wwPDB X-ray Structure Validation Summary Report (i)

Sep 10, 2026 – 03:10 am BST

PDB ID	:	6HQB / pdb_00006hqb
Title	:	Monomeric cyanobacterial photosystem I
Authors	:	Netzer-El, S.Y.; Nelson, N.; Caspy, I.
Deposited on	:	2018-09-24
Resolution	:	4.00 Å(reported)

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

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

The 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:

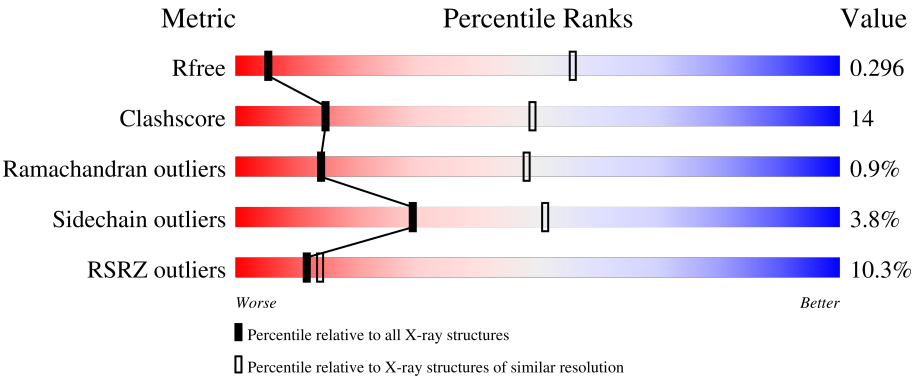
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 4.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	751	9% 75% 25%
2	B	731	9% 76% 24%
3	C	80	9% 62% 36%
4	D	141	11% 77% 21%
5	E	69	3% 77% 19%

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Mol	Chain	Length	Quality of chain
6	F	143	8% 75% 25%
7	I	40	52% 45% 45% 10%
8	J	40	2% 68% 30%
9	K	70	10% 51% 41% 7%
10	L	137	18% 47% 42% 12%
11	M	31	26% 77% 23%

2 Entry composition (i)

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

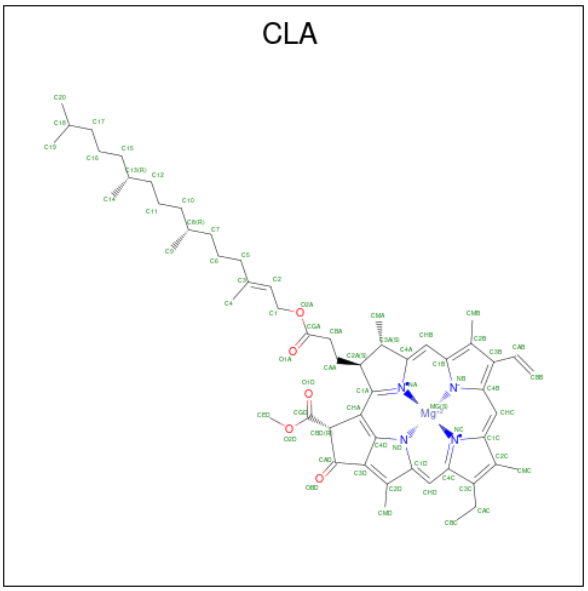
There is a discrepancy between the modelled and reference sequences:

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

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

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

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



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

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

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

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

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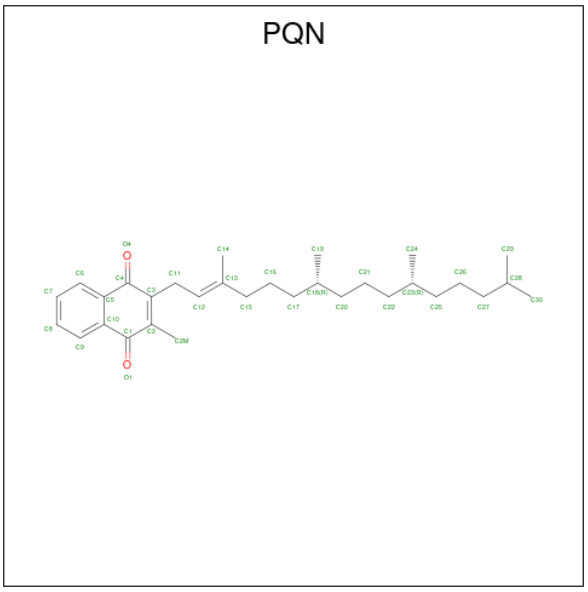
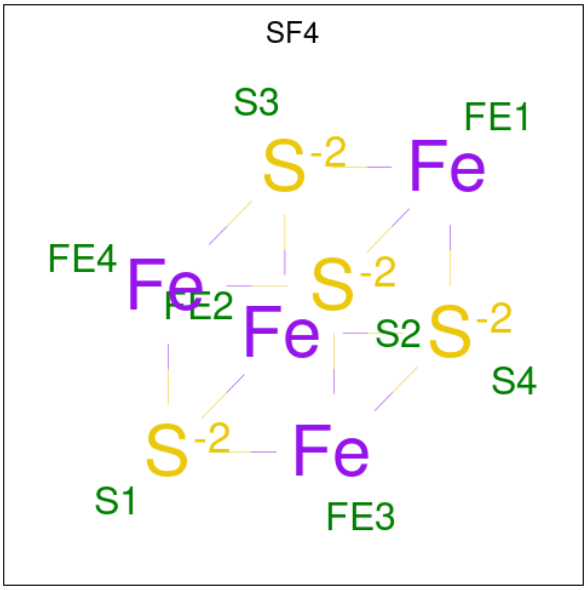
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
12	B	1	Total	C	Mg	N	O	0	0
			49	39	1	4	5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

