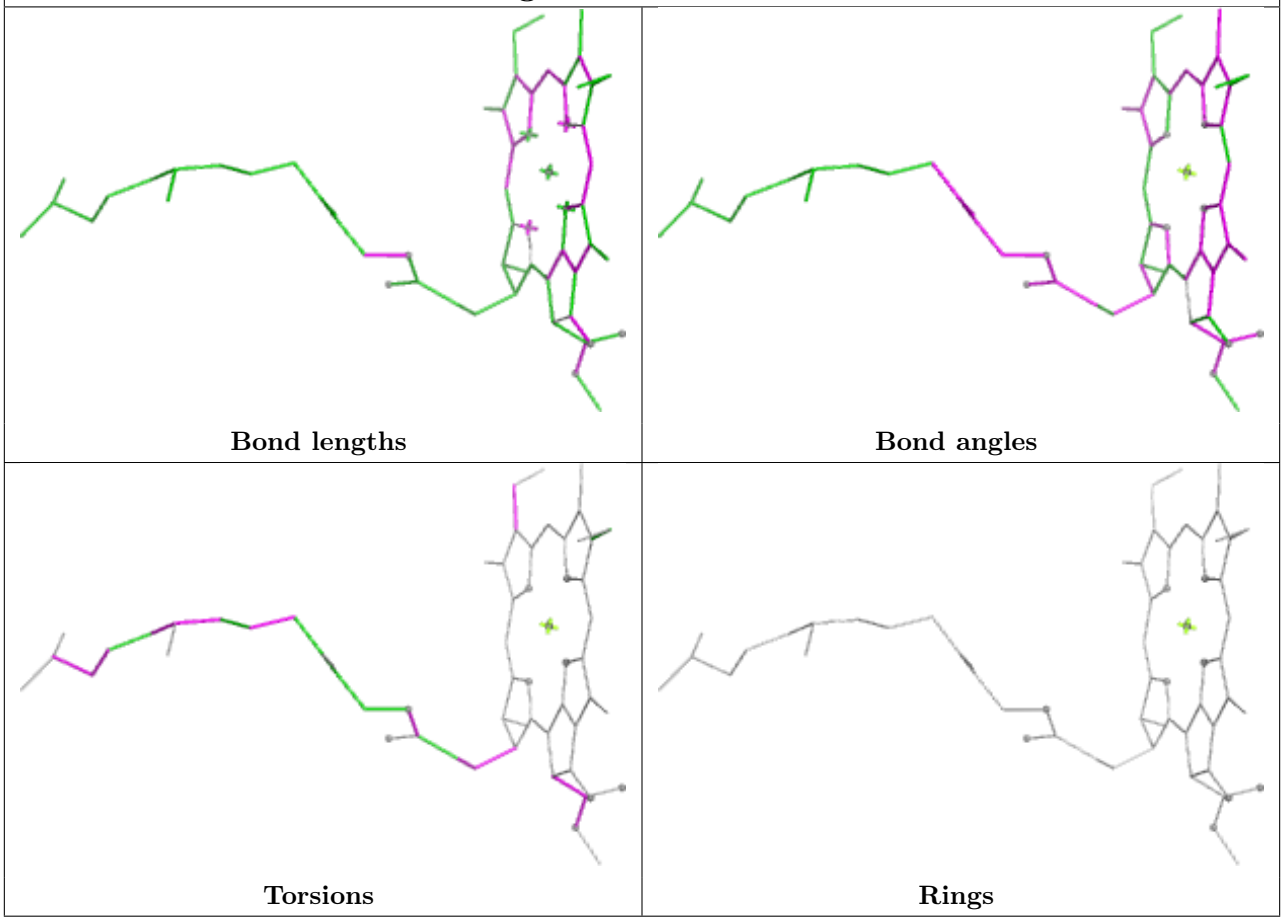


Rings

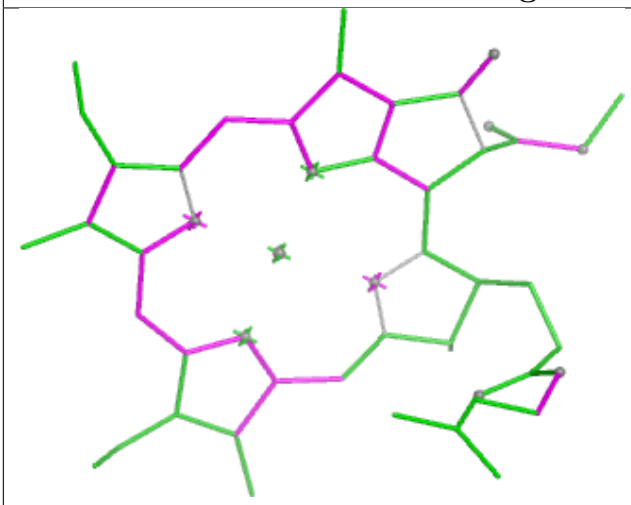
Ligand CLA A 1112



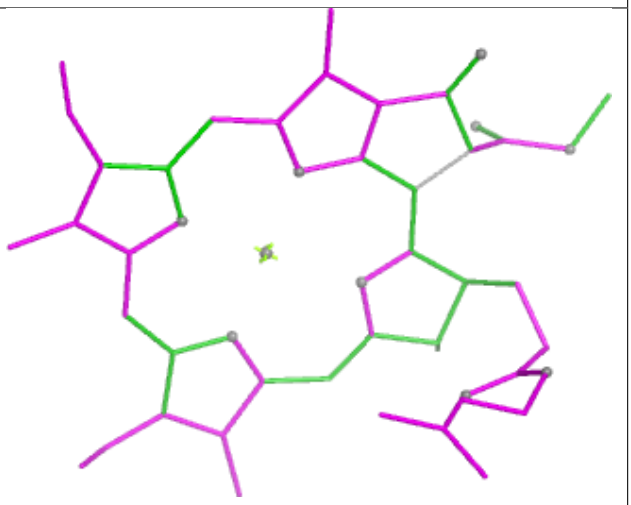
Ligand CLA L 1502



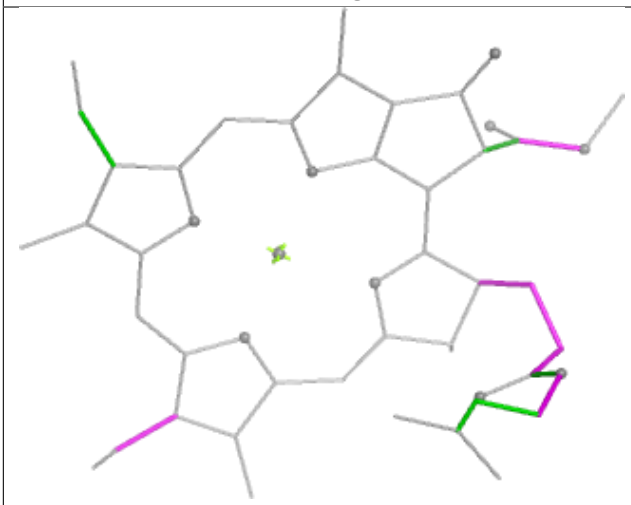
Ligand CLA 1 1012



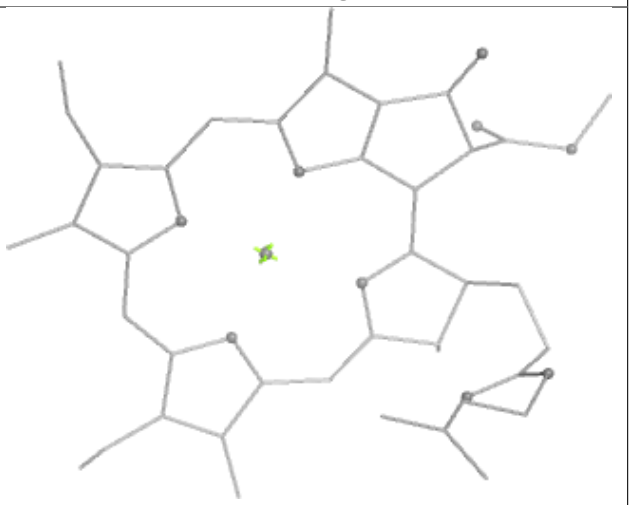
Bond lengths



Bond angles

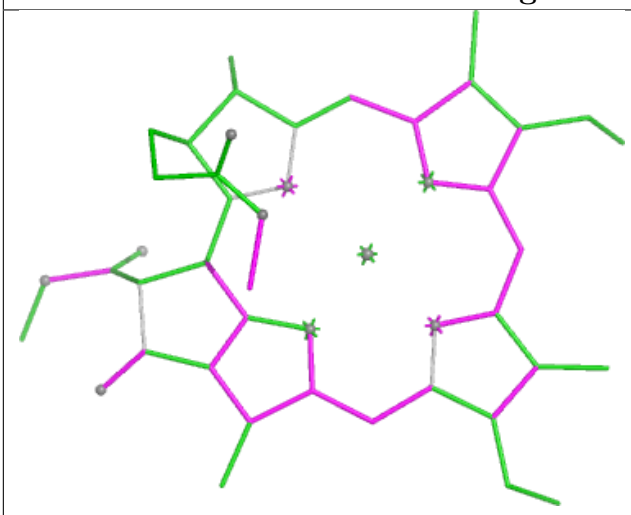


Torsions

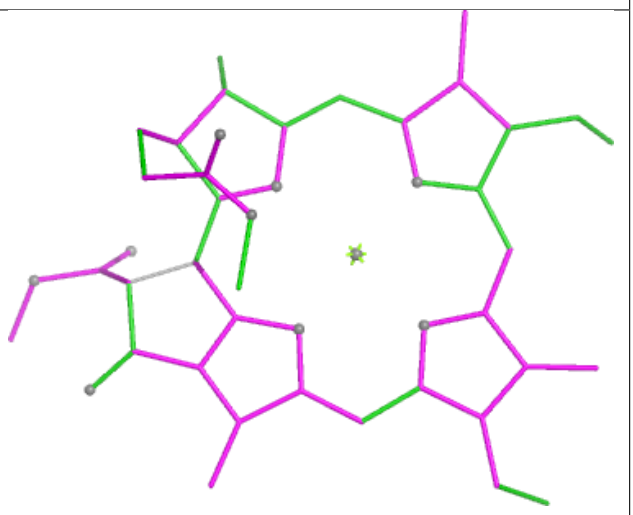


Rings

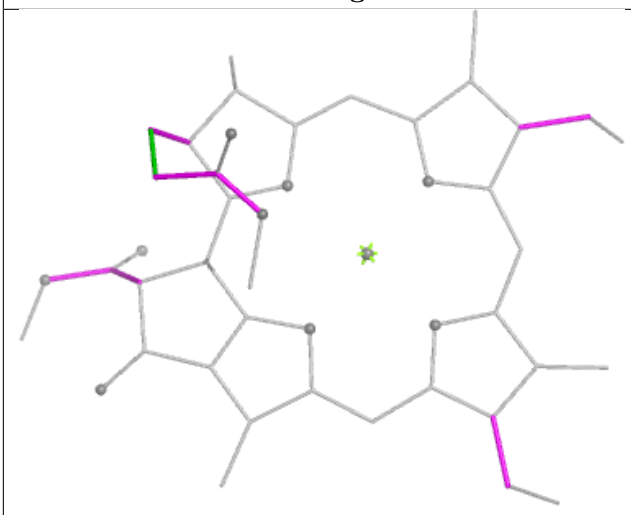
Ligand CLA 4 4016



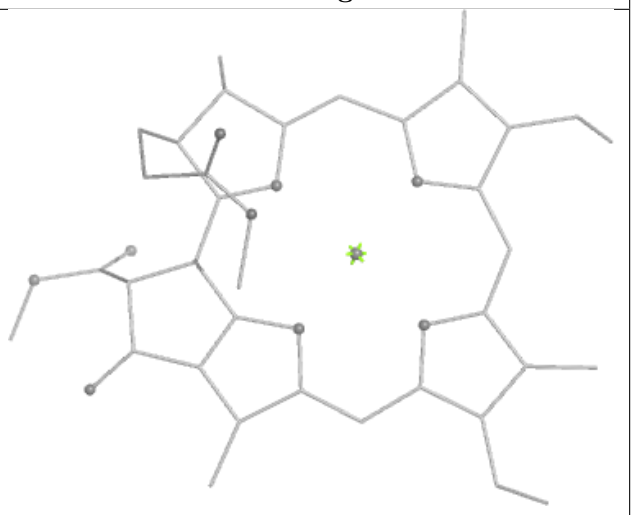
Bond lengths



Bond angles

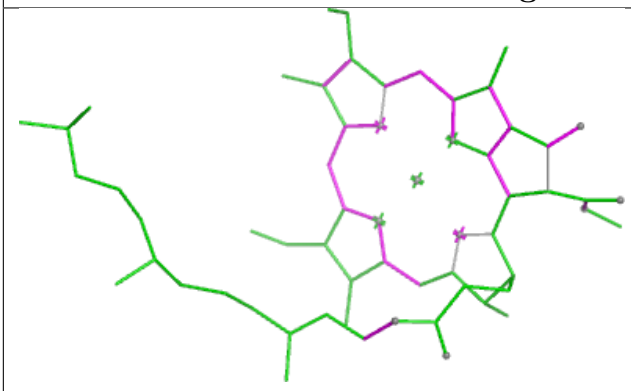


Torsions

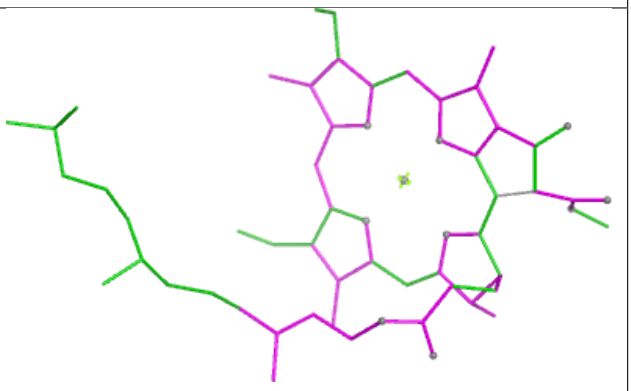


Rings

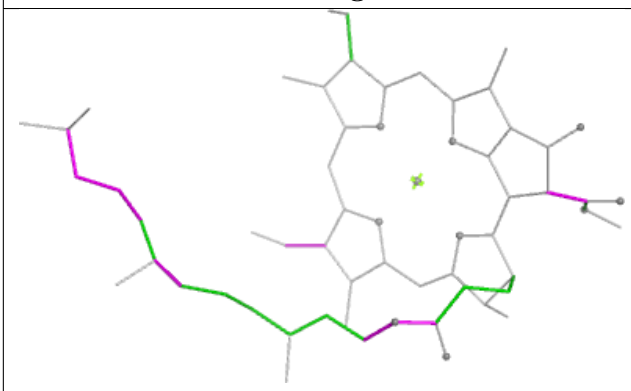
Ligand CLA 4 4004



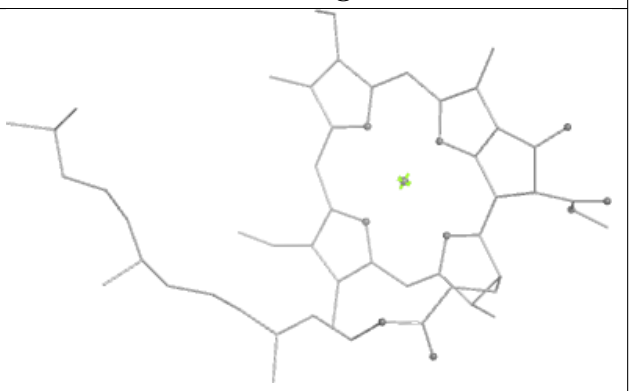
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	742/758 (97%)	0.64	67 (9%) 15 11	56, 92, 150, 244	0
2	B	732/733 (99%)	0.66	63 (8%) 16 12	61, 89, 126, 157	0
3	I	29/30 (96%)	0.81	5 (17%) 4 3	89, 114, 148, 153	0
4	J	41/42 (97%)	0.78	6 (14%) 6 4	70, 80, 116, 164	0
5	F	150/154 (97%)	0.60	17 (11%) 10 7	66, 90, 122, 157	0
6	G	91/97 (93%)	1.43	24 (26%) 1 1	98, 129, 174, 184	0
7	L	160/167 (95%)	1.21	35 (21%) 2 2	86, 123, 172, 197	0
8	C	80/81 (98%)	0.63	7 (8%) 15 11	66, 81, 96, 106	0
9	D	141/147 (95%)	1.34	35 (24%) 2 1	77, 97, 120, 139	0
10	E	66/66 (100%)	0.55	5 (7%) 20 14	65, 91, 136, 183	0
11	H	84/90 (93%)	1.35	23 (27%) 1 1	103, 138, 178, 234	0
12	K	57/129 (44%)	1.48	18 (31%) 1 1	147, 215, 286, 324	0
13	2	207/269 (76%)	1.00	33 (15%) 5 4	85, 130, 180, 270	0
14	4	198/252 (78%)	0.72	22 (11%) 10 7	84, 121, 193, 274	0
15	1	194/202 (96%)	1.50	51 (26%) 1 1	95, 147, 225, 289	0
16	3	215/275 (78%)	1.46	64 (29%) 1 1	111, 179, 317, 368	0
All	All	3187/3492 (91%)	0.90	475 (14%) 5 4	56, 106, 205, 368	0

The worst 5 of 475 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	D	196	VAL	12.0
2	B	82	PHE	11.4
9	D	200	GLU	9.9
2	B	552	ASP	9.5
9	D	206	LYS	8.6

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

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

6.3 Carbohydrates (i)

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
18	CLA	3	3019	27/65	0.45	0.27	158,174,188,189	1
23	LMG	B	5005	38/55	0.63	0.20	76,120,141,143	0
18	CLA	J	1302	50/65	0.66	0.20	137,152,189,196	0
18	CLA	4	4016	46/65	0.68	0.18	126,166,177,183	0
18	CLA	3	3008	48/65	0.69	0.17	180,199,214,217	0
18	CLA	2	2019	27/65	0.71	0.17	148,159,174,174	1
18	CLA	3	3010	60/65	0.73	0.26	122,158,181,196	0
18	CLA	2	2016	50/65	0.75	0.19	114,164,207,211	0
26	LMU	B	8002	35/35	0.76	0.18	162,173,189,191	0
18	CLA	3	3018	50/65	0.78	0.16	173,190,207,213	0
23	LMG	F	5002	37/55	0.78	0.13	84,107,120,126	0
26	LMU	B	8001	35/35	0.78	0.14	104,158,168,172	0
18	CLA	K	1001	46/65	0.78	0.16	147,173,200,209	0
18	CLA	3	3007	50/65	0.79	0.18	175,193,239,246	0
18	CLA	1	1013	46/65	0.80	0.17	127,154,181,185	0
18	CLA	3	3013	46/65	0.80	0.16	127,157,166,176	0
18	CLA	G	1003	60/65	0.81	0.16	97,121,149,153	0
18	CLA	H	1000	46/65	0.82	0.14	119,150,170,176	0
22	BCR	G	2011	40/40	0.82	0.20	112,132,172,174	0
28	CHL	2	2010	47/66	0.82	0.12	111,134,142,143	0
22	BCR	J	6013	40/40	0.83	0.18	74,94,112,116	0
23	LMG	F	5001	23/55	0.83	0.10	86,94,106,109	0
18	CLA	1	1001	60/65	0.83	0.17	122,151,165,171	0
22	BCR	K	2011	40/40	0.84	0.22	125,136,144,147	0
18	CLA	3	3006	50/65	0.84	0.12	125,157,167,170	0
23	LMG	G	2021	41/55	0.84	0.19	138,156,175,176	0
28	CHL	3	3011	56/66	0.84	0.18	144,156,197,200	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	A	1151	50/65	0.85	0.13	99,113,187,189	0
18	CLA	A	1113	46/65	0.85	0.16	119,135,172,187	0
27	LUT	3	3501	42/42	0.85	0.26	202,209,216,218	0
18	CLA	L	1501	50/65	0.85	0.15	106,129,153,159	0
28	CHL	4	4010	47/66	0.85	0.16	105,125,180,187	0
23	LMG	2	2802	35/55	0.85	0.17	108,127,149,152	0
18	CLA	A	1134	55/65	0.86	0.16	112,124,168,172	0
22	BCR	L	6020	40/40	0.86	0.19	98,131,157,164	0
18	CLA	1	1006	50/65	0.86	0.14	125,138,144,148	0
18	CLA	1	1008	46/65	0.86	0.17	112,129,142,150	0
18	CLA	A	1114	46/65	0.86	0.12	107,117,124,136	0
18	CLA	4	4006	50/65	0.86	0.16	110,127,148,156	0
18	CLA	2	2006	55/65	0.86	0.15	105,132,173,174	0
22	BCR	A	6007	40/40	0.87	0.17	77,90,147,151	0
18	CLA	A	1115	46/65	0.87	0.15	107,141,170,178	0
28	CHL	2	2013	46/66	0.87	0.14	110,125,130,135	0
18	CLA	3	3002	46/65	0.87	0.15	173,188,195,222	0
18	CLA	G	1001	55/65	0.87	0.14	119,145,181,184	0
18	CLA	B	1218	65/65	0.88	0.17	86,100,155,160	0
18	CLA	1	1014	46/65	0.88	0.12	83,110,123,143	0
18	CLA	4	4008	46/65	0.88	0.14	93,112,129,137	0
28	CHL	1	1010	47/66	0.88	0.14	125,137,152,155	0
22	BCR	3	3503	40/40	0.88	0.21	119,136,175,177	0
27	LUT	1	1501	42/42	0.89	0.23	115,142,189,197	0
18	CLA	1	1011	50/65	0.89	0.17	126,153,175,185	0
23	LMG	4	4801	35/55	0.89	0.18	104,117,128,132	0
18	CLA	G	1002	46/65	0.89	0.11	142,160,173,181	0
22	BCR	B	6004	40/40	0.89	0.22	105,112,138,144	0
27	LUT	2	2502	42/42	0.89	0.22	102,115,124,131	0
27	LUT	4	4503	42/42	0.89	0.22	110,135,158,160	0
23	LMG	J	5001	55/55	0.90	0.17	62,96,110,122	0
18	CLA	L	1503	50/65	0.90	0.12	106,114,143,149	0
18	CLA	B	1232	55/65	0.90	0.12	80,97,118,122	0
27	LUT	1	1502	42/42	0.90	0.19	85,116,128,129	0
18	CLA	3	3001	50/65	0.90	0.11	147,169,201,206	0
27	LUT	3	3502	42/42	0.90	0.21	133,142,164,166	0
18	CLA	4	4001	60/65	0.90	0.17	113,129,158,160	0
18	CLA	A	1121	55/65	0.90	0.13	104,123,209,211	0
21	LHG	B	5004	21/49	0.90	0.11	86,102,116,119	0
28	CHL	4	4013	47/66	0.90	0.12	98,118,130,134	0
18	CLA	B	1213	60/65	0.90	0.15	85,105,118,126	0
27	LUT	2	2501	42/42	0.90	0.20	121,137,141,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	ZEX	4	4505	42/42	0.90	0.13	85,96,107,114	0
22	BCR	A	6008	40/40	0.91	0.20	76,97,137,139	0
18	CLA	1	1002	46/65	0.91	0.15	120,155,171,194	0
22	BCR	B	6009	40/40	0.91	0.17	63,78,94,95	0
18	CLA	1	1005	55/65	0.91	0.13	84,113,122,124	0
18	CLA	B	1201	50/65	0.91	0.14	80,93,131,134	0
18	CLA	B	1208	55/65	0.91	0.13	82,114,133,137	0
18	CLA	B	1238	65/65	0.91	0.15	70,85,96,116	0
18	CLA	3	3017	46/65	0.91	0.14	101,119,134,145	0
18	CLA	B	1228	60/65	0.91	0.15	63,73,111,114	0
18	CLA	B	1217	46/65	0.91	0.14	96,109,124,127	0
21	LHG	A	5003	40/49	0.91	0.16	101,117,132,134	0
18	CLA	A	1120	60/65	0.91	0.14	95,118,178,182	0
21	LHG	2	2801	24/49	0.91	0.14	109,123,148,152	0
22	BCR	A	6003	40/40	0.91	0.21	79,94,139,140	0
18	CLA	B	1219	60/65	0.91	0.16	82,97,134,135	0
25	DGD	B	7101	61/66	0.91	0.15	62,79,104,113	0
18	CLA	A	1105	51/65	0.92	0.12	66,88,97,100	0
18	CLA	2	2002	46/65	0.92	0.12	137,154,171,183	0
18	CLA	2	2004	65/65	0.92	0.14	84,105,117,125	0
18	CLA	2	2005	55/65	0.92	0.13	93,103,129,135	0
18	CLA	3	3003	60/65	0.92	0.14	137,170,188,190	0
18	CLA	3	3004	60/65	0.92	0.15	125,139,154,155	0
18	CLA	B	1209	46/65	0.92	0.13	100,109,118,145	0
18	CLA	B	1212	55/65	0.92	0.16	109,129,146,154	0
18	CLA	B	1231	60/65	0.92	0.12	65,81,101,104	0
18	CLA	A	1108	46/65	0.92	0.12	85,101,121,126	0
18	CLA	3	3012	50/65	0.92	0.13	117,135,142,144	0
18	CLA	4	4002	50/65	0.92	0.15	107,141,171,211	0
18	CLA	B	1240	65/65	0.92	0.12	66,84,103,108	0
18	CLA	4	4007	60/65	0.92	0.17	110,130,179,183	0
18	CLA	B	1021	65/65	0.92	0.15	61,72,80,83	0
18	CLA	F	1301	45/65	0.92	0.12	61,73,86,101	0
18	CLA	4	4017	65/65	0.92	0.16	93,103,120,121	0
18	CLA	B	1204	55/65	0.92	0.12	80,103,118,124	0
21	LHG	1	1801	49/49	0.92	0.17	94,113,164,170	0
22	BCR	A	6002	40/40	0.92	0.21	82,115,168,169	0
18	CLA	A	1112	65/65	0.92	0.15	101,118,138,140	0
18	CLA	A	1124	55/65	0.92	0.14	59,77,104,116	0
18	CLA	A	1022	65/65	0.92	0.14	58,76,88,99	0
18	CLA	1	1007	46/65	0.92	0.12	112,131,162,181	0
22	BCR	B	6005	40/40	0.92	0.21	87,103,182,184	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	B	1220	65/65	0.92	0.15	61,76,114,118	0
22	BCR	J	6012	40/40	0.92	0.15	67,80,89,91	0
18	CLA	A	1139	65/65	0.92	0.14	56,70,98,104	0
18	CLA	A	1133	55/65	0.93	0.14	83,109,120,126	0
18	CLA	2	2003	55/65	0.93	0.12	103,127,135,158	0
22	BCR	F	6016	40/40	0.93	0.12	66,75,91,94	0
18	CLA	B	1211	65/65	0.93	0.13	93,107,131,136	0
18	CLA	A	1109	65/65	0.93	0.12	71,85,94,101	0
22	BCR	L	6019	40/40	0.93	0.24	88,105,132,135	0
18	CLA	B	1239	65/65	0.93	0.14	69,82,111,116	0
18	CLA	2	2007	60/65	0.93	0.15	116,142,189,195	0
18	CLA	2	2012	55/65	0.93	0.13	86,104,149,153	0
18	CLA	B	1214	59/65	0.93	0.16	71,91,100,108	0
18	CLA	B	1227	65/65	0.93	0.13	60,74,99,105	0
18	CLA	2	2009	50/65	0.93	0.12	100,117,138,139	0
18	CLA	A	1135	51/65	0.93	0.14	72,92,114,117	0
18	CLA	A	1137	55/65	0.93	0.13	71,85,125,126	0
18	CLA	4	4003	65/65	0.93	0.13	84,106,135,143	0
18	CLA	4	4004	60/65	0.93	0.14	76,99,112,118	0
18	CLA	B	1234	60/65	0.93	0.15	64,77,106,108	0
18	CLA	A	1126	65/65	0.93	0.15	65,79,87,97	0
27	LUT	I	6018	42/42	0.93	0.15	101,109,116,121	0
18	CLA	A	1131	65/65	0.93	0.16	79,93,103,112	0
18	CLA	4	4012	65/65	0.93	0.14	92,104,117,120	0
27	LUT	4	4501	42/42	0.93	0.15	107,121,142,149	0
27	LUT	4	4502	42/42	0.93	0.16	88,106,117,121	0
18	CLA	A	1118	46/65	0.93	0.13	99,108,127,131	0
18	CLA	A	1129	50/65	0.93	0.11	71,93,115,126	0
18	CLA	A	1101	65/65	0.93	0.12	58,72,90,113	0
18	CLA	B	1222	65/65	0.93	0.15	58,74,103,110	0
18	CLA	1	1004	65/65	0.93	0.14	98,114,122,125	0
18	CLA	L	1502	60/65	0.93	0.13	86,116,125,130	0
28	CHL	2	2011	48/66	0.93	0.14	108,124,129,136	0
18	CLA	B	1012	65/65	0.93	0.15	51,69,85,92	0
18	CLA	B	1207	65/65	0.93	0.14	78,102,122,129	0
22	BCR	B	6006	40/40	0.93	0.19	94,115,164,164	0
28	CHL	1	1009	56/66	0.93	0.12	92,105,113,130	0
18	CLA	B	1216	65/65	0.93	0.14	73,86,105,108	0
22	BCR	B	6010	40/40	0.93	0.15	64,73,96,100	0
22	BCR	I	6020	40/40	0.93	0.16	85,97,110,111	0
18	CLA	A	1123	65/65	0.94	0.16	70,88,93,96	0
18	CLA	B	1221	65/65	0.94	0.14	66,78,115,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	A	1119	65/65	0.94	0.14	78,95,107,115	0
18	CLA	B	1223	65/65	0.94	0.14	59,78,90,96	0
18	CLA	A	1102	50/65	0.94	0.11	58,69,95,104	0
18	CLA	A	1110	55/65	0.94	0.15	97,114,138,143	0
24	CA	B	6000	1/1	0.94	0.09	100,100,100,100	0
18	CLA	A	1127	65/65	0.94	0.15	69,83,95,99	0
18	CLA	1	1003	55/65	0.94	0.14	100,122,134,142	0
18	CLA	2	2001	60/65	0.94	0.16	114,134,167,169	0
18	CLA	A	1111	60/65	0.94	0.13	75,91,112,118	0
18	CLA	A	1132	65/65	0.94	0.14	79,94,120,129	0
18	CLA	B	1236	55/65	0.94	0.14	56,69,117,124	0
18	CLA	A	1104	65/65	0.94	0.13	55,73,81,85	0
18	CLA	A	1237	60/65	0.94	0.14	75,94,113,116	0
18	CLA	1	1012	50/65	0.94	0.11	103,125,130,132	0
18	CLA	B	1224	65/65	0.94	0.15	65,83,100,107	0
18	CLA	B	1226	65/65	0.94	0.14	65,76,97,103	0
18	CLA	A	1106	65/65	0.94	0.13	59,74,90,106	0
18	CLA	A	1136	56/65	0.94	0.12	84,98,115,119	0
18	CLA	B	1023	65/65	0.94	0.12	57,70,94,105	0
22	BCR	F	6014	40/40	0.94	0.12	54,64,73,74	0
18	CLA	A	1107	65/65	0.94	0.13	60,77,94,105	0
18	CLA	3	3005	55/65	0.94	0.14	107,131,144,157	0
17	CL0	A	1011	65/65	0.94	0.13	52,70,82,84	0
18	CLA	A	1122	65/65	0.94	0.15	76,96,122,139	0
18	CLA	F	1302	50/65	0.94	0.09	67,84,114,124	0
18	CLA	4	4005	60/65	0.94	0.13	84,97,106,120	0
18	CLA	A	1116	60/65	0.94	0.14	89,119,137,142	0
21	LHG	A	7001	49/49	0.95	0.13	56,72,84,92	0
18	CLA	A	1130	50/65	0.95	0.13	83,100,123,127	0
18	CLA	A	1013	65/65	0.95	0.12	49,62,74,90	0
18	CLA	2	2008	50/65	0.95	0.13	109,138,148,156	0
18	CLA	A	1117	65/65	0.95	0.16	85,98,110,114	0
18	CLA	B	1215	60/65	0.95	0.13	82,91,102,109	0
18	CLA	A	1103	65/65	0.95	0.12	66,83,104,107	0
18	CLA	B	1225	65/65	0.95	0.14	66,81,98,105	0
22	BCR	A	6017	40/40	0.95	0.16	71,86,105,122	0
18	CLA	B	1235	65/65	0.95	0.09	54,68,78,92	0
18	CLA	B	1205	65/65	0.95	0.15	90,103,116,152	0
18	CLA	B	1202	65/65	0.95	0.14	71,82,91,104	0
18	CLA	B	1230	58/65	0.95	0.10	58,74,83,86	0
28	CHL	4	4011	51/66	0.95	0.13	117,131,149,154	0
18	CLA	B	1206	65/65	0.95	0.12	86,104,112,127	0

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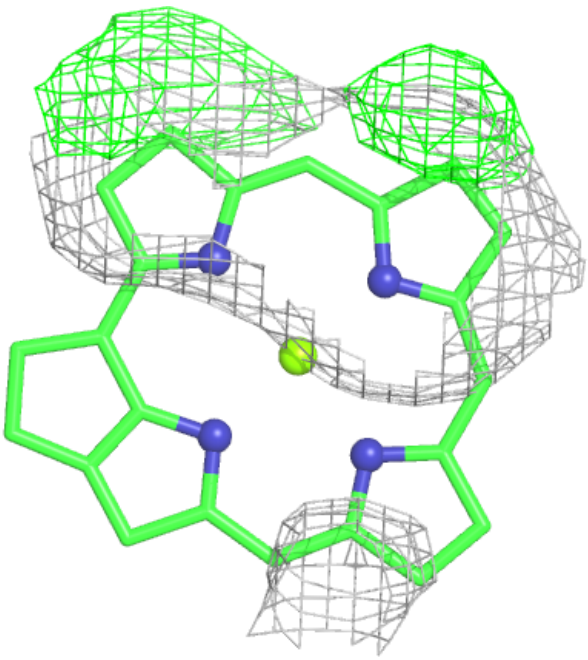
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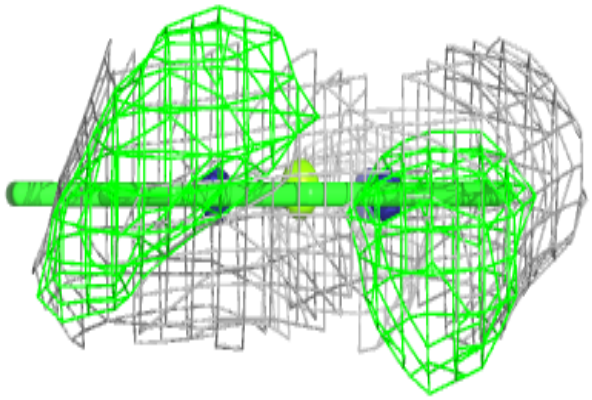
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
18	CLA	A	1128	65/65	0.95	0.12	56,66,74,85	0
18	CLA	A	1140	65/65	0.95	0.12	58,66,78,106	0
20	PQN	A	5001	33/33	0.95	0.12	53,63,76,85	0
18	CLA	A	1125	60/65	0.95	0.12	79,94,102,114	0
18	CLA	A	1138	65/65	0.96	0.11	55,65,75,82	0
22	BCR	A	6011	40/40	0.96	0.13	61,73,88,96	0
18	CLA	B	1229	65/65	0.96	0.11	60,72,82,84	0
18	CLA	B	1203	65/65	0.96	0.11	68,82,97,104	0
20	PQN	B	5002	33/33	0.96	0.11	54,72,91,93	0
18	CLA	B	1210	65/65	0.96	0.14	81,94,107,113	0
18	CLA	4	4009	50/65	0.96	0.11	85,94,116,131	0
19	SF4	C	3003	8/8	0.97	0.05	89,106,119,126	0
19	SF4	C	3002	8/8	0.97	0.05	73,103,107,107	0
19	SF4	A	3001	8/8	0.98	0.04	69,95,97,99	0

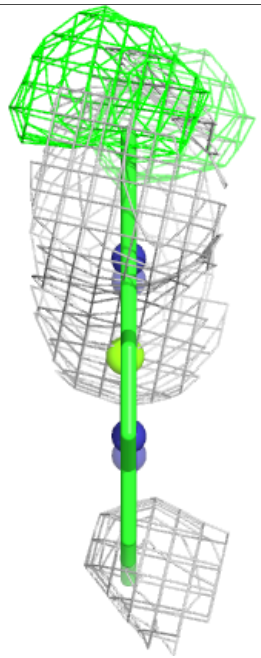
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA 3 3019:

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

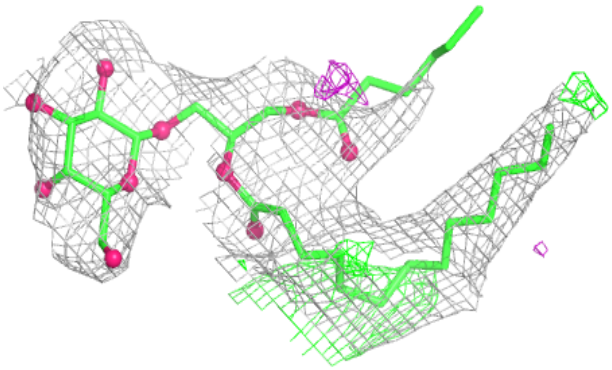


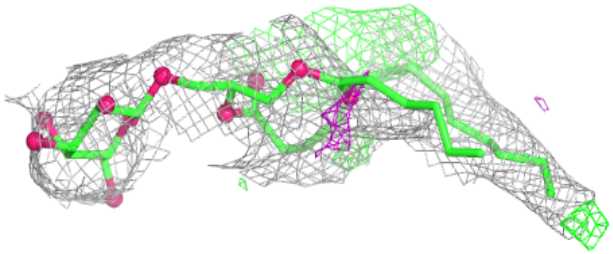


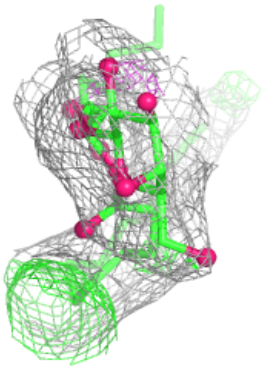


Electron density around LMG B 5005:

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

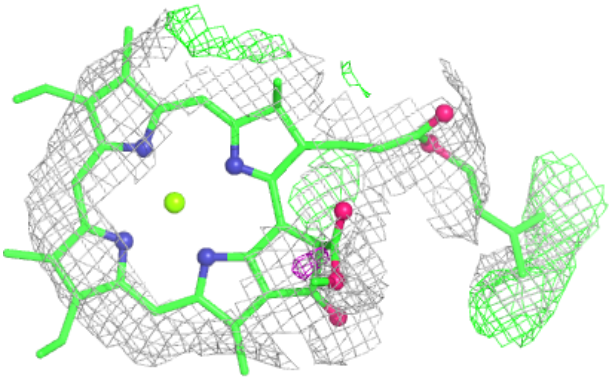


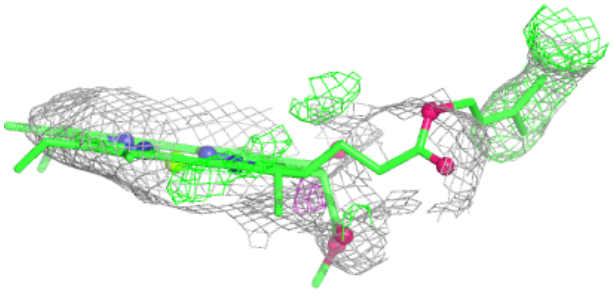


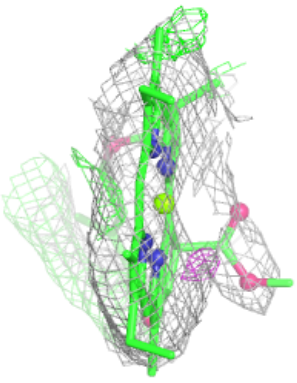


Electron density around CLA J 1302:

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

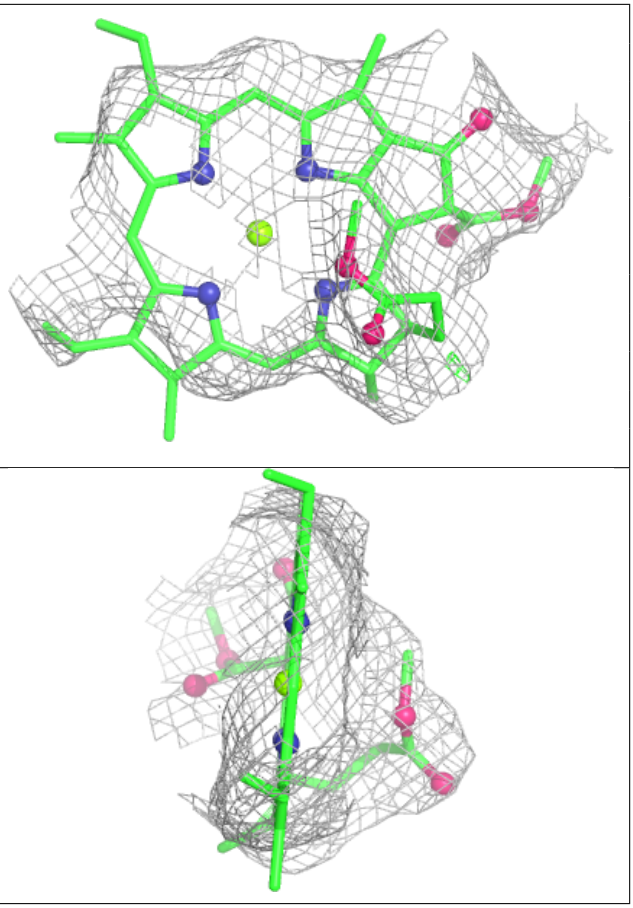


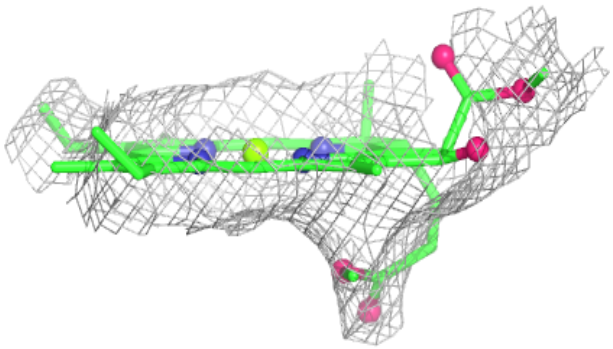




Electron density around CLA 4 4016:

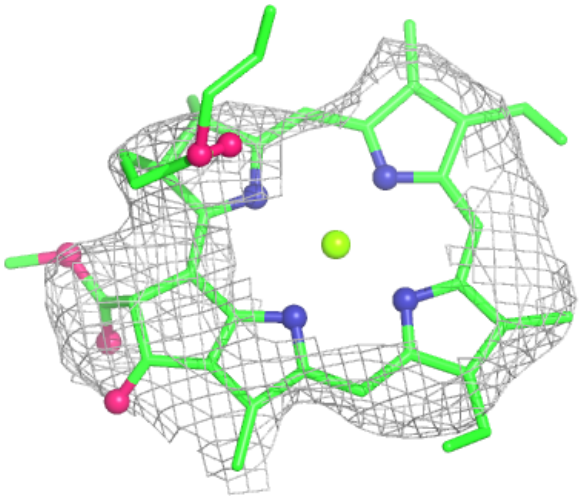
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

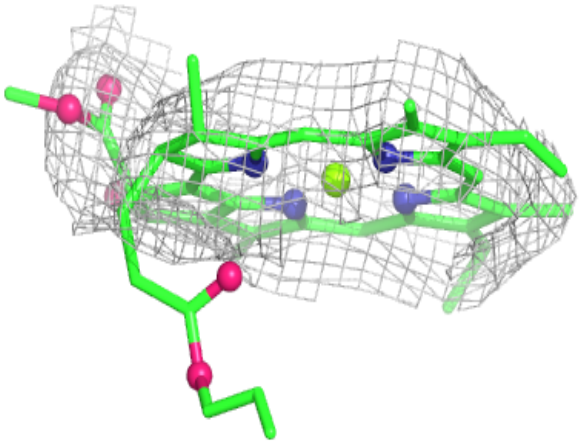




Electron density around CLA 3 3008:

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

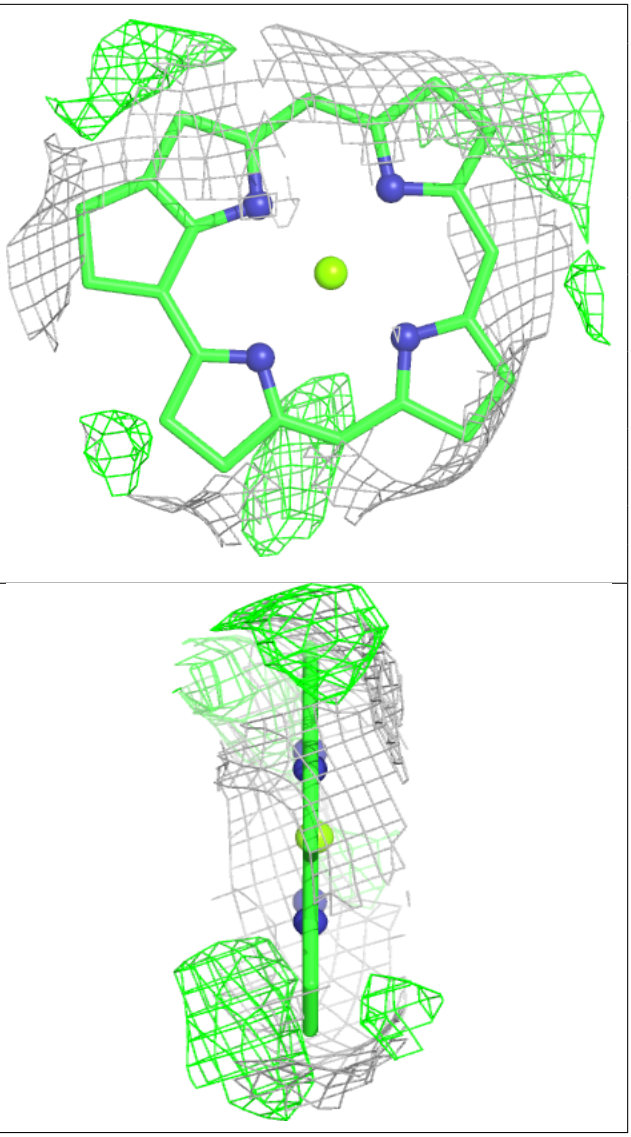






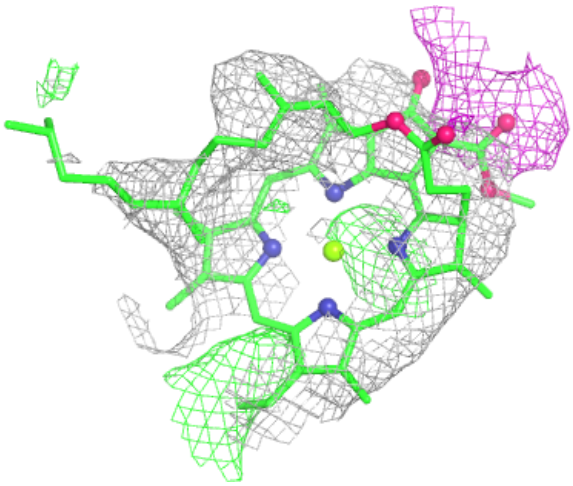
Electron density around CLA 2 2019:

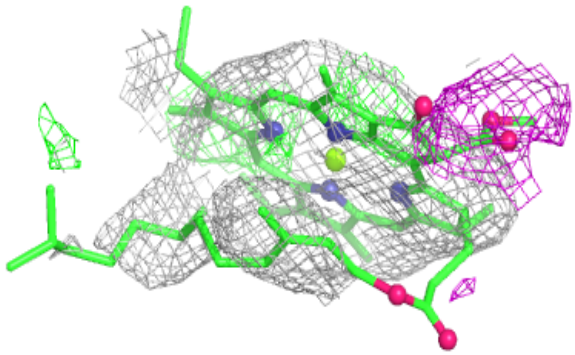
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

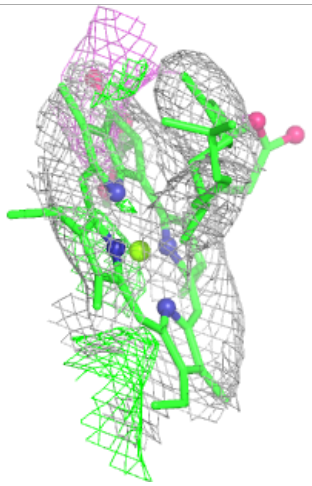


Electron density around CLA 3 3010:

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

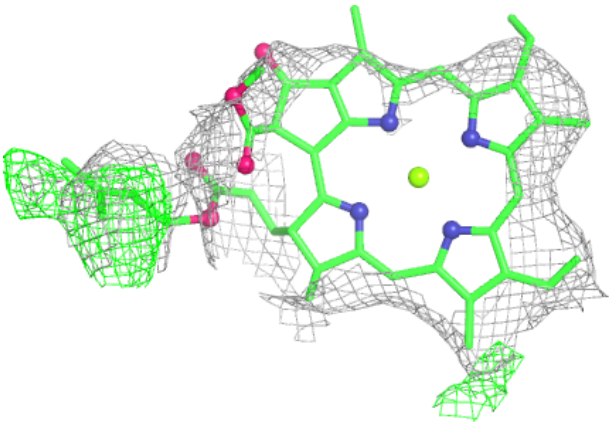


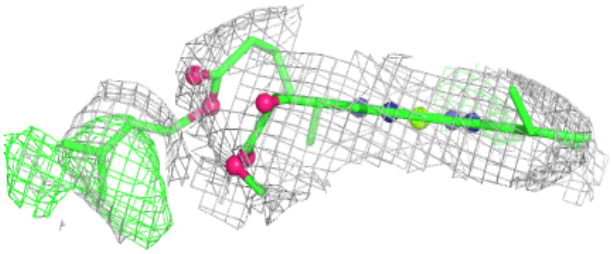


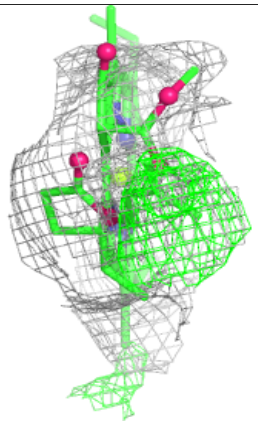


Electron density around CLA 2 2016:

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

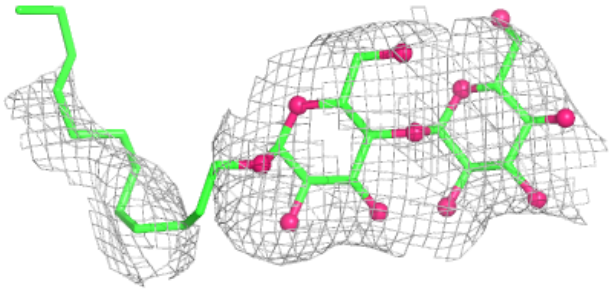


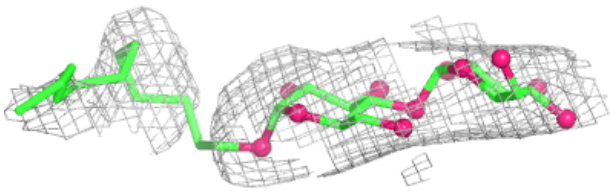




Electron density around LMU B 8002:

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

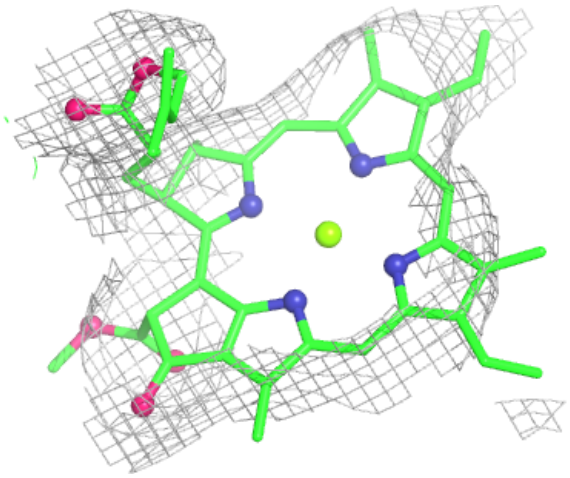


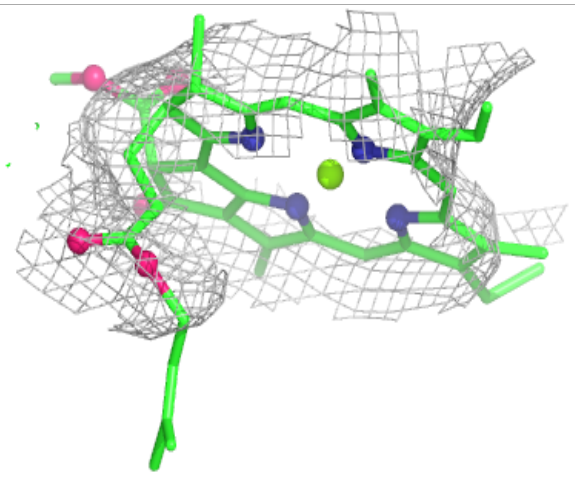


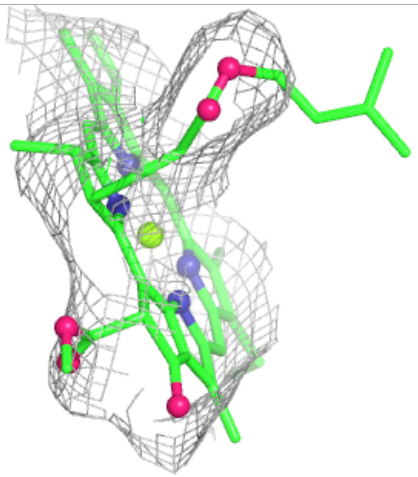


Electron density around CLA 3 3018:

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

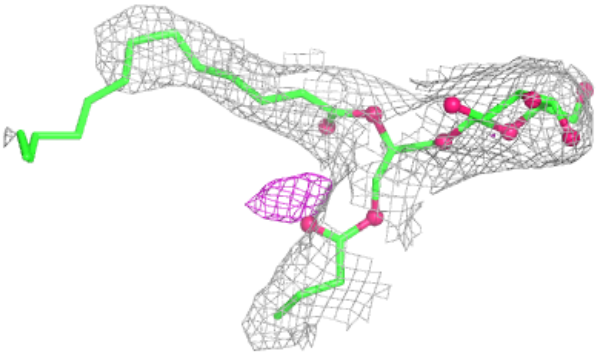


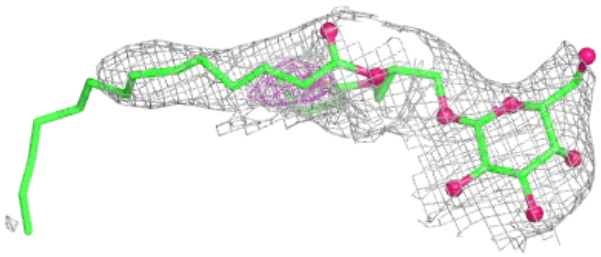




Electron density around LMG F 5002:

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

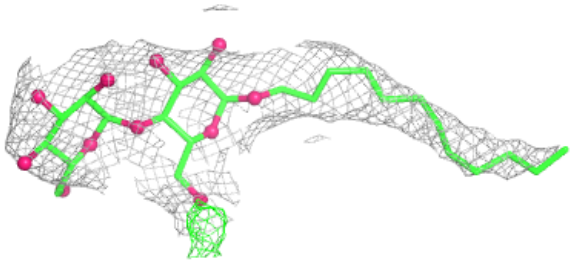


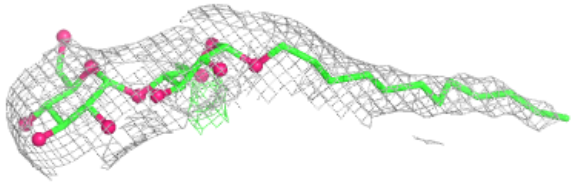


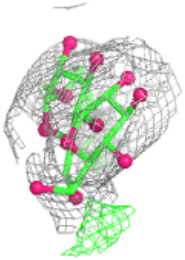


Electron density around LMU B 8001:

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

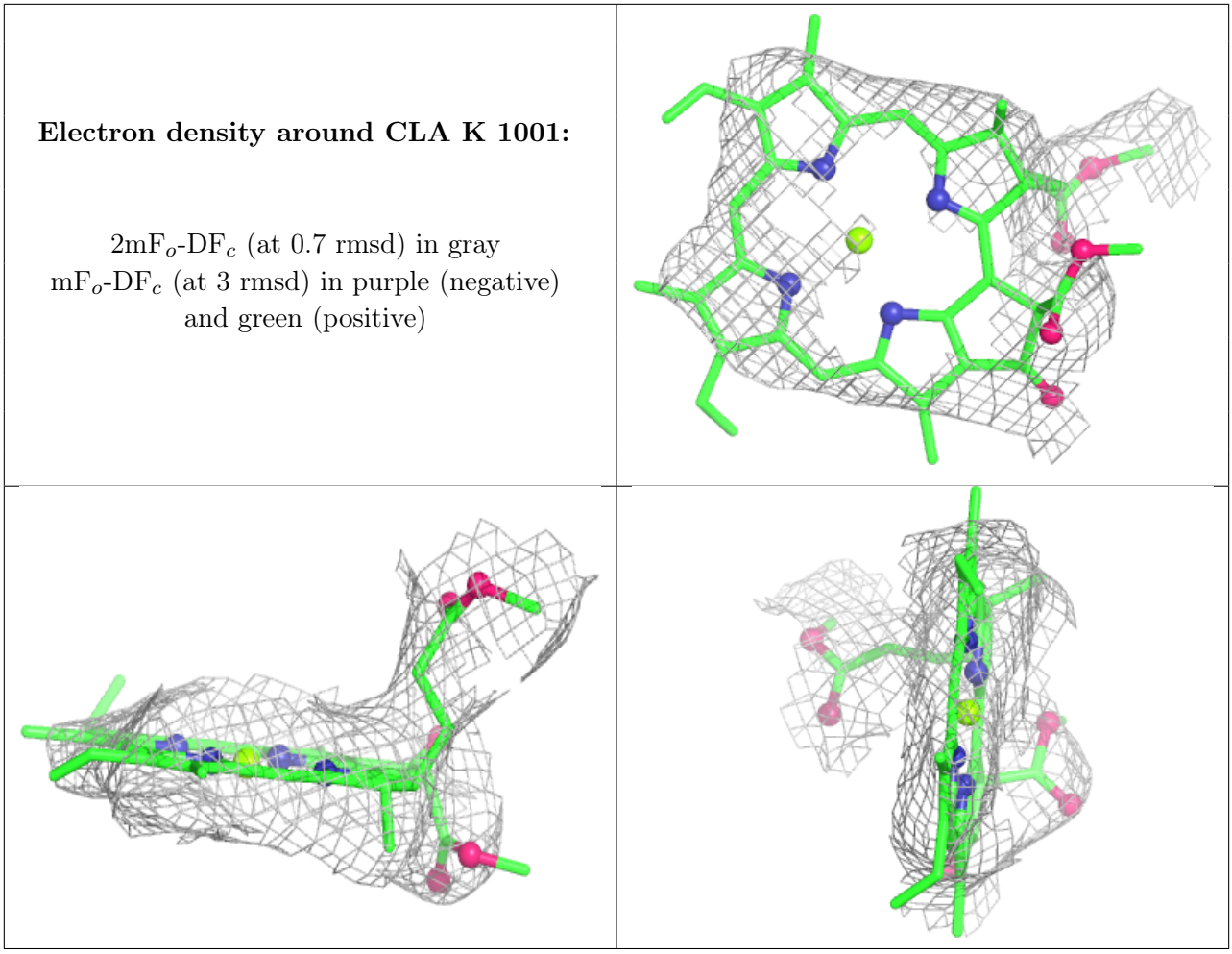






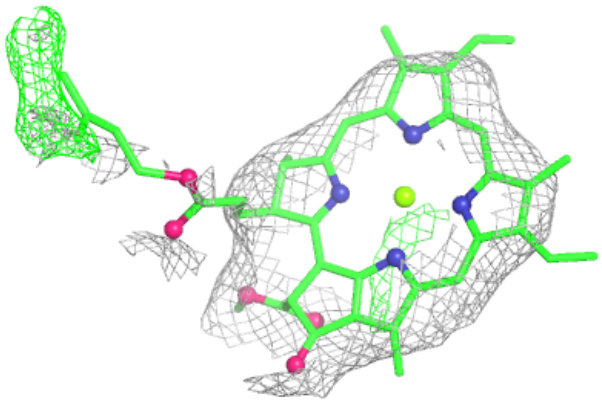
Electron density around CLA K 1001:

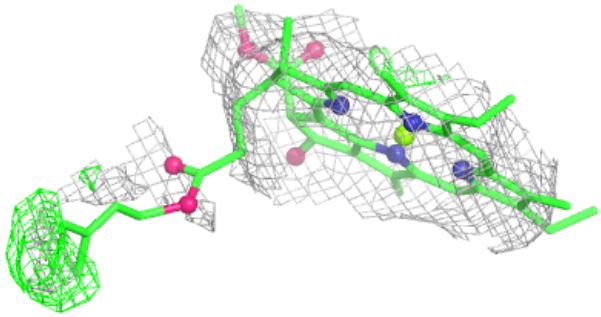
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

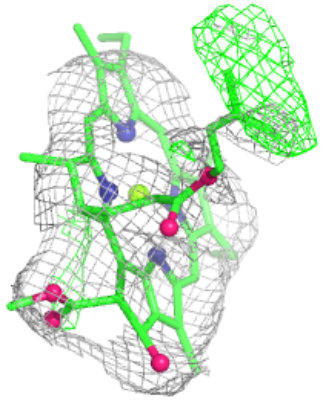


Electron density around CLA 3 3007:

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

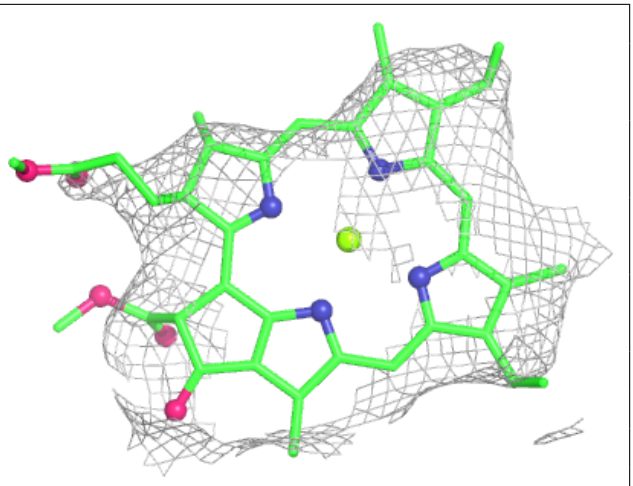


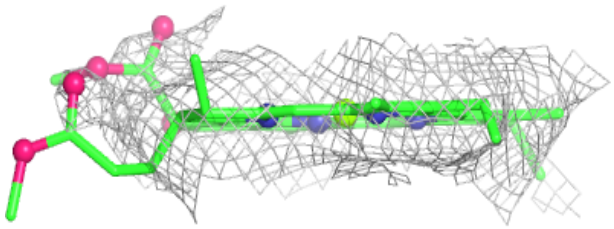


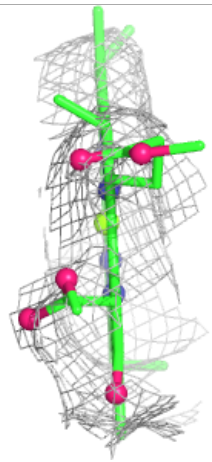


Electron density around CLA 1 1013:

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

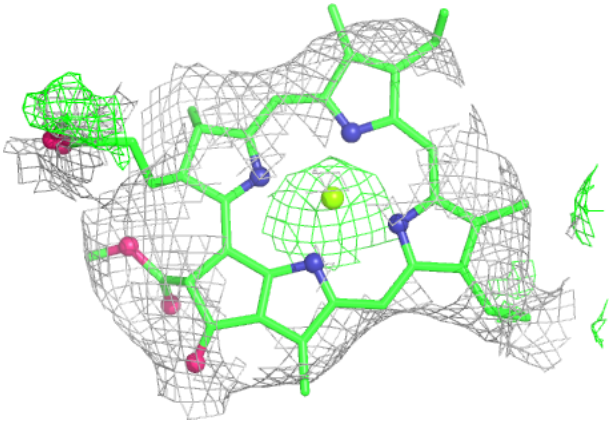


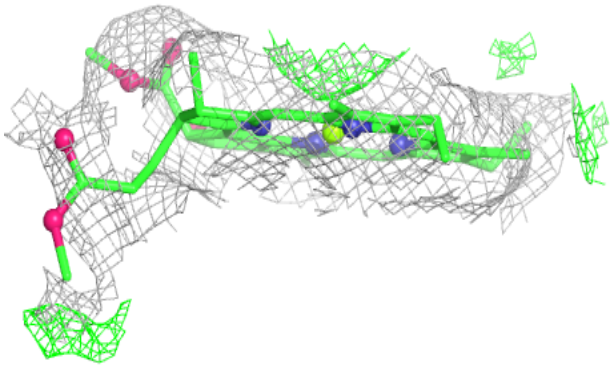


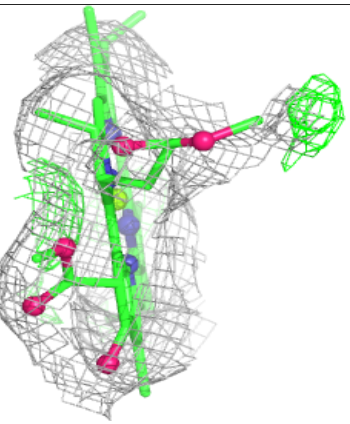


Electron density around CLA 3 3013:

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

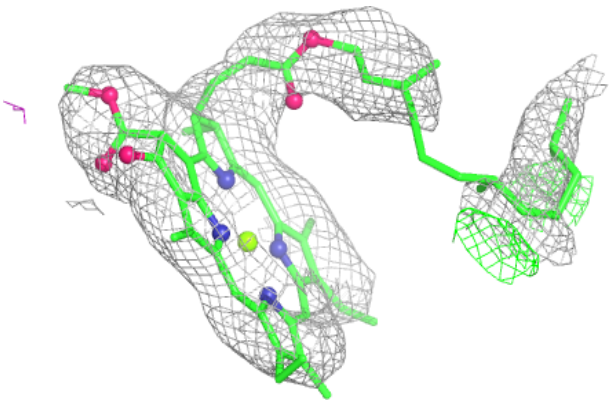


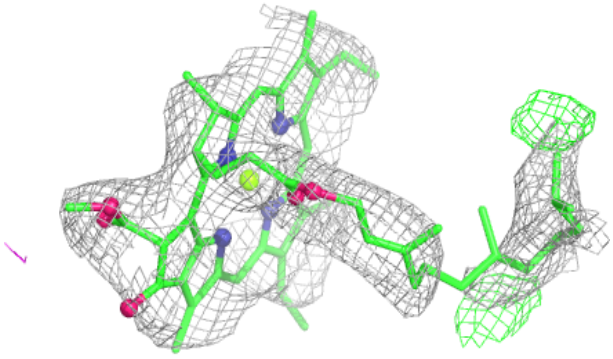


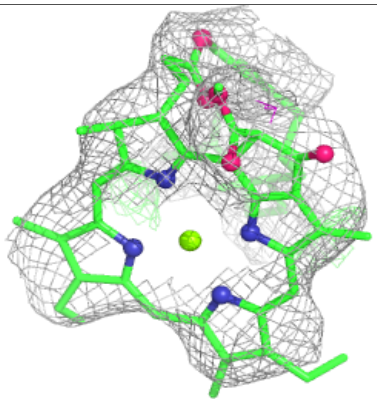


Electron density around CLA G 1003:

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

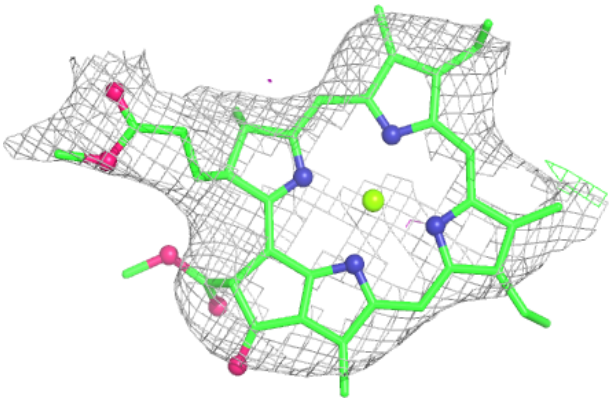


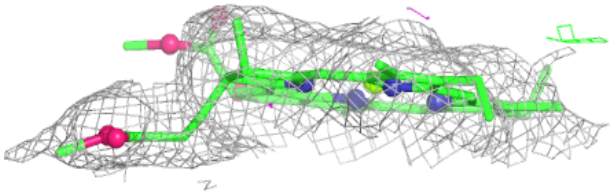


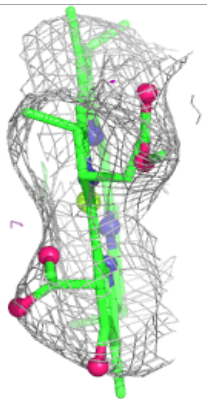


Electron density around CLA H 1000:

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

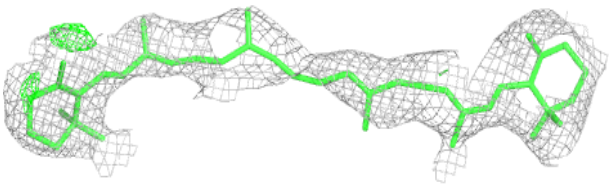


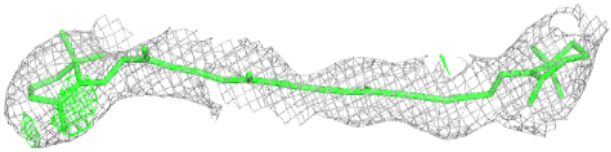


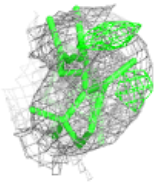


Electron density around BCR G 2011:

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

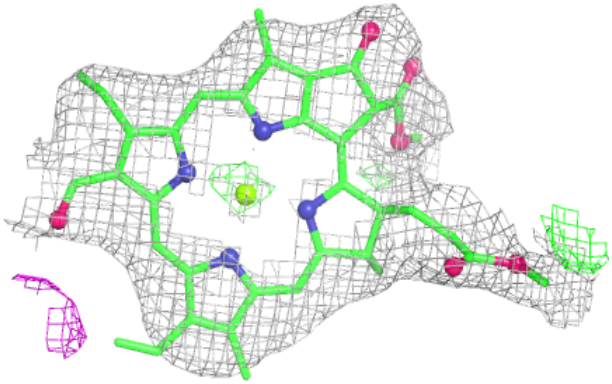


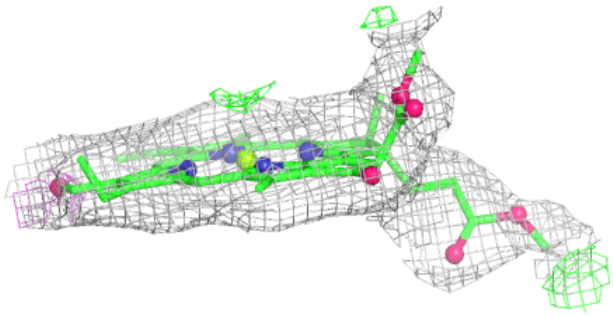


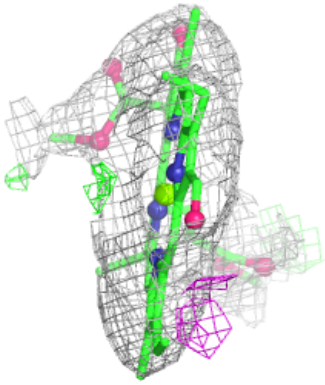


Electron density around CHL 2 2010:

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

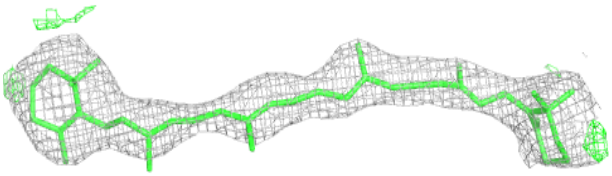


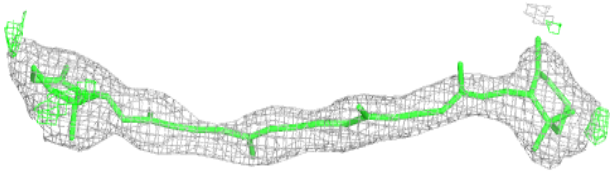


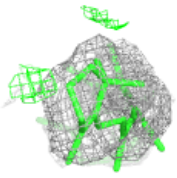


Electron density around BCR J 6013:

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



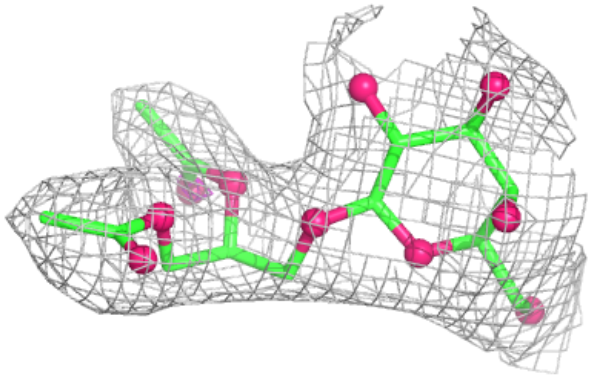


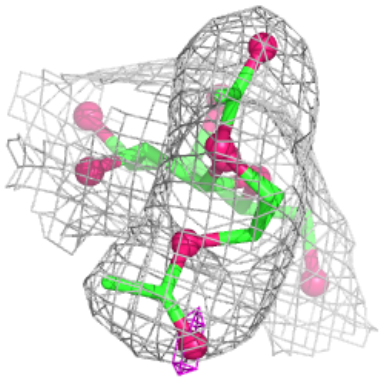


Electron density around LMG F 5001:

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

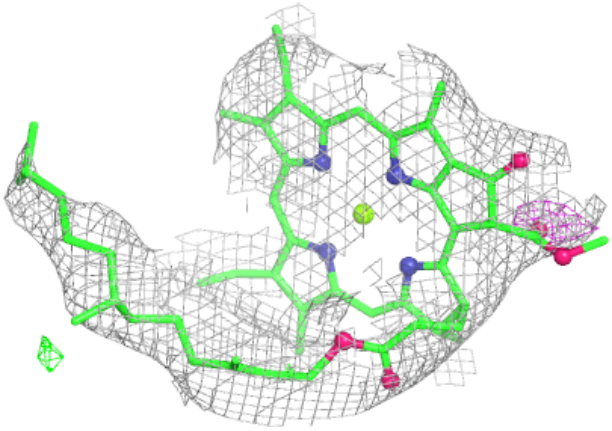


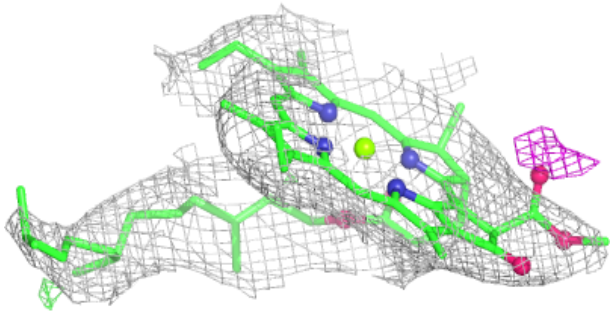


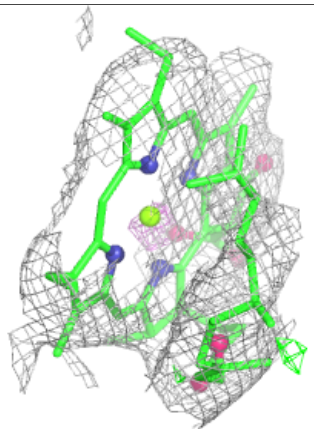


Electron density around CLA 1 1001:

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

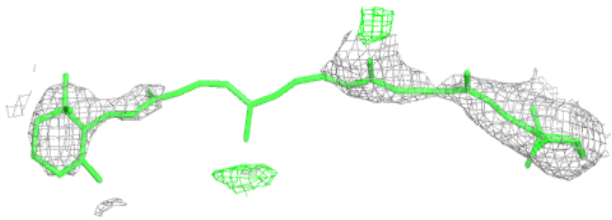


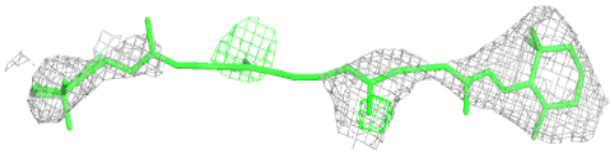


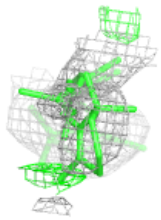


Electron density around BCR K 2011:

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

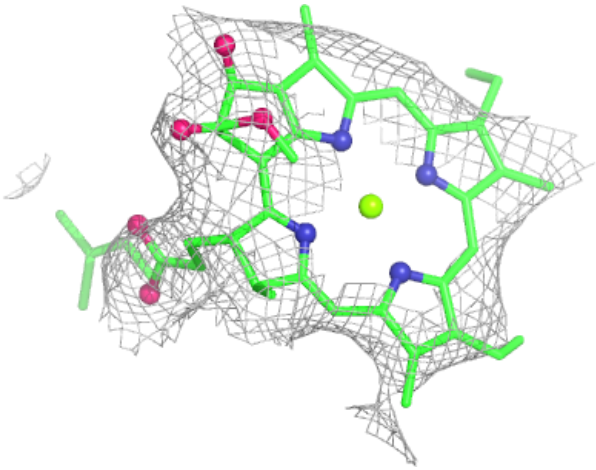


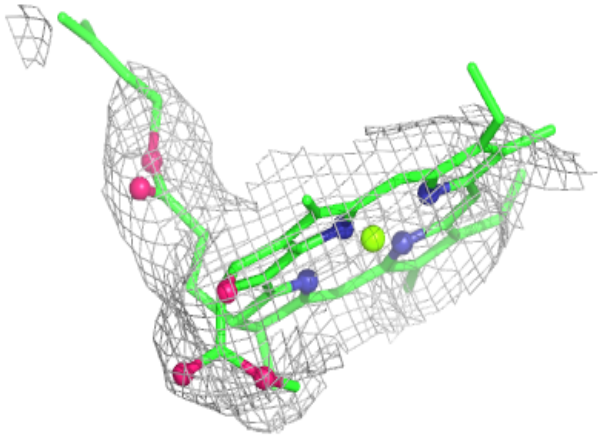


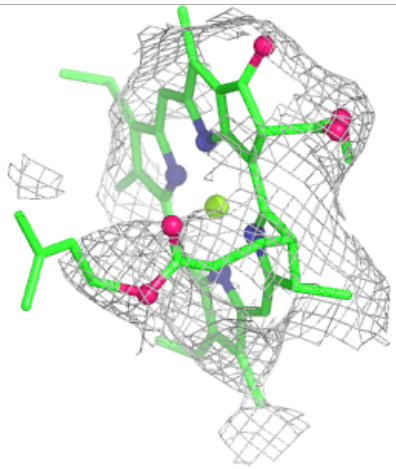


Electron density around CLA 3 3006:

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



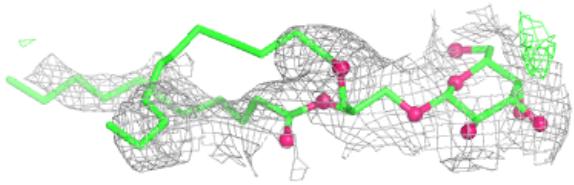


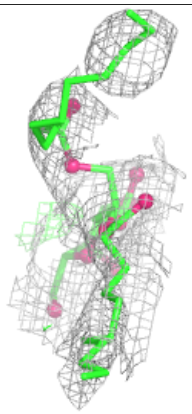


Electron density around LMG G 2021:

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

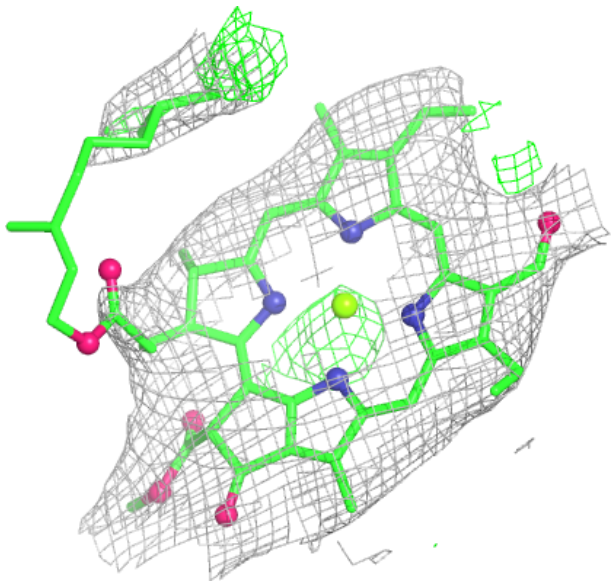


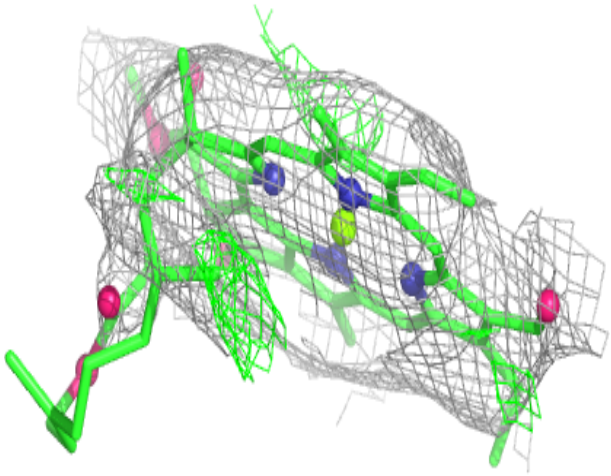


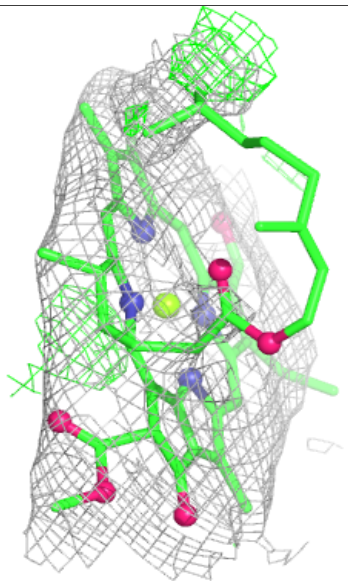


Electron density around CHL 3 3011:

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

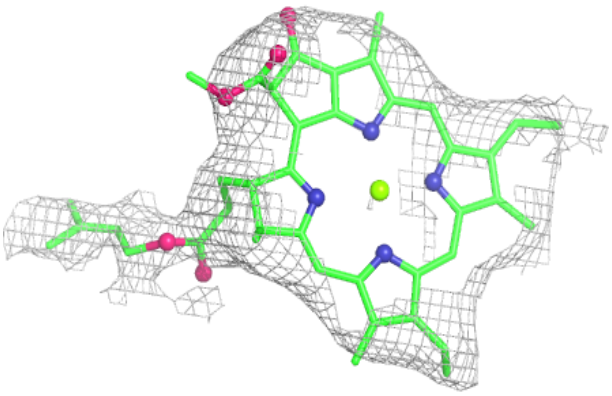


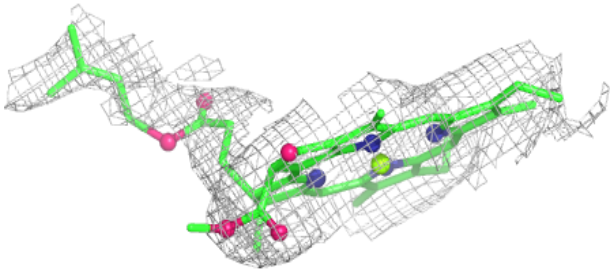


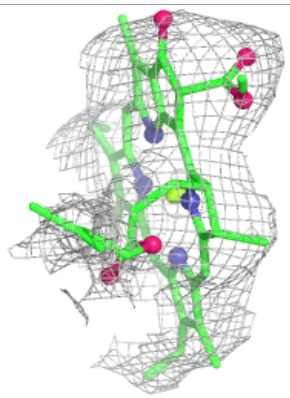


Electron density around CLA A 1151:

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

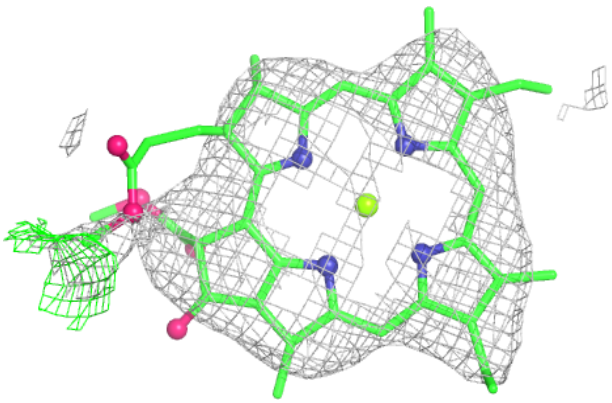


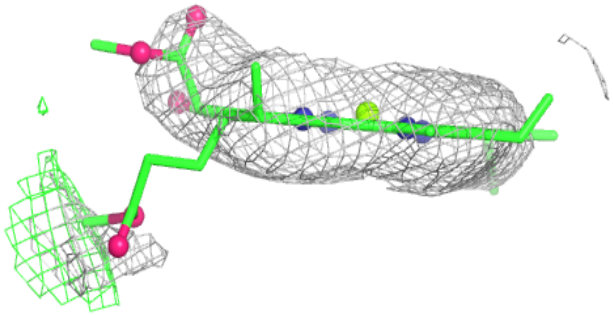


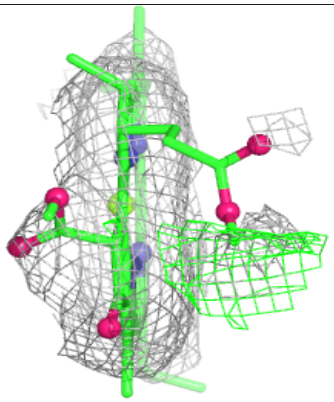


Electron density around CLA A 1113:

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

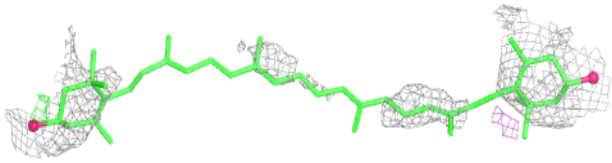


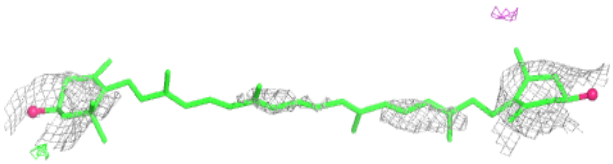


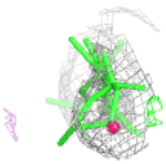


Electron density around LUT 3 3501:

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

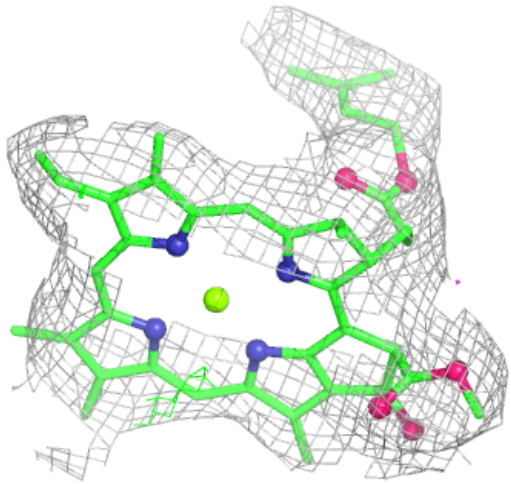


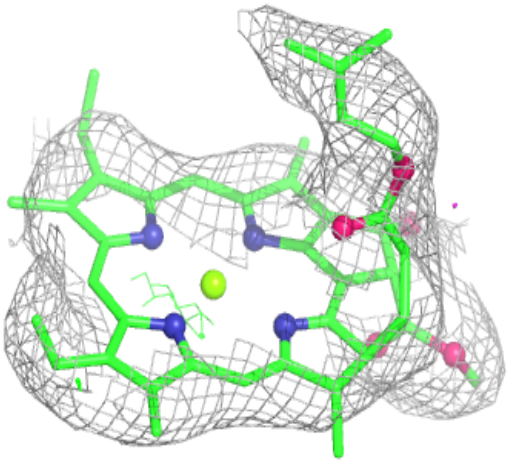


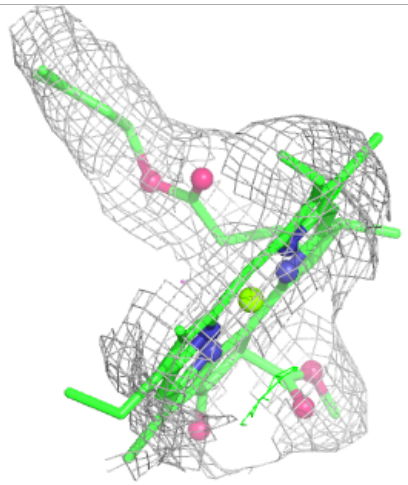


Electron density around CLA L 1501:

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

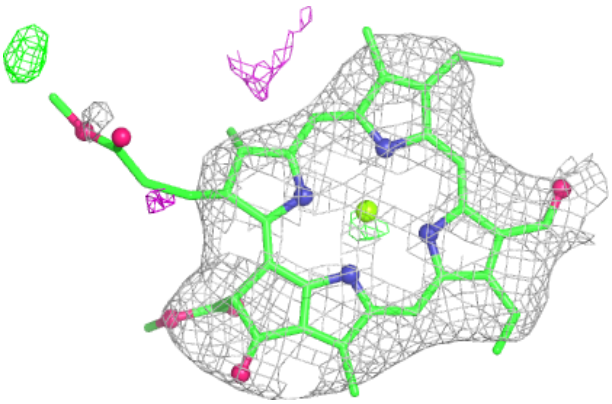


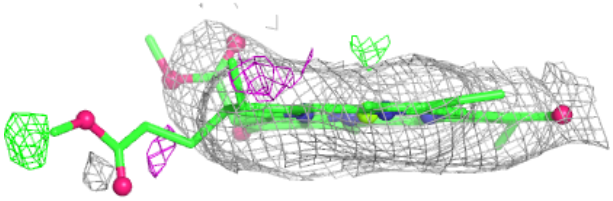


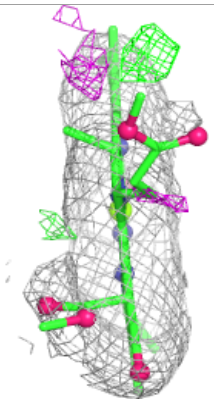


Electron density around CHL 4 4010:

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

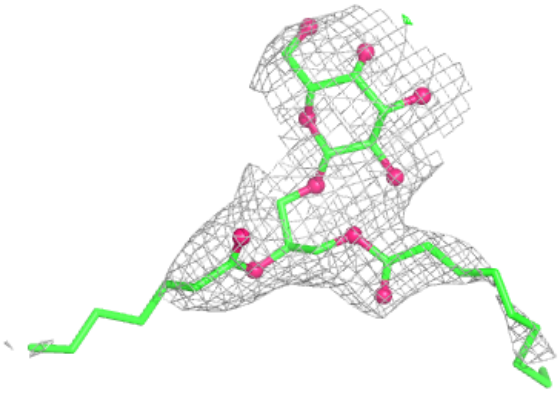


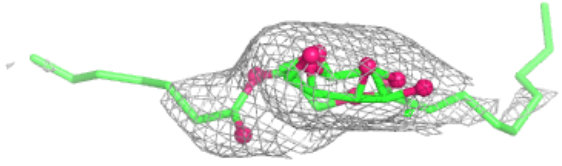


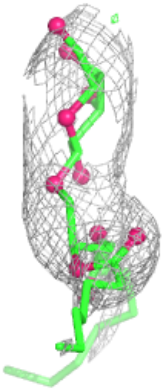


Electron density around LMG 2 2802:

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

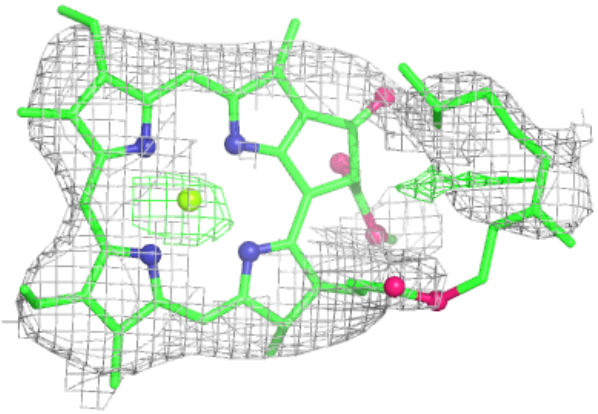


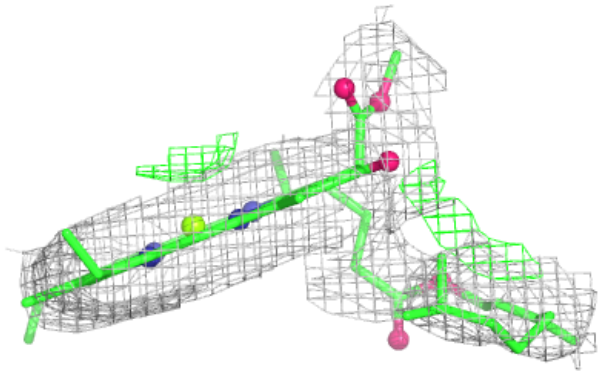


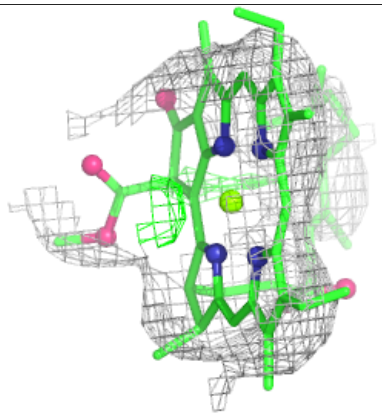


Electron density around CLA A 1134:

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

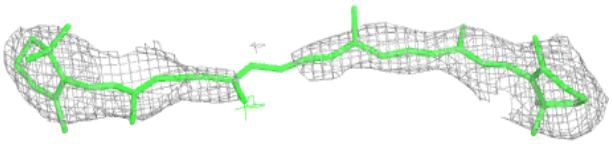


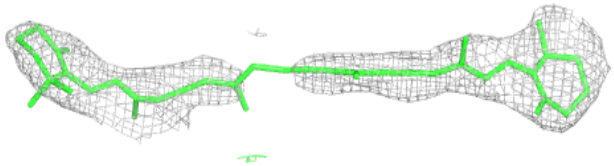


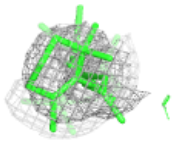


Electron density around BCR L 6020:

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

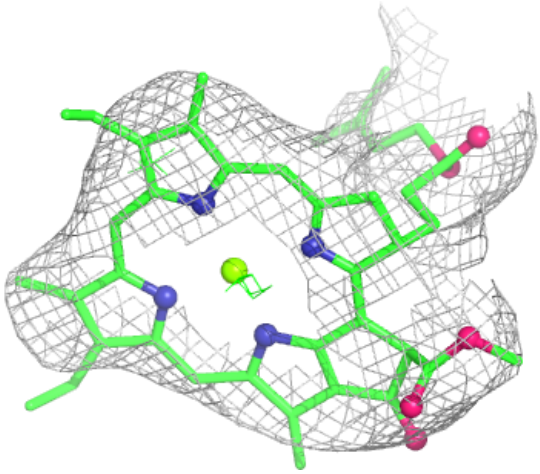


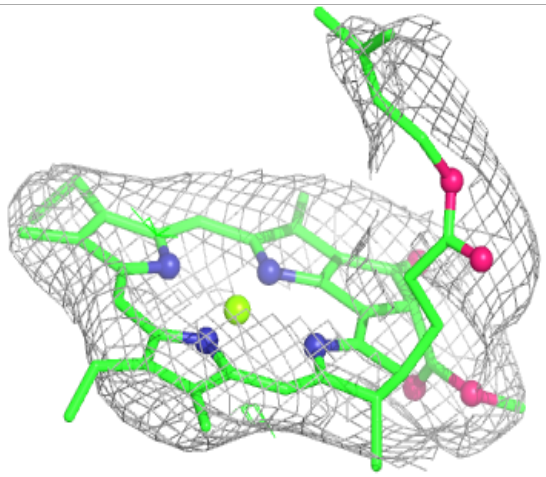


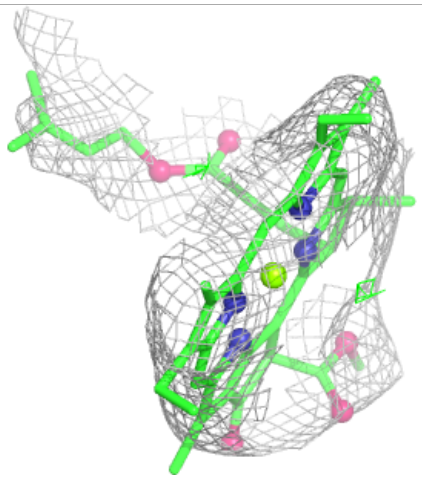


Electron density around CLA 1 1006:

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

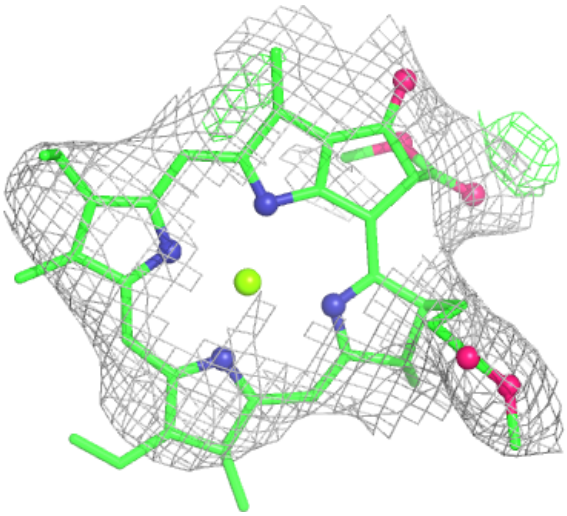


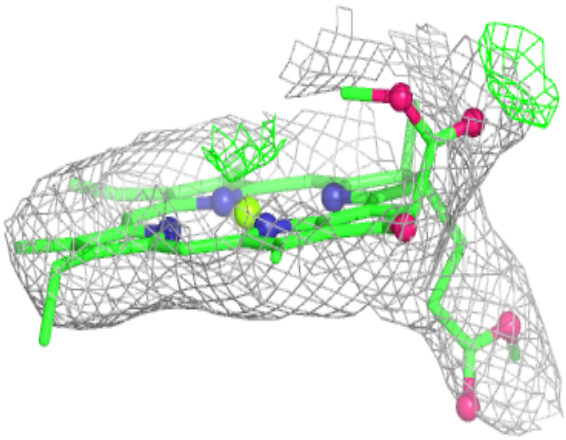


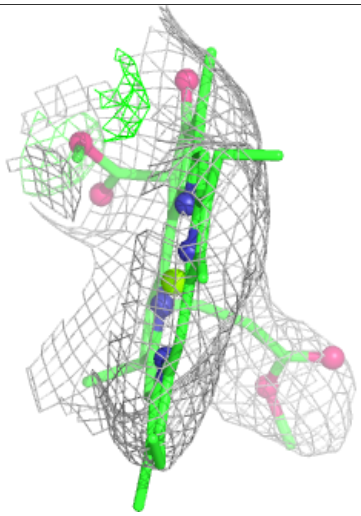


Electron density around CLA 1 1008:

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

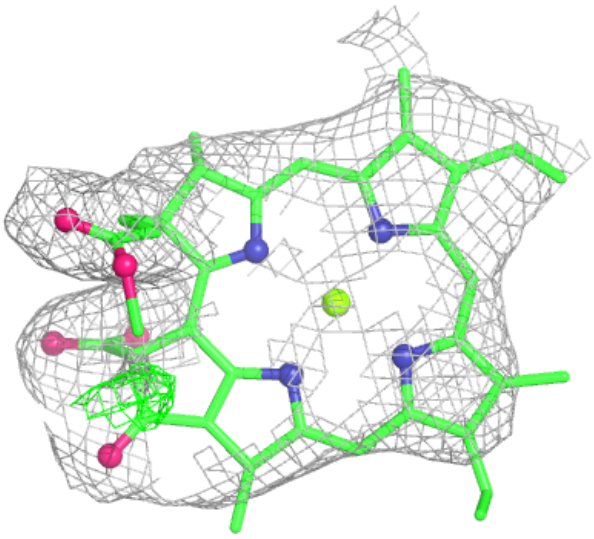


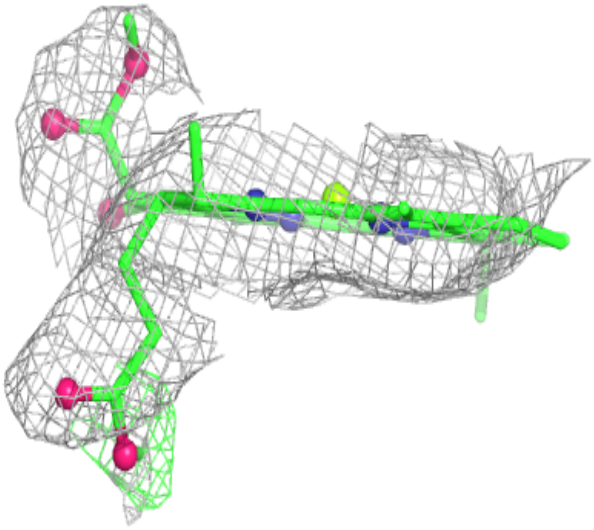


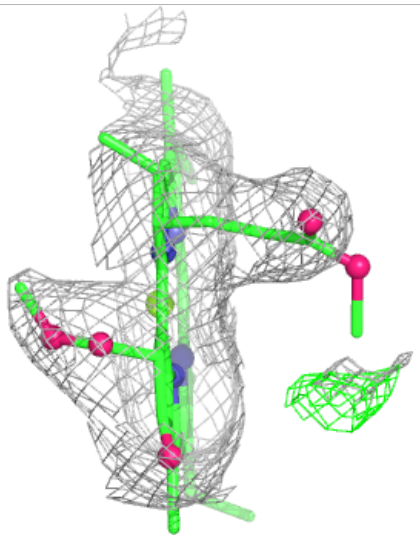


Electron density around CLA A 1114:

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

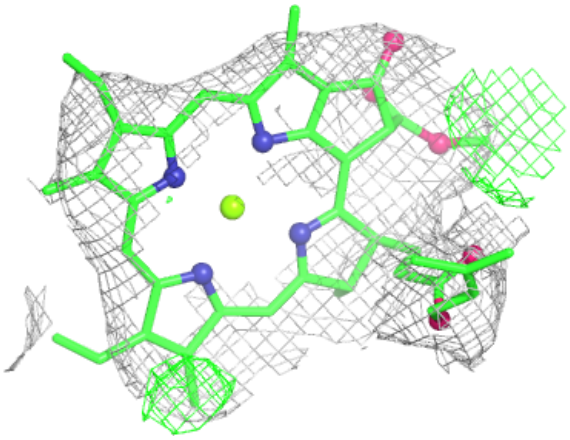


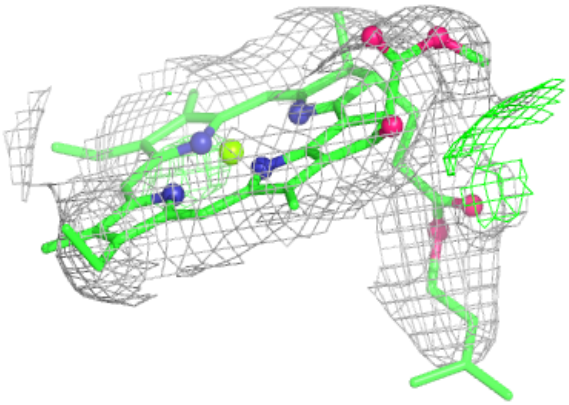


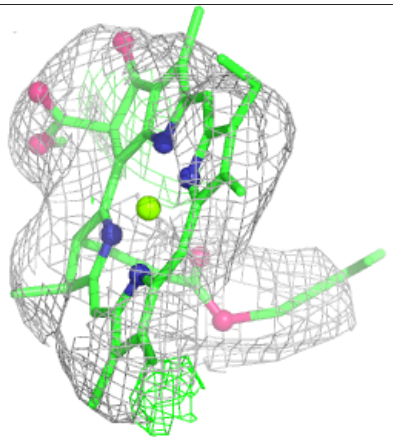


Electron density around CLA 4 4006:

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

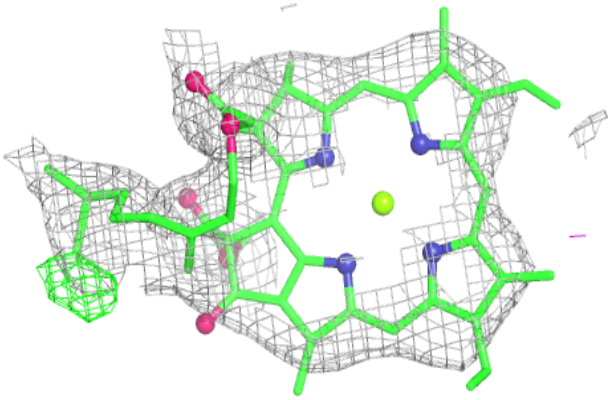


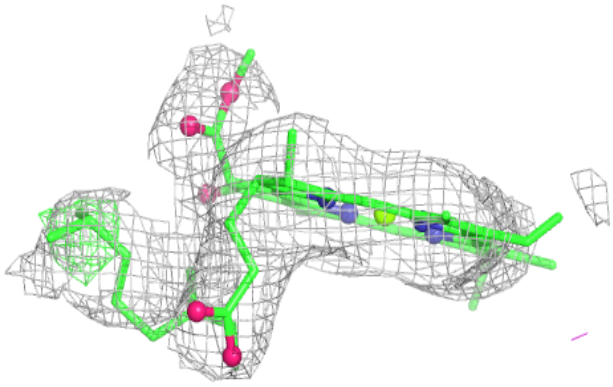


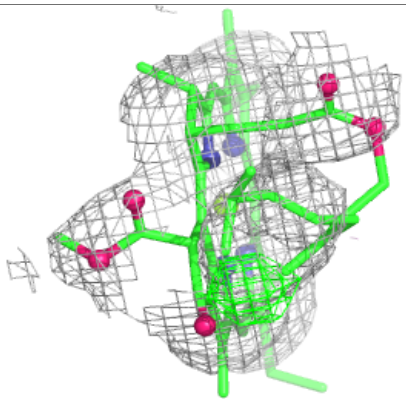


Electron density around CLA 2 2006:

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

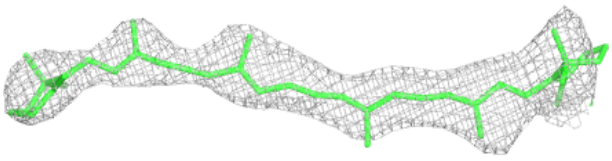


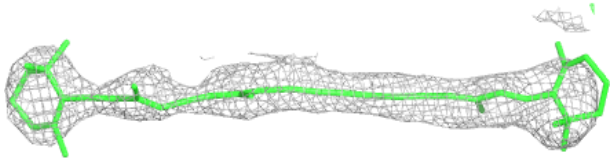


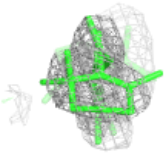


Electron density around BCR A 6007:

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

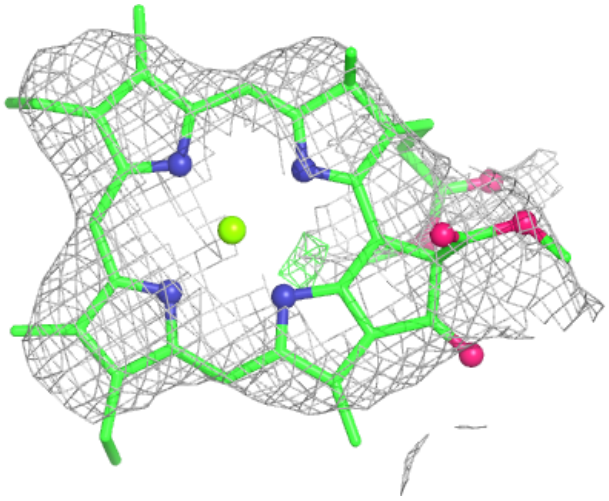


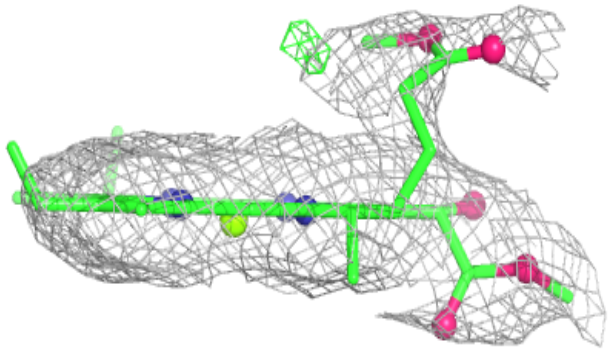


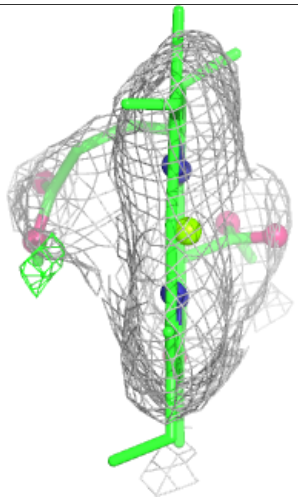


Electron density around CLA A 1115:

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

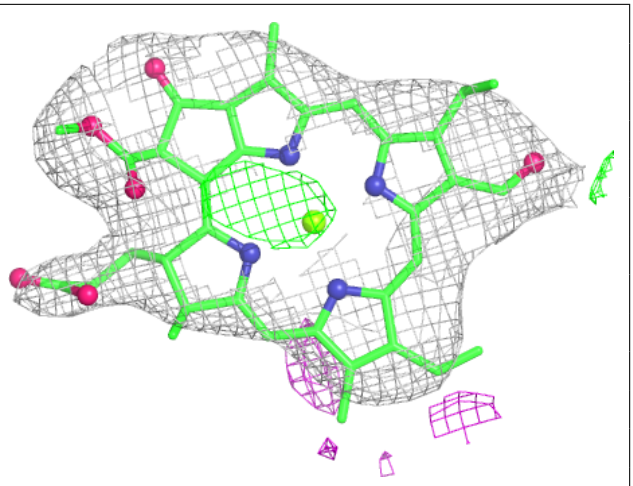


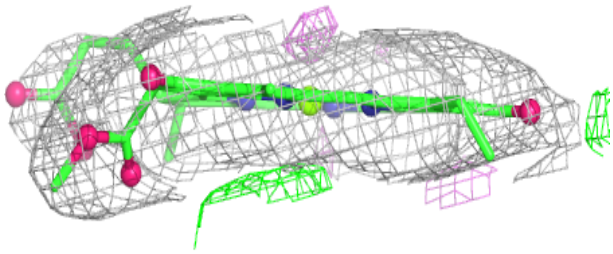


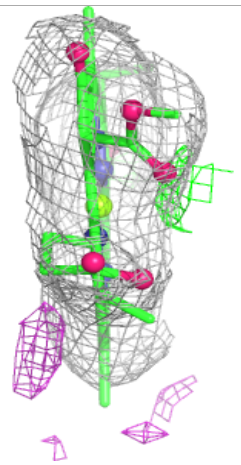


Electron density around CHL 2 2013:

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

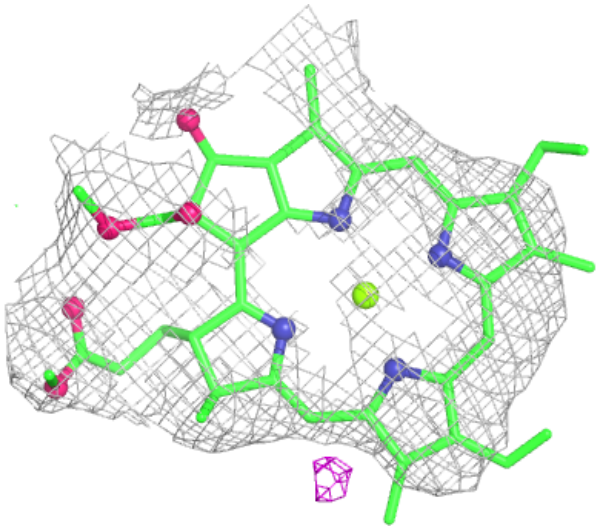


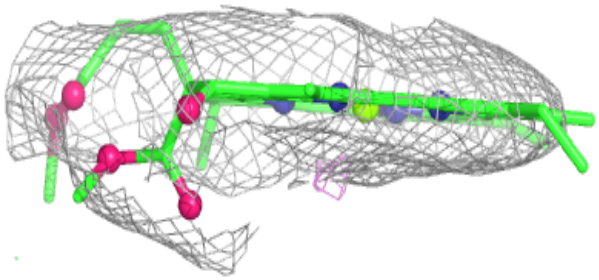


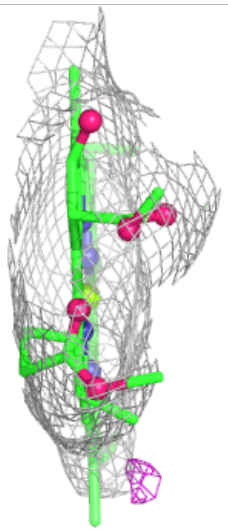


Electron density around CLA 3 3002:

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

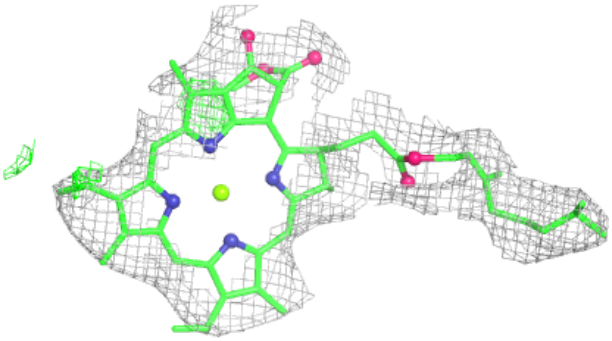


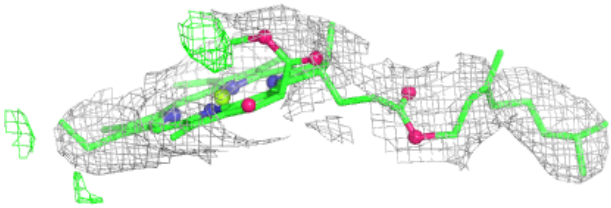


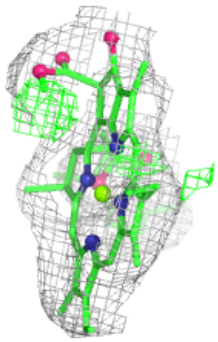


Electron density around CLA G 1001:

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

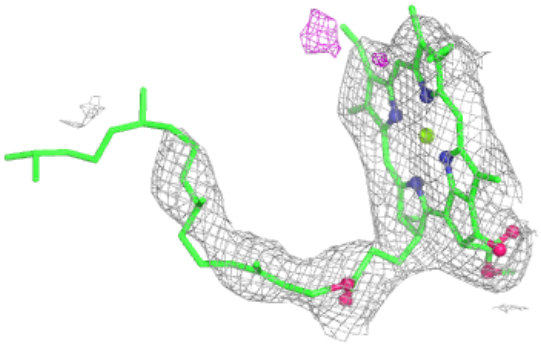


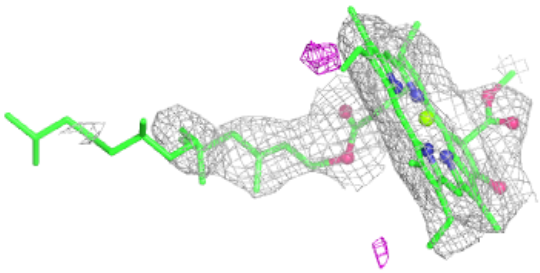


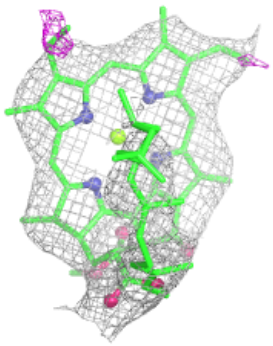


Electron density around CLA B 1218:

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

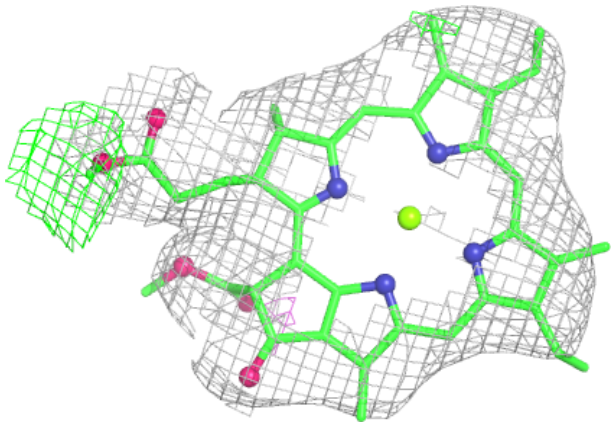


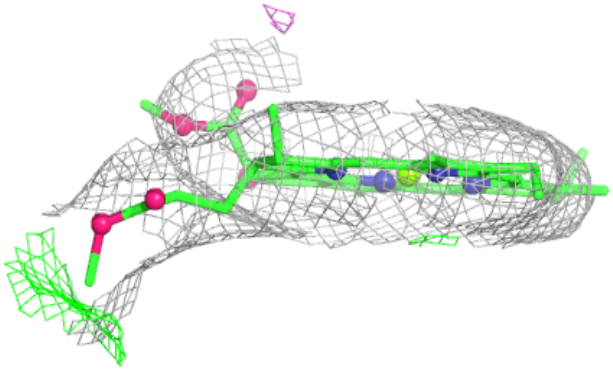


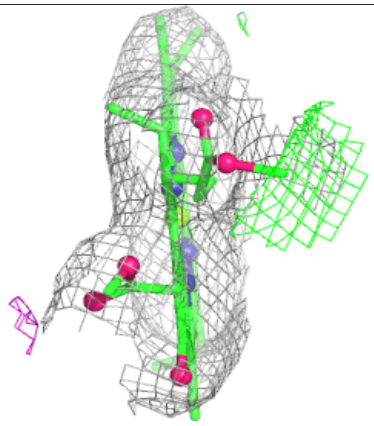


Electron density around CLA 1 1014:

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

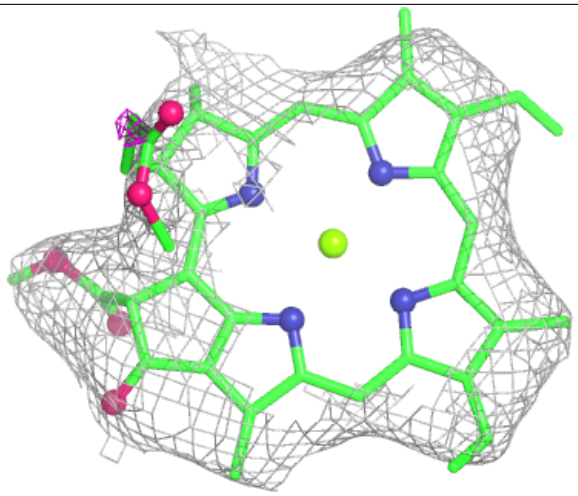


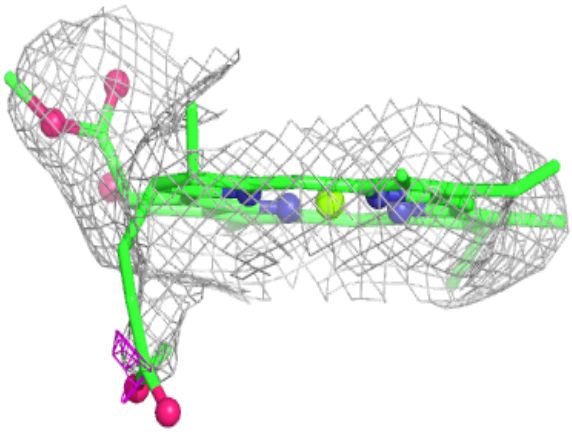


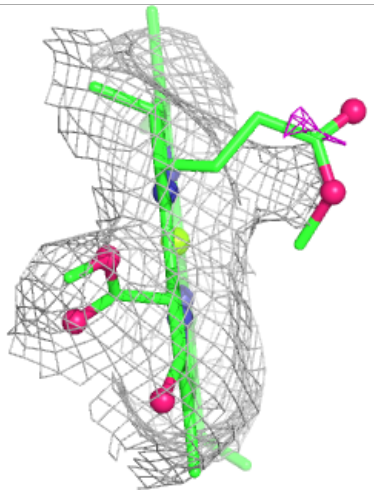


Electron density around CLA 4 4008:

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

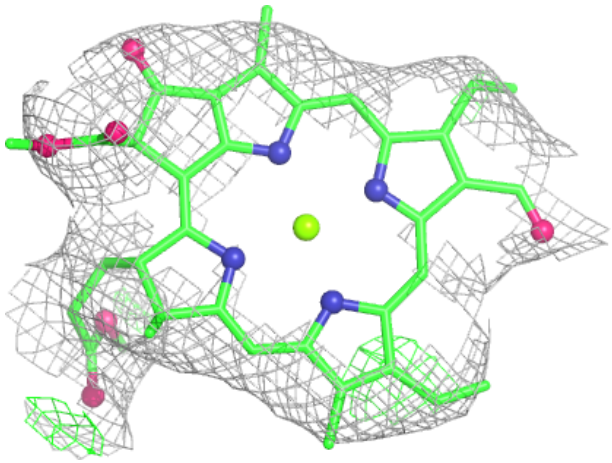


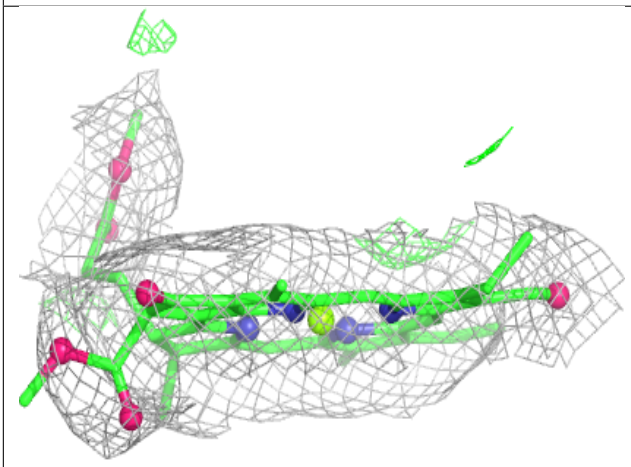




Electron density around CHL 1 1010:

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

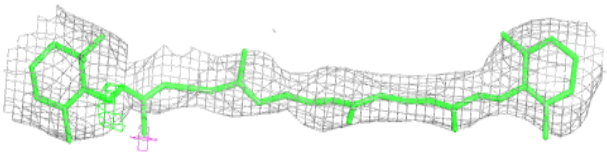


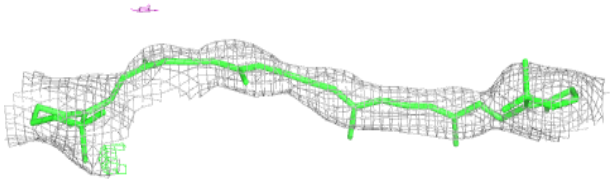


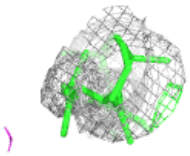


Electron density around BCR 3 3503:

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

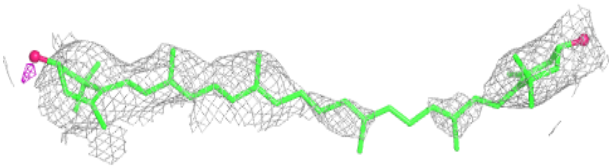


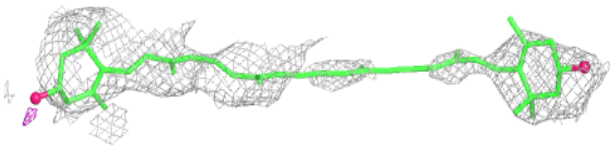


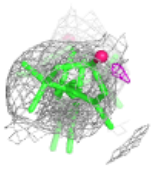


Electron density around LUT 1 1501:

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

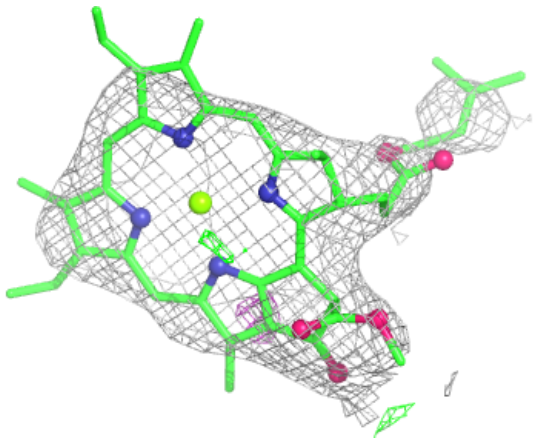


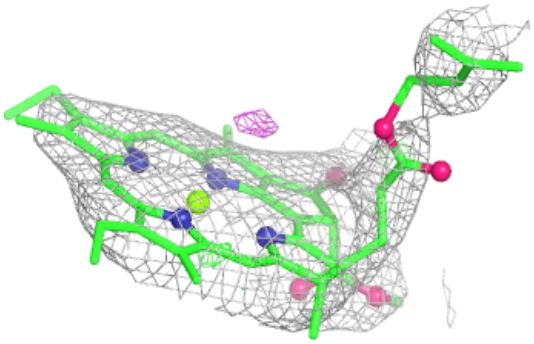


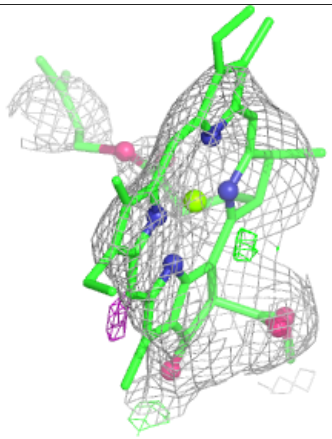


Electron density around CLA 1 1011:

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

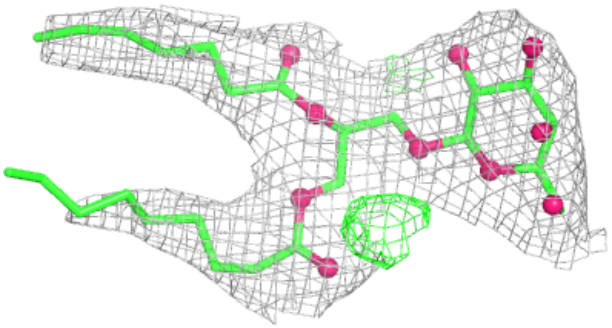


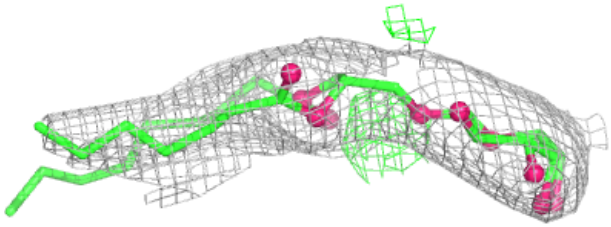


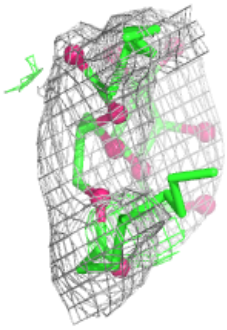


Electron density around LMG 4 4801:

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

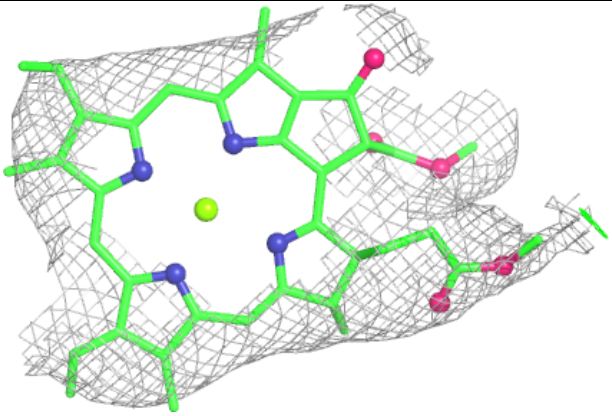


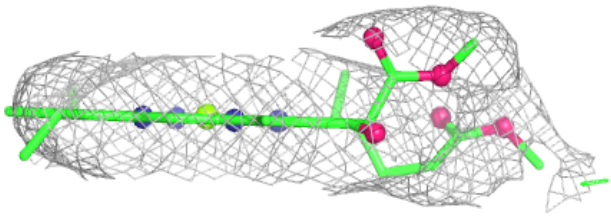


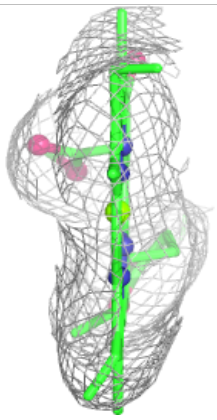


Electron density around CLA G 1002:

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

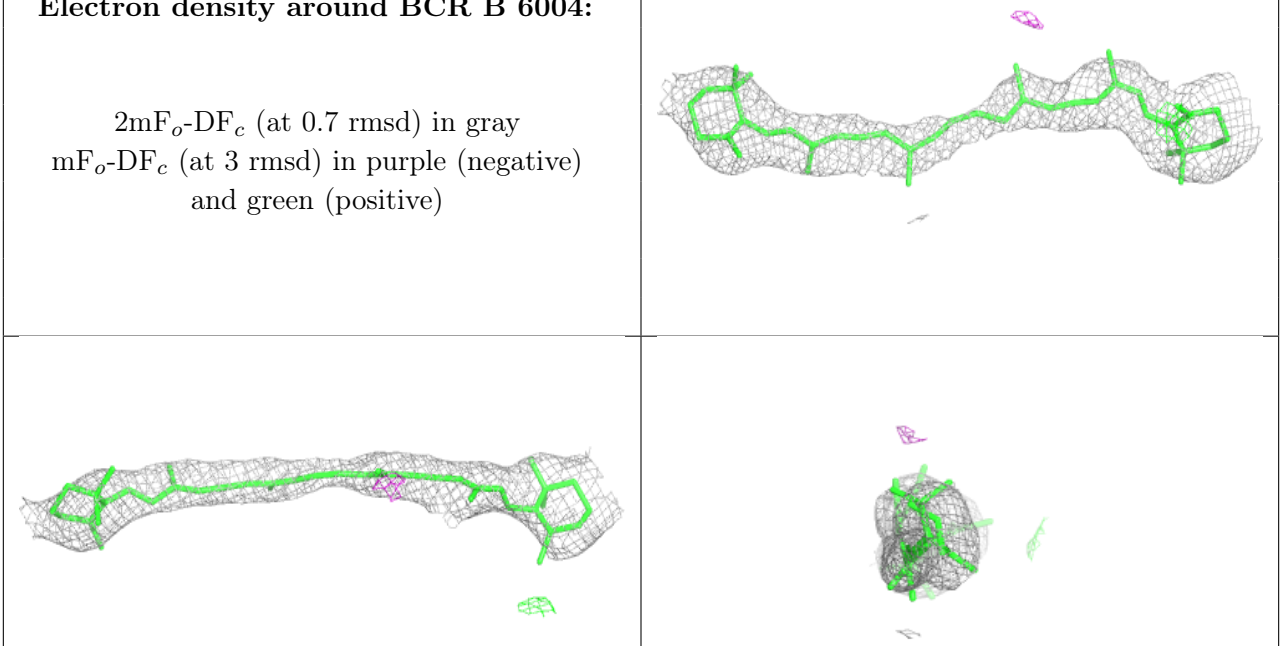






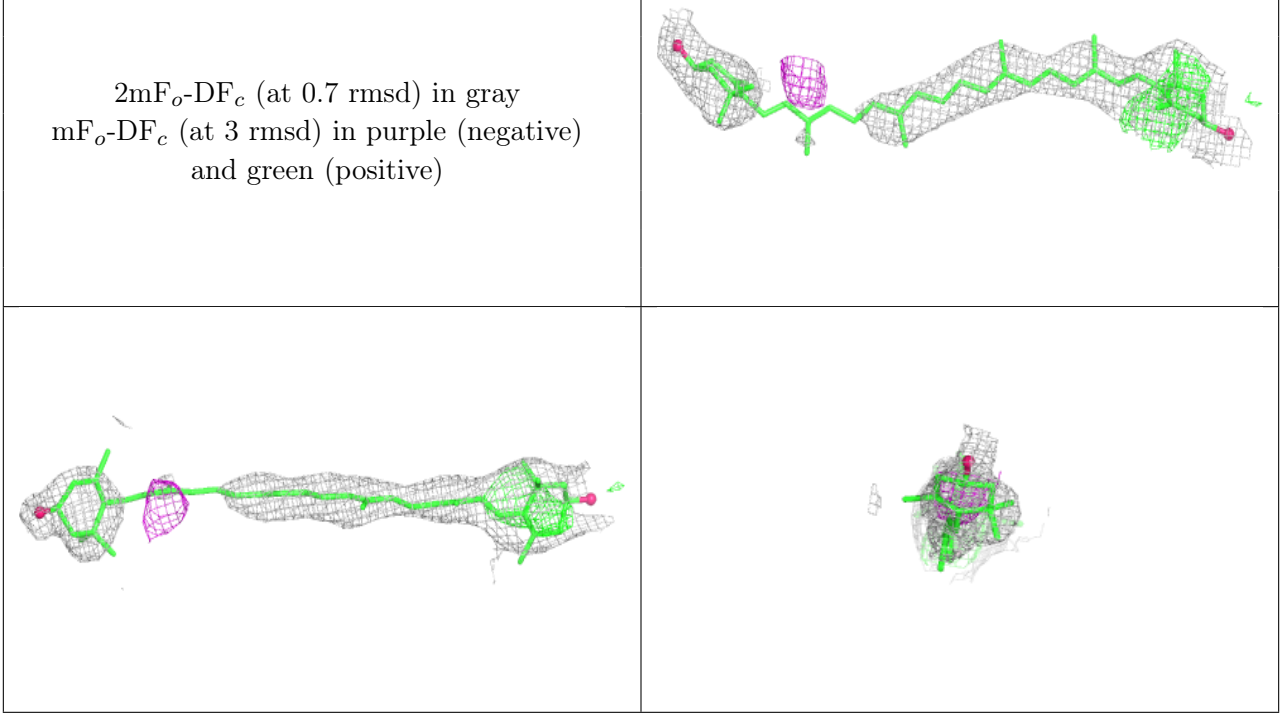
Electron density around BCR B 6004:

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



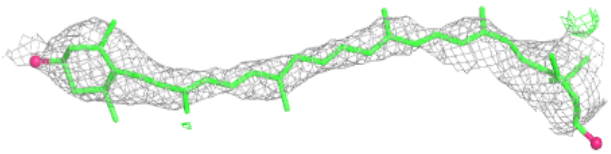
Electron density around LUT 2 2502:

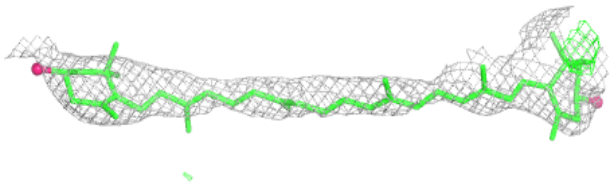
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

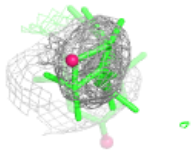


Electron density around LUT 4 4503:

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

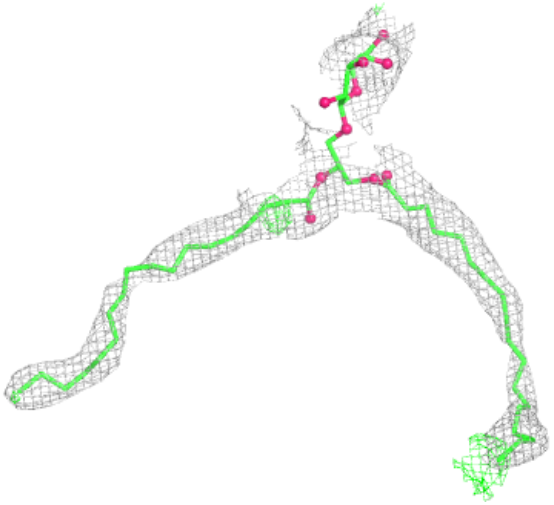


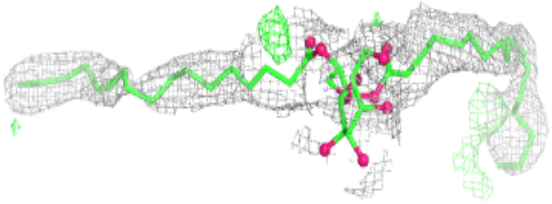


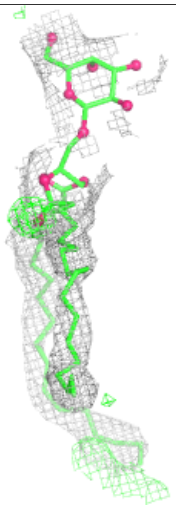


Electron density around LMG J 5001:

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

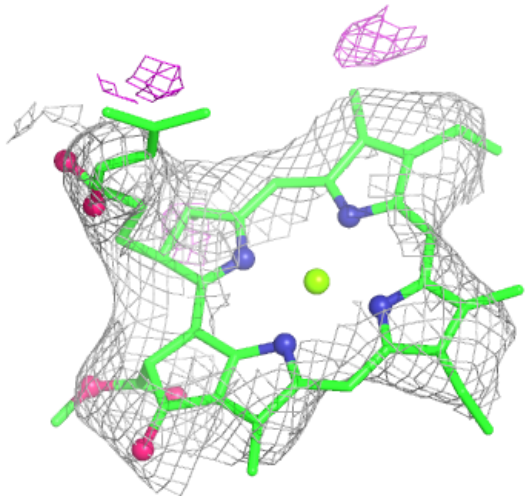


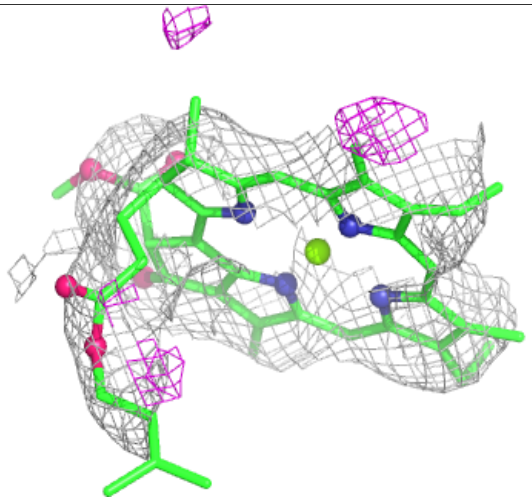


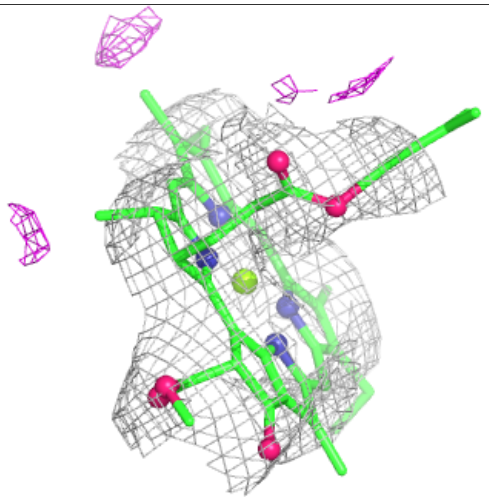


Electron density around CLA L 1503:

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

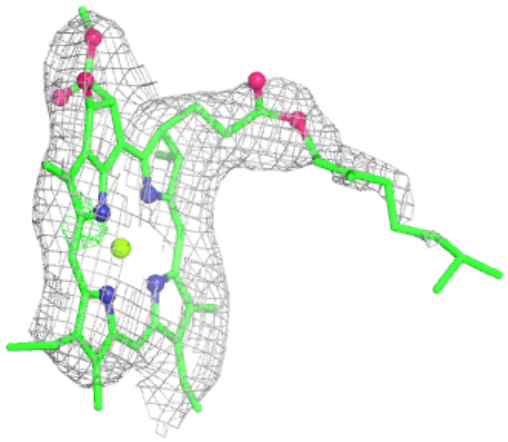


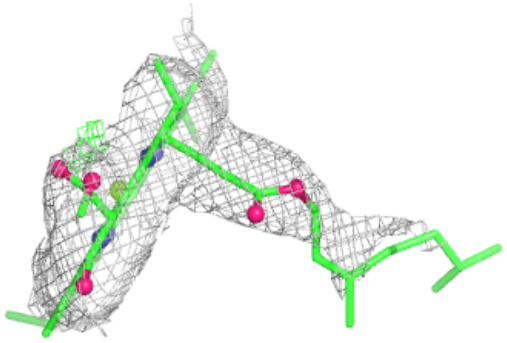


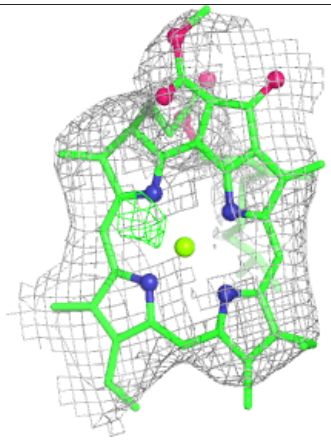


Electron density around CLA B 1232:

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

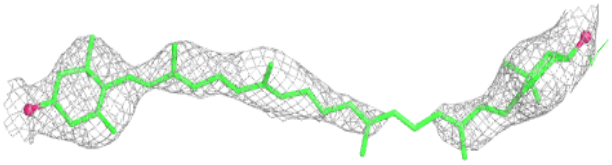


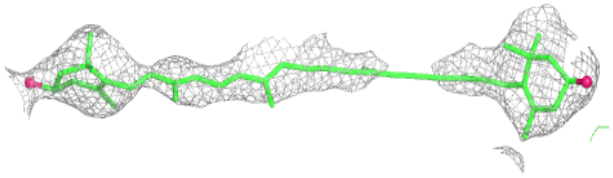


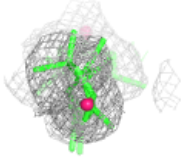


Electron density around LUT 1 1502:

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

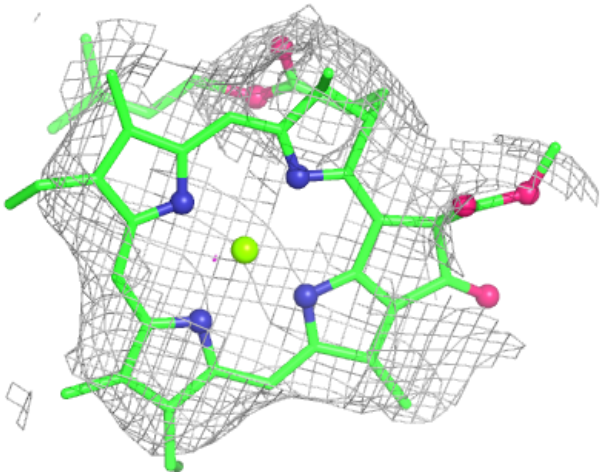


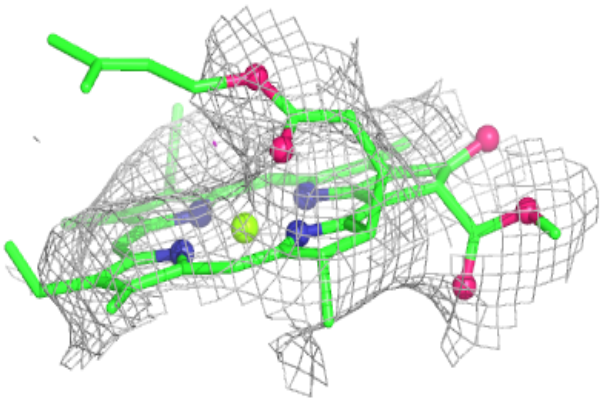


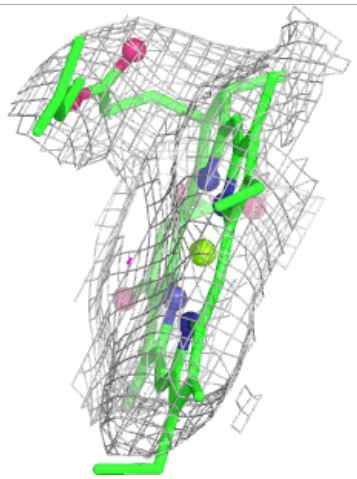


Electron density around CLA 3 3001:

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

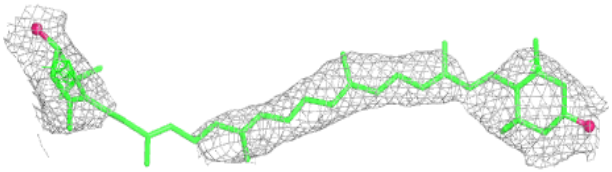


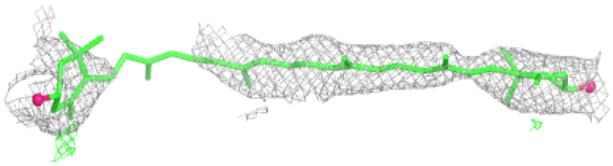


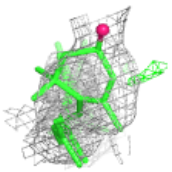


Electron density around LUT 3 3502:

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

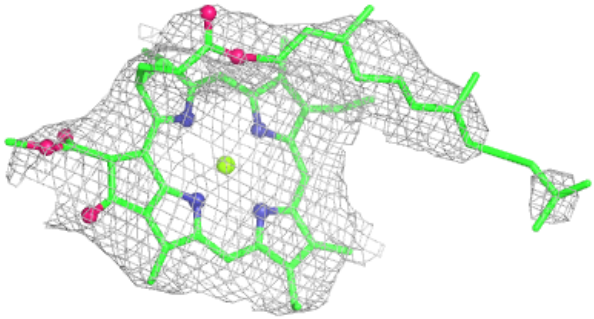


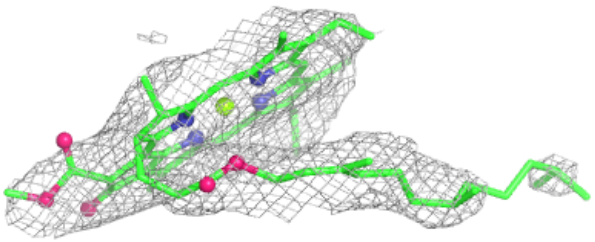


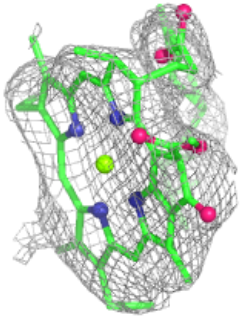


Electron density around CLA 4 4001:

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

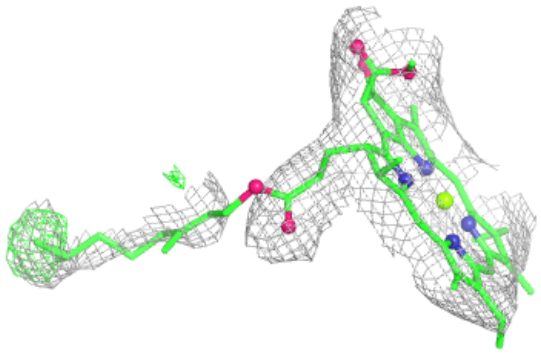


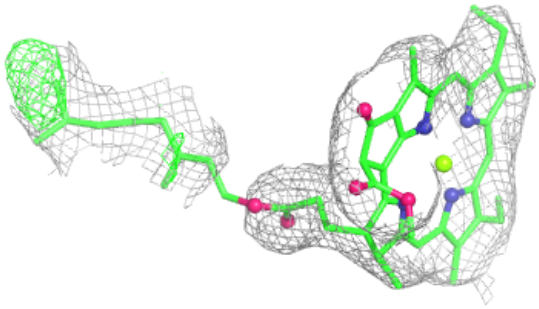


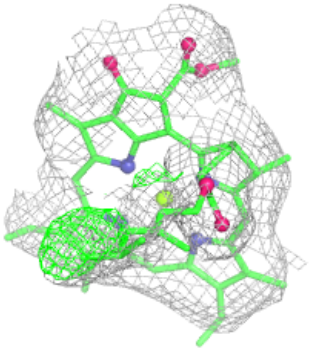


Electron density around CLA A 1121:

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

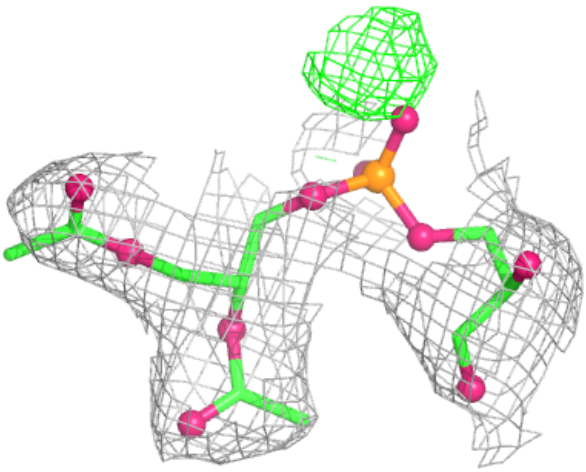


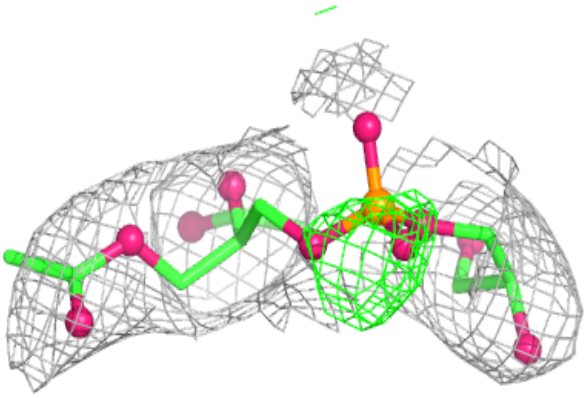


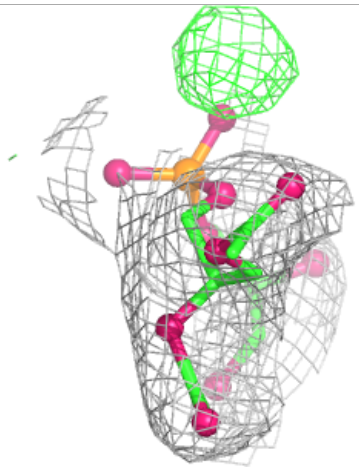


Electron density around LHG B 5004:

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

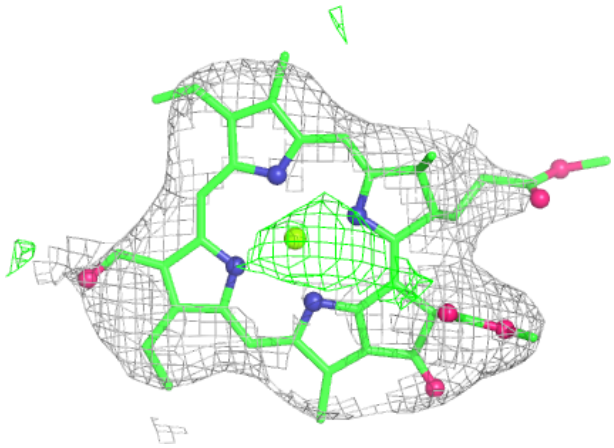


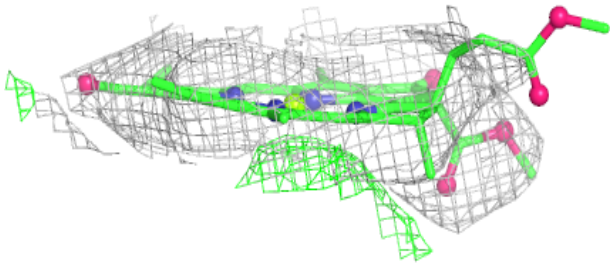


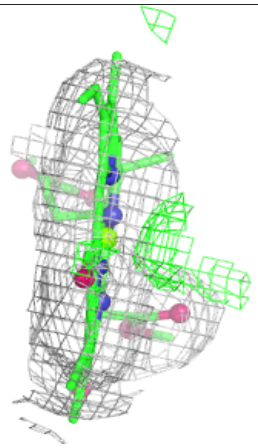


Electron density around CHL 4 4013:

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

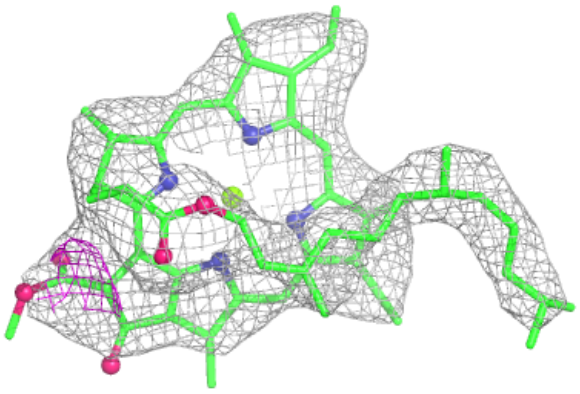


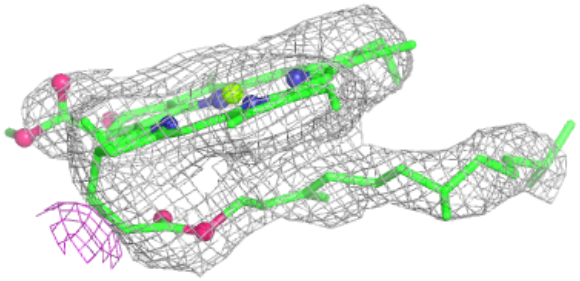


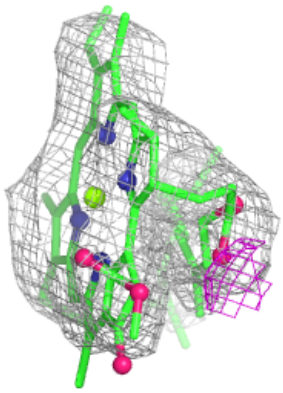


Electron density around CLA B 1213:

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

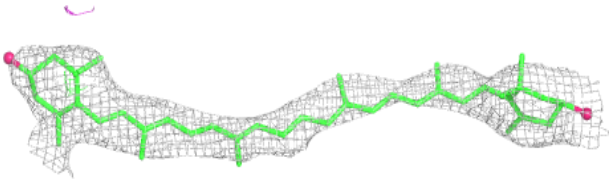


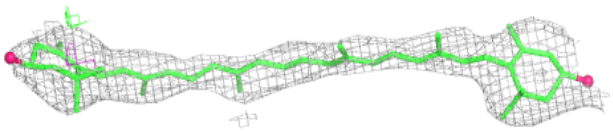




Electron density around LUT 2 2501:

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

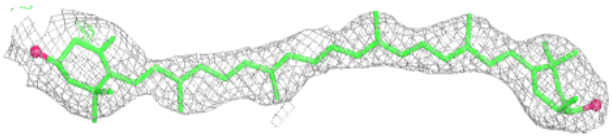


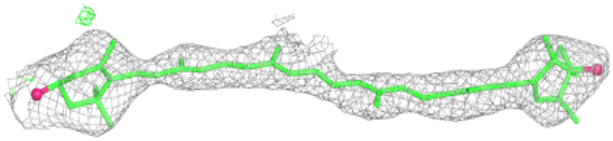


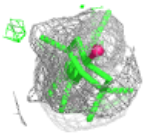


Electron density around ZEX 4 4505:

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

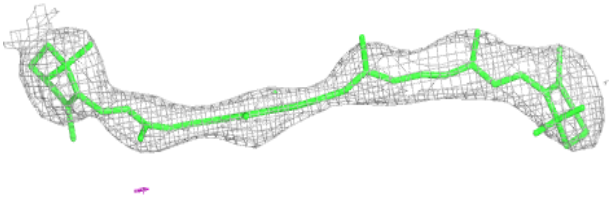


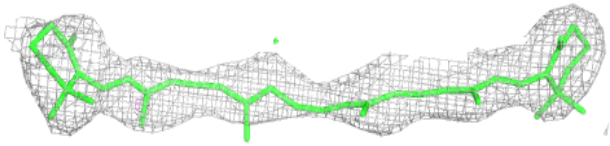


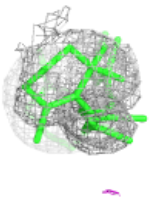


Electron density around BCR A 6008:

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

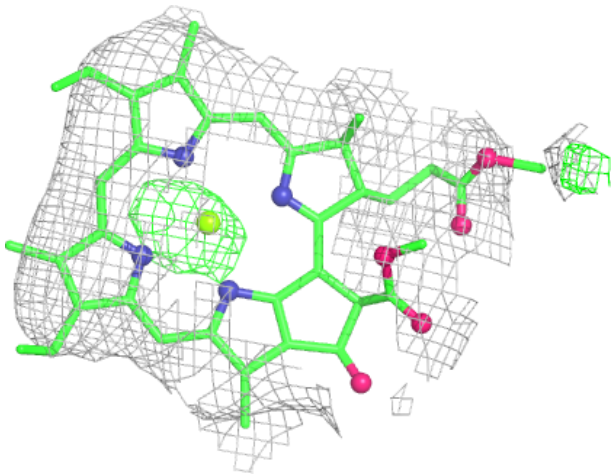


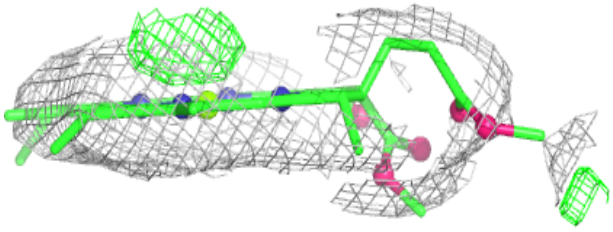


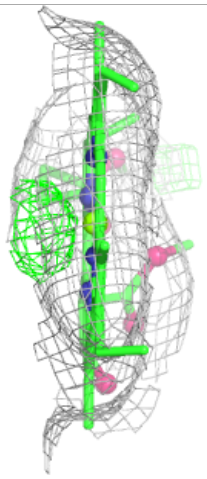


Electron density around CLA 1 1002:

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

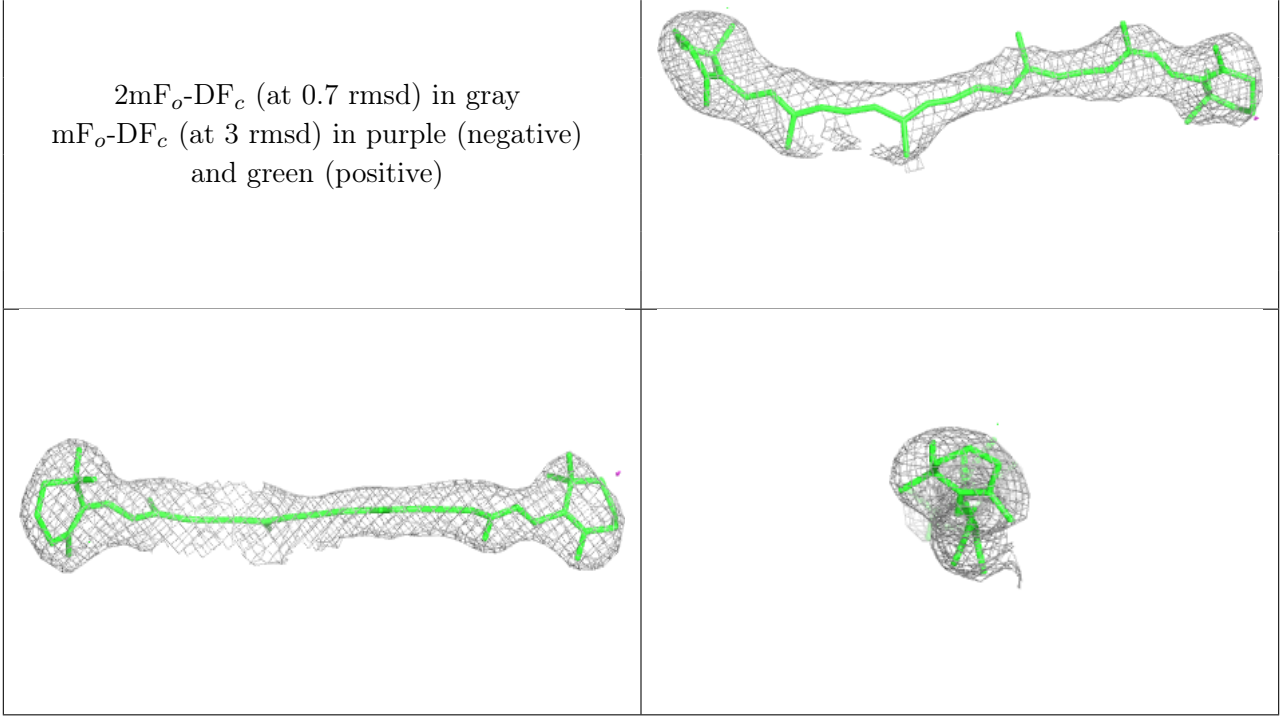






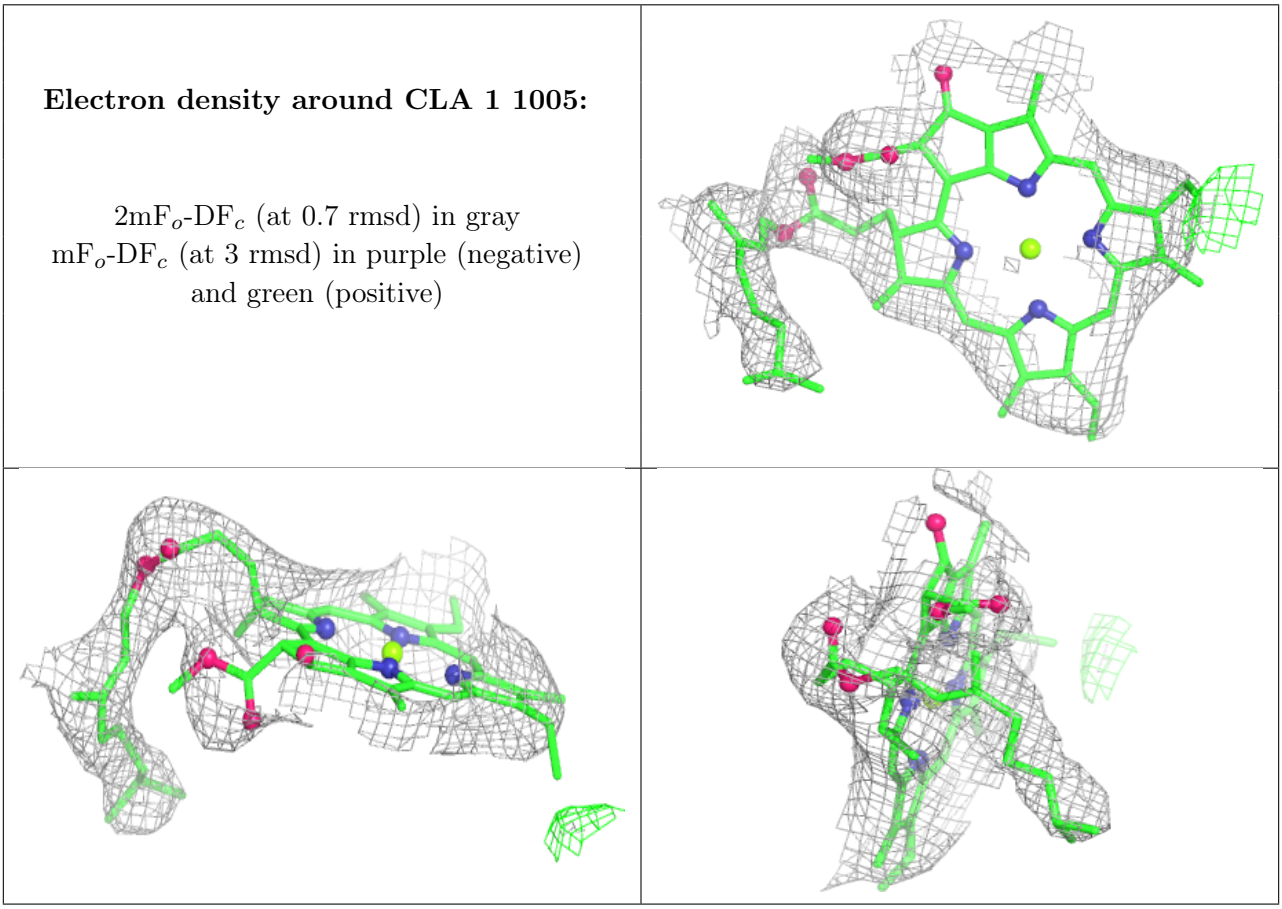
Electron density around BCR B 6009:

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



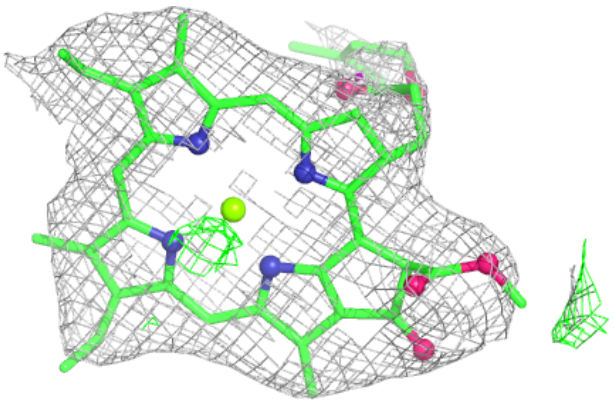
Electron density around CLA 1 1005:

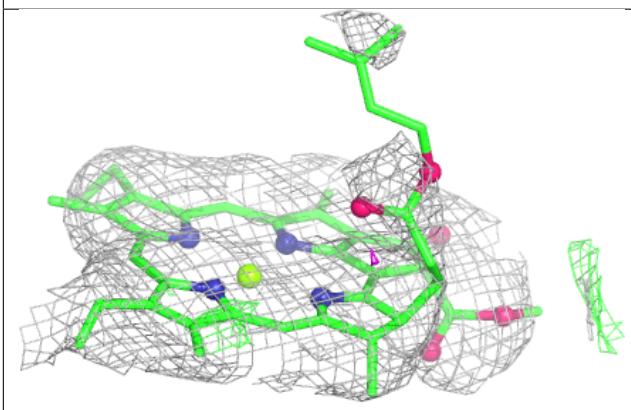
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

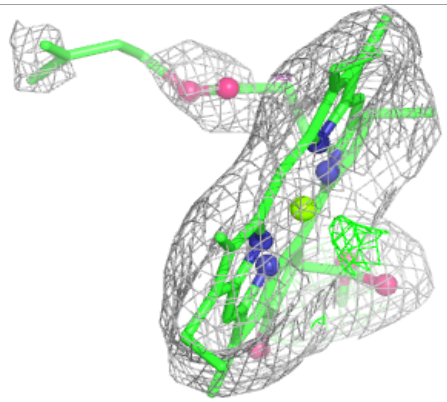


Electron density around CLA B 1201:

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

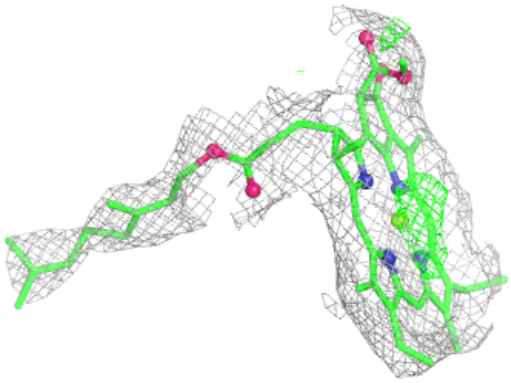


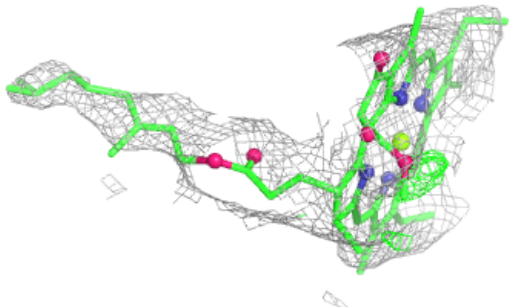


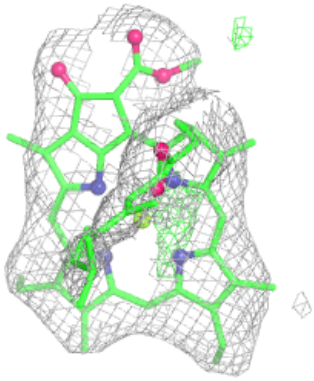


Electron density around CLA B 1208:

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

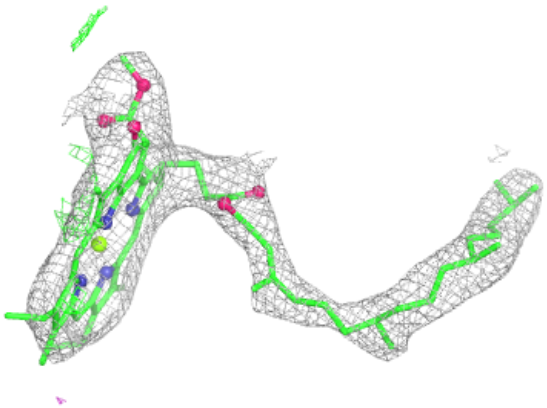


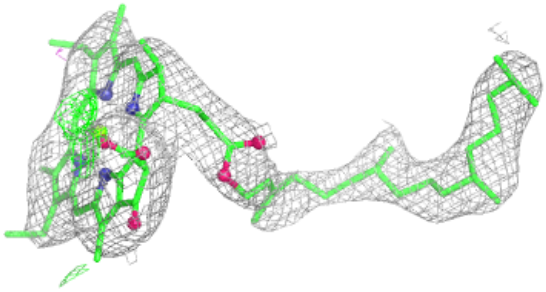


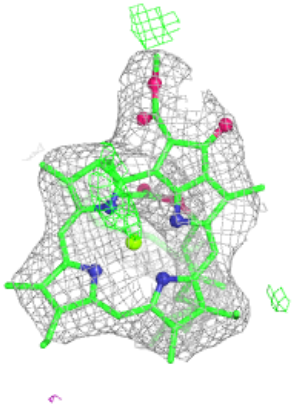


Electron density around CLA B 1238:

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

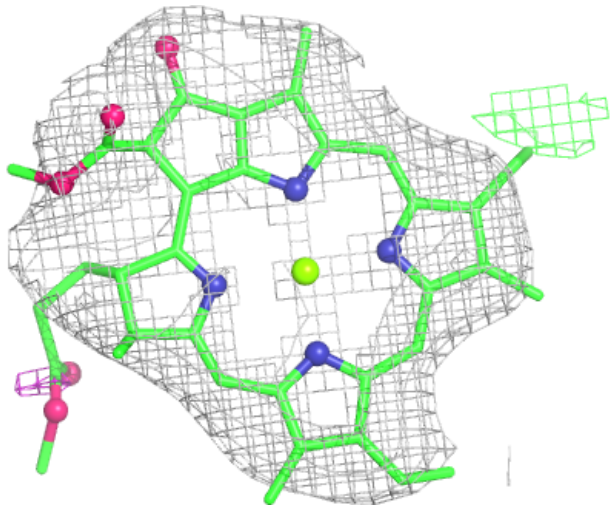


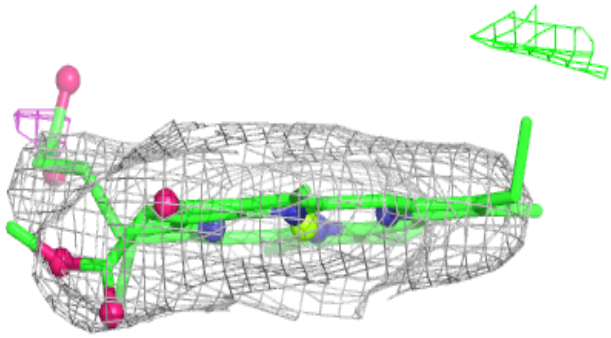


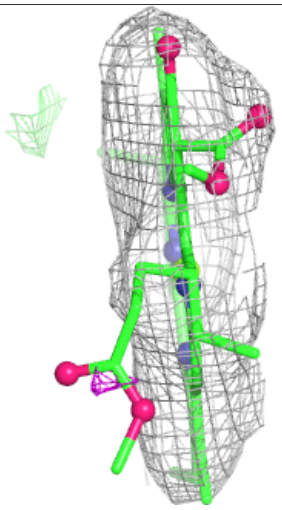


Electron density around CLA 3 3017:

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

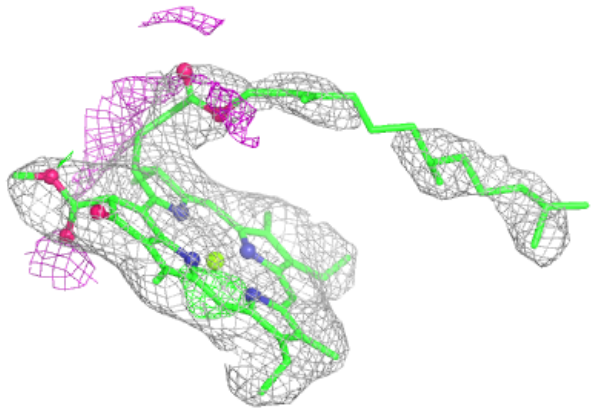


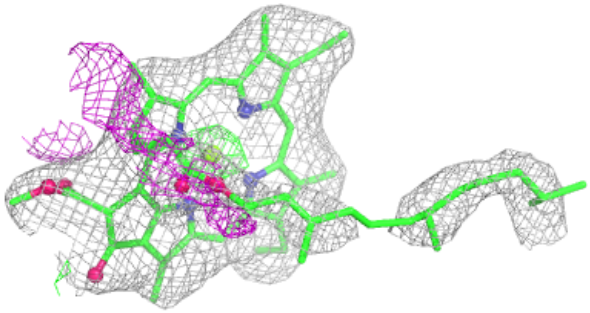


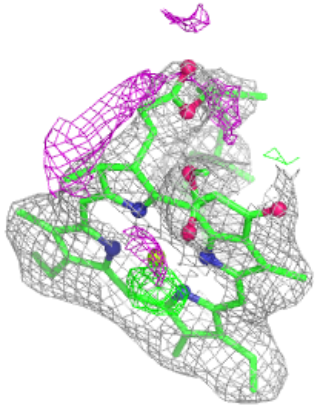


Electron density around CLA B 1228:

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

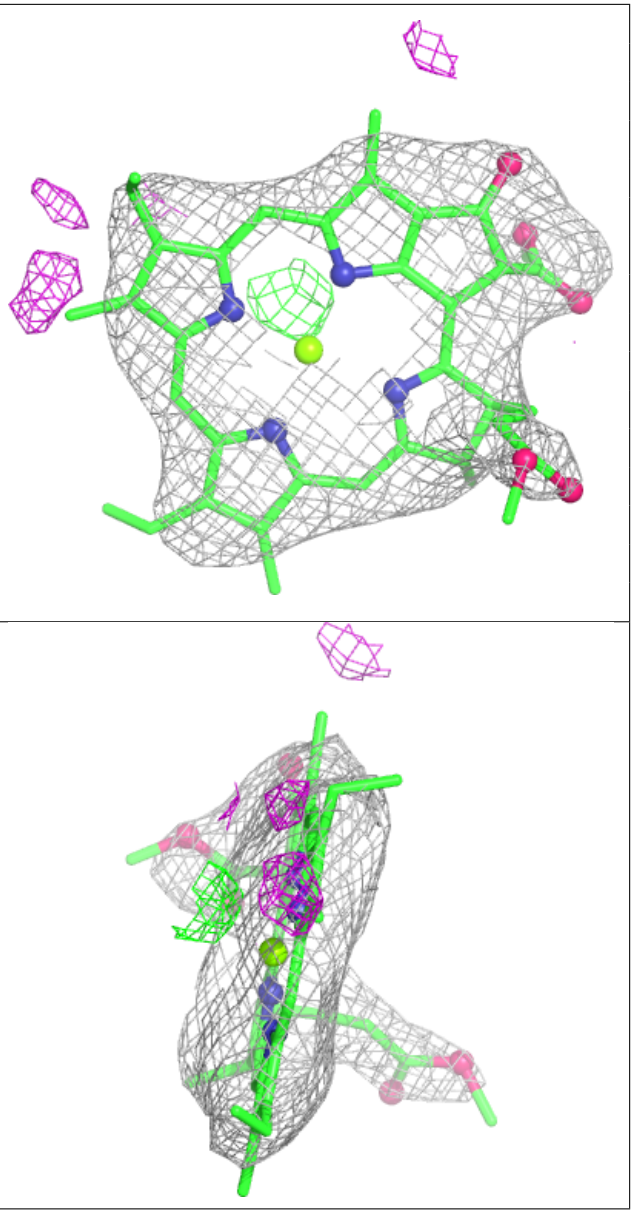






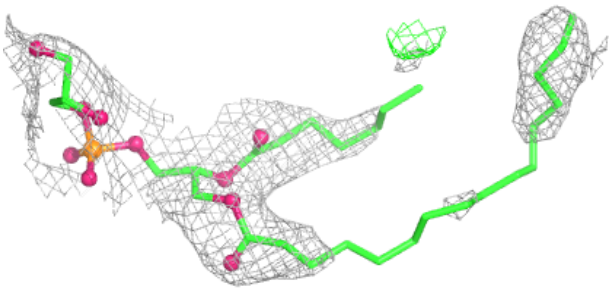
Electron density around CLA B 1217:

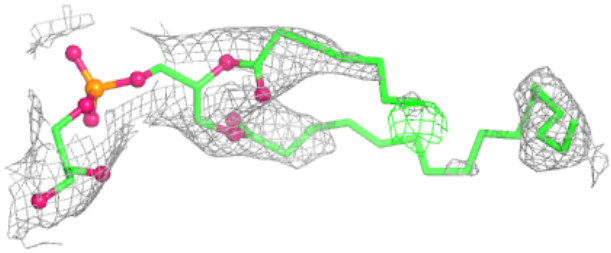
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

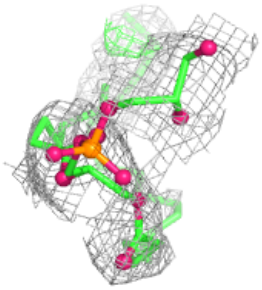


Electron density around LHG A 5003:

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

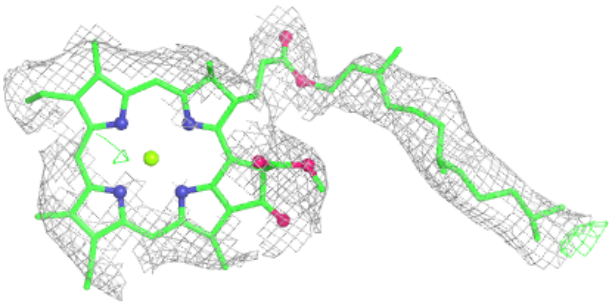


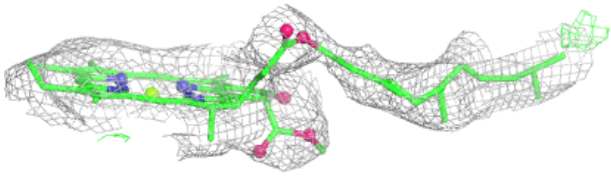


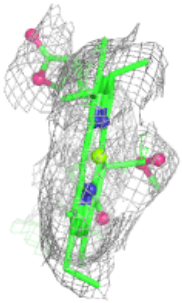


Electron density around CLA A 1120:

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

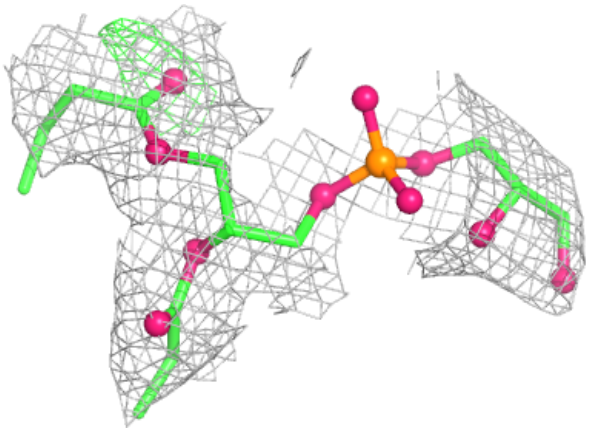


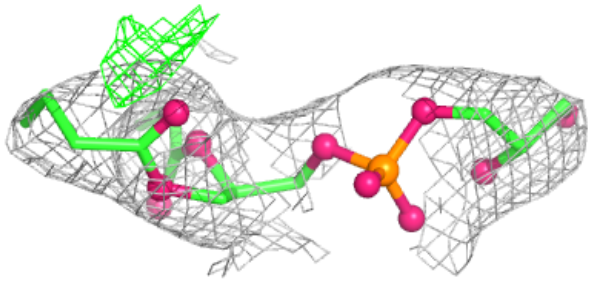


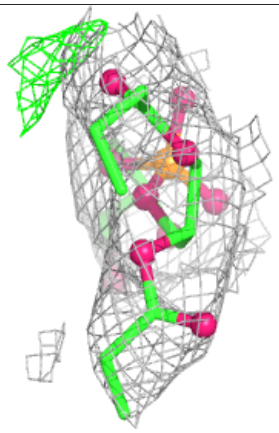


Electron density around LHG 2 2801:

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

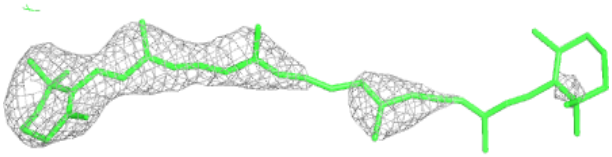


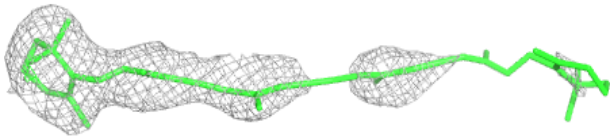


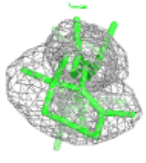


Electron density around BCR A 6003:

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

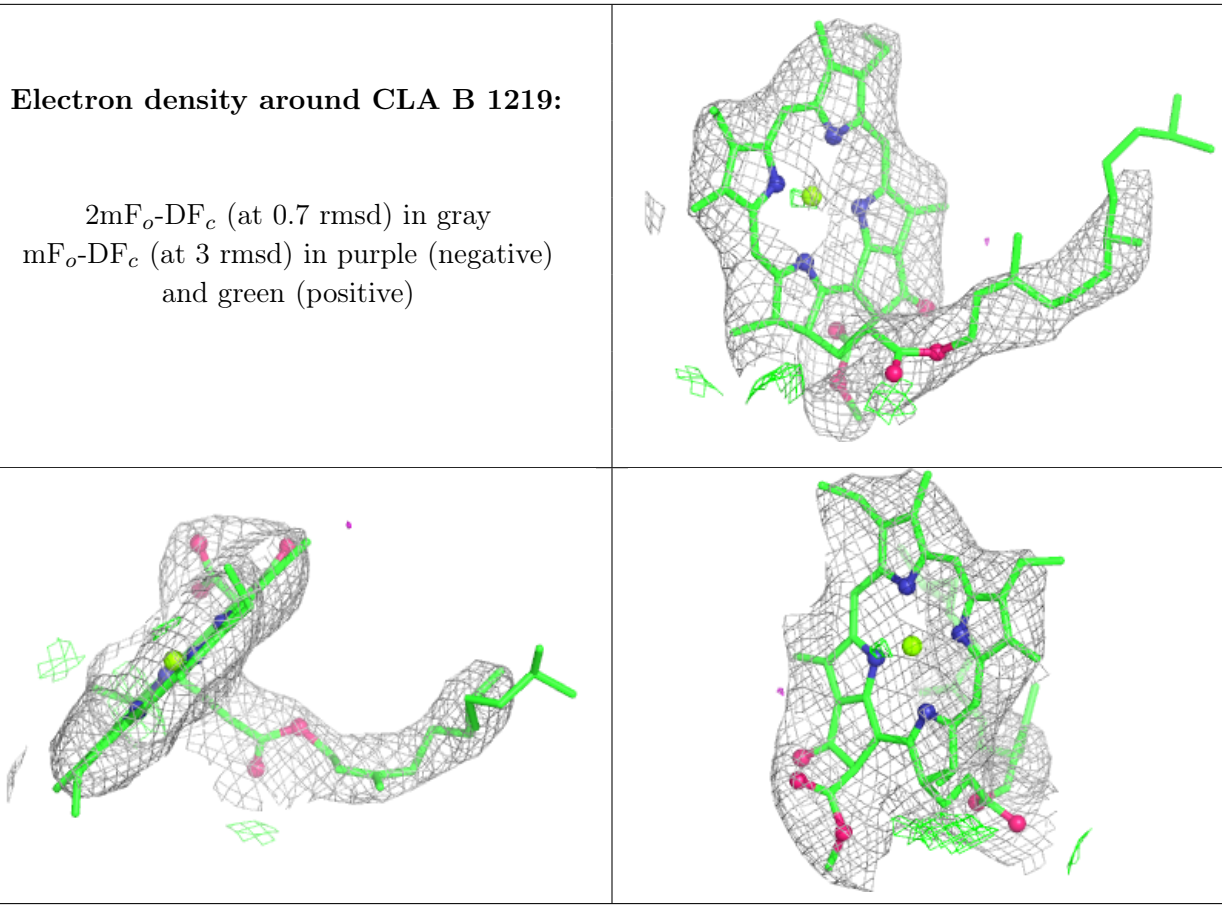






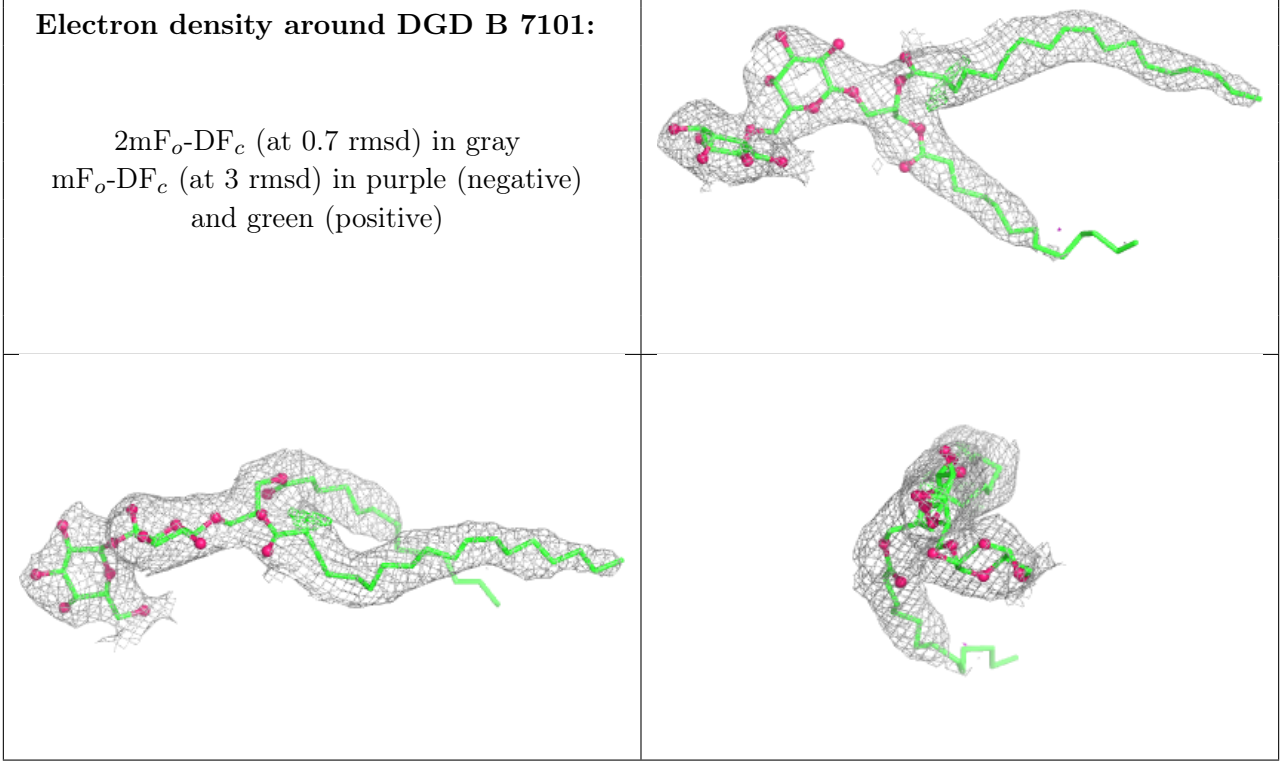
Electron density around CLA B 1219:

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



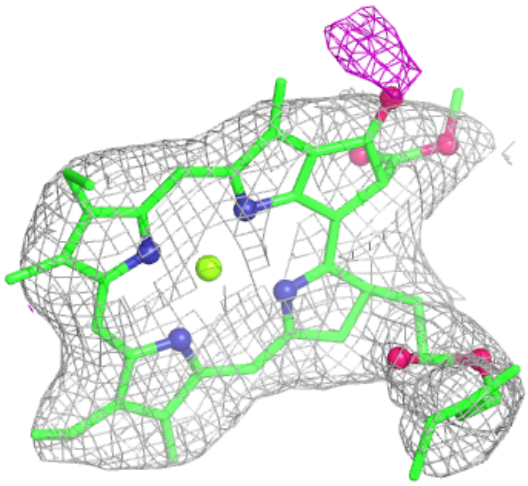
Electron density around DGD B 7101:

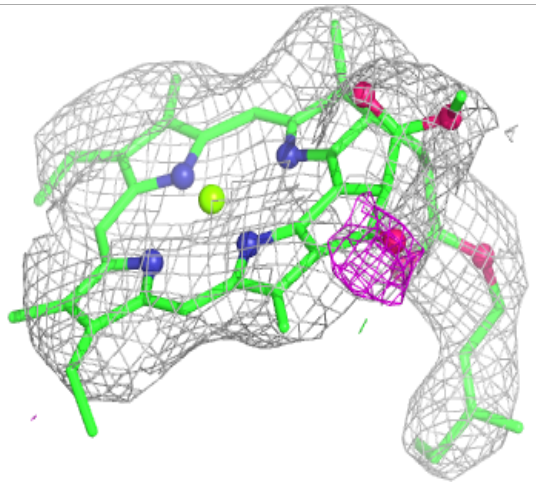
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

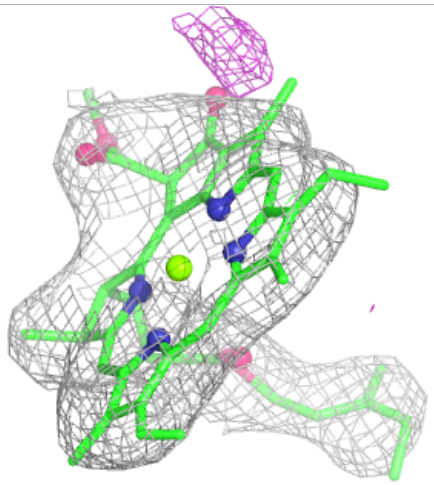


Electron density around CLA A 1105:

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

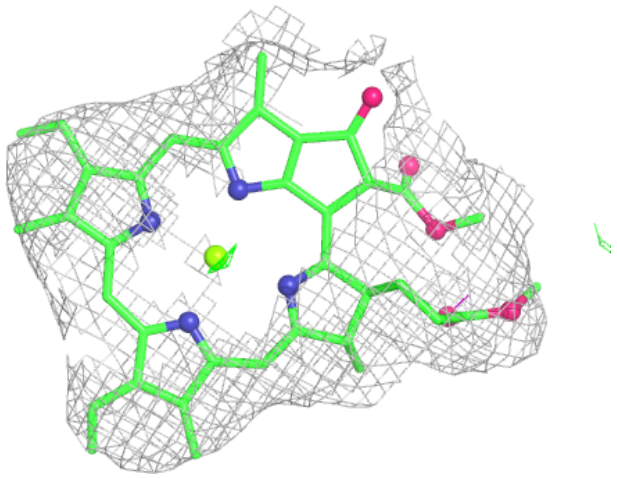


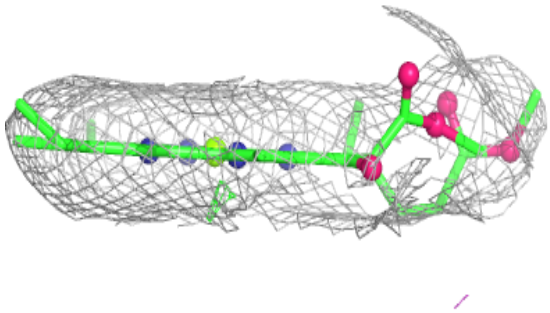


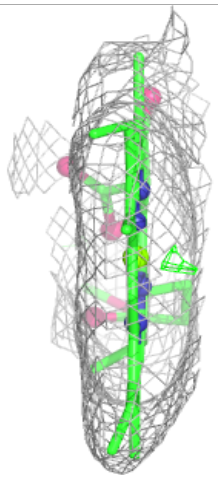


Electron density around CLA 2 2002:

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

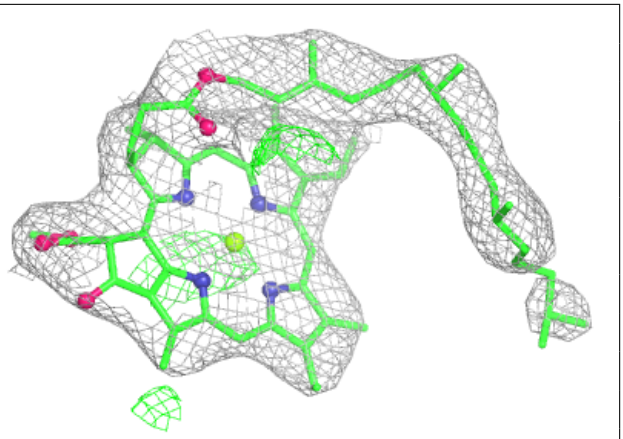


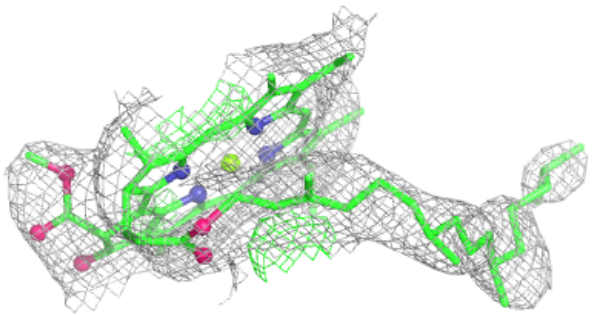


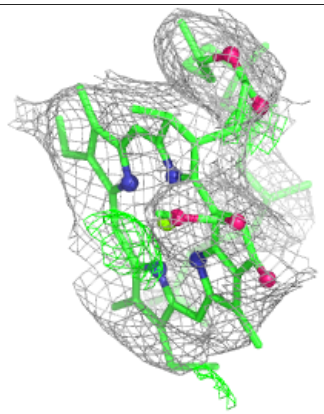


Electron density around CLA 2 2004:

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

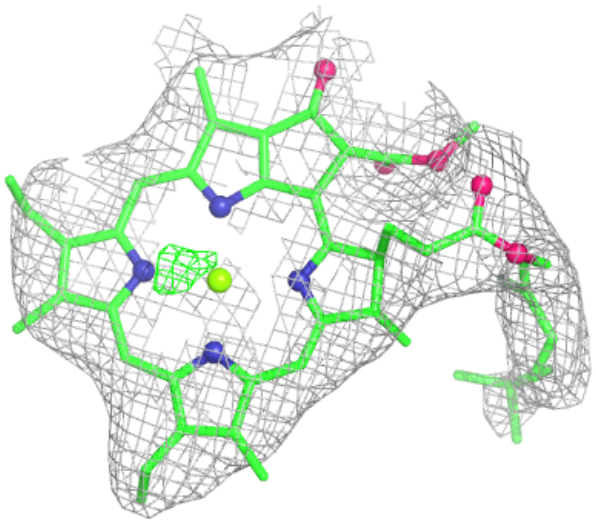


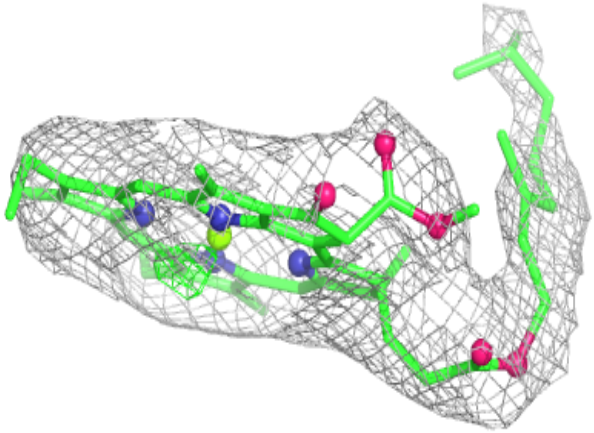


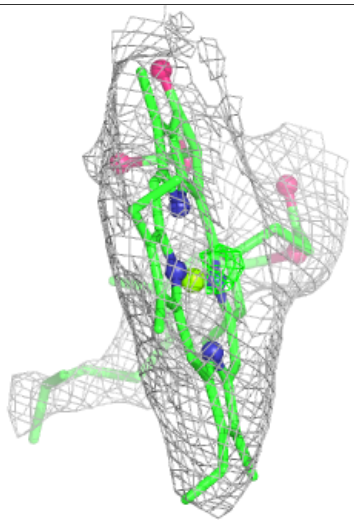


Electron density around CLA 2 2005:

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

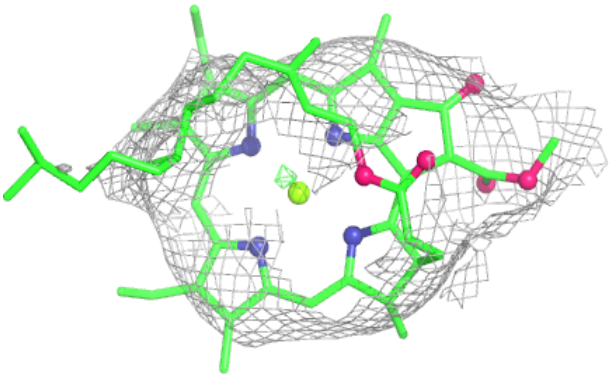


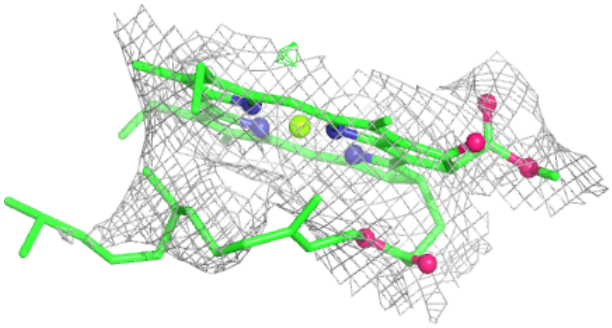


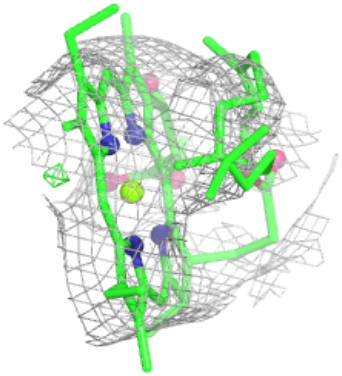


Electron density around CLA 3 3003:

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

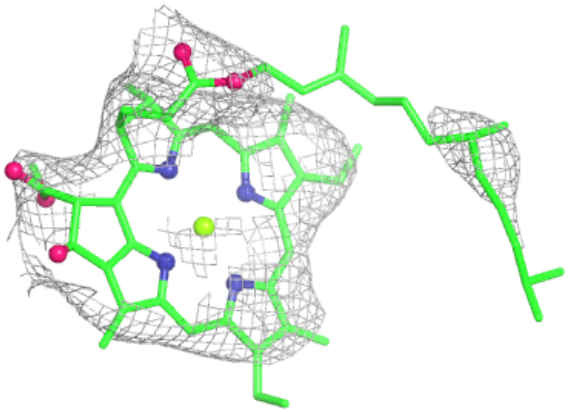


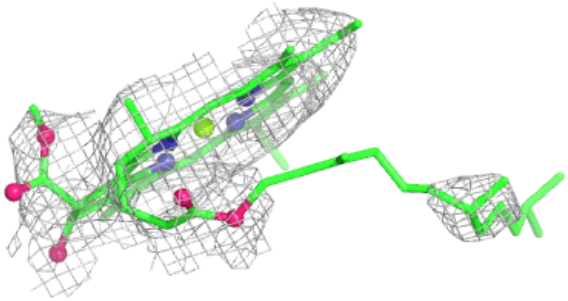


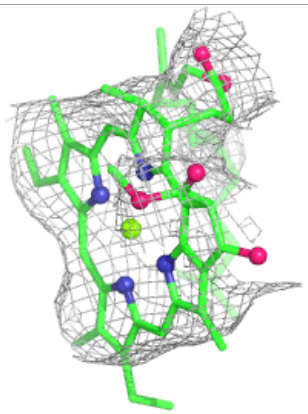


Electron density around CLA 3 3004:

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

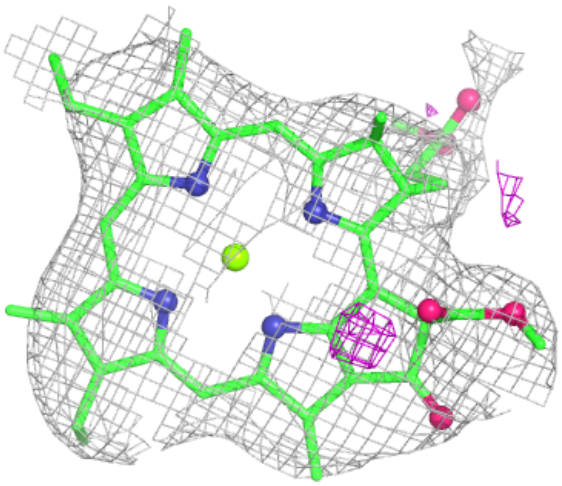


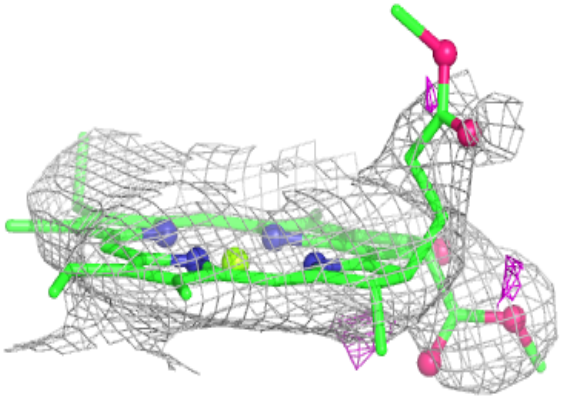


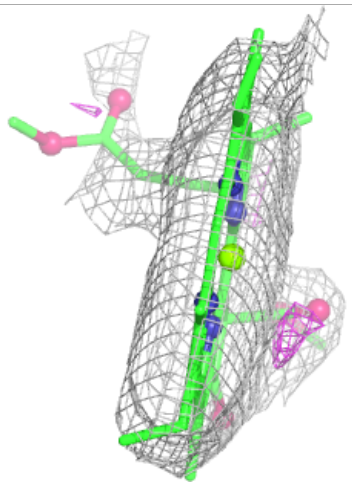


Electron density around CLA B 1209:

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

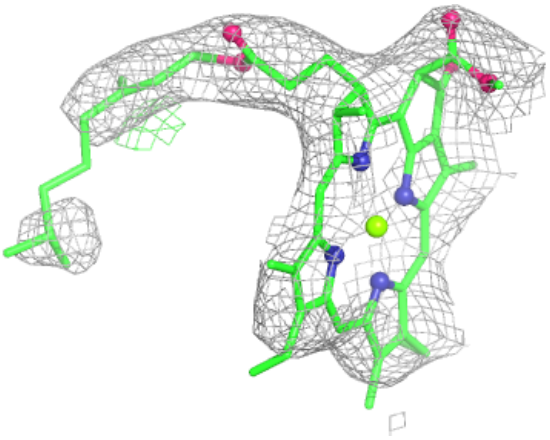




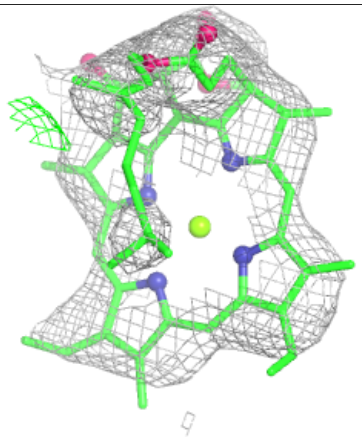


Electron density around CLA B 1212:

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

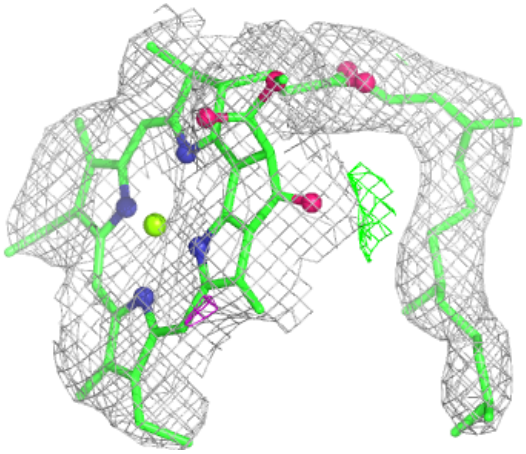


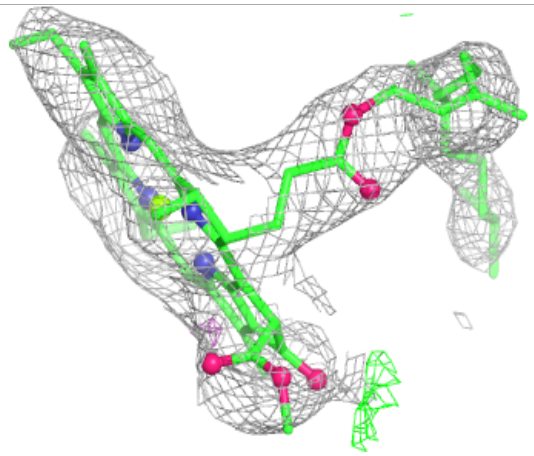


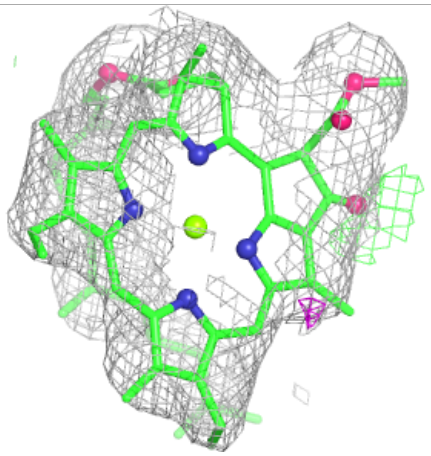


Electron density around CLA B 1231:

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

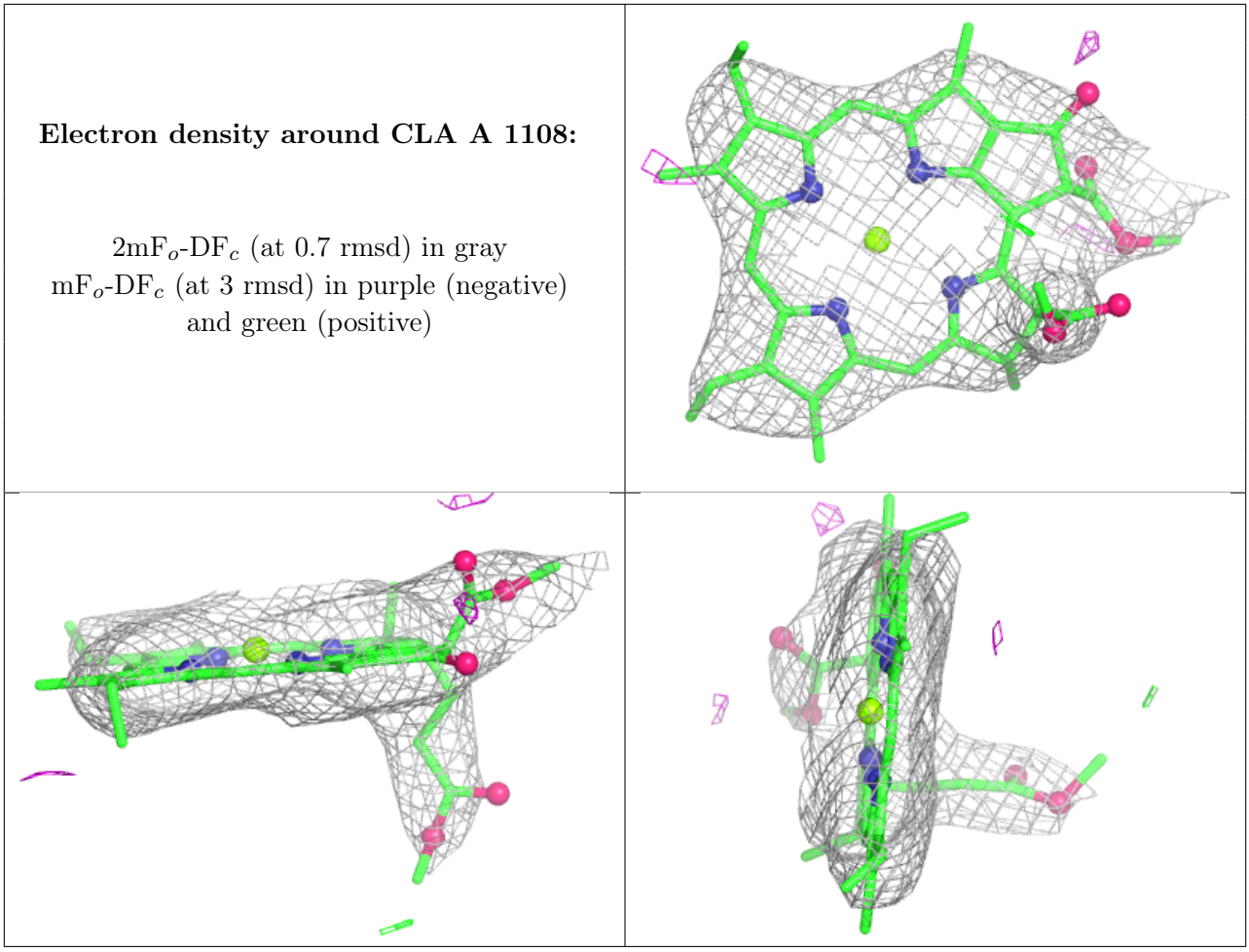






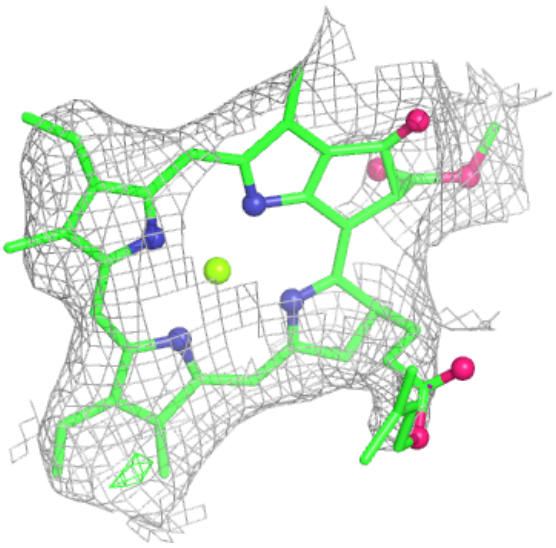
Electron density around CLA A 1108:

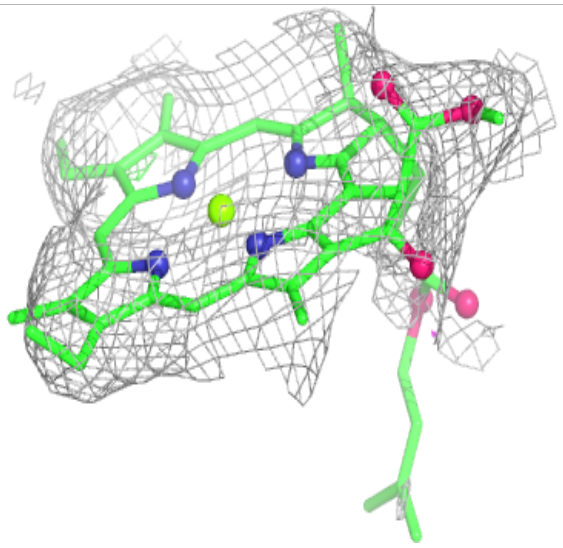
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 3 3012:

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

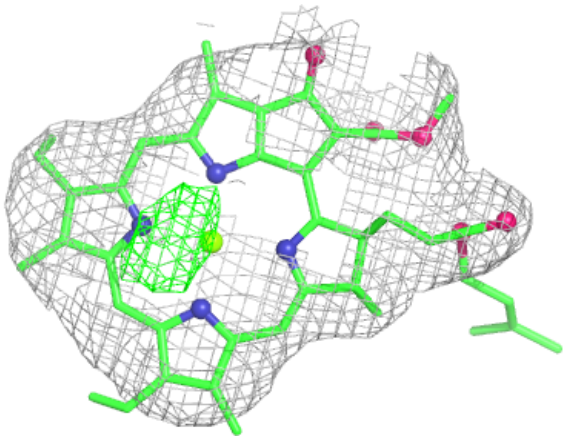


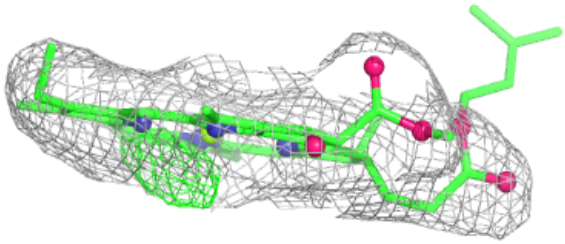


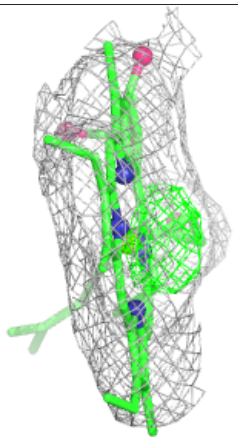


Electron density around CLA 4 4002:

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

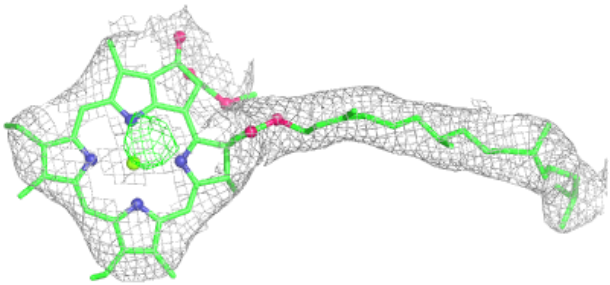


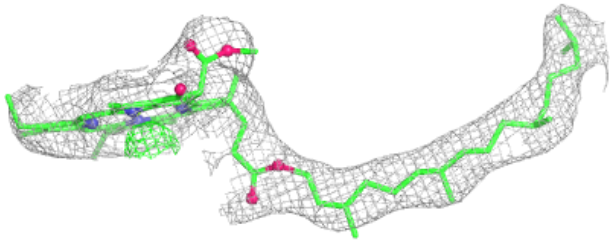


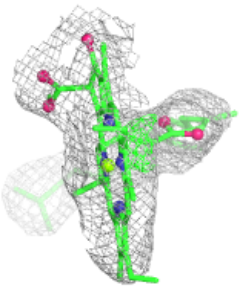


Electron density around CLA B 1240:

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

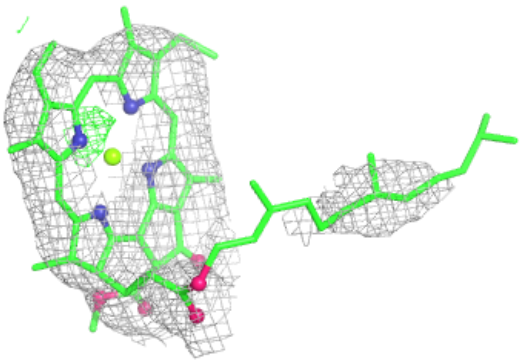


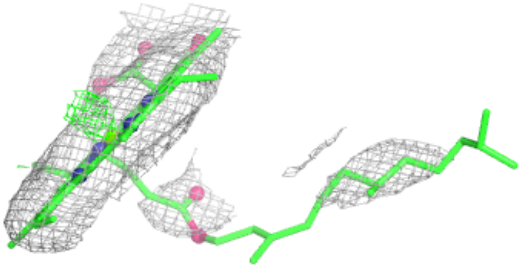


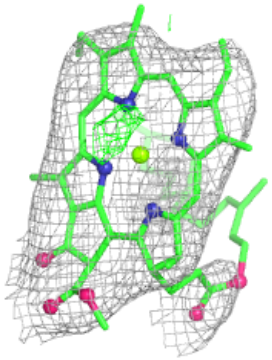


Electron density around CLA 4 4007:

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

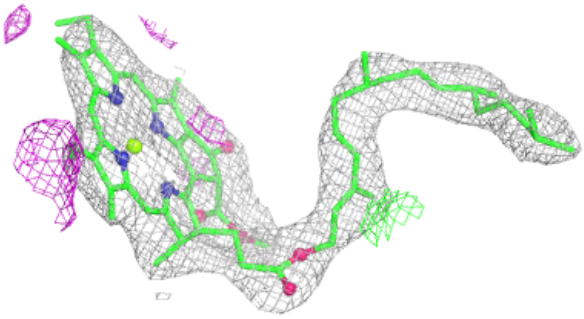


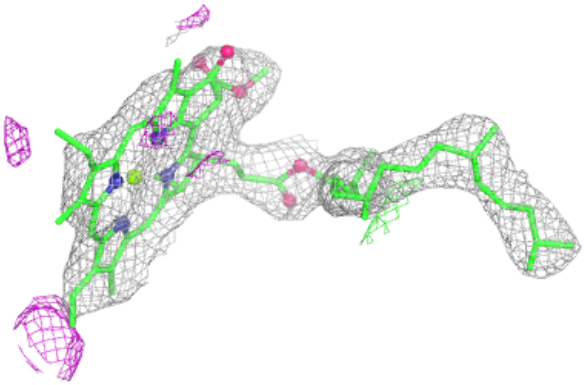


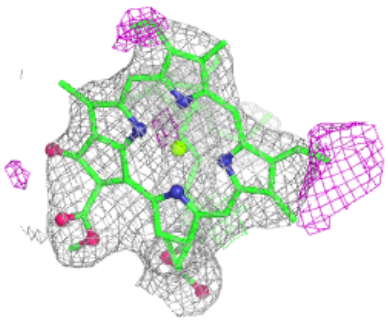


Electron density around CLA B 1021:

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

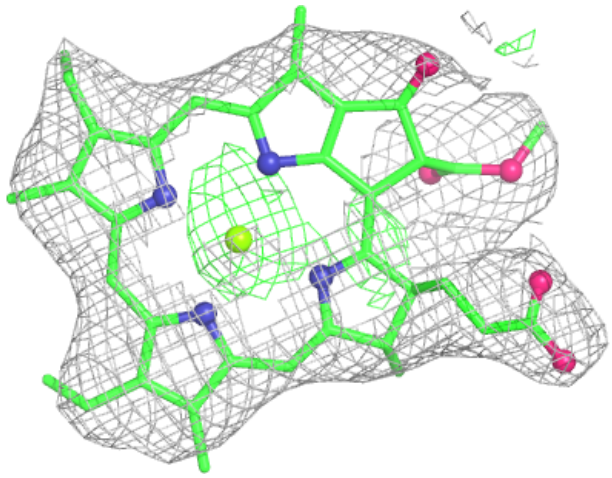


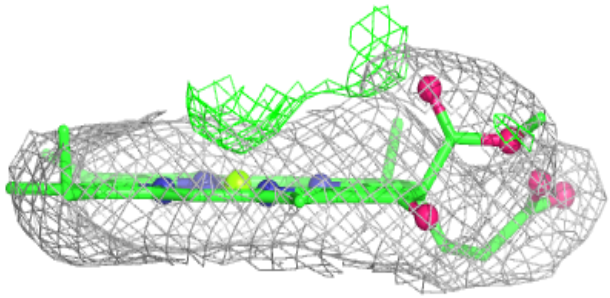


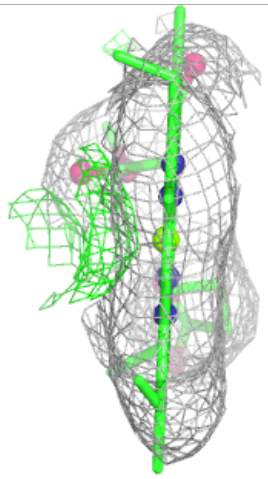


Electron density around CLA F 1301:

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

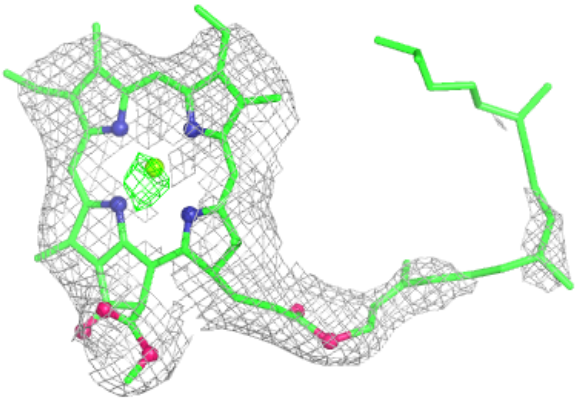


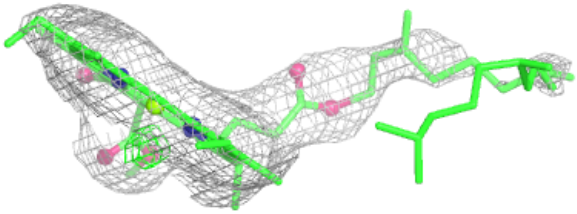


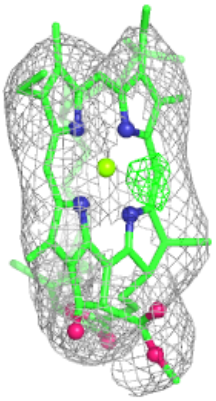


Electron density around CLA 4 4017:

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

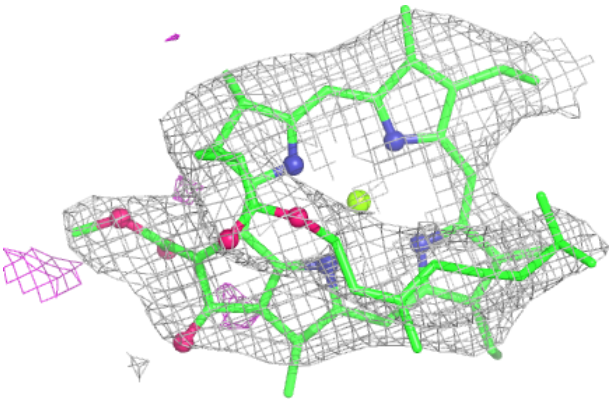


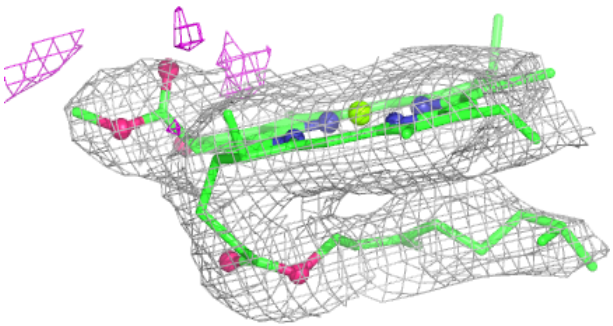


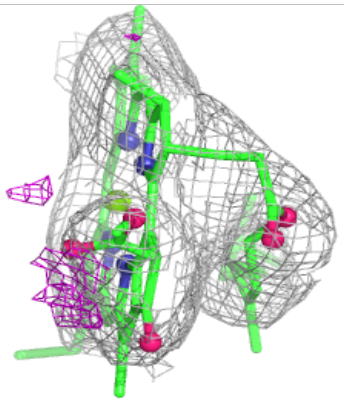


Electron density around CLA B 1204:

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

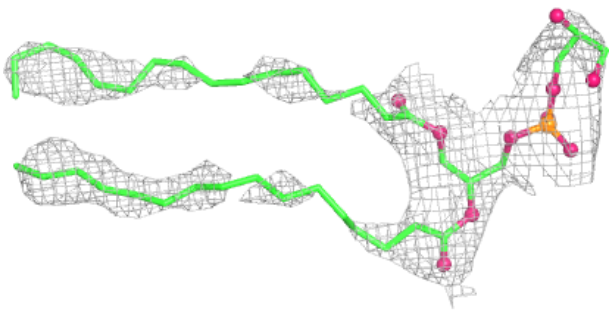


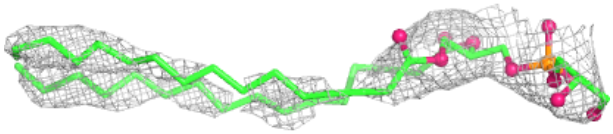




Electron density around LHG 1 1801:

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

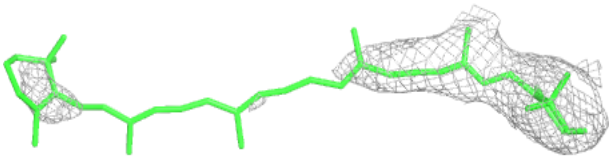


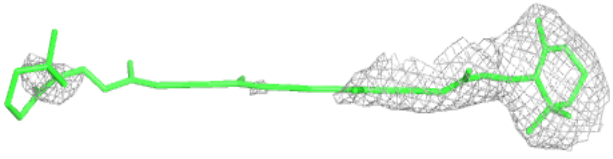


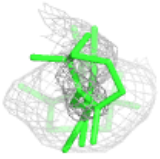


Electron density around BCR A 6002:

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

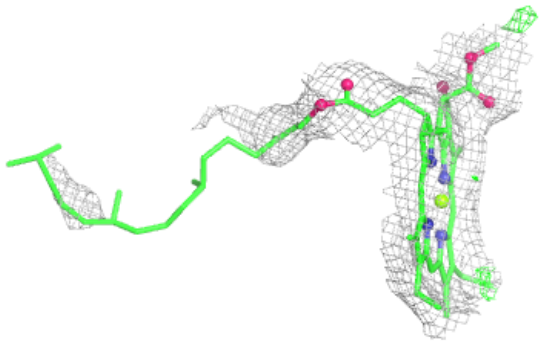


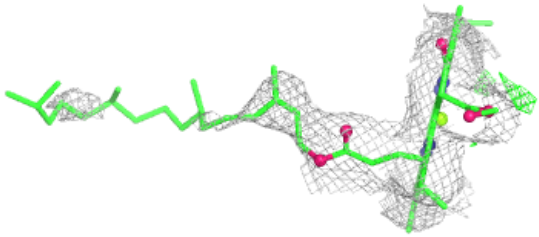


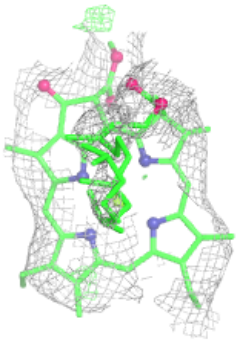


Electron density around CLA A 1112:

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

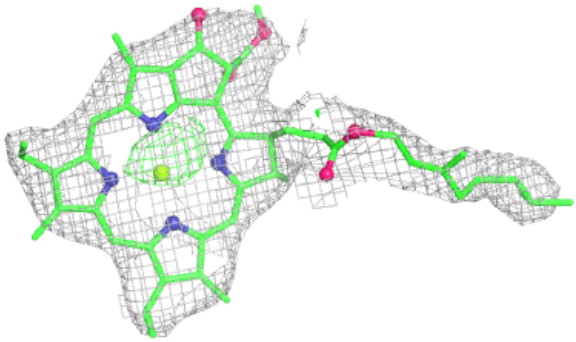


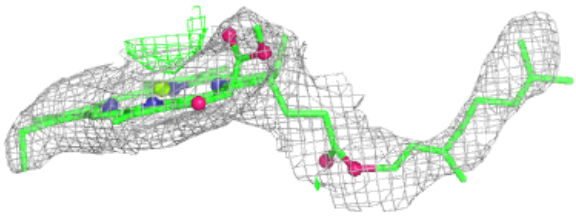


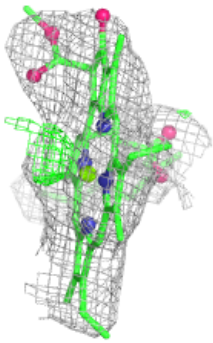


Electron density around CLA A 1124:

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

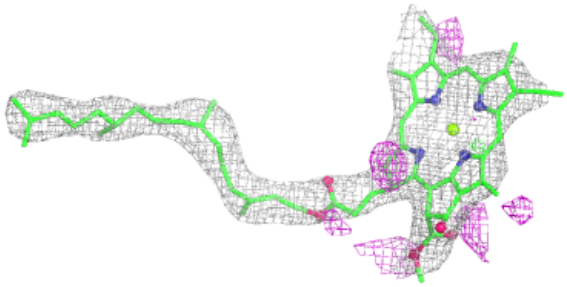


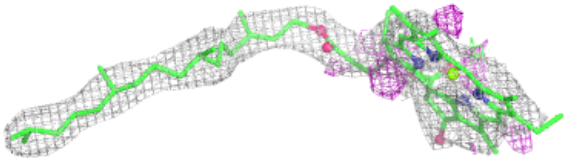


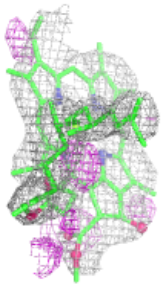


Electron density around CLA A 1022:

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

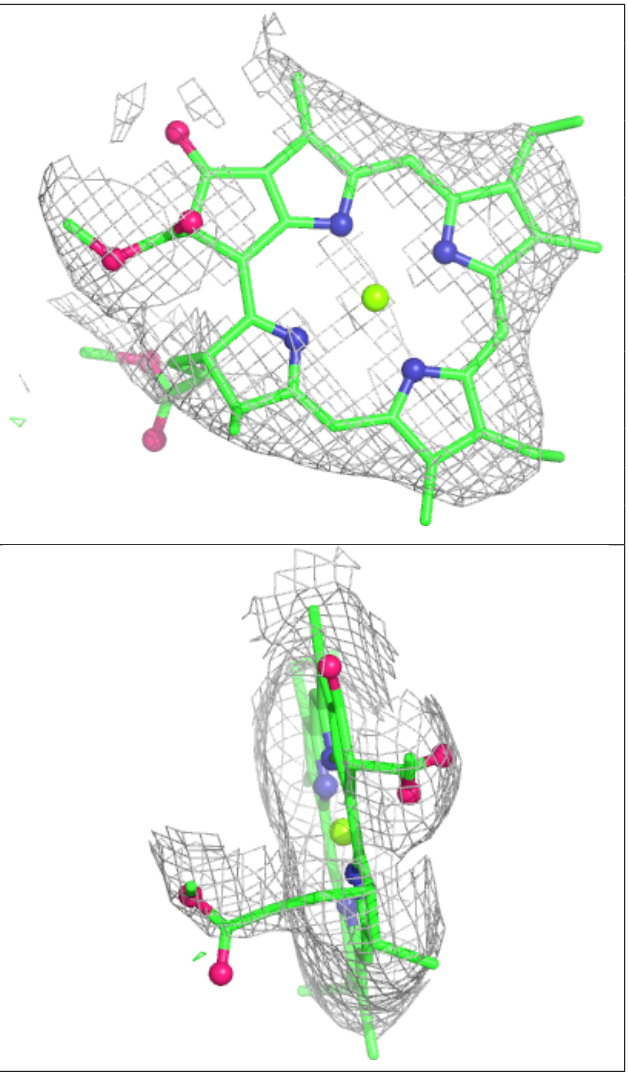


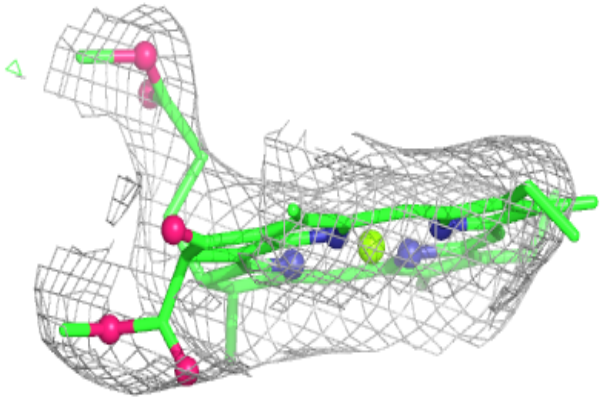




Electron density around CLA 1 1007:

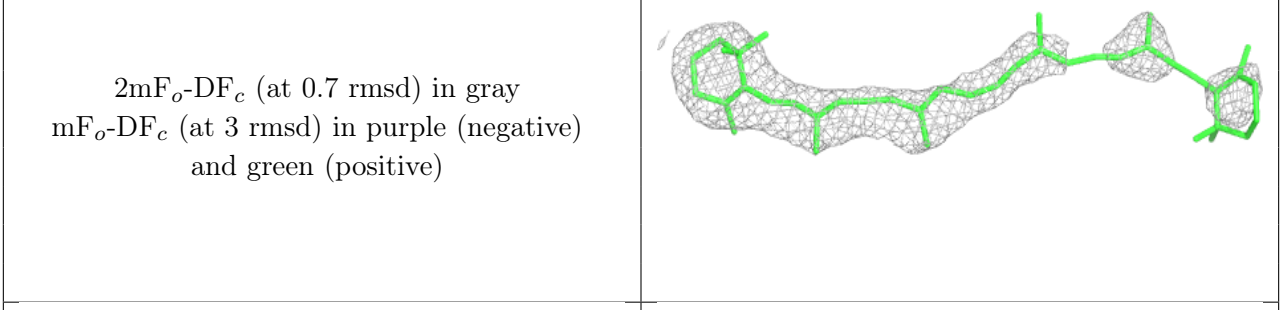
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

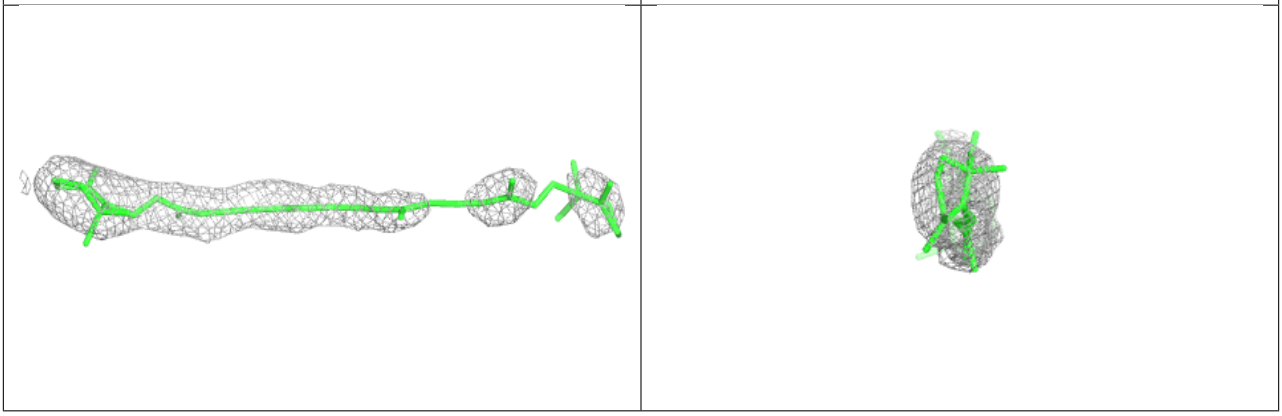




Electron density around BCR B 6005:

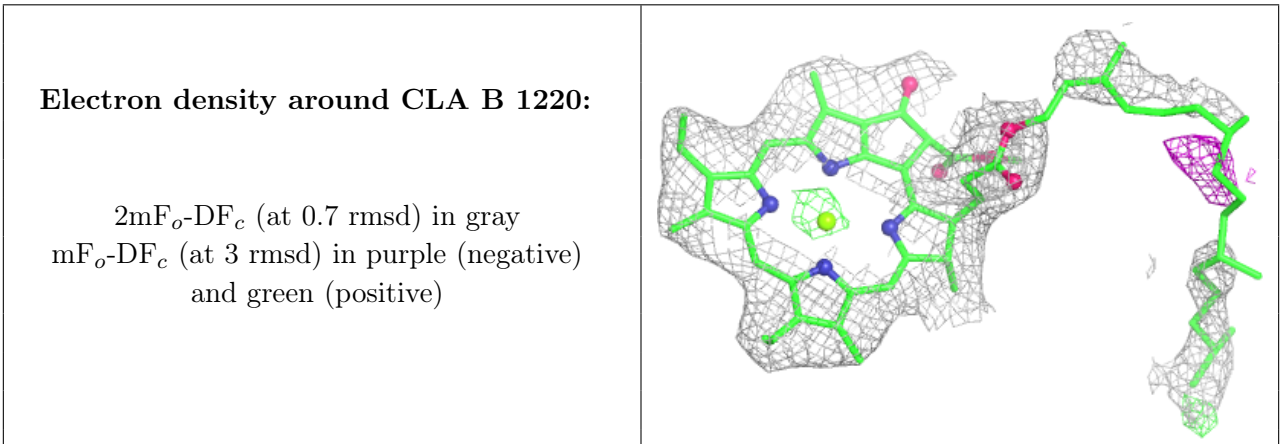
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

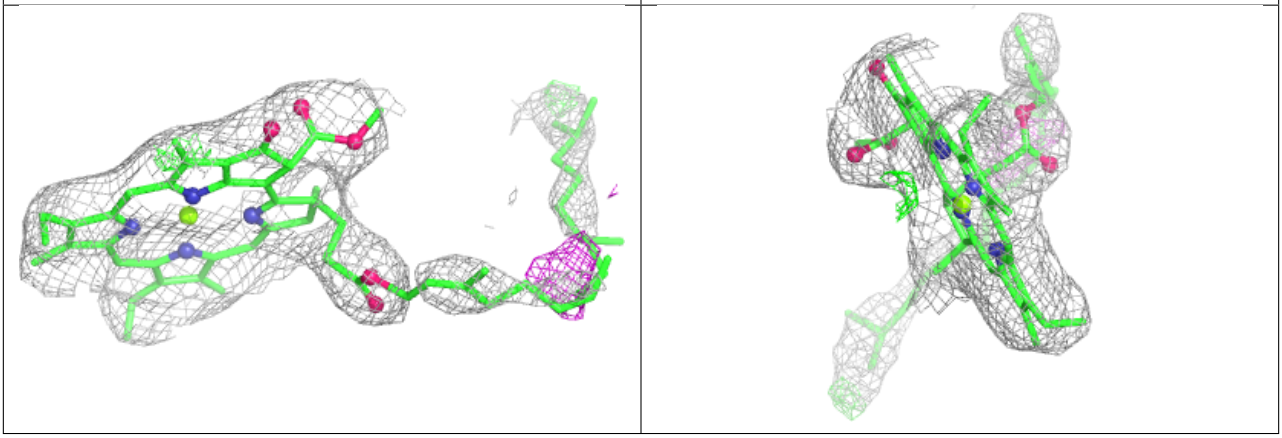




Electron density around CLA B 1220:

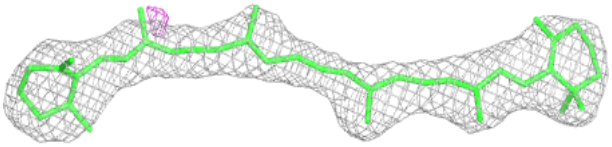
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

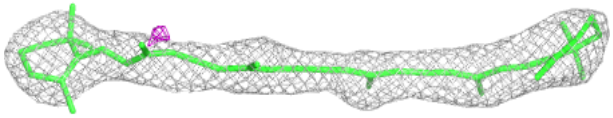


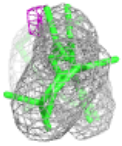


Electron density around BCR J 6012:

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

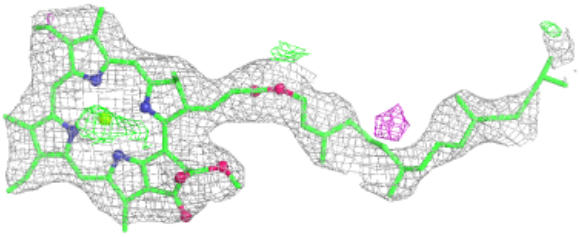


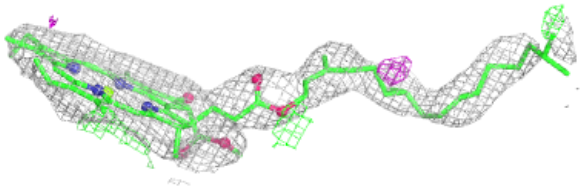




Electron density around CLA A 1139:

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

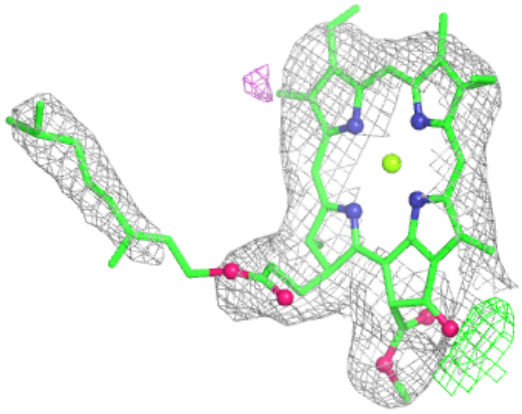


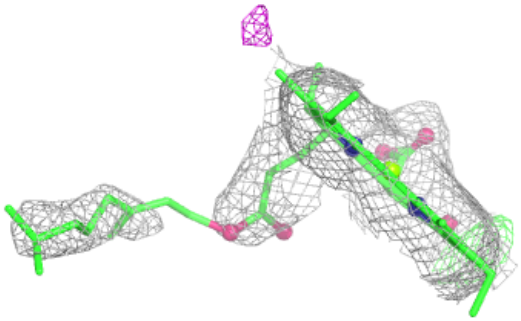


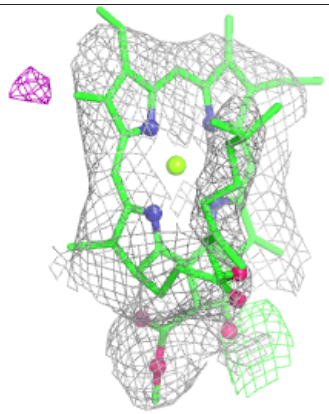


Electron density around CLA A 1133:

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

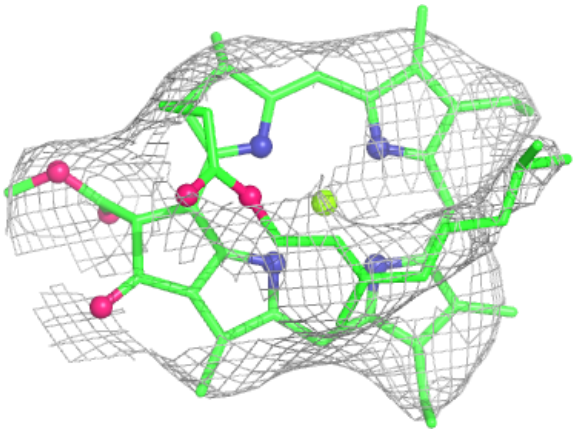


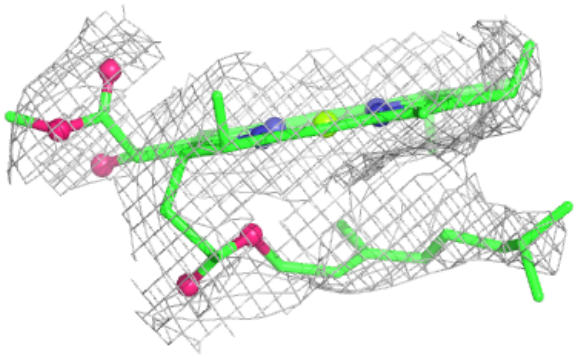


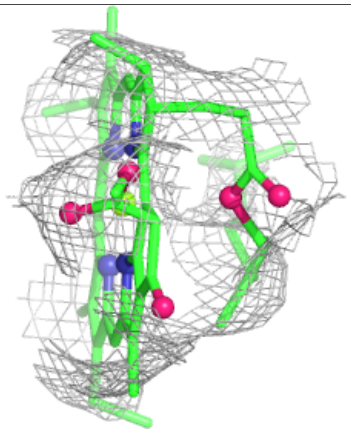


Electron density around CLA 2 2003:

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

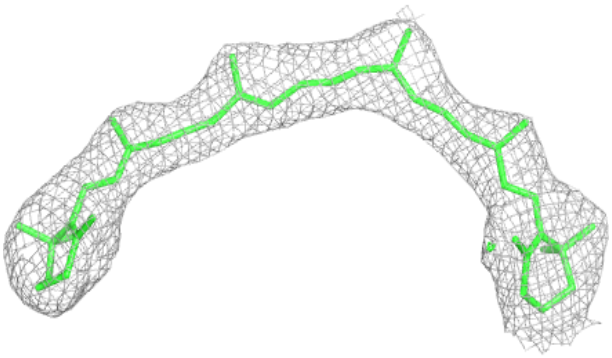


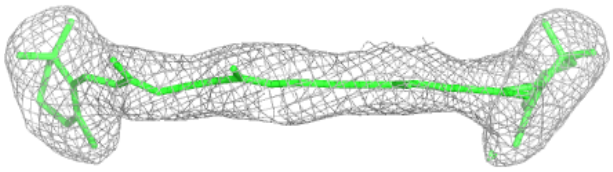


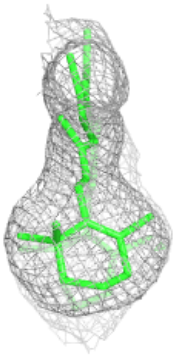


Electron density around BCR F 6016:

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

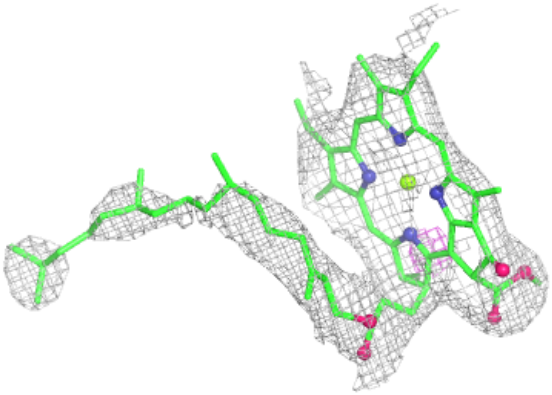


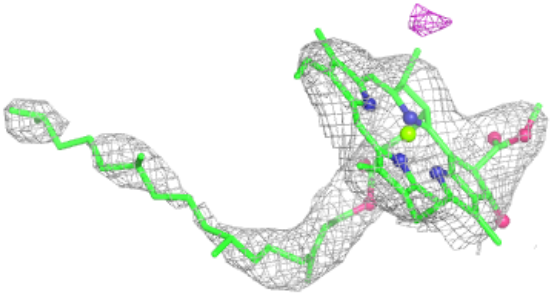


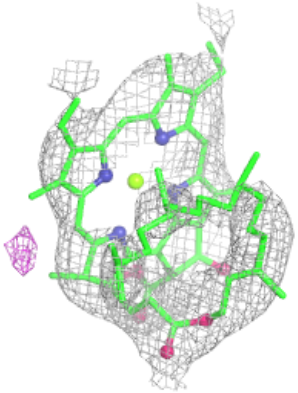


Electron density around CLA B 1211:

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

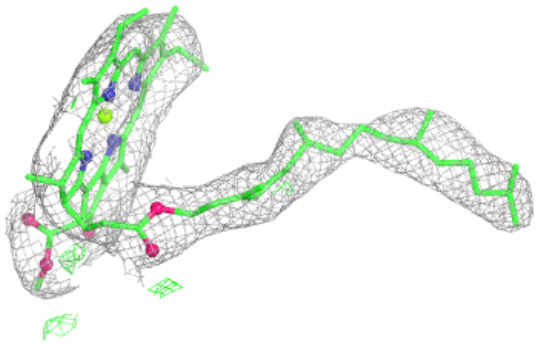


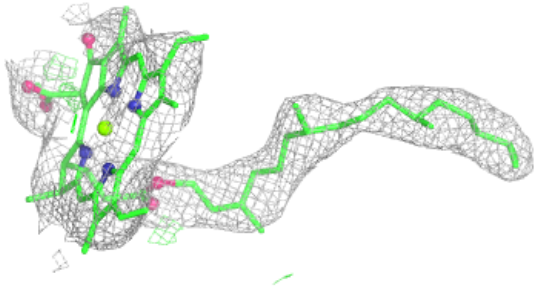


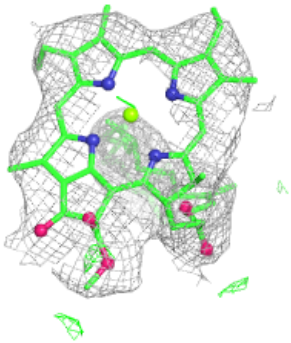


Electron density around CLA A 1109:

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

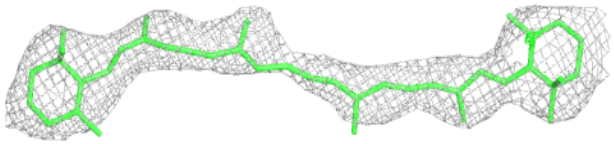


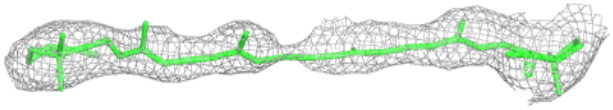


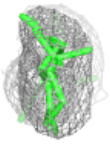


Electron density around BCR L 6019:

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

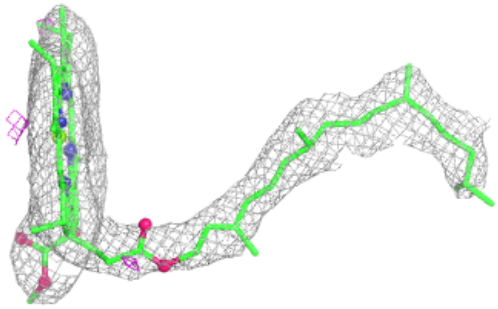


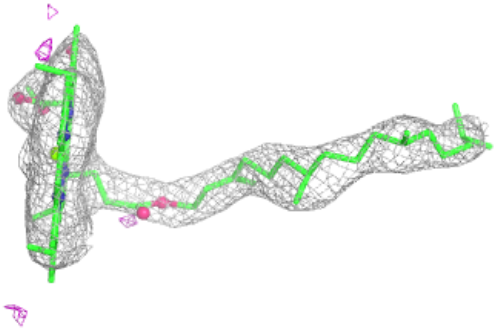


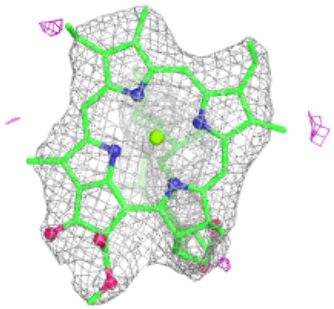


Electron density around CLA B 1239:

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

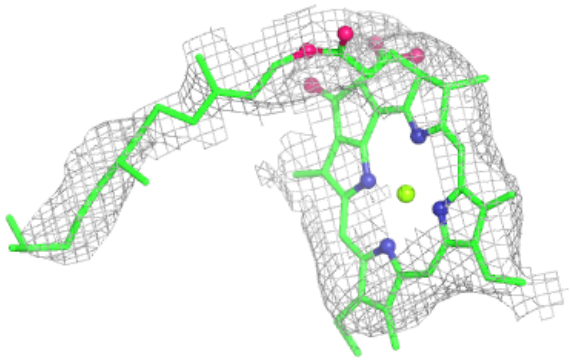


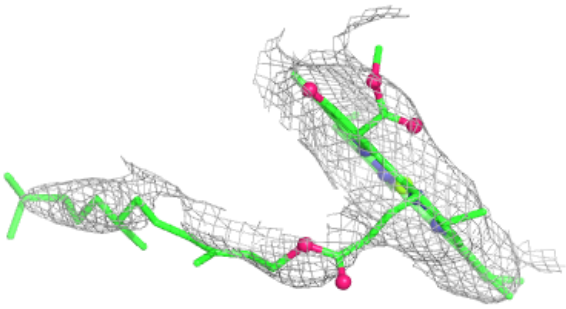


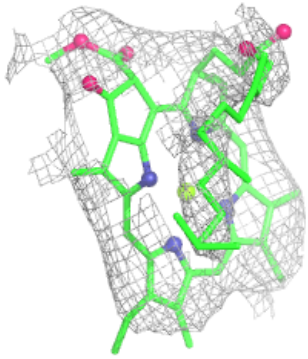


Electron density around CLA 2 2007:

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

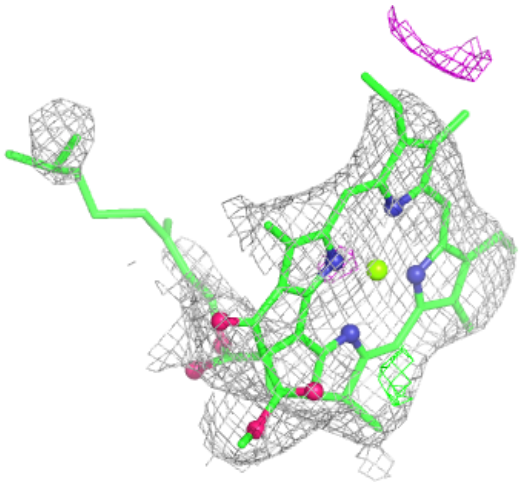


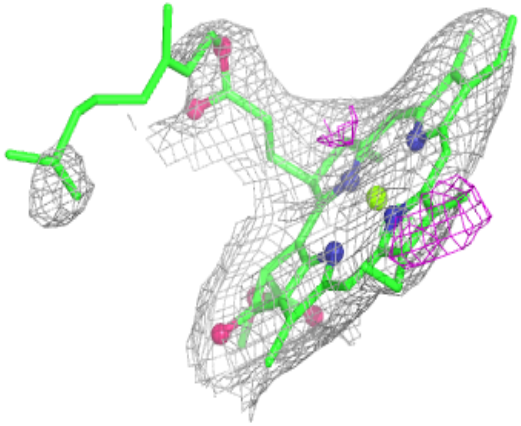


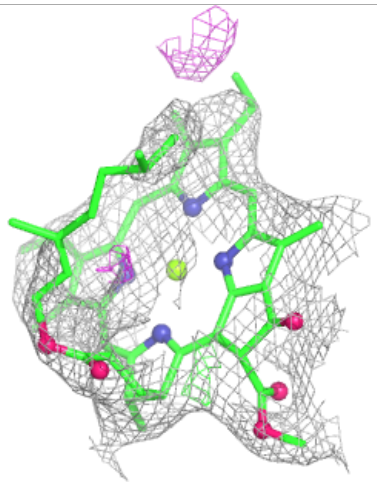


Electron density around CLA 2 2012:

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

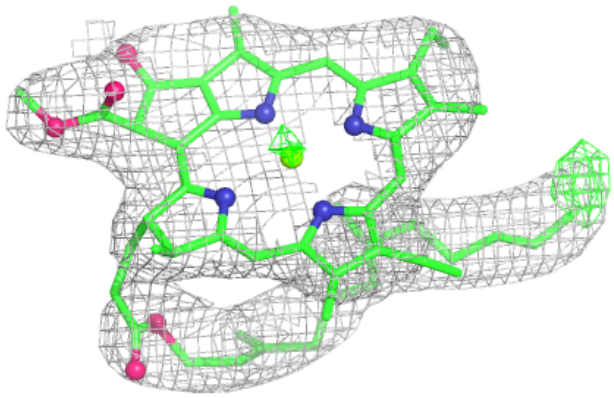


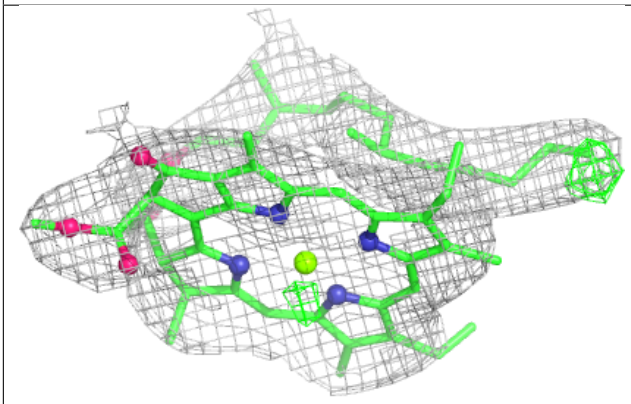


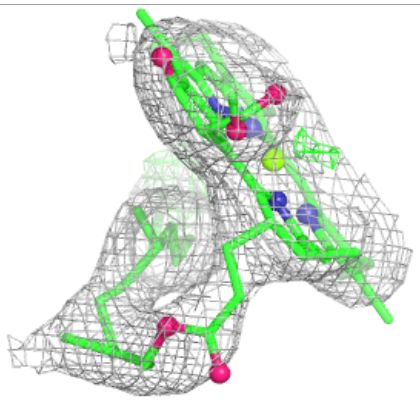


Electron density around CLA B 1214:

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

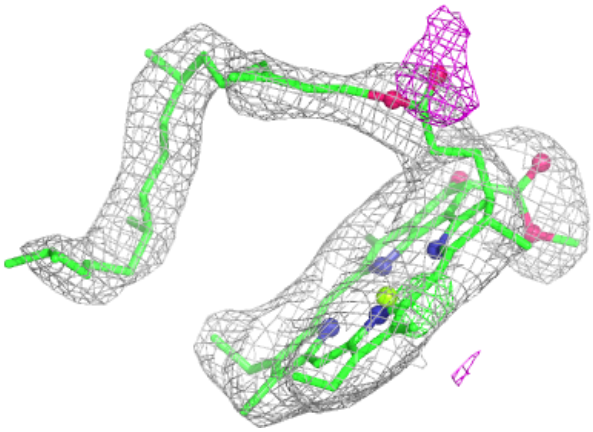


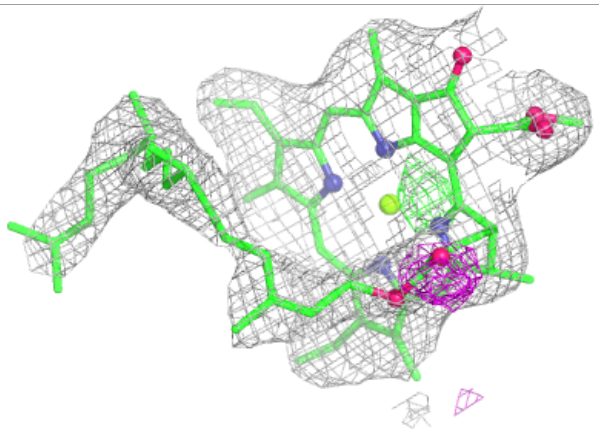


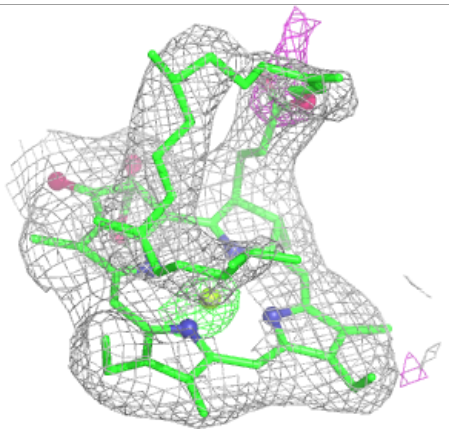


Electron density around CLA B 1227:

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

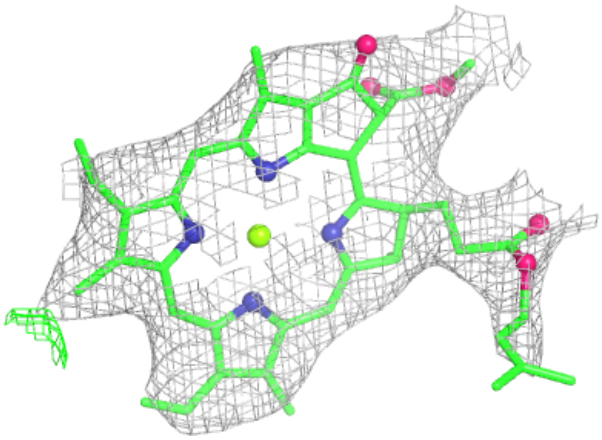


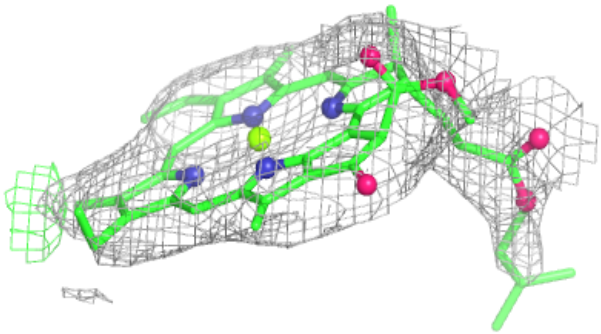


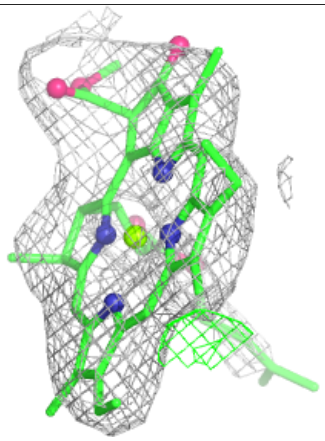


Electron density around CLA 2 2009:

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

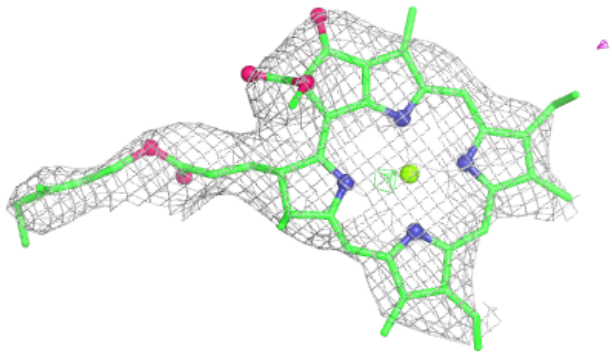


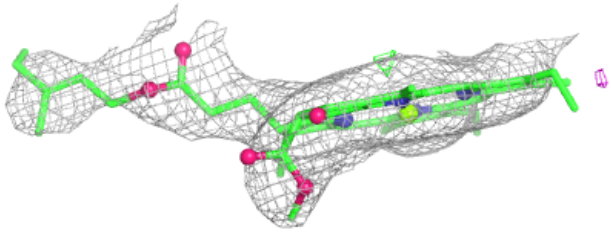


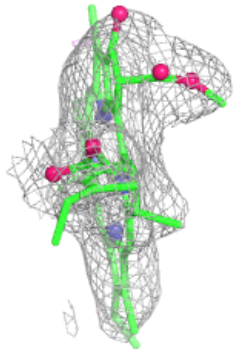


Electron density around CLA A 1135:

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

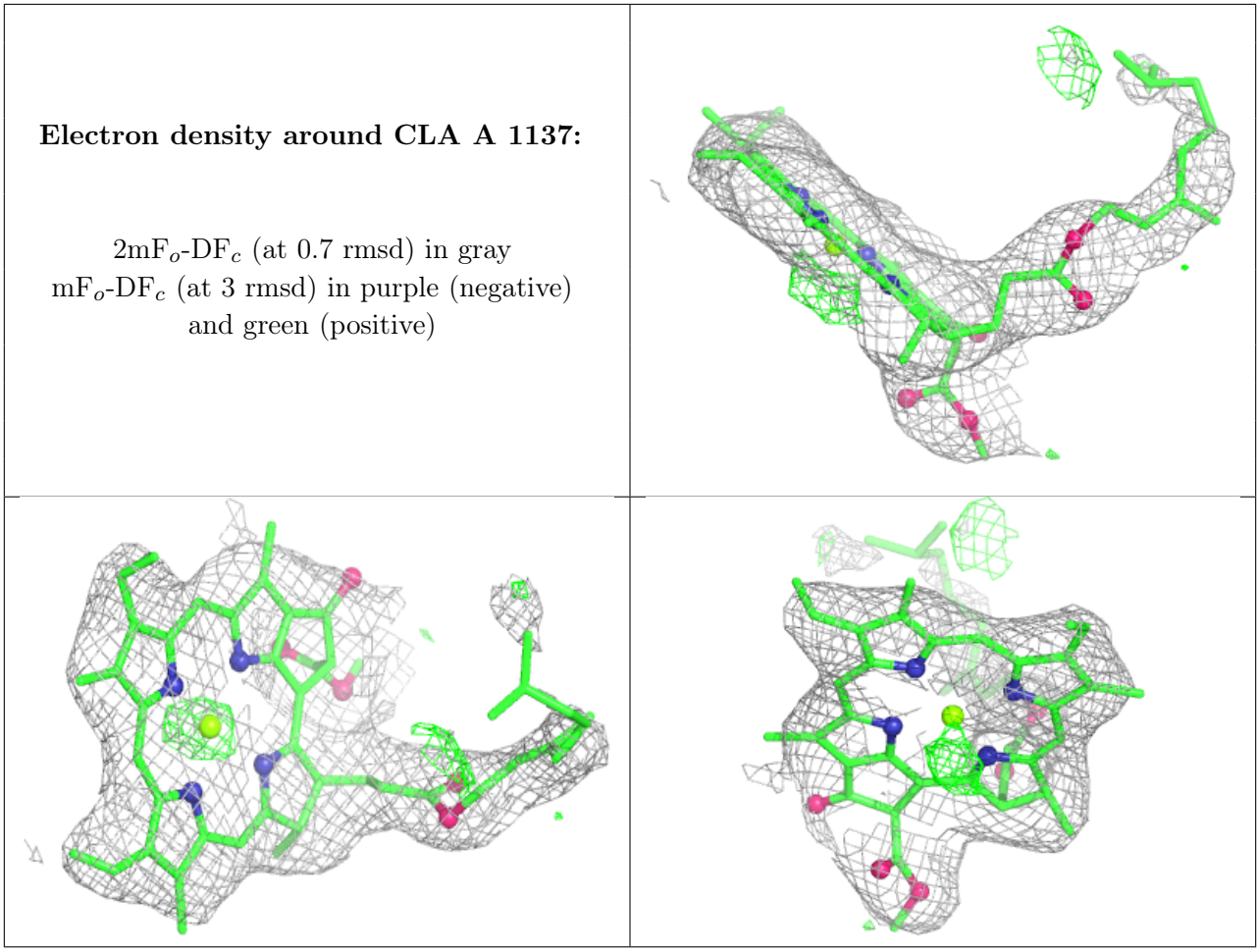






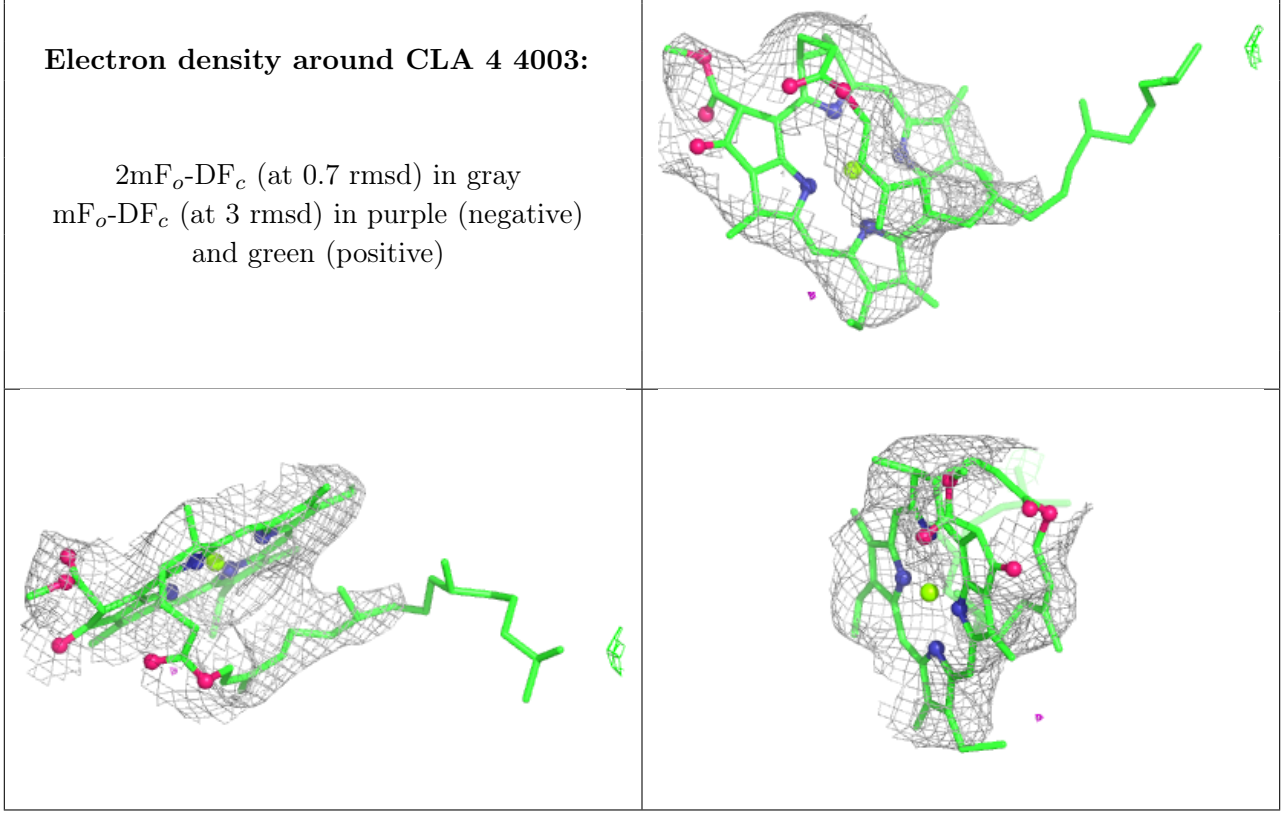
Electron density around CLA A 1137:

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



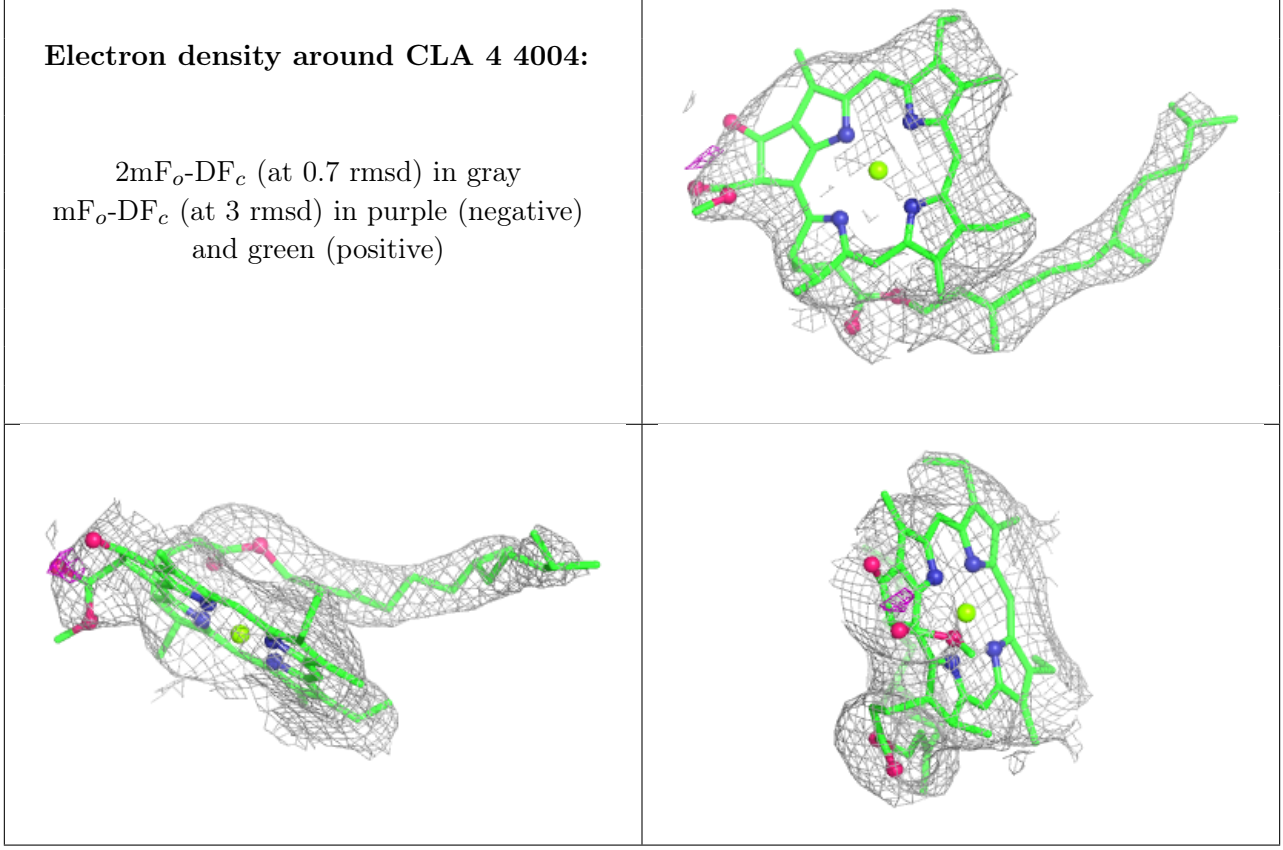
Electron density around CLA 4 4003:

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



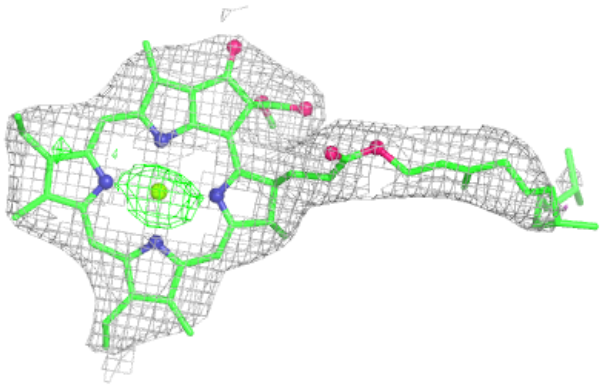
Electron density around CLA 4 4004:

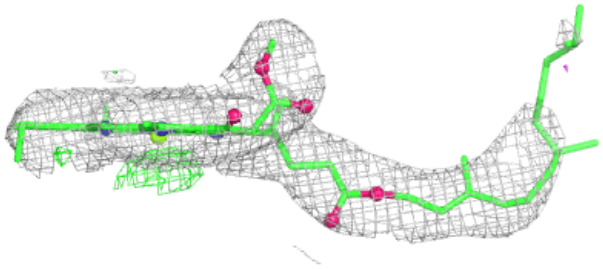
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 1234:

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

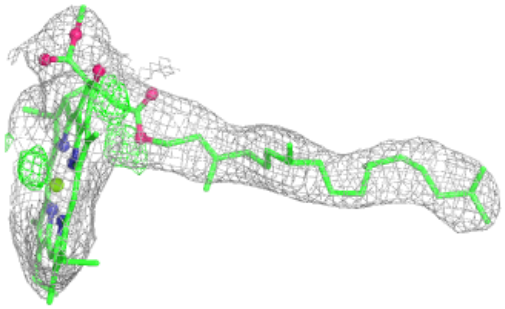


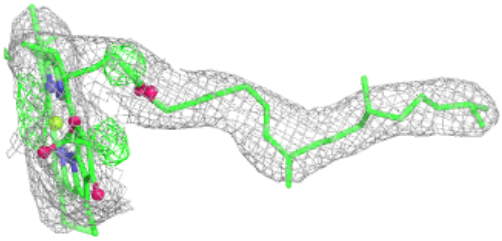


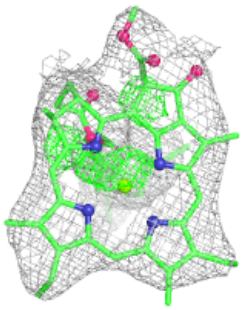


Electron density around CLA A 1126:

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

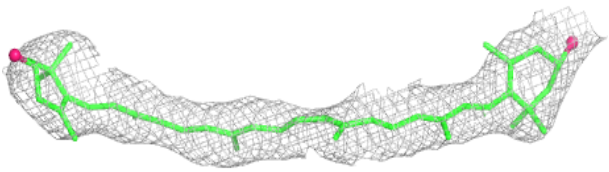


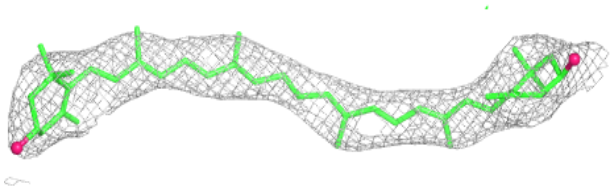


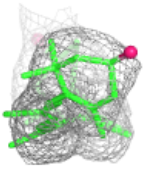


Electron density around LUT I 6018:

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

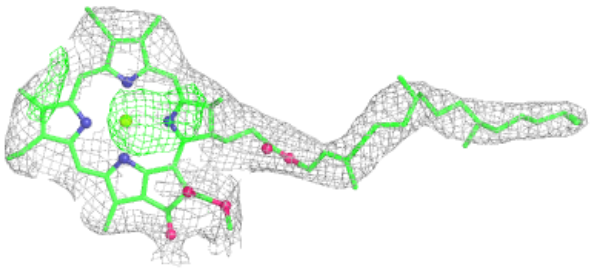


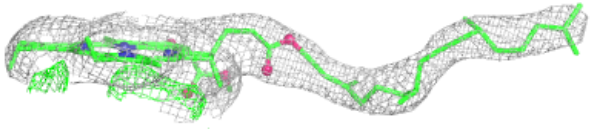


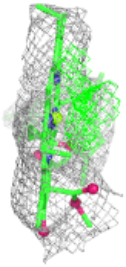


Electron density around CLA A 1131:

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

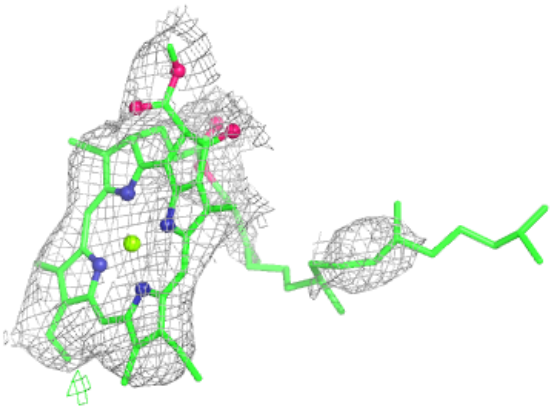


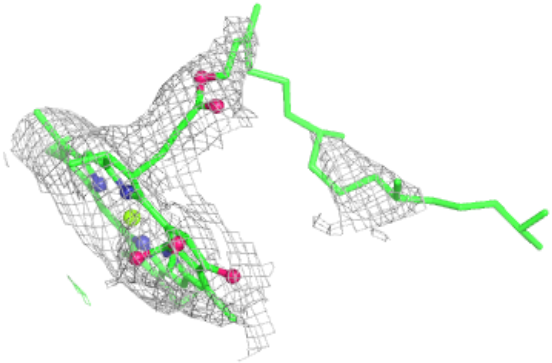


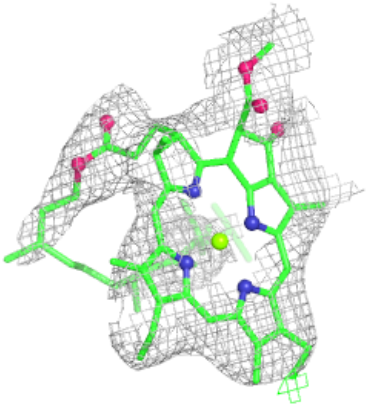


Electron density around CLA 4 4012:

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

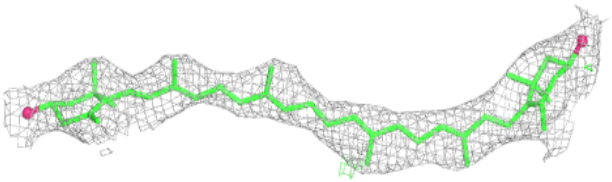


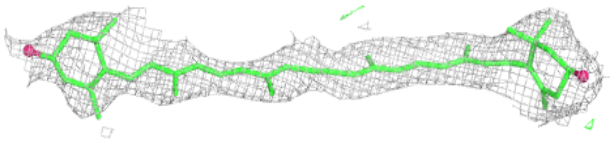


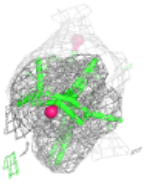


Electron density around LUT 4 4501:

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

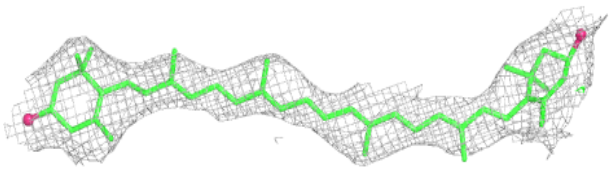


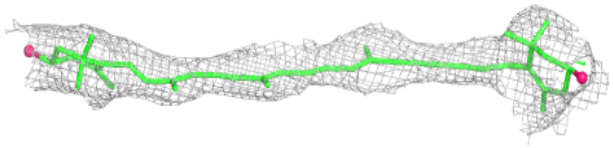


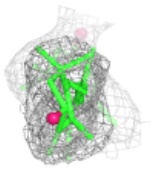


Electron density around LUT 4 4502:

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

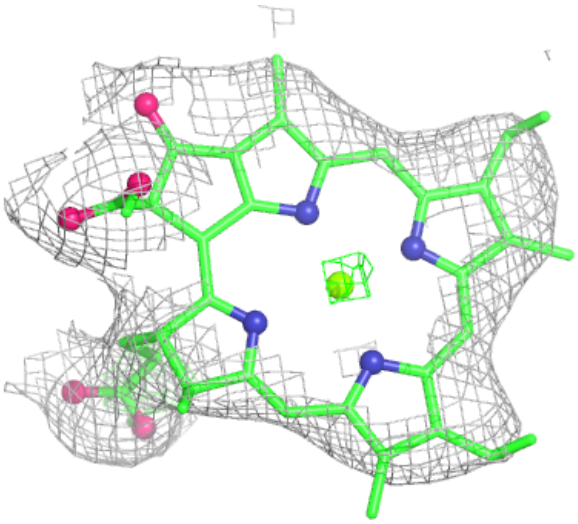


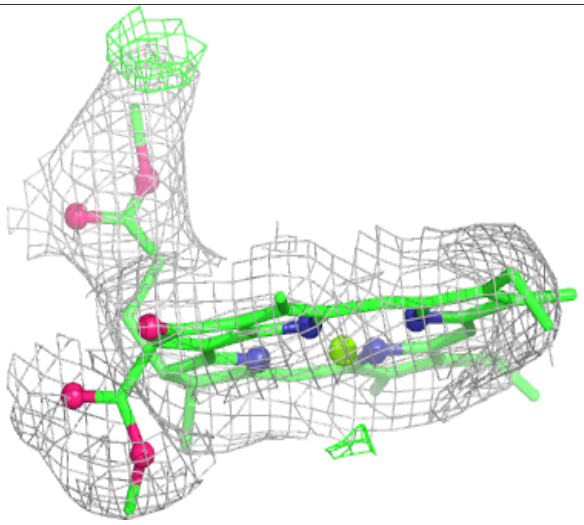


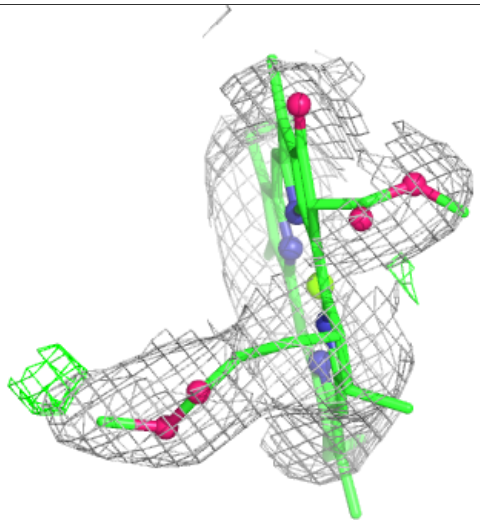


Electron density around CLA A 1118:

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

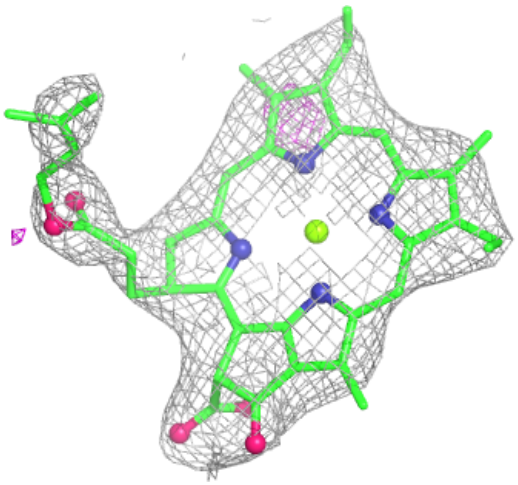


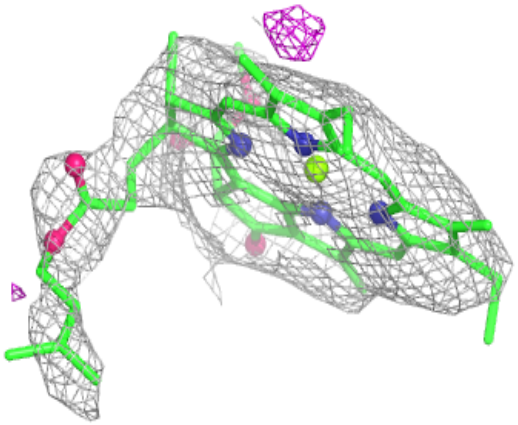


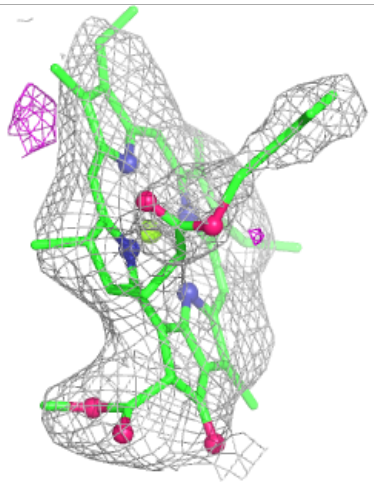


Electron density around CLA A 1129:

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

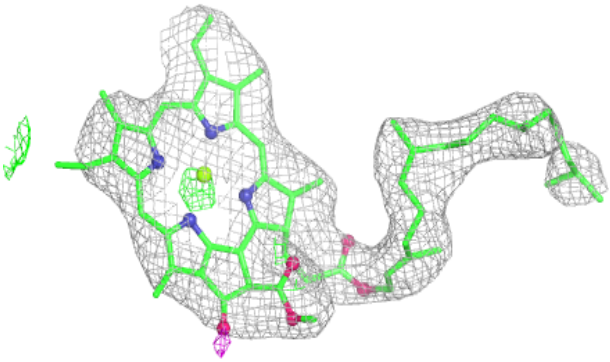


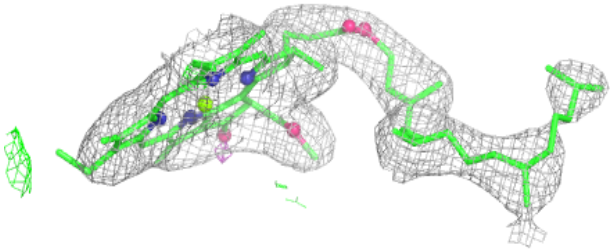


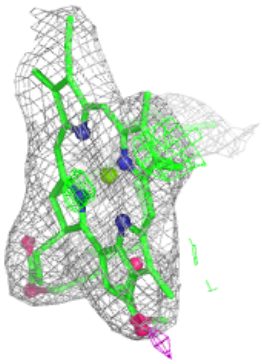


Electron density around CLA A 1101:

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

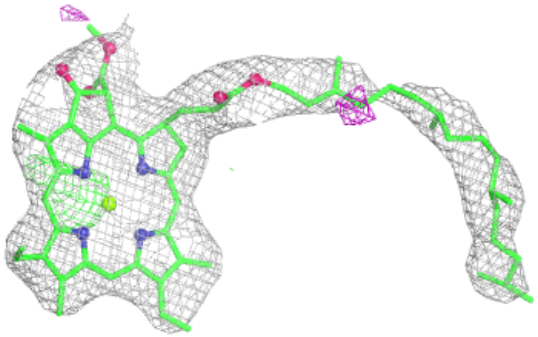


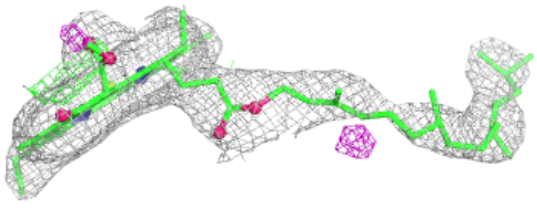


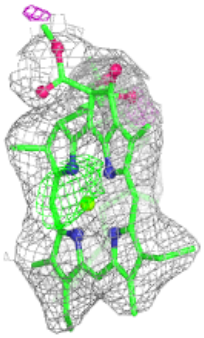


Electron density around CLA B 1222:

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

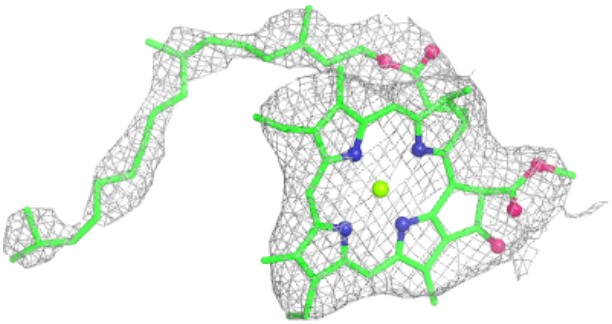


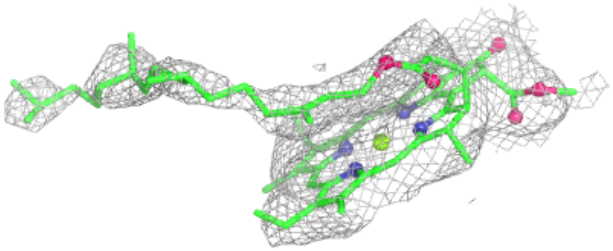


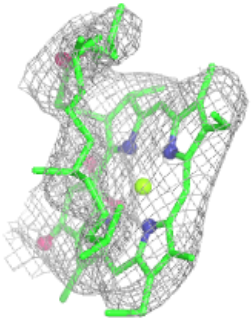


Electron density around CLA 1 1004:

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

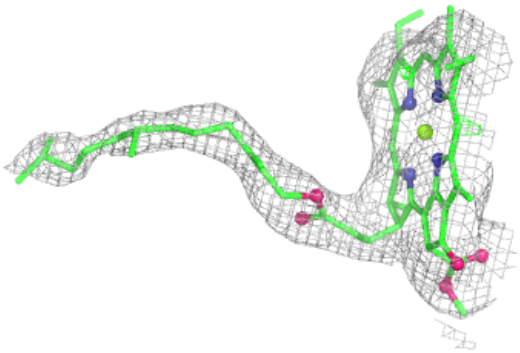


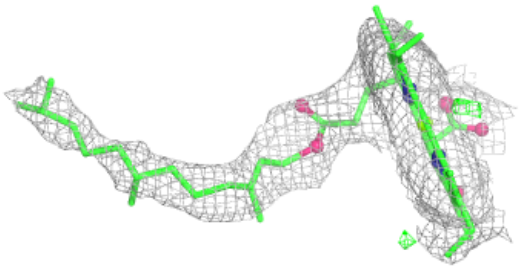


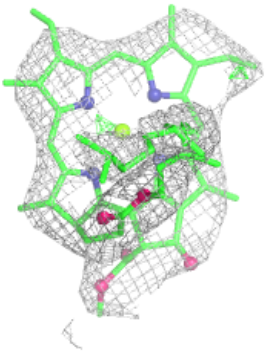


Electron density around CLA L 1502:

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

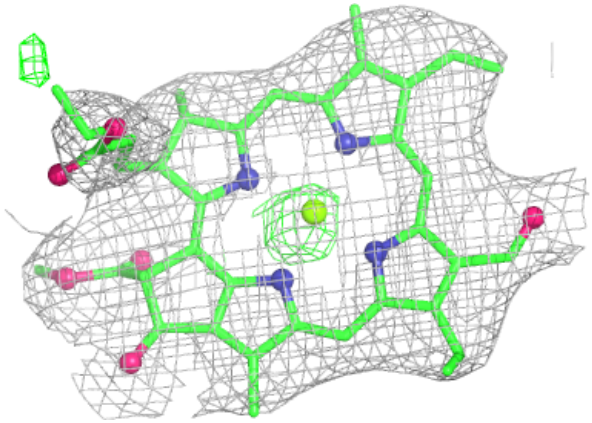


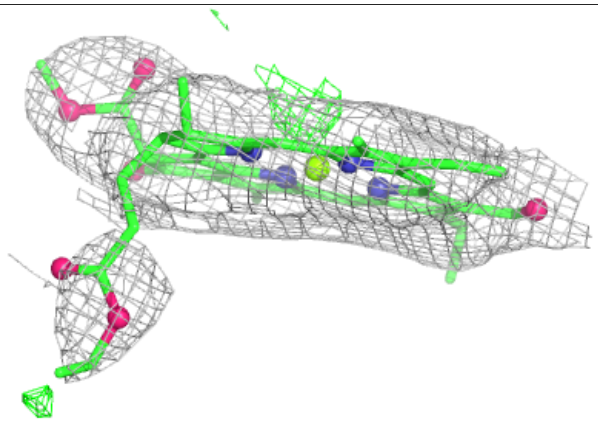


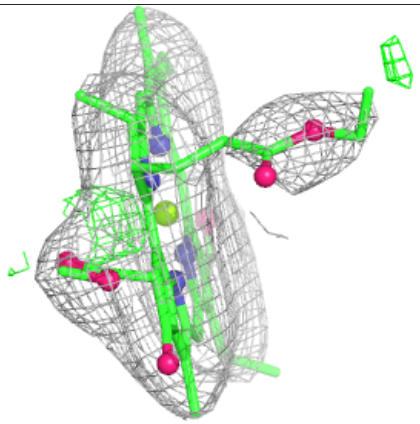


Electron density around CHL 2 2011:

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

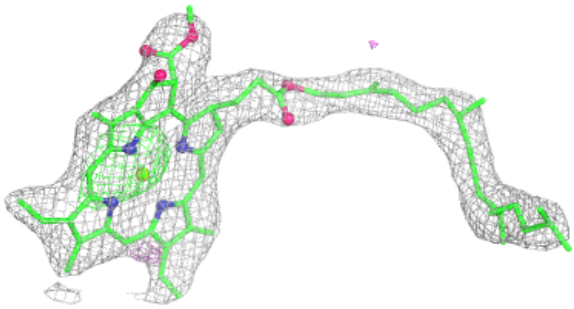


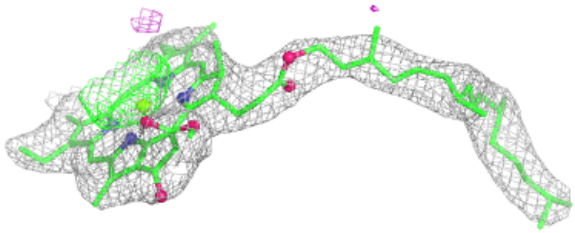


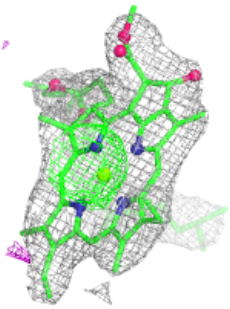


Electron density around CLA B 1012:

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

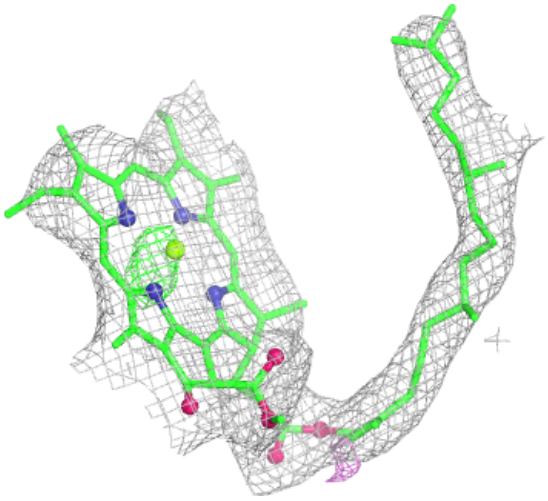


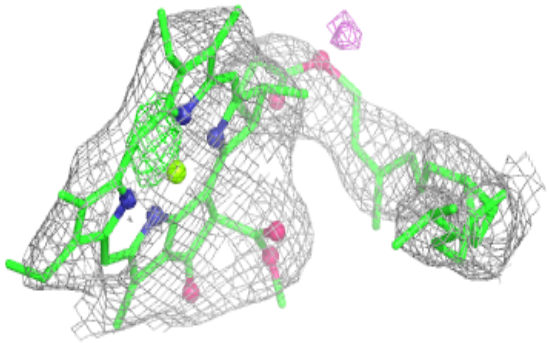


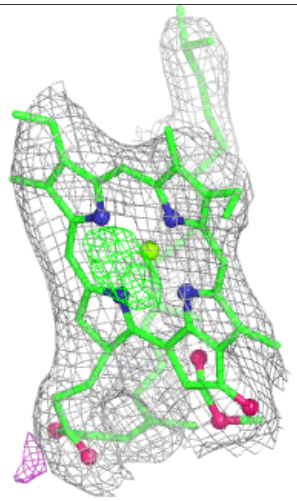


Electron density around CLA B 1207:

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

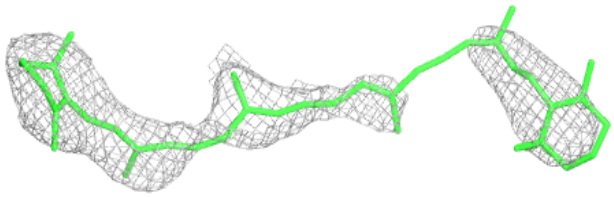


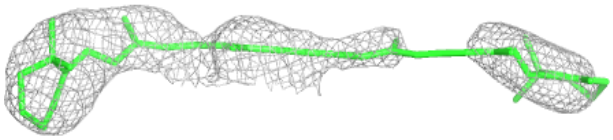


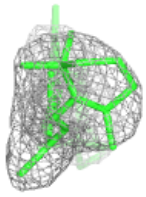


Electron density around BCR B 6006:

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

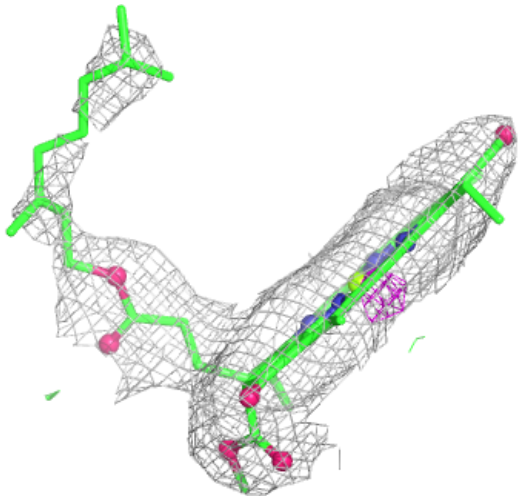


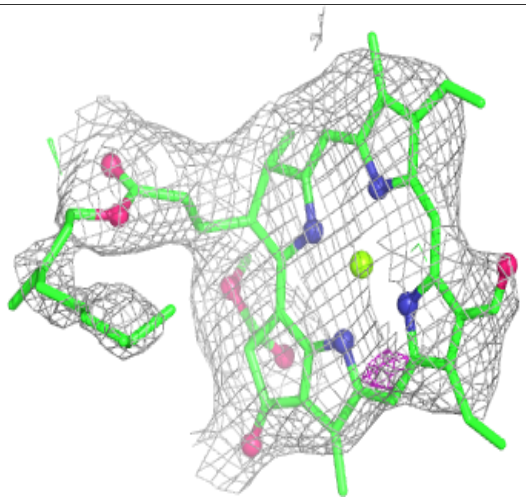


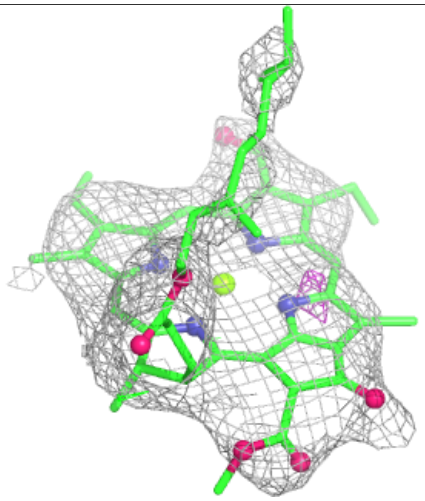


Electron density around CHL 1 1009:

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

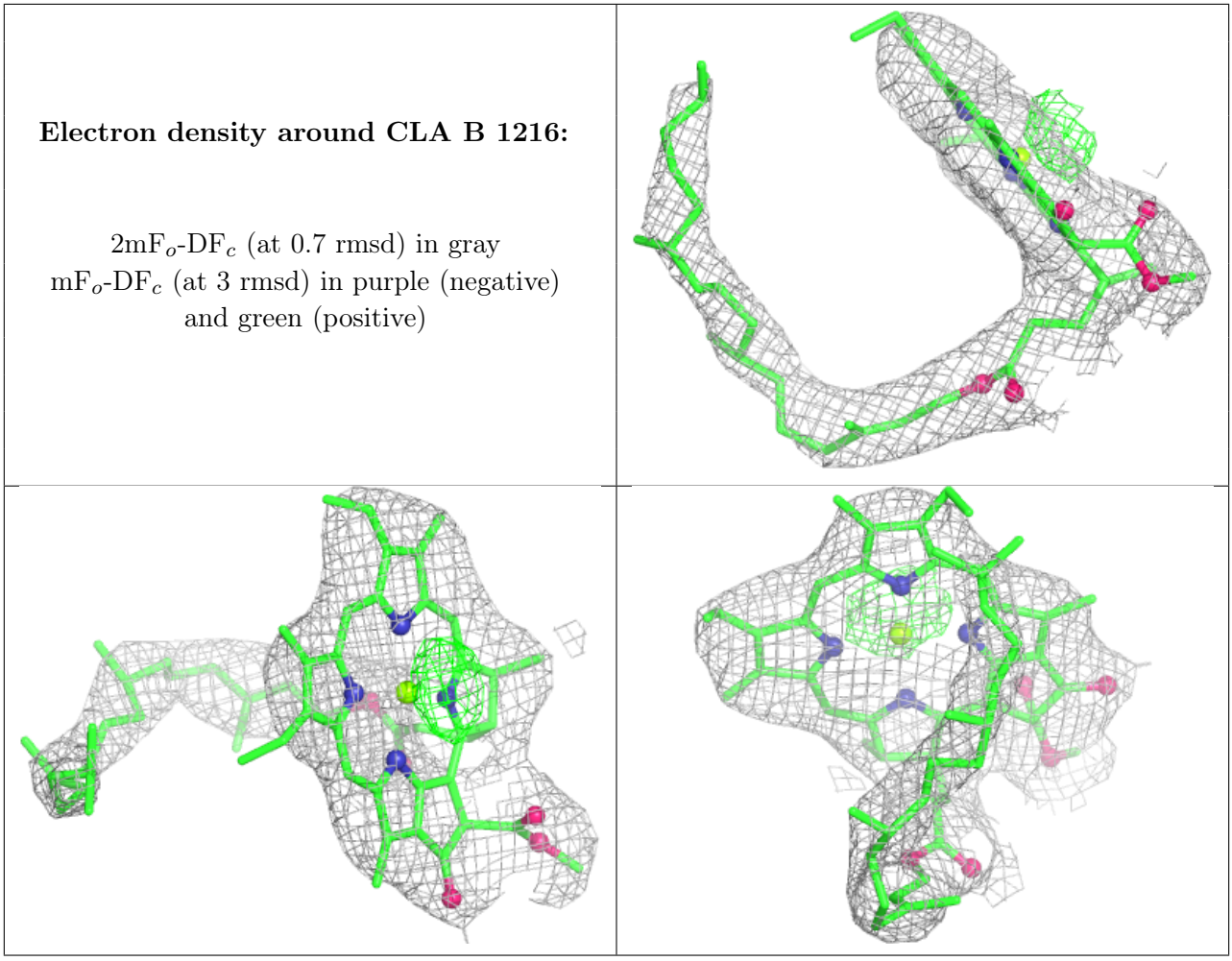






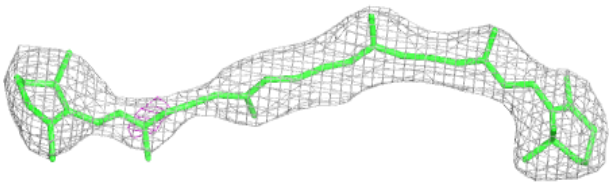
Electron density around CLA B 1216:

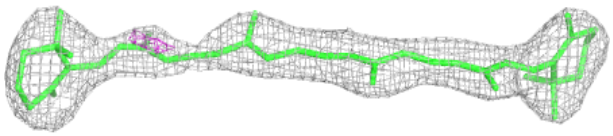
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

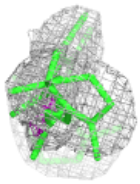


Electron density around BCR B 6010:

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

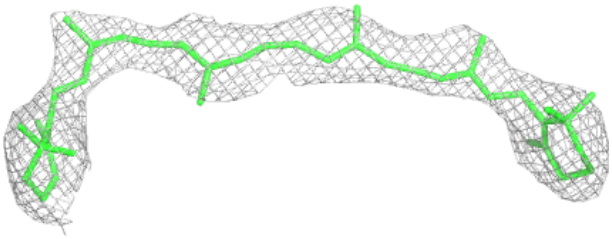


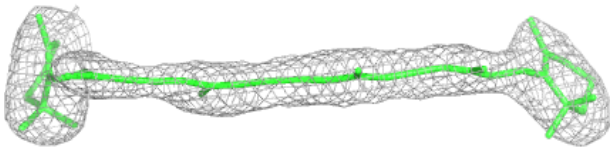


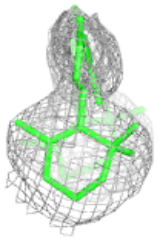


Electron density around BCR I 6020:

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

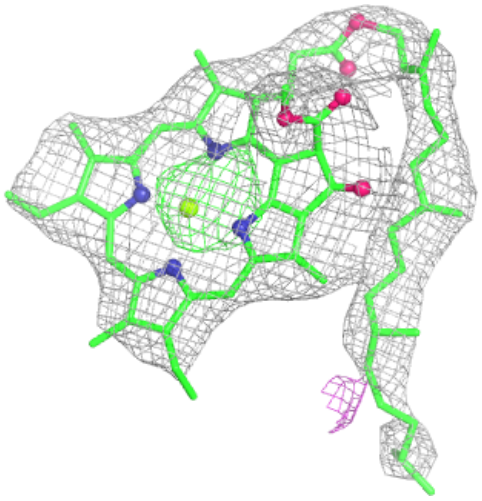


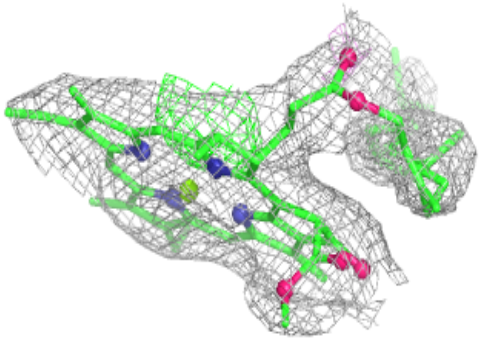


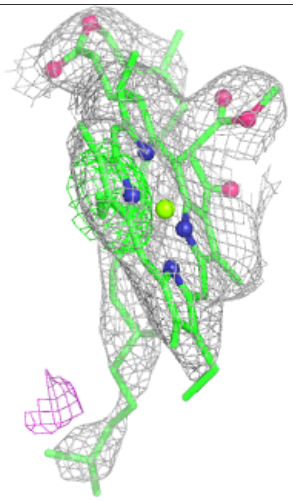


Electron density around CLA A 1123:

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

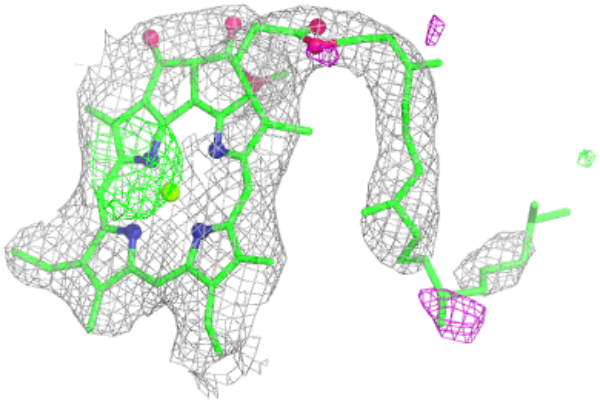


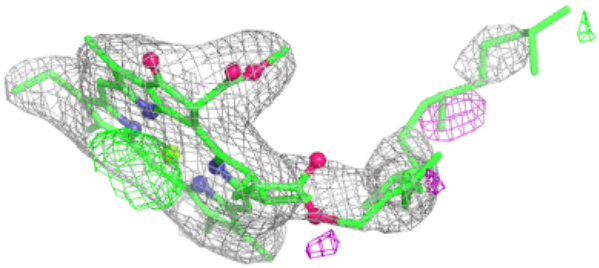


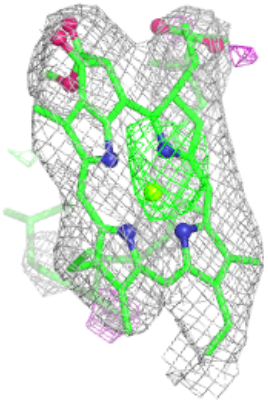


Electron density around CLA B 1221:

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

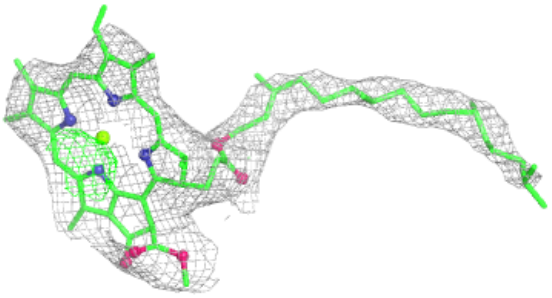




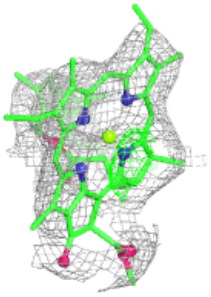


Electron density around CLA A 1119:

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

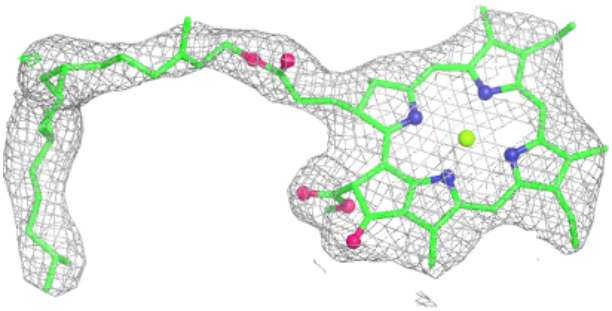


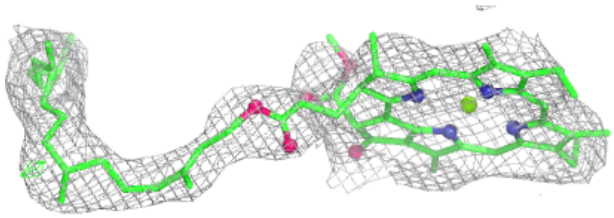


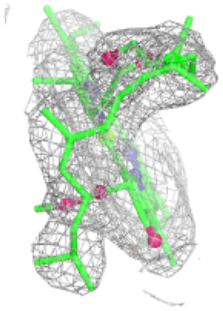


Electron density around CLA B 1223:

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

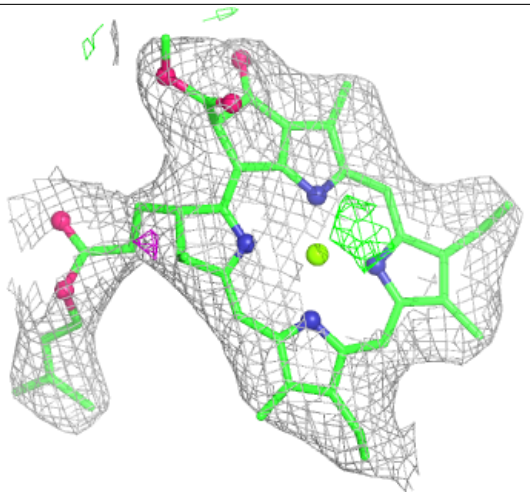


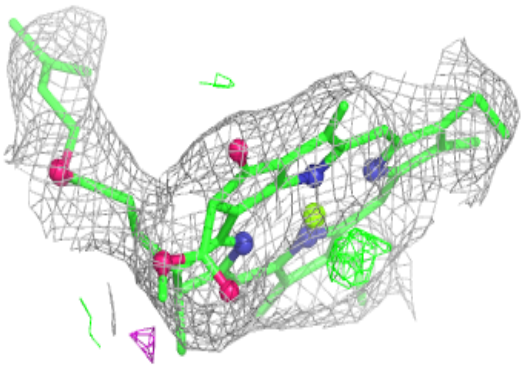


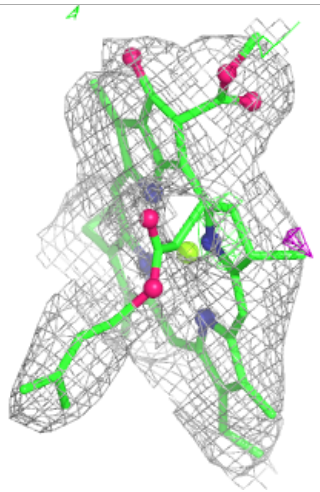


Electron density around CLA A 1102:

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

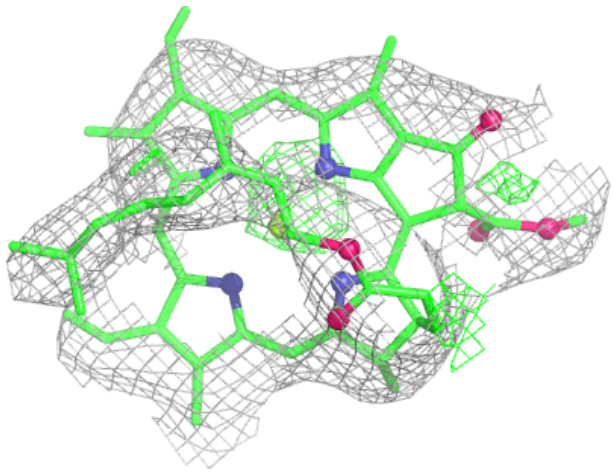


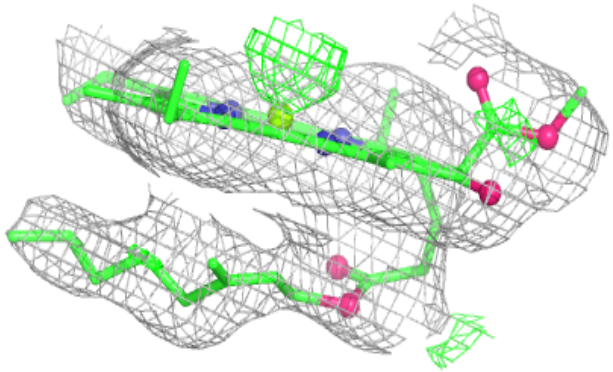


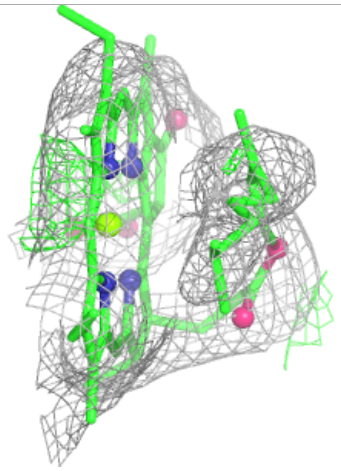


Electron density around CLA A 1110:

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

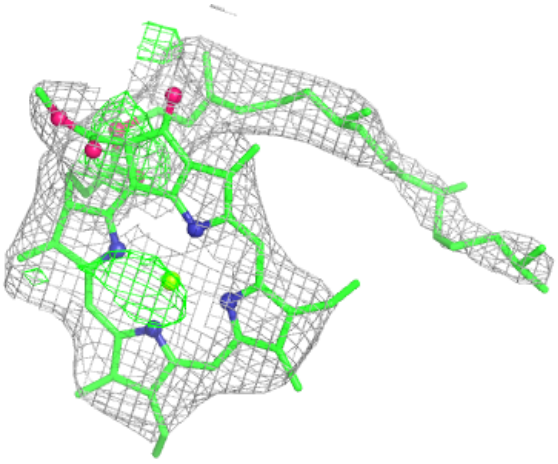


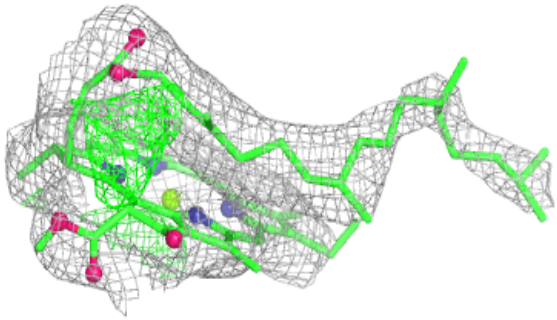


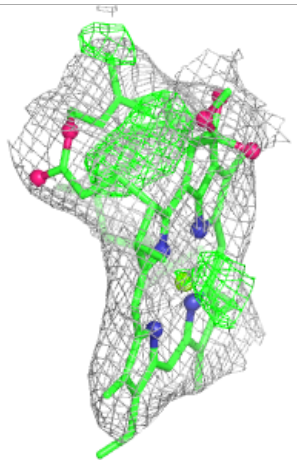


Electron density around CLA A 1127:

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

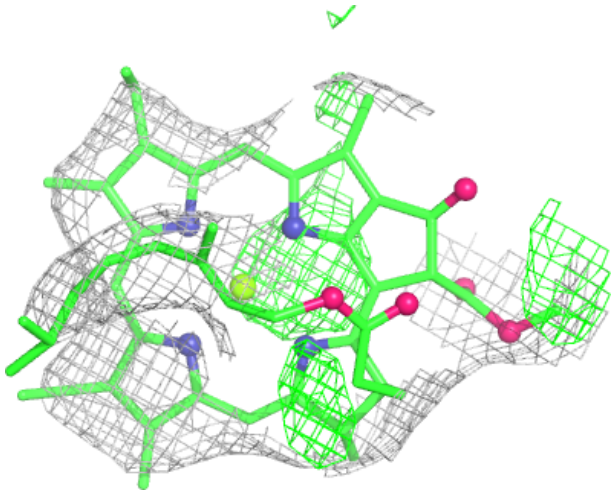


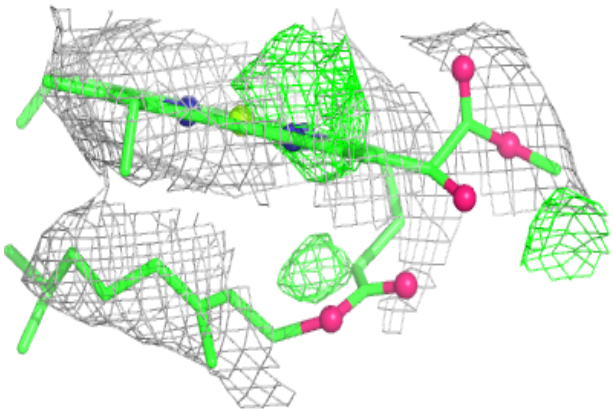


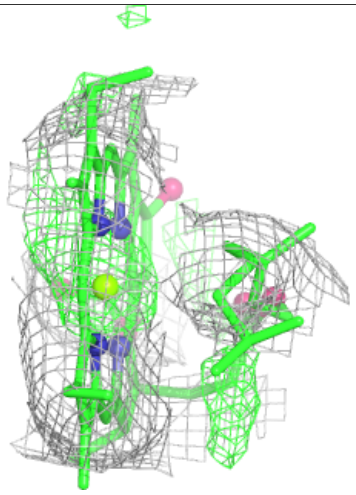


Electron density around CLA 1 1003:

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

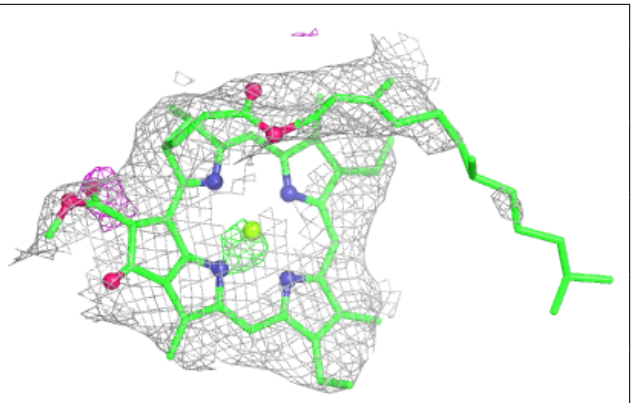


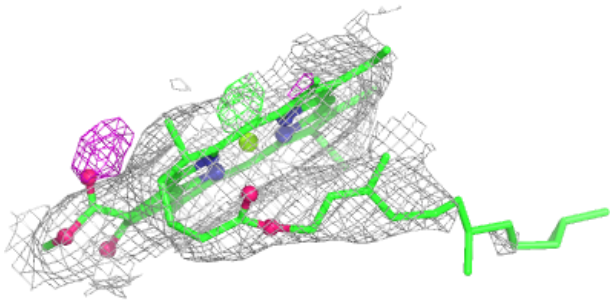


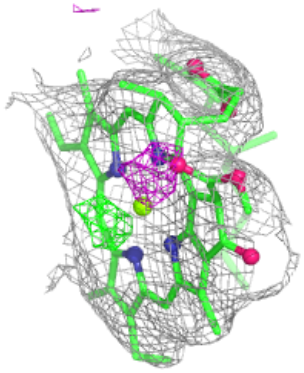


Electron density around CLA 2 2001:

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

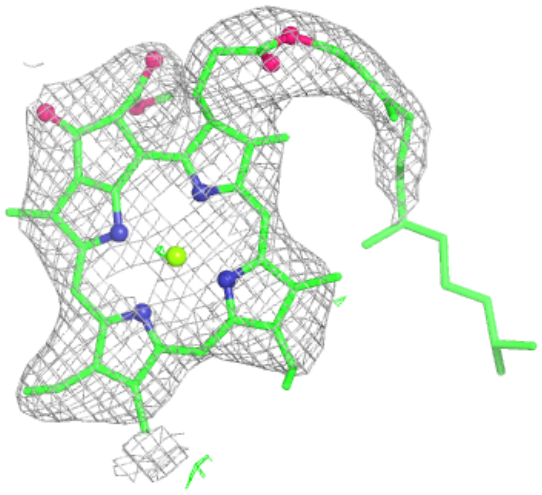


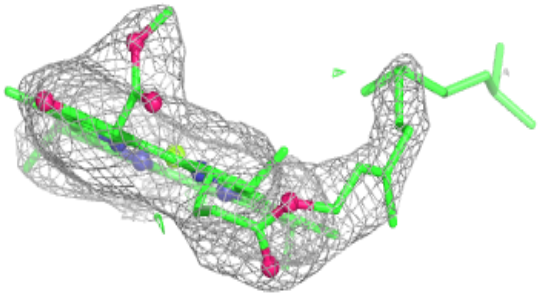


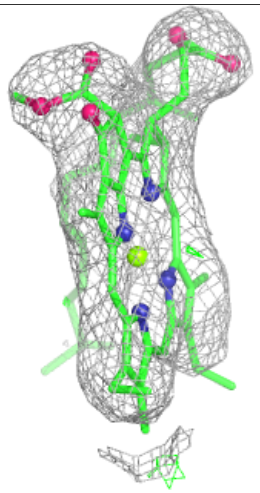


Electron density around CLA A 1111:

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

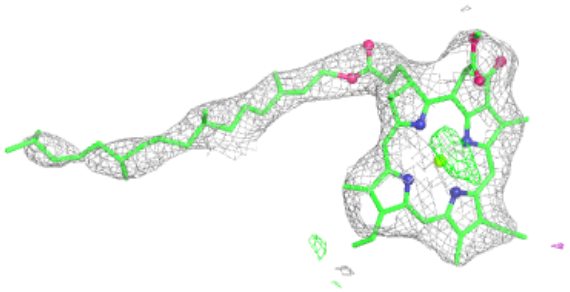




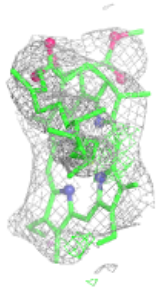


Electron density around CLA A 1132:

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

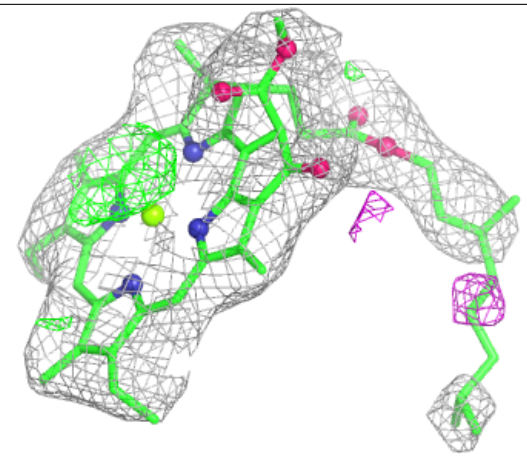


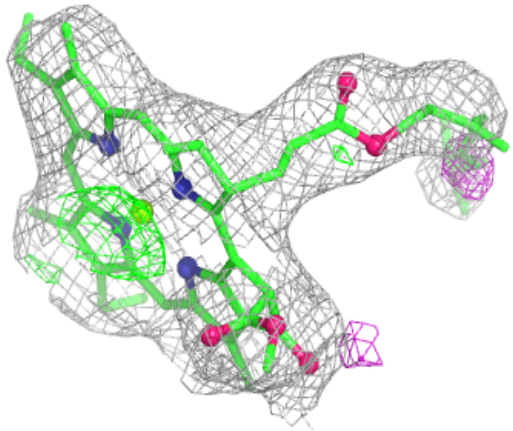


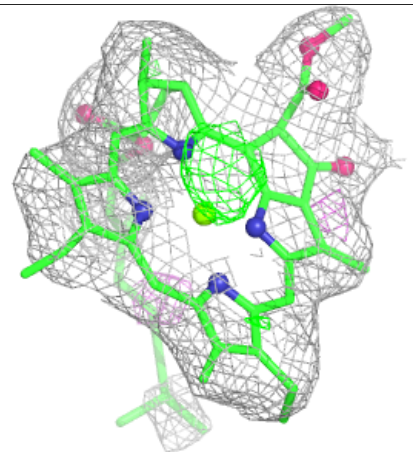


Electron density around CLA B 1236:

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

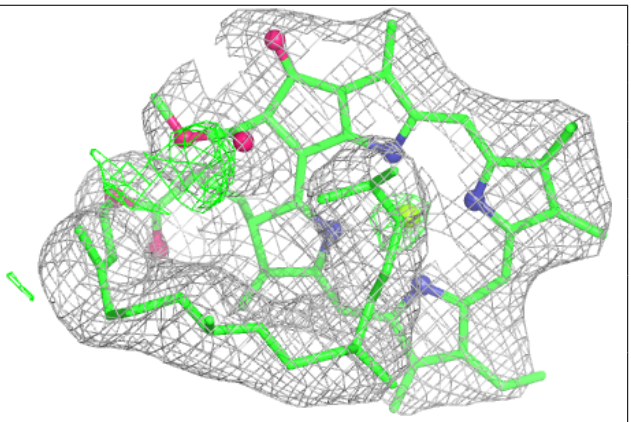


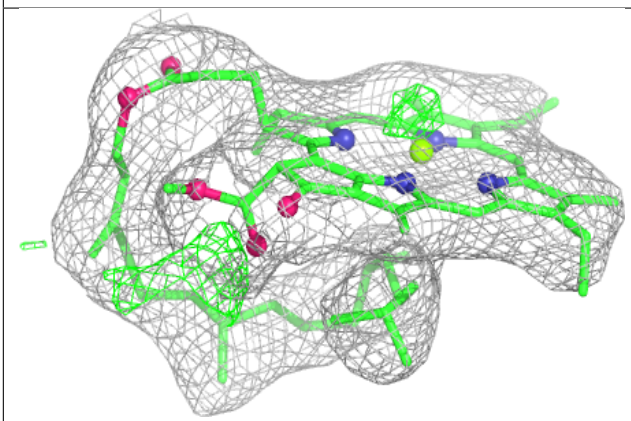


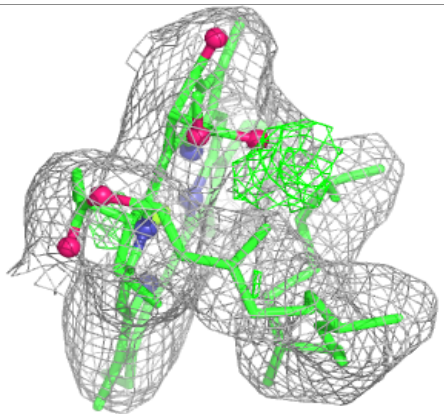


Electron density around CLA A 1104:

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

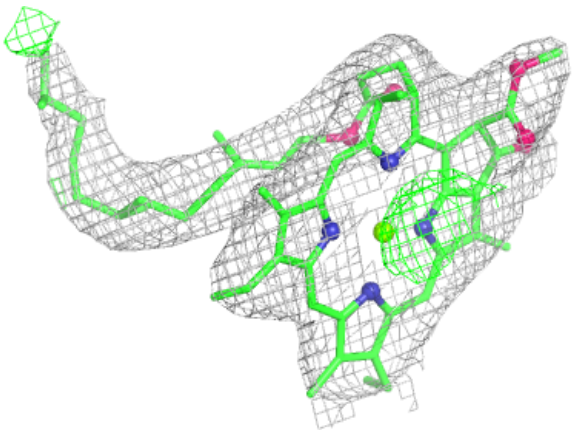


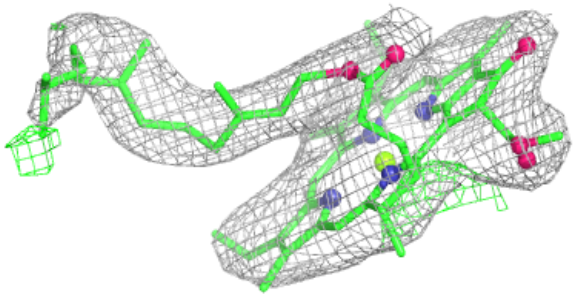


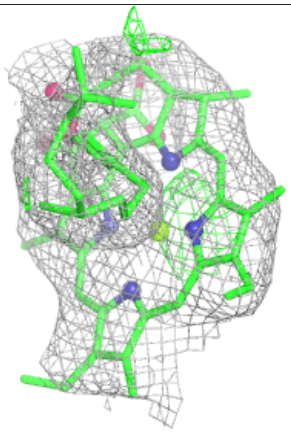


Electron density around CLA A 1237:

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

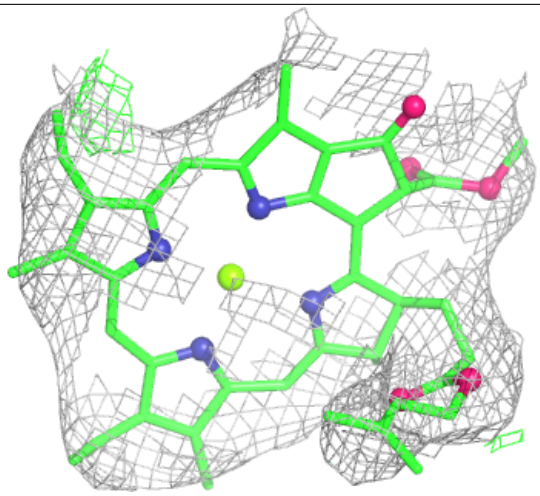


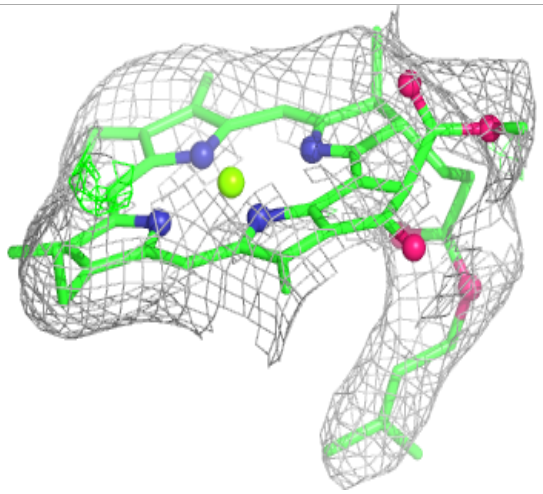




Electron density around CLA 1 1012:

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

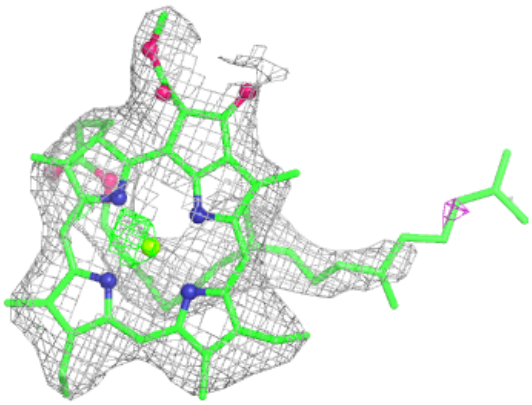


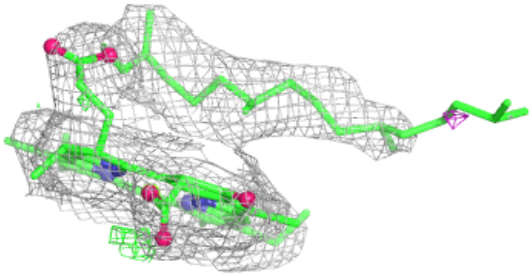


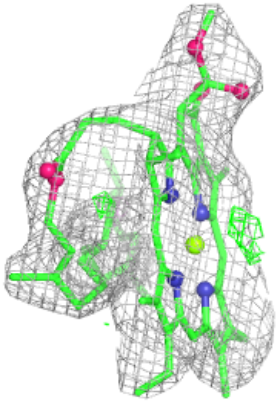


Electron density around CLA B 1224:

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

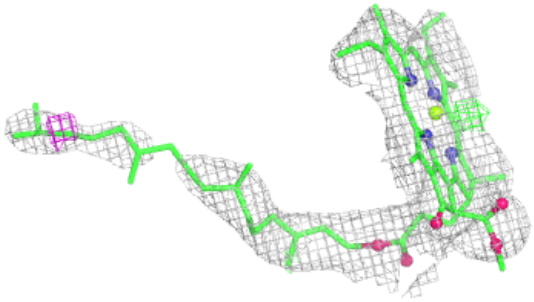


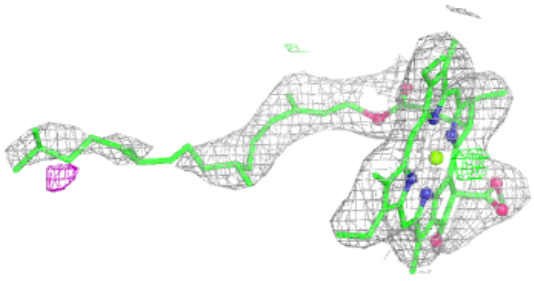


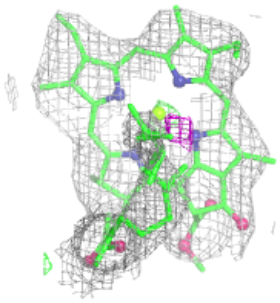


Electron density around CLA B 1226:

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

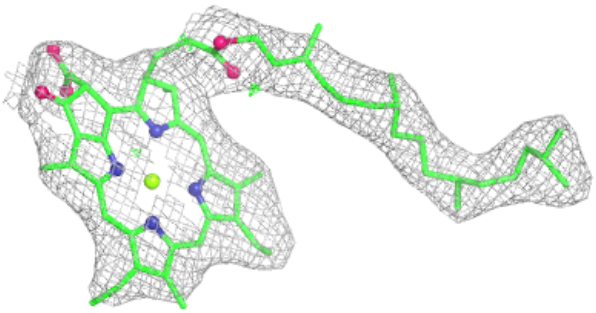


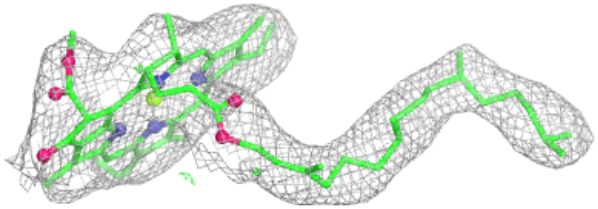


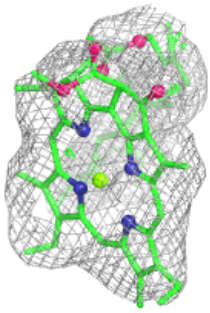


Electron density around CLA A 1106:

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

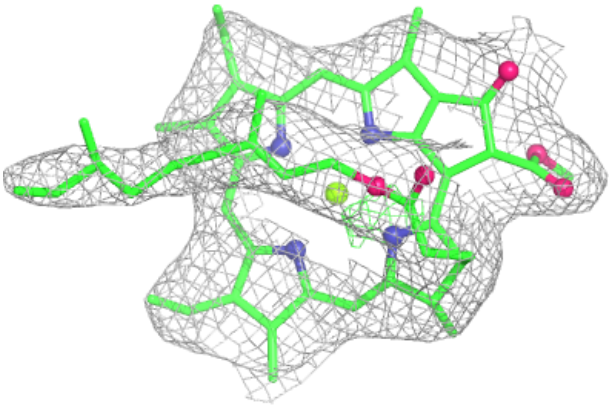


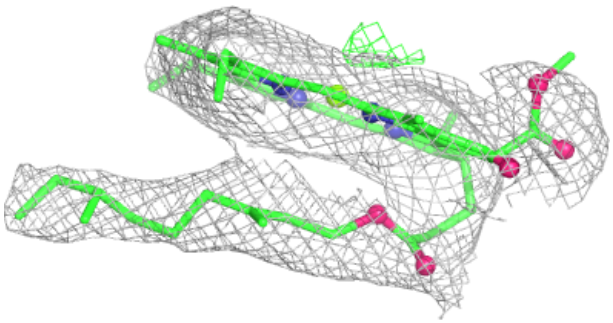


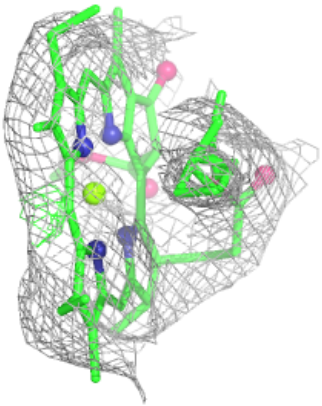


Electron density around CLA A 1136:

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

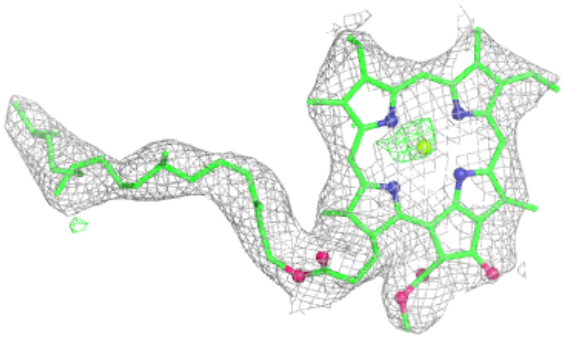


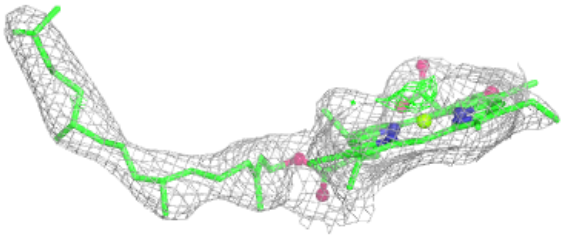


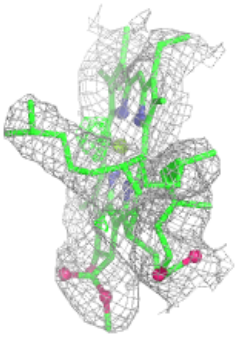


Electron density around CLA B 1023:

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

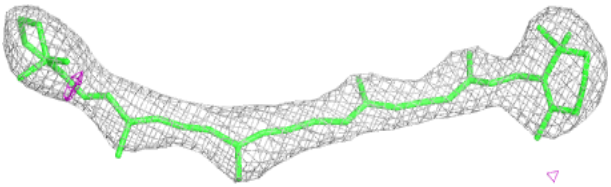


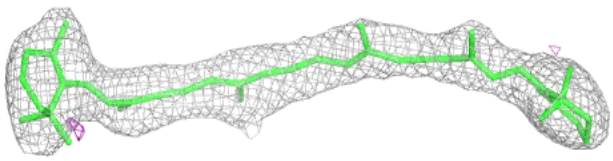


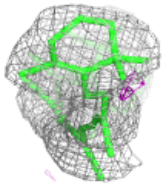


Electron density around BCR F 6014:

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

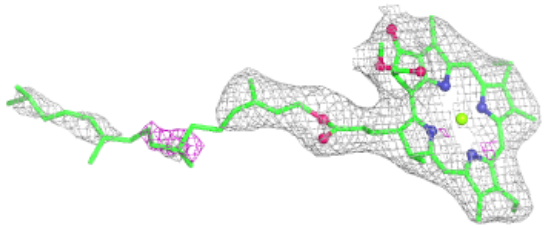


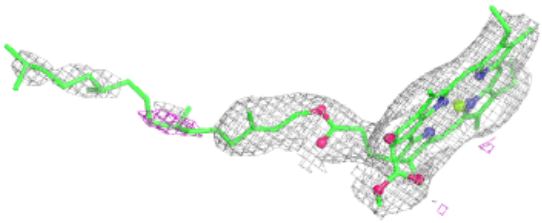


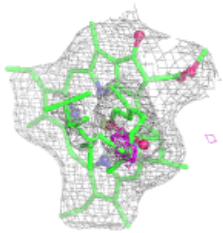


Electron density around CLA A 1107:

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

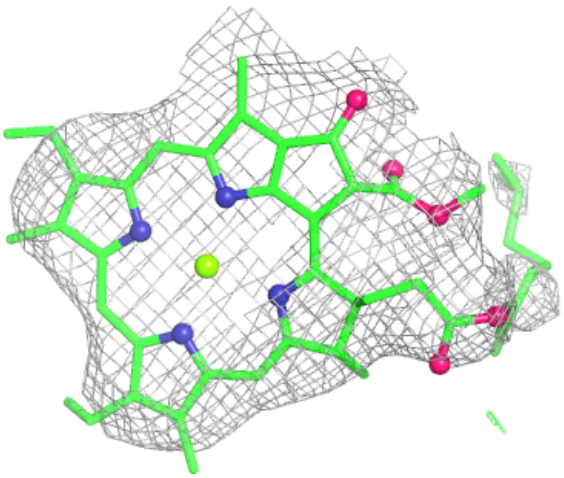


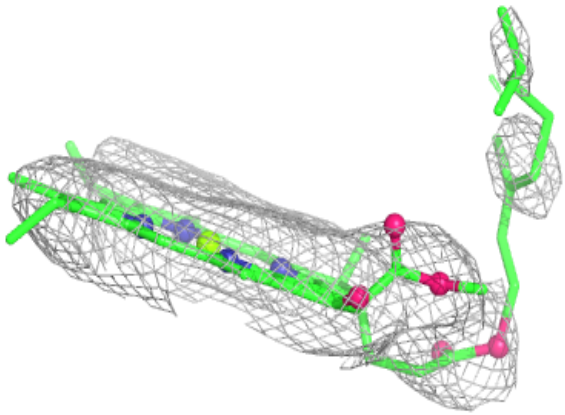


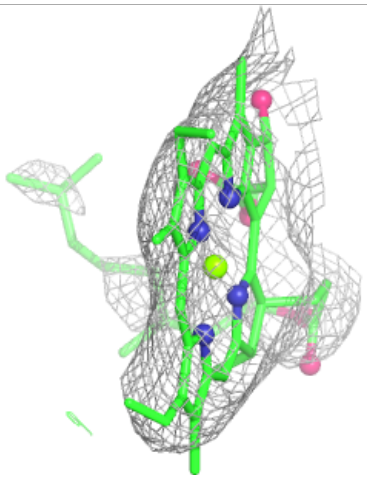


Electron density around CLA 3 3005:

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

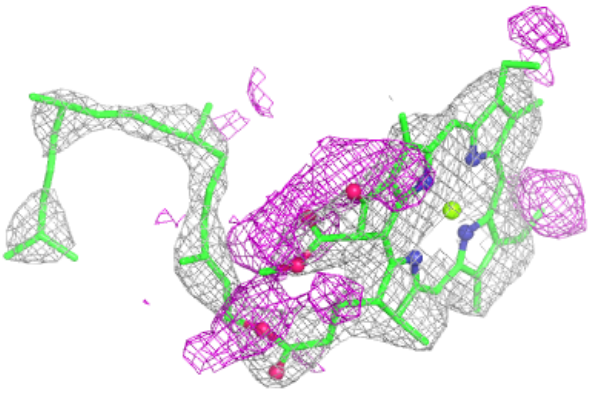


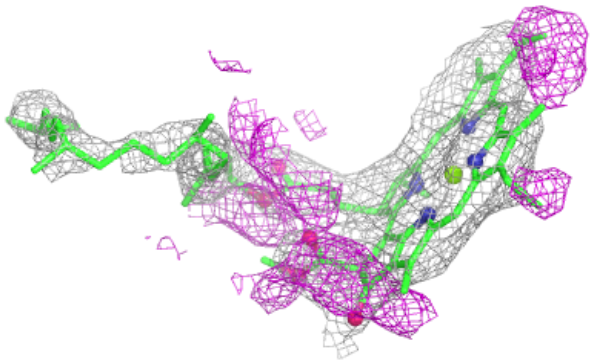


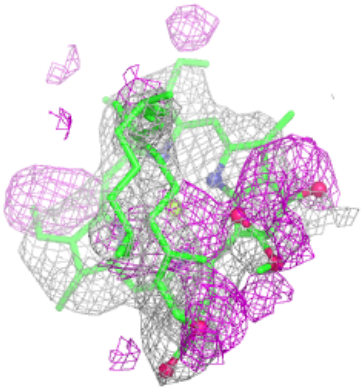


Electron density around CL0 A 1011:

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

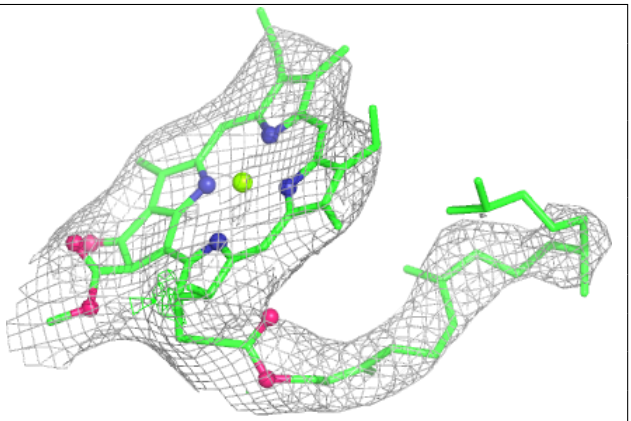


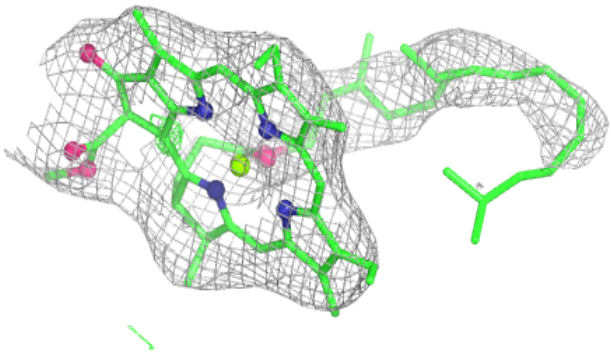


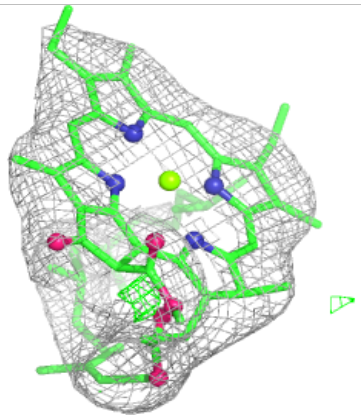


Electron density around CLA A 1122:

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

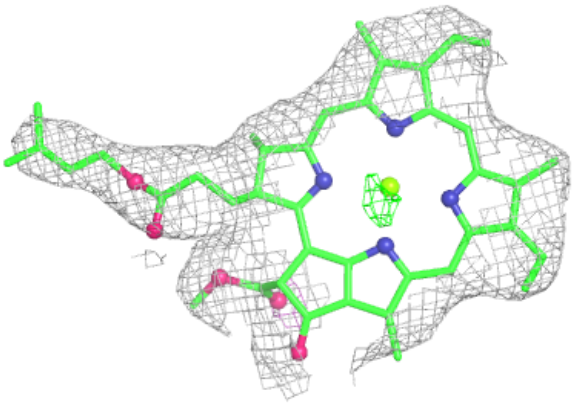


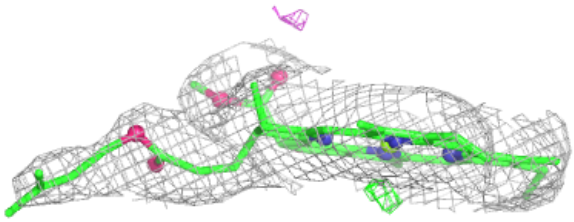


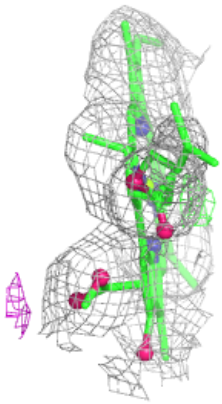


Electron density around CLA F 1302:

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

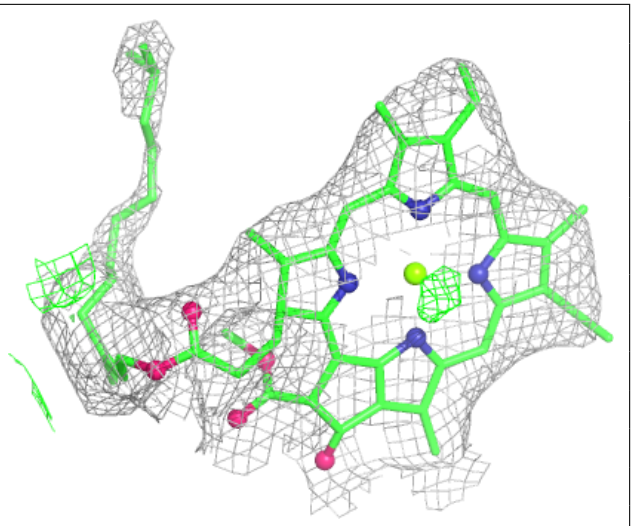


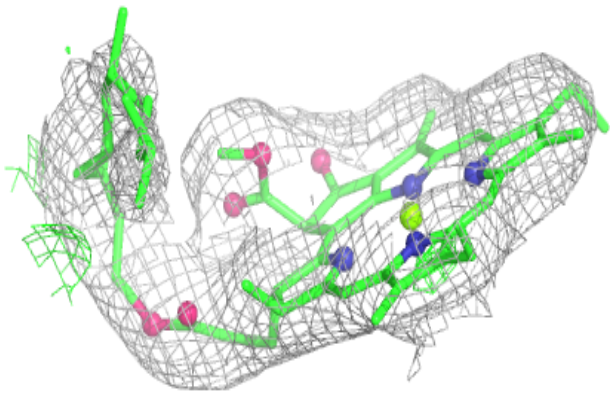


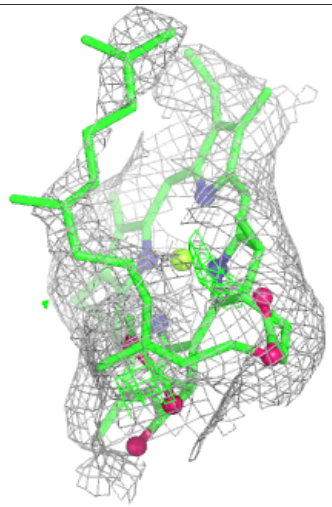


Electron density around CLA 4 4005:

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

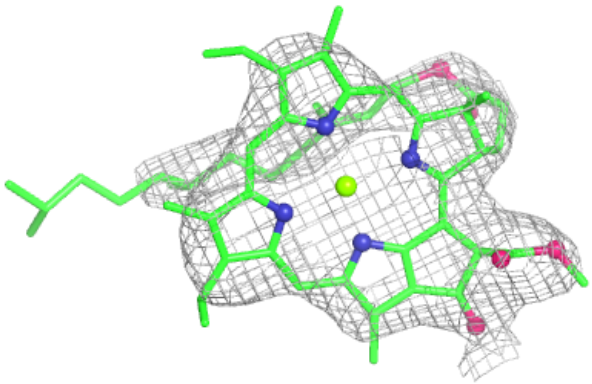


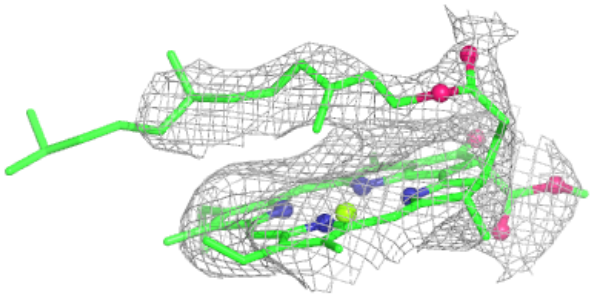


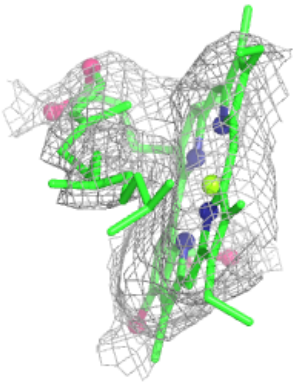


Electron density around CLA A 1116:

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

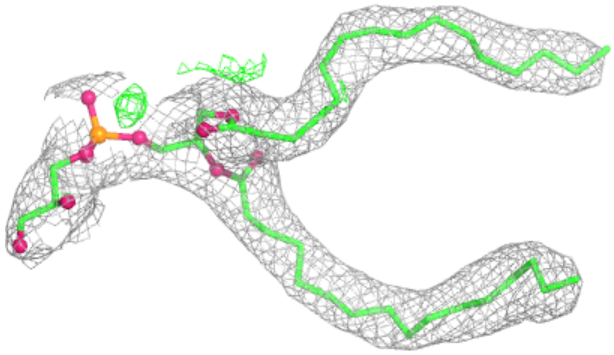


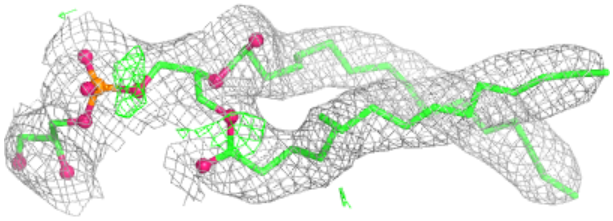


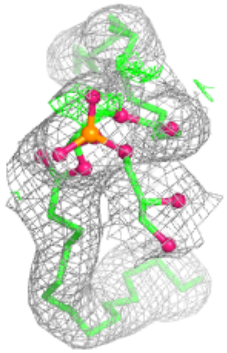


Electron density around LHG A 7001:

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

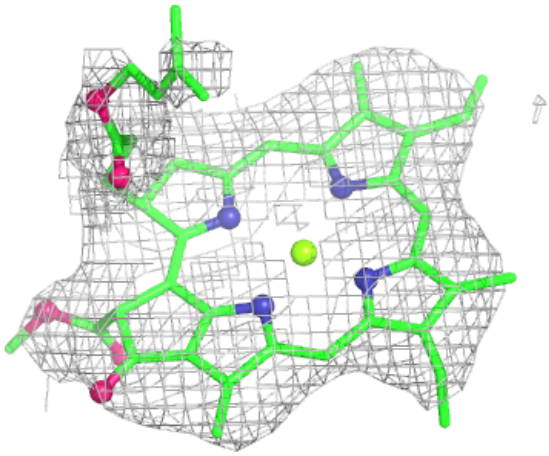


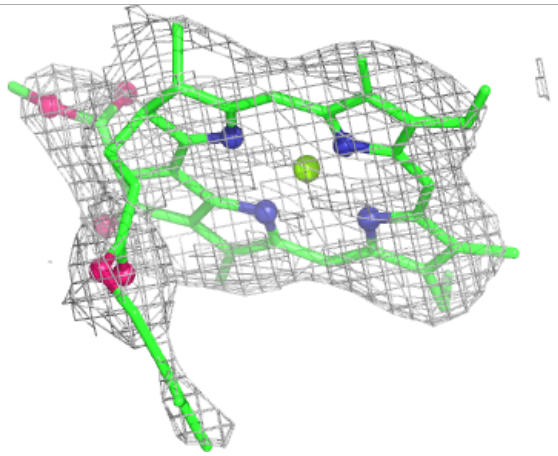


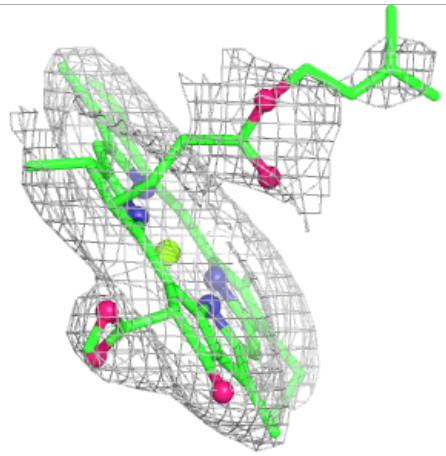


Electron density around CLA A 1130:

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

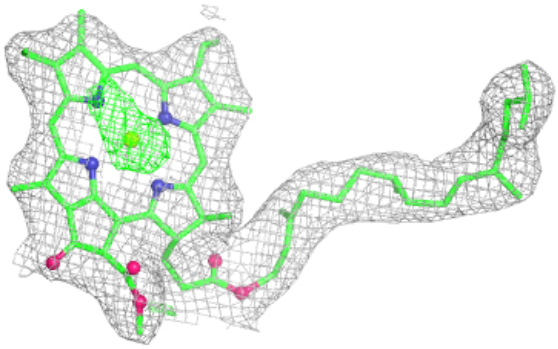


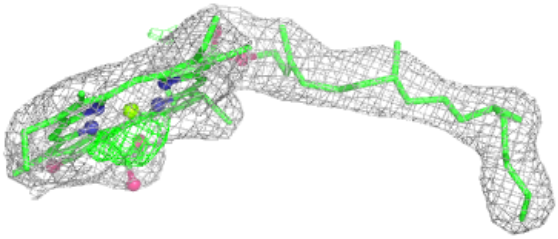


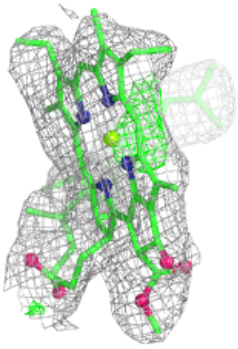


Electron density around CLA A 1013:

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

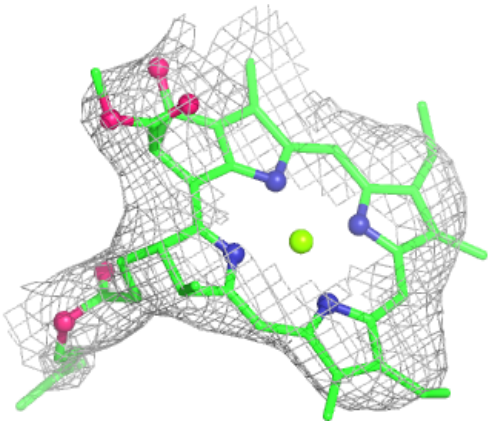


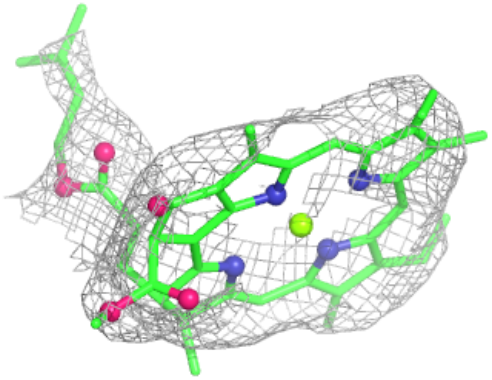


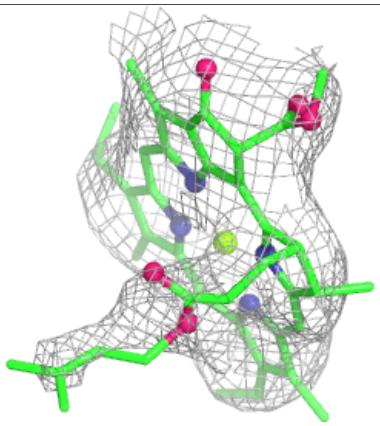


Electron density around CLA 2 2008:

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

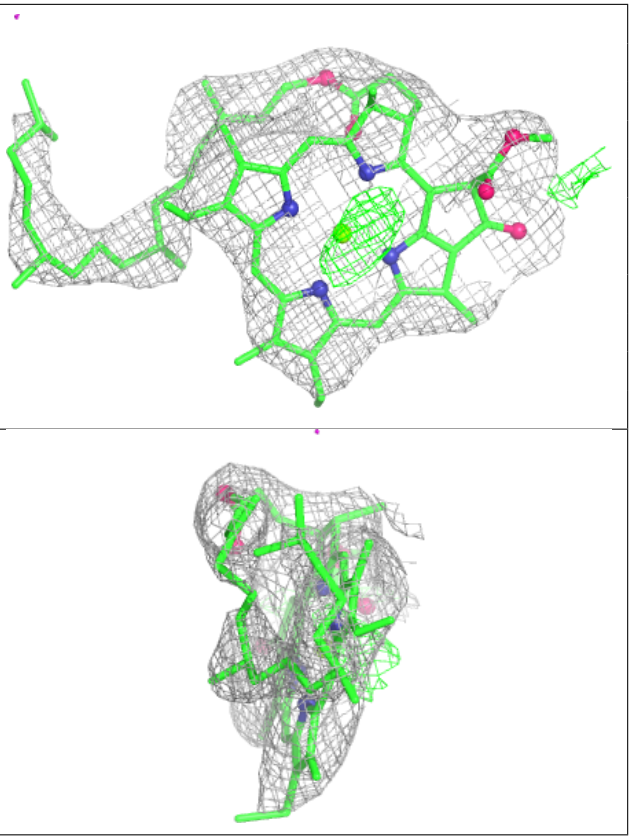






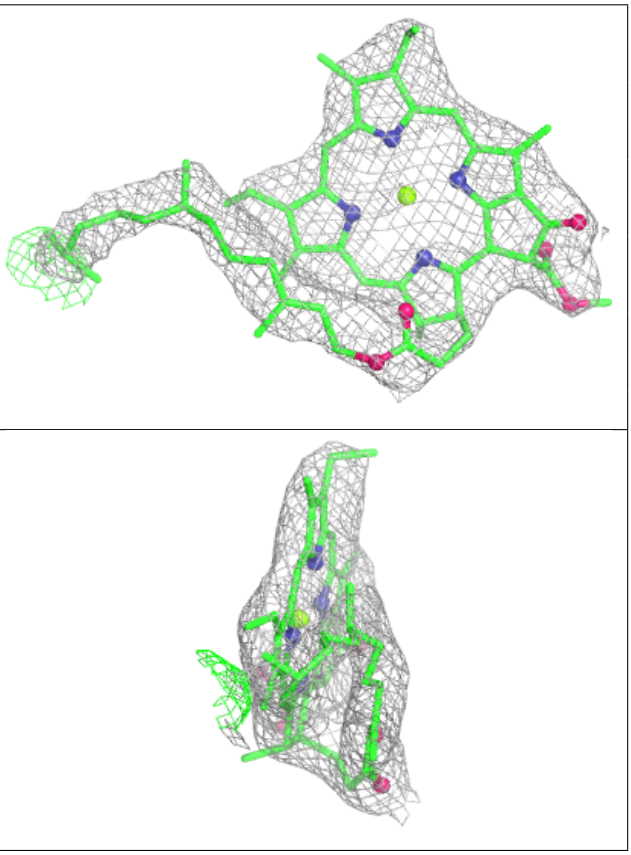
Electron density around CLA A 1117:

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



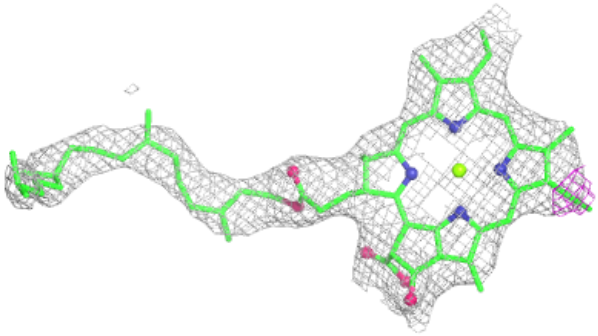
Electron density around CLA B 1215:

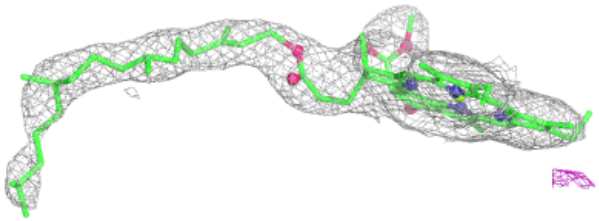
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

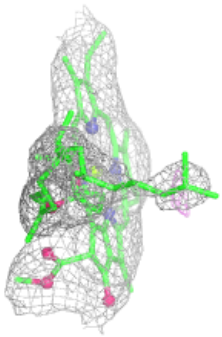


Electron density around CLA A 1103:

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

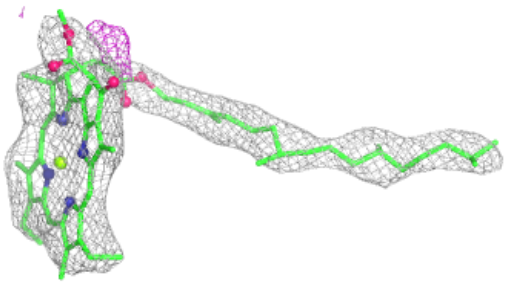


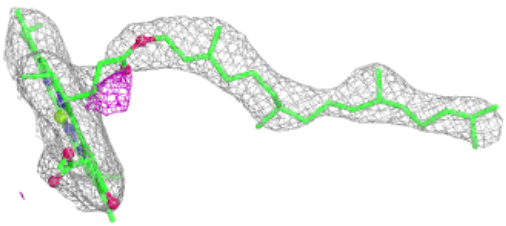


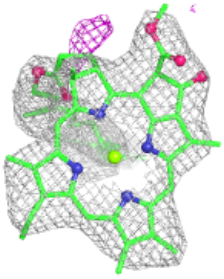


Electron density around CLA B 1225:

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

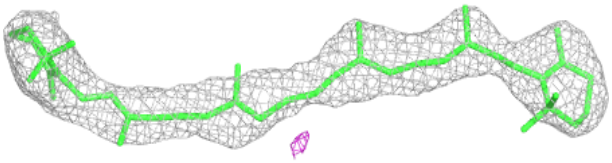


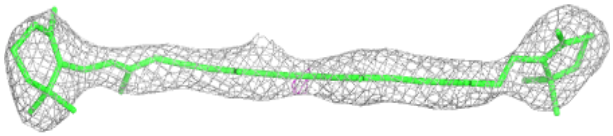


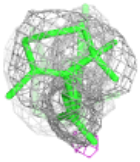


Electron density around BCR A 6017:

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

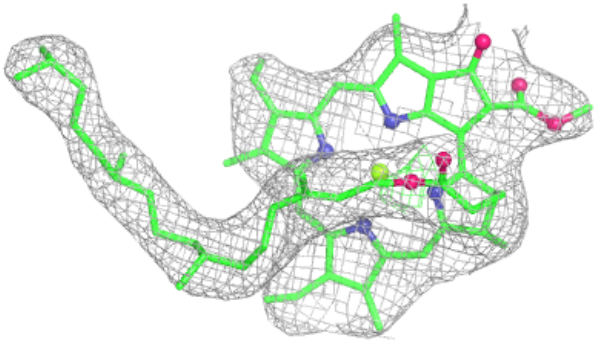


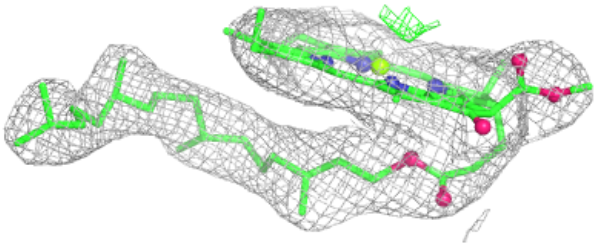


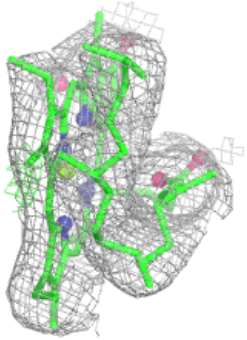


Electron density around CLA B 1235:

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

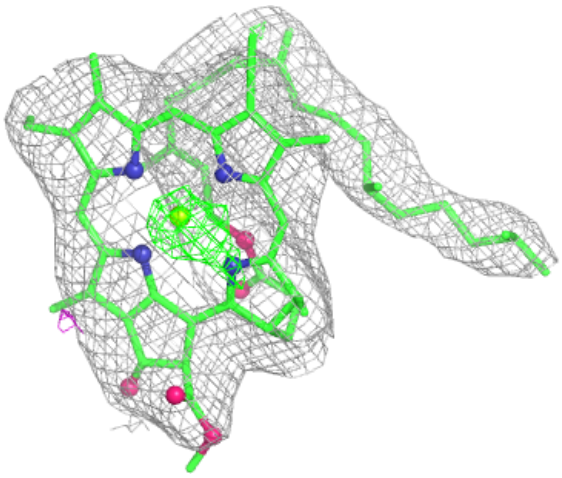


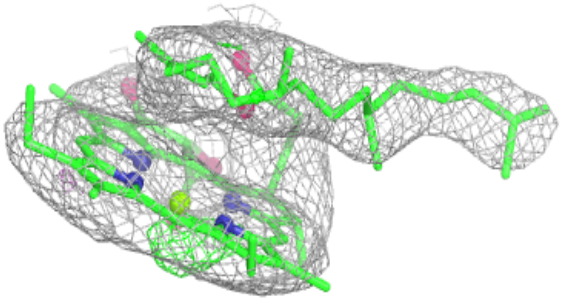


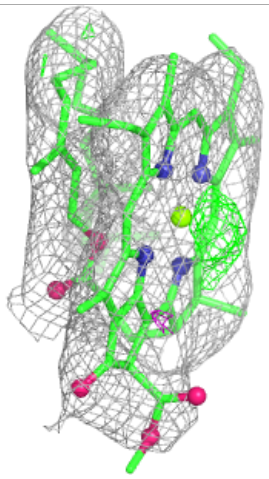


Electron density around CLA B 1205:

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

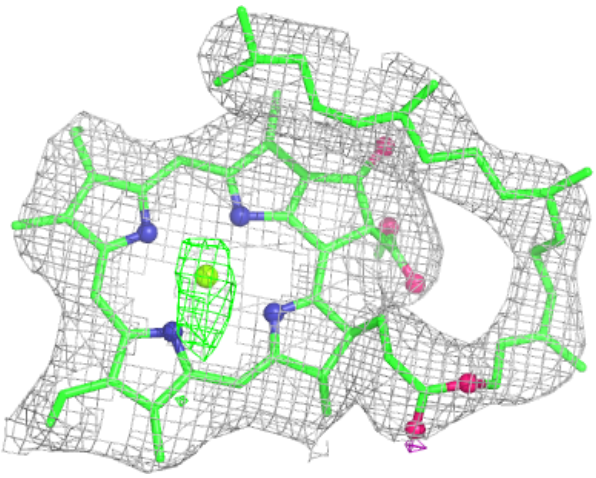


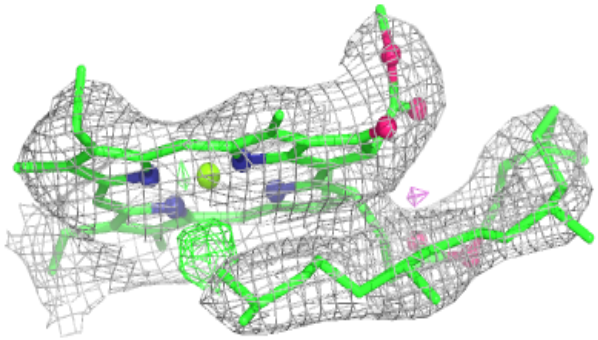


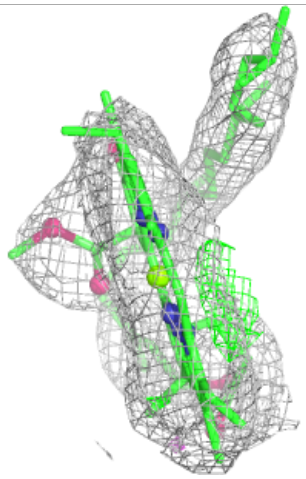


Electron density around CLA B 1202:

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

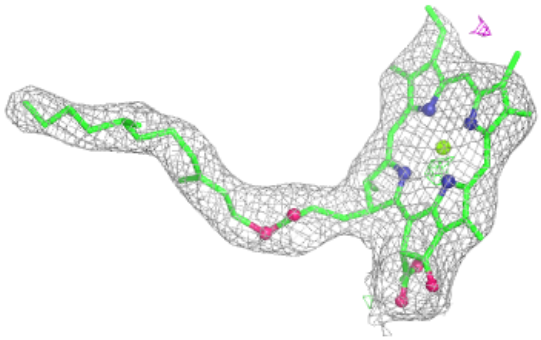


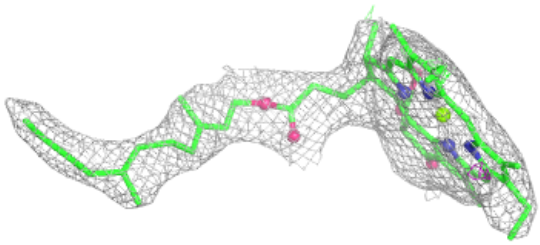


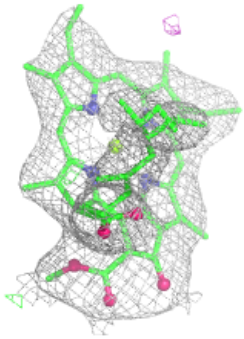


Electron density around CLA B 1230:

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

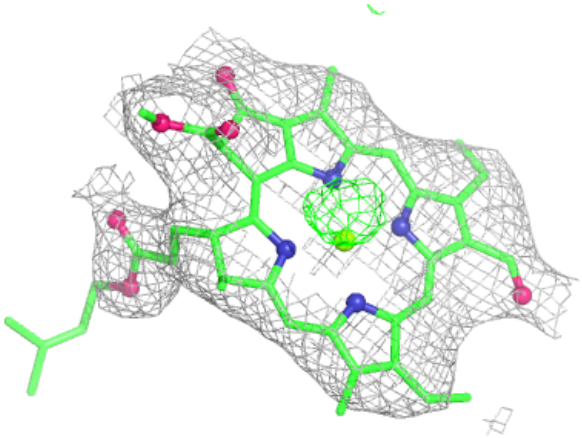


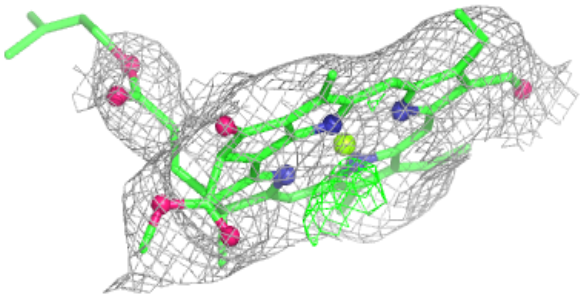


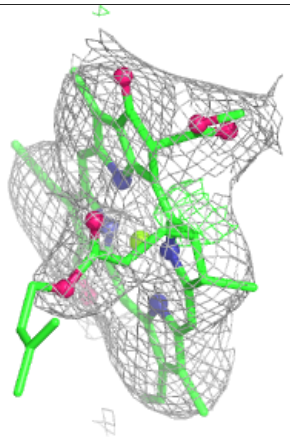


Electron density around CHL 4 4011:

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

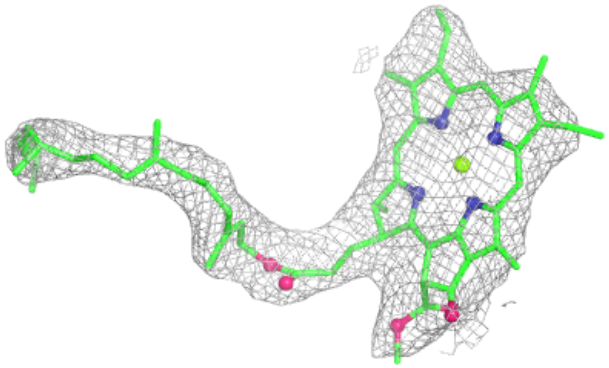


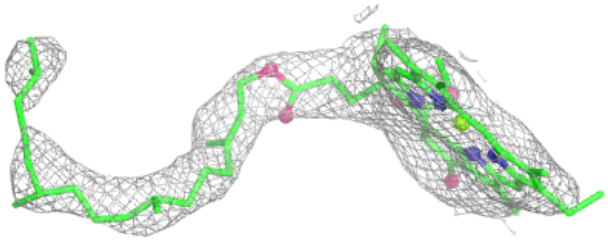


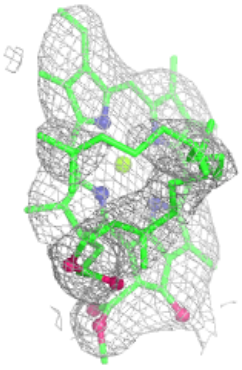


Electron density around CLA B 1206:

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

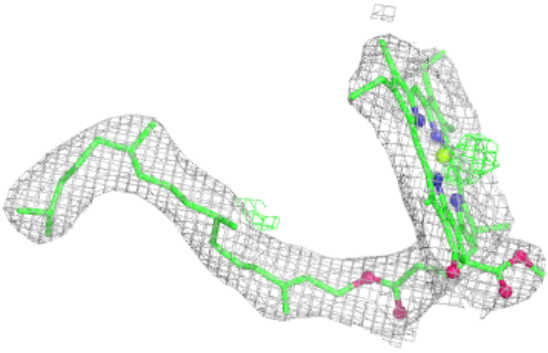


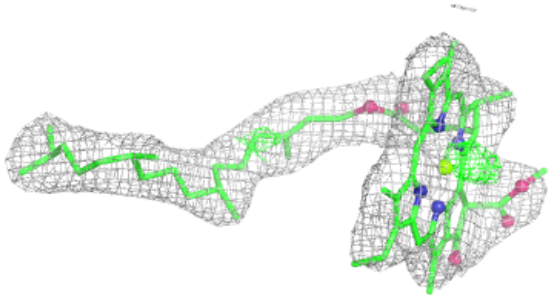


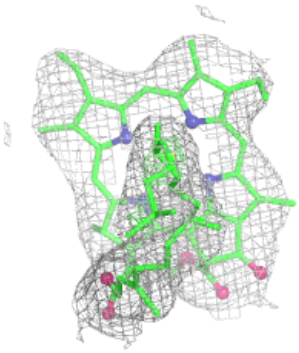


Electron density around CLA A 1128:

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

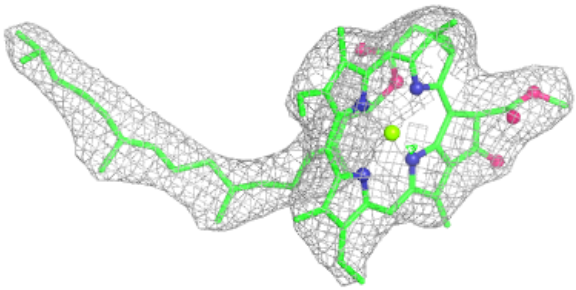


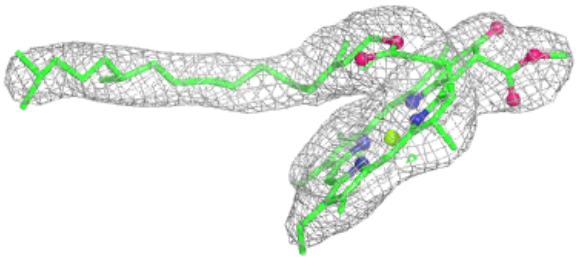


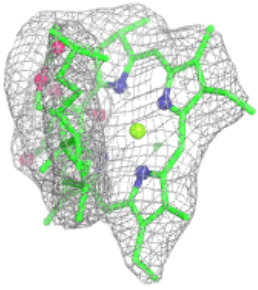


Electron density around CLA A 1140:

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

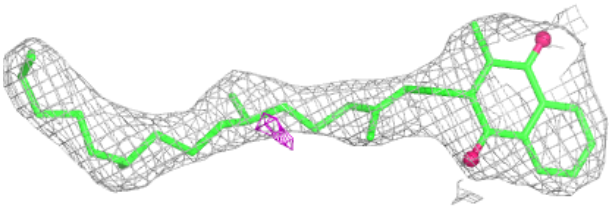


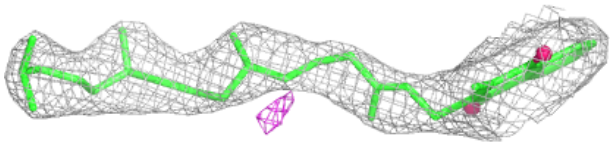


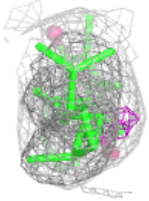


Electron density around PQN A 5001:

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

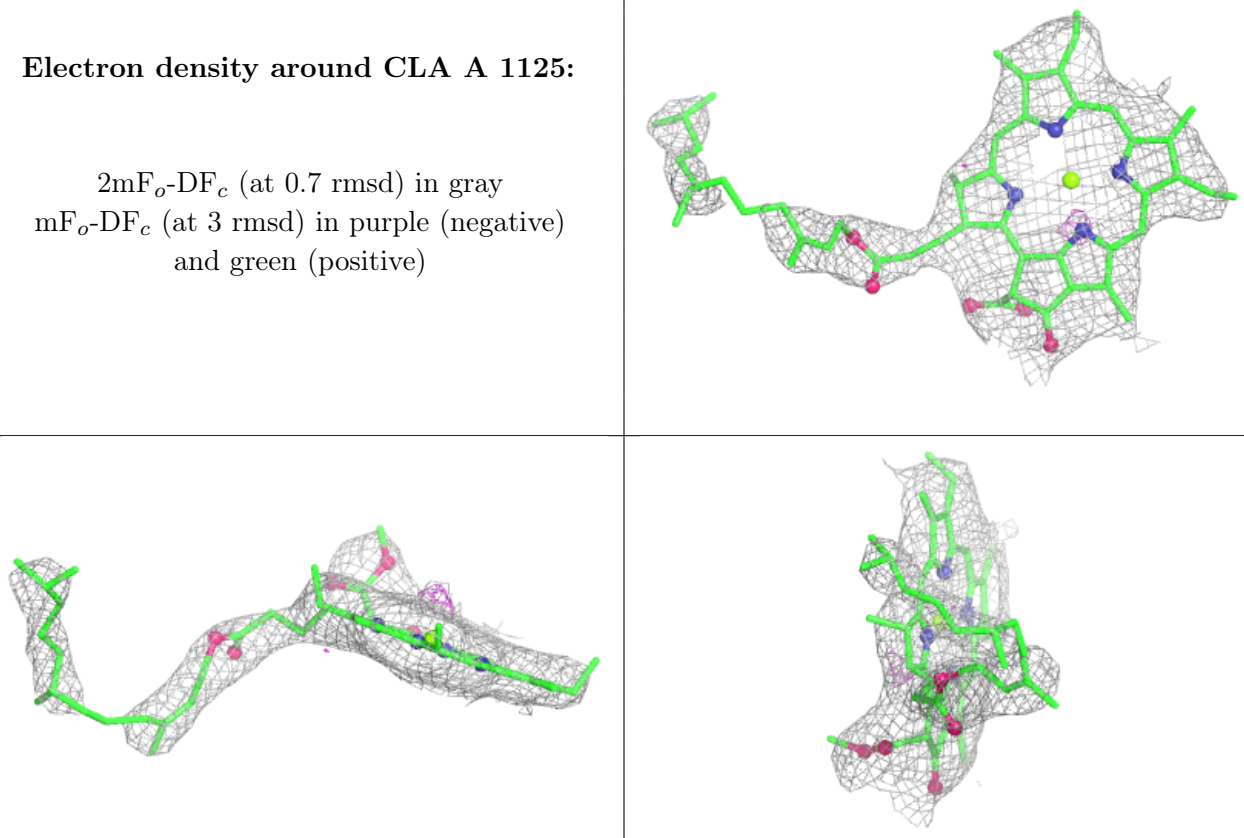






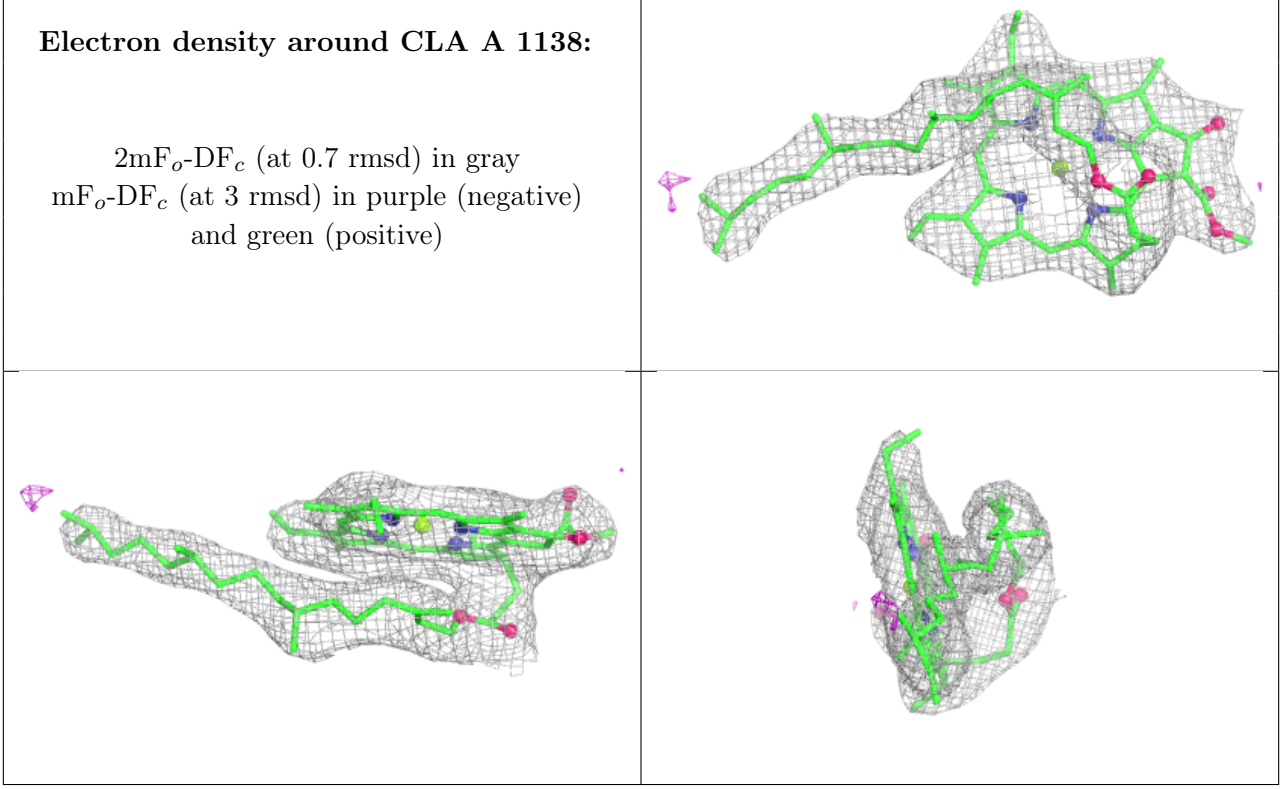
Electron density around CLA A 1125:

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



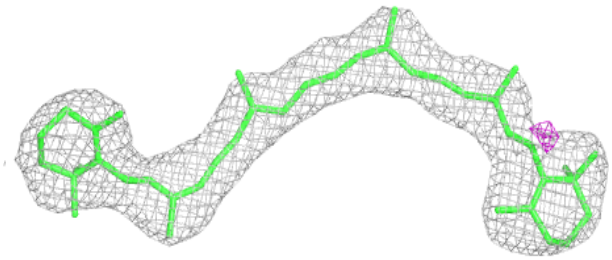
Electron density around CLA A 1138:

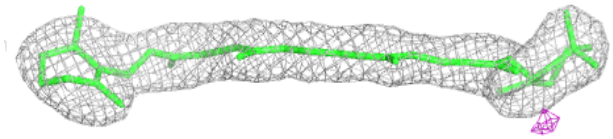
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

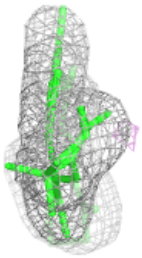


Electron density around BCR A 6011:

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

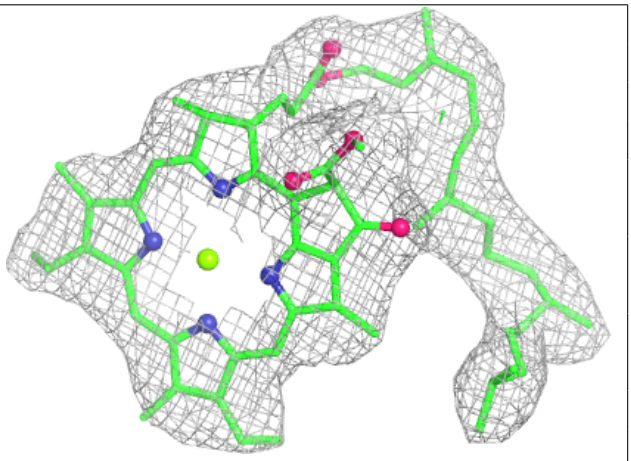


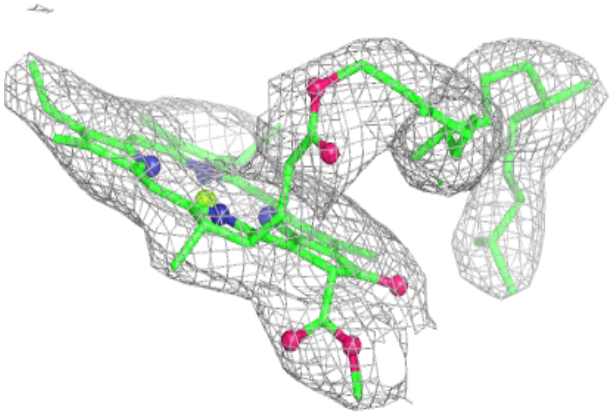


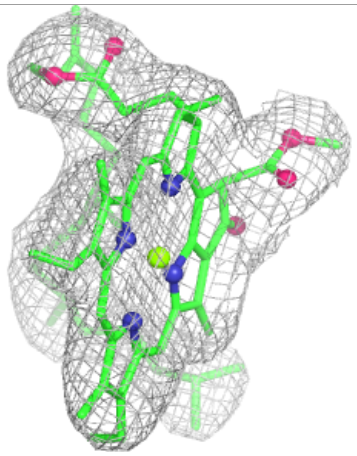


Electron density around CLA B 1229:

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

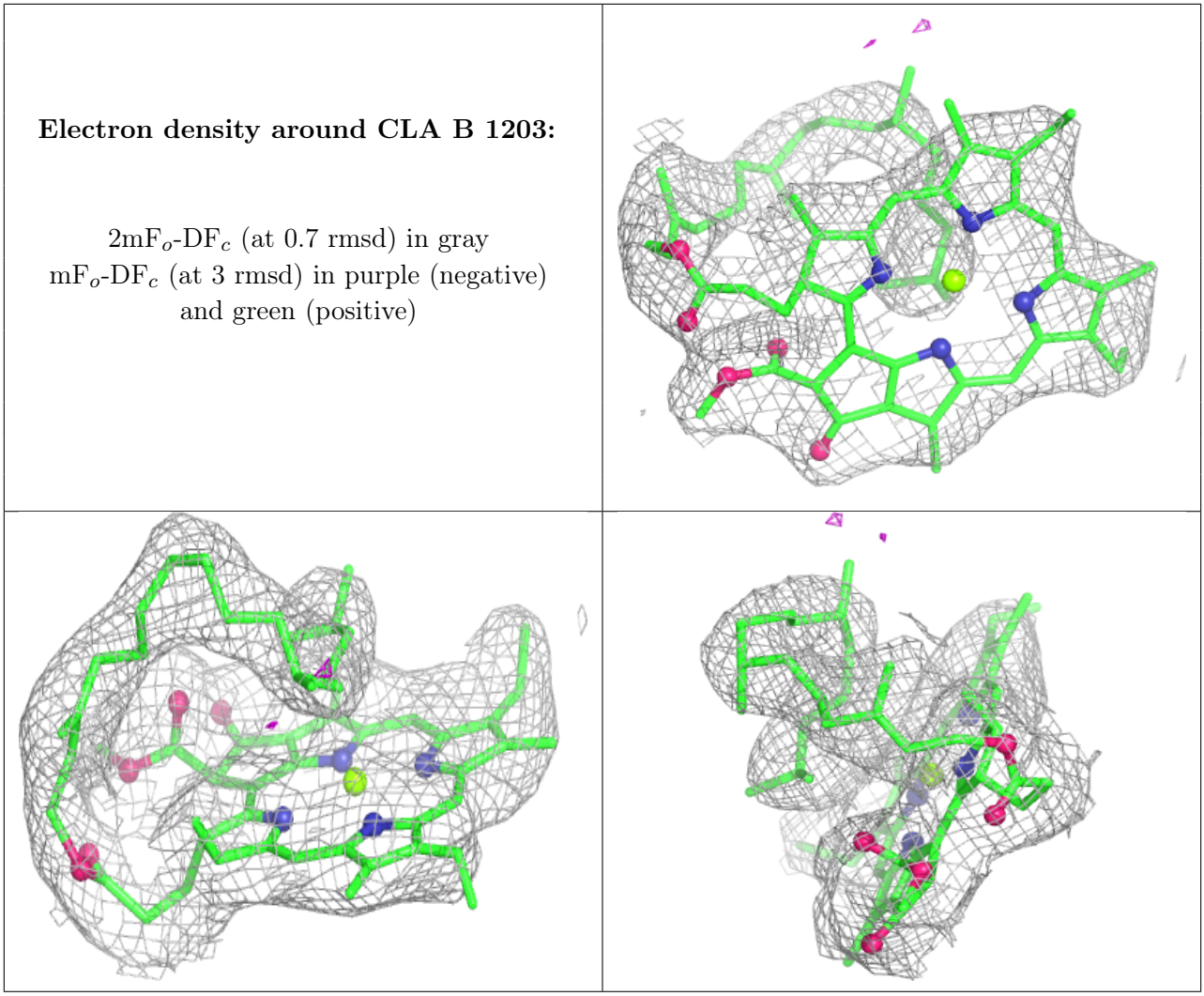






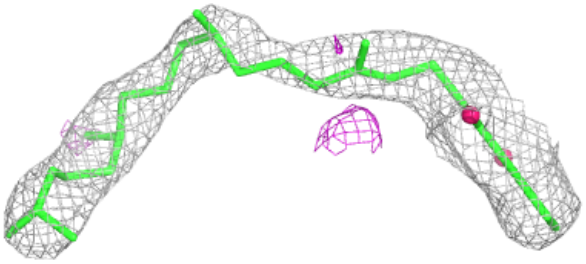
Electron density around CLA B 1203:

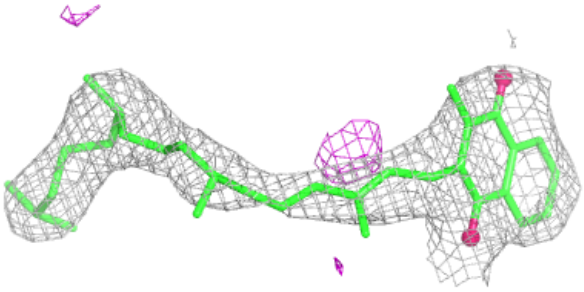
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

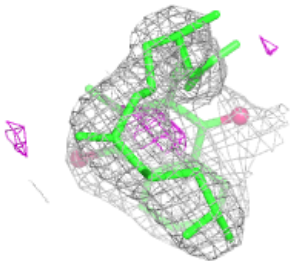


Electron density around PQN B 5002:

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

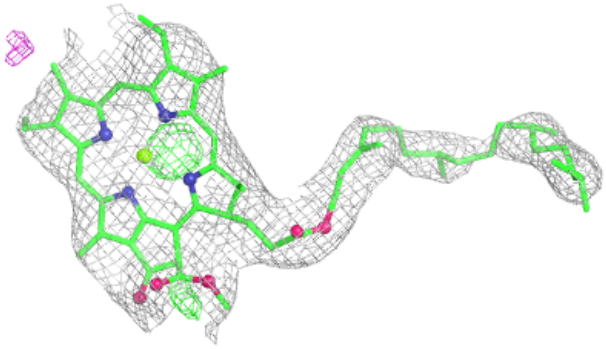


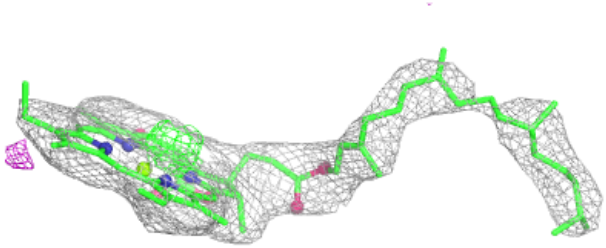


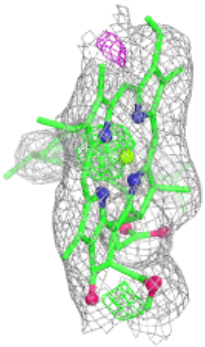


Electron density around CLA B 1210:

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

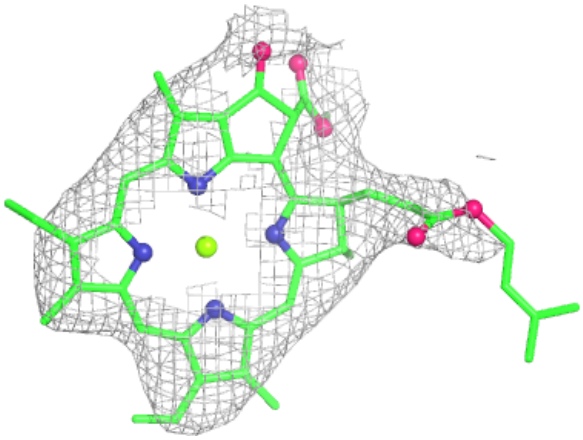


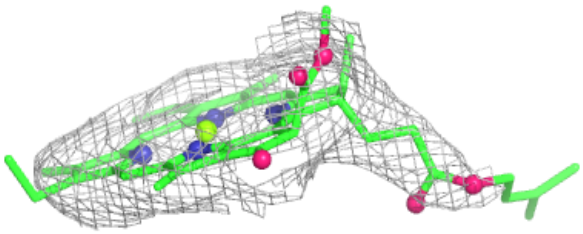


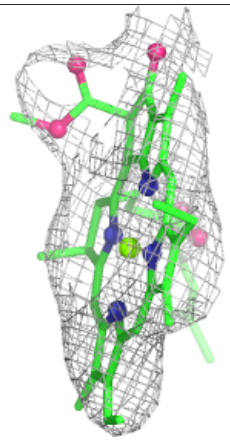


Electron density around CLA 4 4009:

$2mF_o$-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.