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

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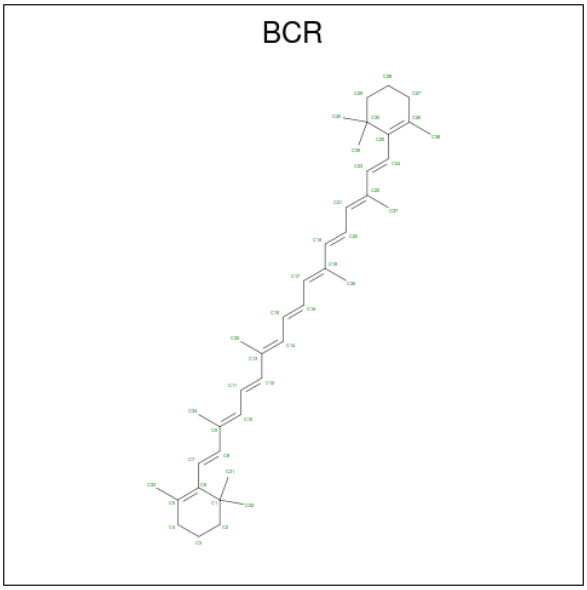
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	C	1	Total Fe S 8 4 4	0	0

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

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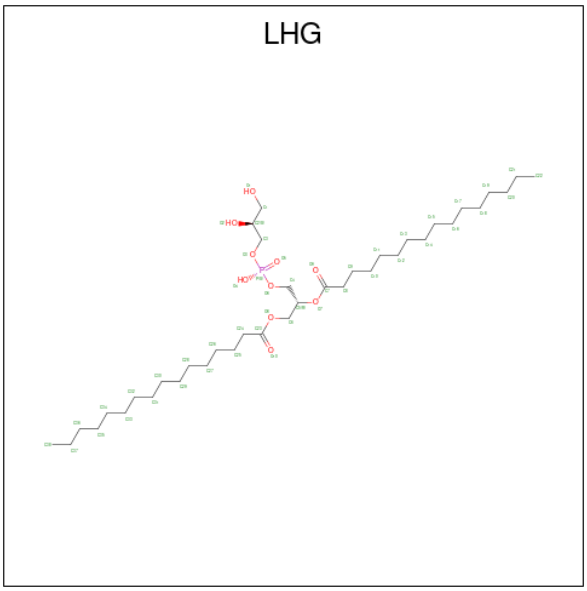
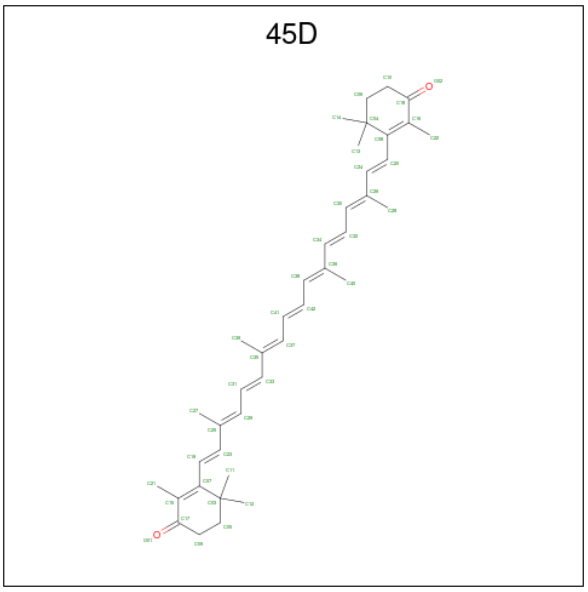
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	F	1	Total C 40 40	0	0
15	I	1	Total C 40 40	0	0
15	J	1	Total C 40 40	0	0
15	K	1	Total C 40 40	0	0

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



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

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

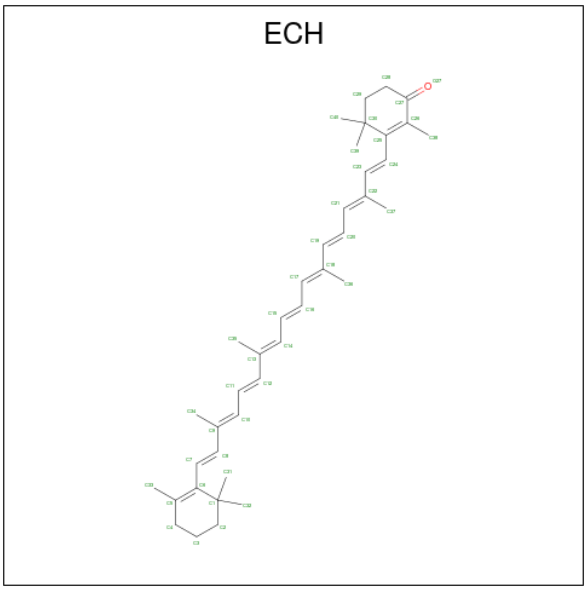


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	1	Total C O 42 40 2	0	0

- Molecule 18 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

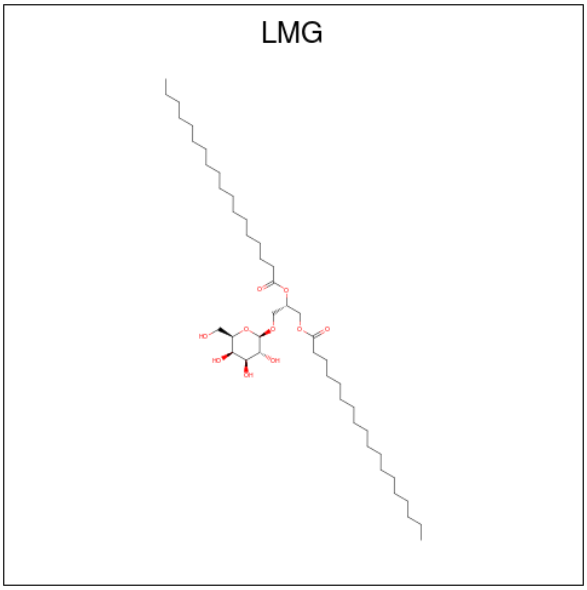
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	B	1	Total Cl 1 1	0	0

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



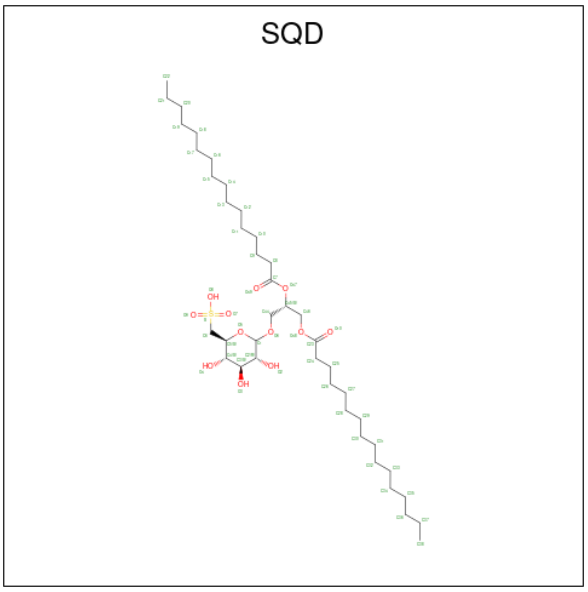
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	B	1	Total	C	O	0	0
			41	40	1		
19	M	1	Total	C	O	0	0
			41	40	1		

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



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

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

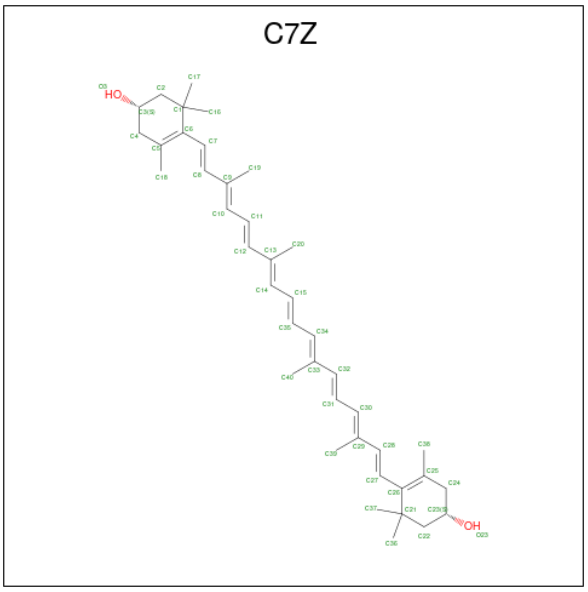


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	B	1	Total	C	O	S	0	0
			54	41	12	1		
21	F	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 22 is CALCIUM ION (CCD ID: CA) (formula: Ca).

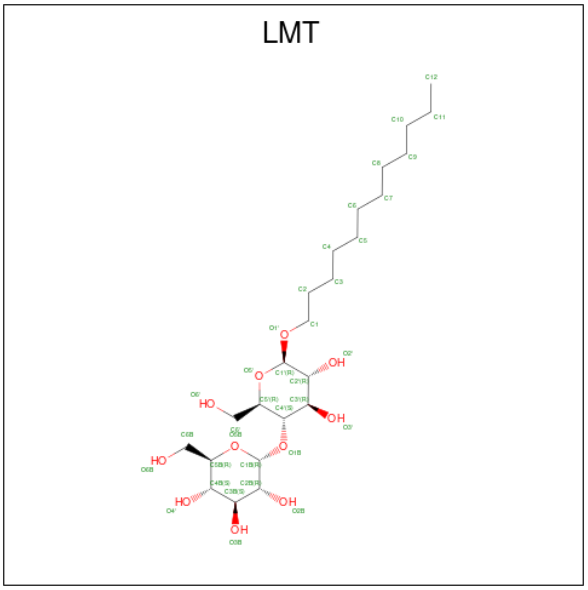
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	B	1	Total	Ca	0	0
			1	1		
22	L	1	Total	Ca	0	0
			1	1		

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



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

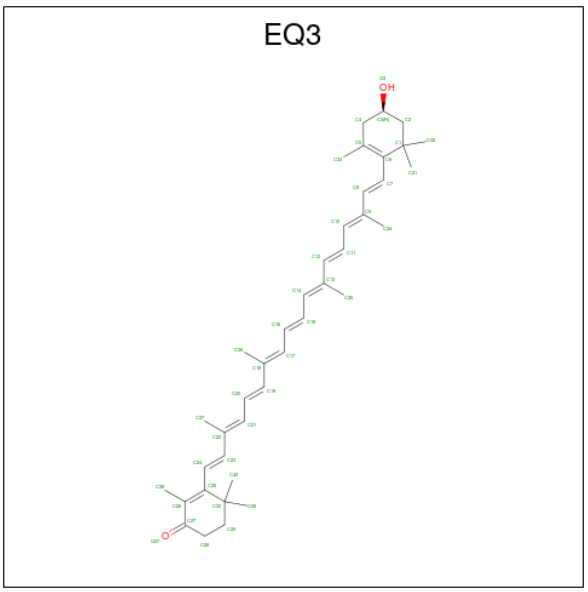
- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



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

- Molecule 25 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula:

$C_{40}H_{54}O_2$).



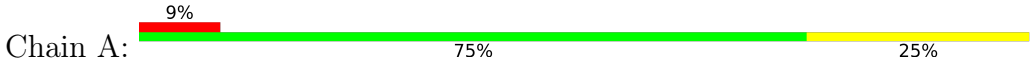
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	I	1	Total C O 42 40 2	0	0

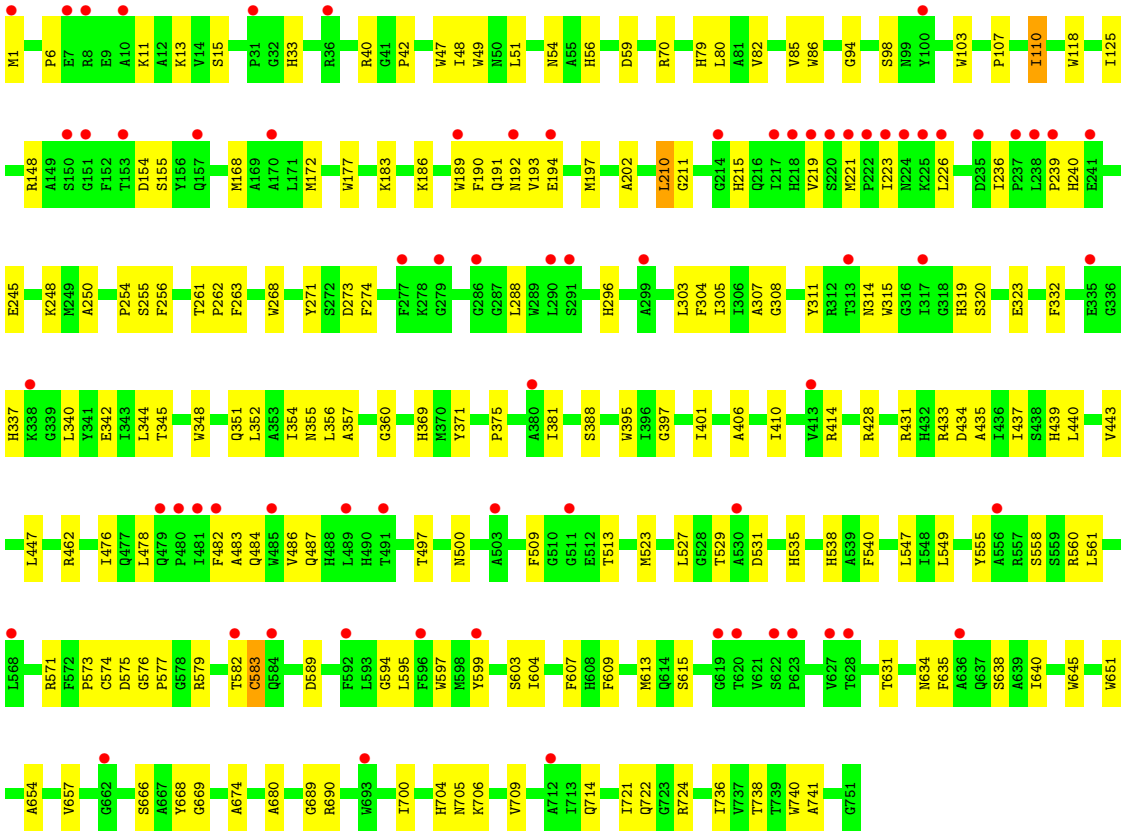
3 Residue-property plots (i)

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

• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

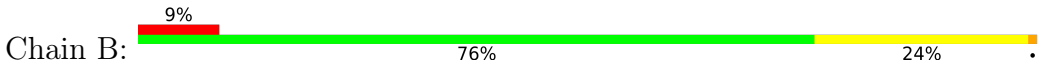
Chain A:

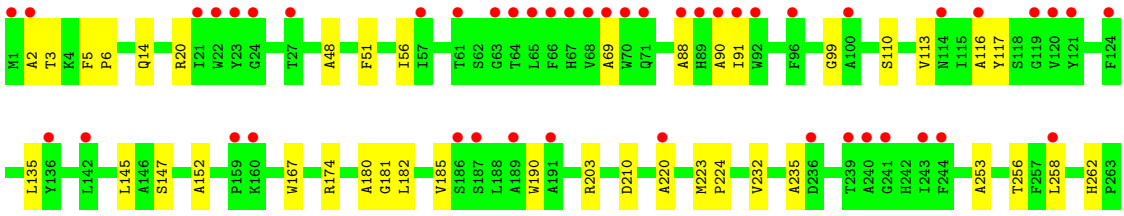


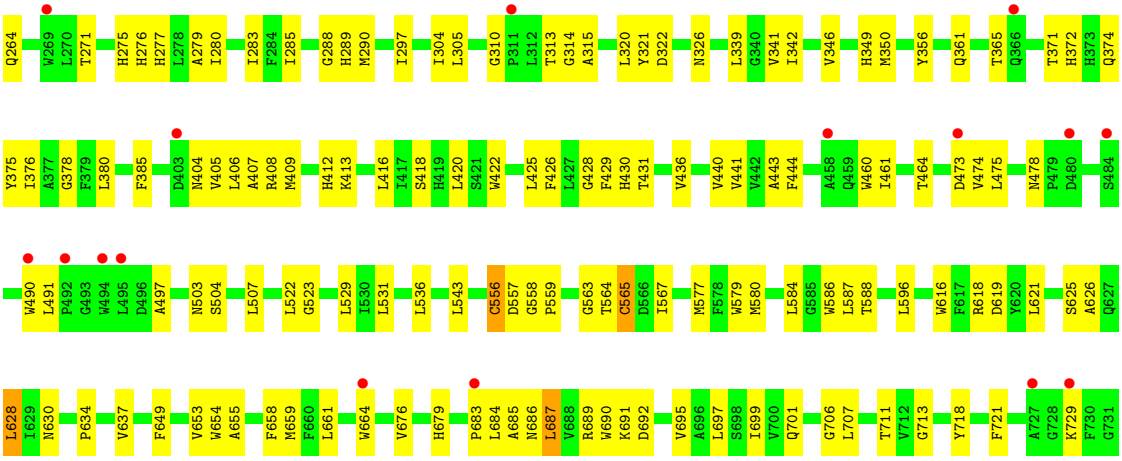


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:

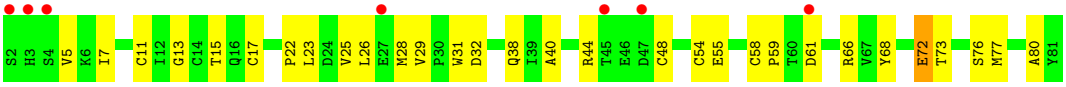




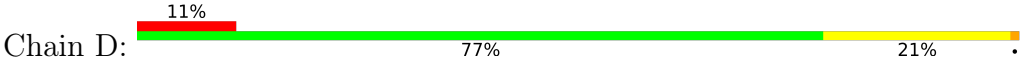


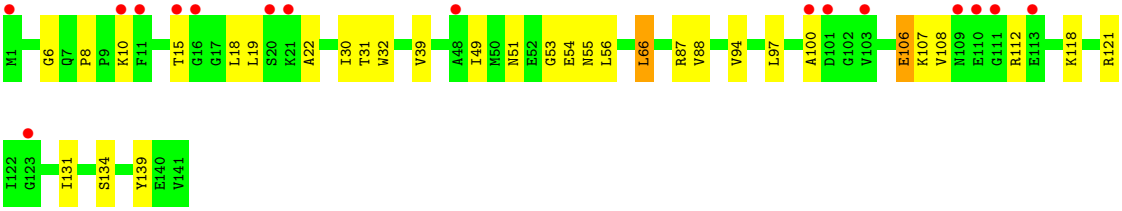
• Molecule 3: Photosystem I iron-sulfur center



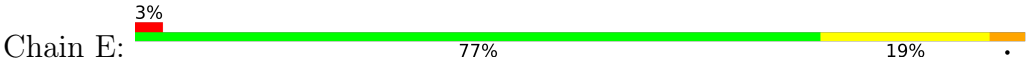


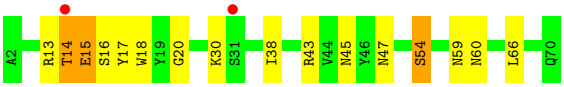
• Molecule 4: Photosystem I reaction center subunit II





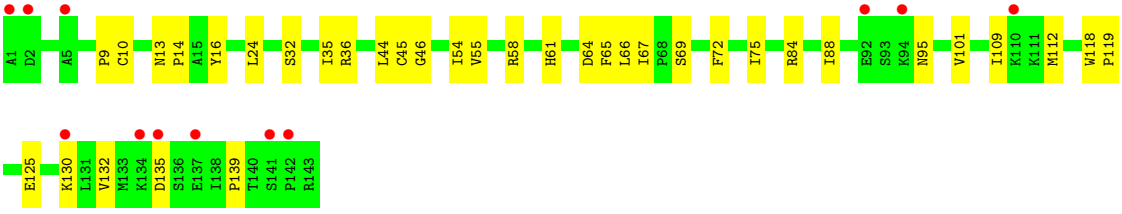
• Molecule 5: Photosystem I reaction center subunit IV





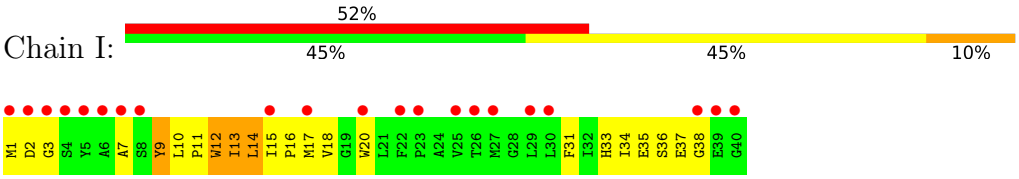
• Molecule 6: Photosystem I reaction center subunit III





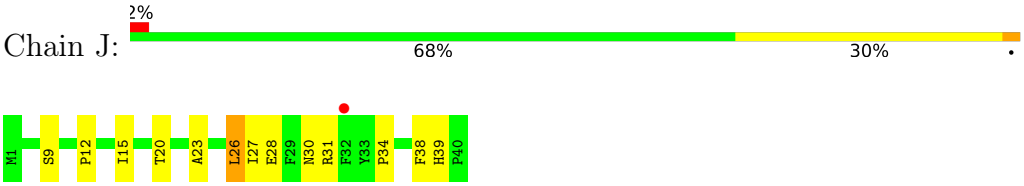
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I:



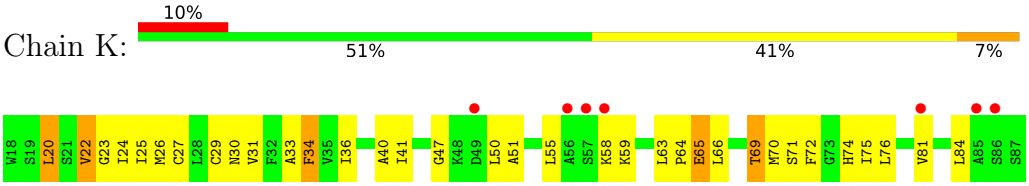
• Molecule 8: Photosystem I reaction center subunit IX

Chain J:



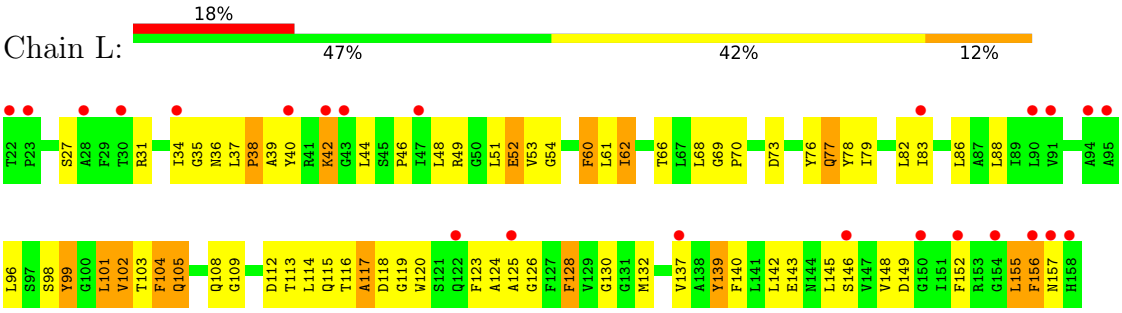
• Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain K:



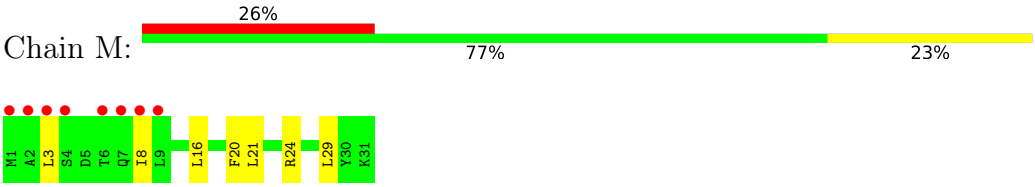
• Molecule 10: Photosystem I reaction center subunit XI

Chain L:



• Molecule 11: Photosystem I reaction center subunit XII

Chain M:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	124.32Å 178.66Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 4.00 49.29 – 4.00	Depositor EDS
% Data completeness (in resolution range)	88.7 (49.29-4.00) 88.6 (49.29-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.04 (at 4.00Å)	Xtriage
Refinement program	PHENIX (1.14_3228: ???)	Depositor
R, R_{free}	0.255 , 0.295 0.258 , 0.296	Depositor DCC
R_{free} test set	756 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 68.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.028 for -h,l,k	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	23566	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ECH, SQD, LMT, EQ3, 45D, C7Z, SF4, LMG, CL, LHG, BCR, CA, CLA, 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	0.11	0/6075	0.26	0/8278
2	B	0.11	0/5994	0.27	0/8195
3	C	0.11	0/610	0.29	0/826
4	D	0.09	0/1126	0.26	0/1517
5	E	0.10	0/552	0.27	0/745
6	F	0.12	0/1143	0.29	0/1553
7	I	0.18	0/322	0.44	0/438
8	J	0.10	0/328	0.26	0/443
9	K	0.13	0/520	0.33	0/700
10	L	0.14	0/1057	0.41	0/1434
11	M	0.11	0/241	0.26	0/326
All	All	0.11	0/17968	0.29	0/24455

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5876	0	5739	153	0
2	B	5783	0	5565	145	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	600	0	589	23	0
4	D	1102	0	1101	17	0
5	E	543	0	525	14	0
6	F	1113	0	1110	23	0
7	I	311	0	304	18	0
8	J	319	0	328	14	0
9	K	510	0	534	30	0
10	L	1030	0	1011	60	0
11	M	238	0	260	7	0
12	A	2326	0	2027	147	0
12	B	2152	0	1801	125	0
12	F	98	0	76	3	0
12	J	98	0	76	2	0
12	K	94	0	71	1	0
12	L	49	0	38	4	0
13	A	33	0	46	2	0
13	B	33	0	46	4	0
14	A	8	0	0	1	0
14	C	16	0	0	1	0
15	A	200	0	265	21	0
15	B	200	0	264	9	0
15	F	40	0	53	10	0
15	I	40	0	52	5	0
15	J	40	0	53	9	0
15	K	40	0	53	6	0
16	A	98	0	148	5	0
16	B	70	0	83	9	0
17	B	42	0	52	5	0
18	B	1	0	0	0	0
19	B	41	0	54	4	0
19	M	41	0	54	5	0
20	B	110	0	172	7	0
21	B	54	0	77	0	0
21	F	54	0	77	3	0
22	B	1	0	0	0	0
22	L	1	0	0	0	0
23	F	42	0	0	1	0
23	J	42	0	0	0	0
24	F	35	0	45	1	0
25	I	42	0	0	1	0
All	All	23566	0	22749	640	0

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

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

The worst 5 of 640 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD11	15:A:4001:BCR:H10C	1.42	1.01
12:B:1207:CLA:HBC3	15:I:4018:BCR:H21C	1.44	0.96
10:L:35:GLY:HA2	10:L:40:TYR:HB3	1.52	0.92
12:A:1125:CLA:HED1	12:A:1133:CLA:HAB	1.58	0.86
1:A:395:TRP:CD1	12:A:1126:CLA:HAB	2.11	0.85

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	749/751 (100%)	694 (93%)	52 (7%)	3 (0%)	30 65
2	B	729/731 (100%)	685 (94%)	43 (6%)	1 (0%)	48 81
3	C	78/80 (98%)	68 (87%)	9 (12%)	1 (1%)	9 41
4	D	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	9 39
5	E	67/69 (97%)	59 (88%)	6 (9%)	2 (3%)	3 26
6	F	141/143 (99%)	132 (94%)	7 (5%)	2 (1%)	9 39
7	I	38/40 (95%)	29 (76%)	6 (16%)	3 (8%)	1 12
8	J	38/40 (95%)	36 (95%)	2 (5%)	0	100 100
9	K	68/70 (97%)	61 (90%)	6 (9%)	1 (2%)	8 38
10	L	135/137 (98%)	104 (77%)	25 (18%)	6 (4%)	2 20
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100 100
All	All	2211/2233 (99%)	2022 (92%)	168 (8%)	21 (1%)	14 48

5 of 21 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	602/603 (100%)	591 (98%)	11 (2%)	51 68
2	B	583/583 (100%)	567 (97%)	16 (3%)	39 60
3	C	68/68 (100%)	66 (97%)	2 (3%)	37 58
4	D	116/116 (100%)	112 (97%)	4 (3%)	32 55
5	E	58/58 (100%)	55 (95%)	3 (5%)	21 44
6	F	119/119 (100%)	117 (98%)	2 (2%)	53 68
7	I	32/32 (100%)	28 (88%)	4 (12%)	4 20
8	J	35/35 (100%)	34 (97%)	1 (3%)	37 58
9	K	53/54 (98%)	47 (89%)	6 (11%)	5 22
10	L	102/102 (100%)	82 (80%)	20 (20%)	1 9
11	M	25/25 (100%)	25 (100%)	0	100 100
All	All	1793/1795 (100%)	1724 (96%)	69 (4%)	29 51

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	L	102	VAL
10	L	108	GLN
10	L	149	ASP
2	B	687	LEU
2	B	686	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	373	HIS
5	E	47	ASN
2	B	438	ASN
9	K	30	ASN
2	B	627	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 130 ligands modelled in this entry, 3 are monoatomic - leaving 127 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	CLA	A	1120	-	53,57,73	1.21	7 (13%)	62,93,113	1.90	13 (20%)
12	CLA	A	1104	-	53,57,73	1.21	6 (11%)	62,93,113	1.86	12 (19%)
12	CLA	A	1124	-	53,57,73	1.20	6 (11%)	62,93,113	1.91	12 (19%)
12	CLA	A	1105	1	69,73,73	1.07	6 (8%)	83,113,113	1.76	14 (16%)
12	CLA	B	1240	-	53,57,73	1.22	7 (13%)	62,93,113	1.93	13 (20%)
12	CLA	B	1217	2	53,57,73	1.21	6 (11%)	62,93,113	1.93	13 (20%)
12	CLA	B	1230	-	53,57,73	1.21	6 (11%)	62,93,113	1.96	13 (20%)
12	CLA	B	1204	-	53,57,73	1.22	6 (11%)	62,93,113	1.86	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	A	1115	1	60,64,73	1.14	6 (10%)	72,102,113	1.82	15 (20%)
12	CLA	B	1232	-	53,57,73	1.21	6 (11%)	62,93,113	1.92	14 (22%)
12	CLA	J	1302	8	53,57,73	1.20	6 (11%)	62,93,113	1.91	12 (19%)
12	CLA	B	1021	-	69,73,73	1.08	6 (8%)	83,113,113	1.68	11 (13%)
16	LHG	B	5004	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
12	CLA	A	1106	-	69,73,73	1.07	6 (8%)	83,113,113	1.73	14 (16%)
12	CLA	A	1121	-	53,57,73	1.20	6 (11%)	62,93,113	1.94	13 (20%)
12	CLA	A	1127	-	53,57,73	1.21	6 (11%)	62,93,113	1.89	13 (20%)
12	CLA	B	1202	-	69,73,73	1.06	6 (8%)	83,113,113	1.72	13 (15%)
12	CLA	B	1218	2	53,57,73	1.21	6 (11%)	62,93,113	1.89	12 (19%)
23	C7Z	J	4015	-	43,43,43	5.34	18 (41%)	58,60,60	5.20	31 (53%)
16	LHG	B	5006	2	20,20,48	0.59	0	23,26,54	1.48	2 (8%)
20	LMG	B	5005	-	55,55,55	1.14	6 (10%)	63,63,63	1.06	3 (4%)
15	BCR	I	4018	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	20 (35%)
12	CLA	B	1203	2	53,57,73	1.21	6 (11%)	62,93,113	1.81	12 (19%)
19	ECH	M	4021	-	42,42,42	0.85	1 (2%)	55,58,58	2.62	14 (25%)
12	CLA	A	1113	-	53,57,73	1.21	6 (11%)	62,93,113	1.87	12 (19%)
17	45D	B	4011	-	43,43,43	3.57	16 (37%)	54,60,60	2.15	17 (31%)
12	CLA	B	1222	-	54,58,73	1.20	6 (11%)	65,95,113	1.94	13 (20%)
12	CLA	B	1234	2	64,68,73	1.13	6 (9%)	77,107,113	1.78	13 (16%)
12	CLA	B	1201	2	53,57,73	1.21	6 (11%)	62,93,113	1.88	13 (20%)
12	CLA	B	1022	-	64,68,73	1.12	6 (9%)	77,107,113	1.77	14 (18%)
15	BCR	B	4005	-	41,41,41	1.85	4 (9%)	56,56,56	4.43	14 (25%)
12	CLA	A	1112	-	53,57,73	1.20	6 (11%)	62,93,113	1.91	13 (20%)
13	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.09	3 (7%)
15	BCR	J	4013	-	41,41,41	1.87	4 (9%)	56,56,56	4.35	15 (26%)
21	SQD	F	5001	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
12	CLA	A	1110	-	53,57,73	1.21	6 (11%)	62,93,113	1.88	12 (19%)
12	CLA	A	1011	1	59,63,73	1.17	6 (10%)	71,101,113	1.87	15 (21%)
12	CLA	A	1109	12	69,73,73	1.06	6 (8%)	83,113,113	1.70	14 (16%)
12	CLA	A	1129	-	53,57,73	1.21	6 (11%)	62,93,113	1.88	12 (19%)
15	BCR	A	4008	-	41,41,41	1.84	4 (9%)	56,56,56	4.38	17 (30%)
25	EQ3	I	4020	-	43,43,43	4.21	25 (58%)	56,60,60	2.37	20 (35%)
12	CLA	A	1130	-	53,57,73	1.21	6 (11%)	62,93,113	1.87	12 (19%)
15	BCR	B	4017	-	41,41,41	1.85	4 (9%)	56,56,56	4.45	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	A	1116	-	53,57,73	1.23	6 (11%)	62,93,113	1.93	12 (19%)
12	CLA	B	1239	-	53,57,73	1.20	6 (11%)	62,93,113	1.86	12 (19%)
15	BCR	A	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.39	16 (28%)
12	CLA	F	1301	-	53,57,73	1.22	6 (11%)	62,93,113	1.87	12 (19%)
15	BCR	A	4003	-	41,41,41	1.85	4 (9%)	56,56,56	4.29	16 (28%)
12	CLA	B	1205	2	53,57,73	1.22	6 (11%)	62,93,113	1.95	14 (22%)
12	CLA	K	1402	-	53,57,73	1.21	6 (11%)	62,93,113	1.96	15 (24%)
15	BCR	F	4014	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	14 (25%)
20	LMG	B	5002	-	55,55,55	1.13	6 (10%)	63,63,63	1.02	2 (3%)
12	CLA	A	1117	-	53,57,73	1.21	6 (11%)	62,93,113	1.87	13 (20%)
12	CLA	A	1108	-	53,57,73	1.21	6 (11%)	62,93,113	1.87	12 (19%)
12	CLA	B	1221	-	53,57,73	1.22	7 (13%)	62,93,113	1.90	13 (20%)
12	CLA	A	1136	-	53,57,73	1.21	6 (11%)	62,93,113	1.91	12 (19%)
14	SF4	A	3001	-	0,12,12	-	-	-		
19	ECH	B	4006	-	42,42,42	0.85	1 (2%)	55,58,58	2.46	12 (21%)
12	CLA	B	1208	2	53,57,73	1.21	6 (11%)	62,93,113	1.84	12 (19%)
12	CLA	L	1502	-	53,57,73	1.21	7 (13%)	62,93,113	1.97	12 (19%)
12	CLA	A	1140	1	69,73,73	1.06	6 (8%)	83,113,113	1.69	13 (15%)
12	CLA	B	1226	-	53,57,73	1.24	6 (11%)	62,93,113	1.86	12 (19%)
12	CLA	A	1103	1	53,57,73	1.20	6 (11%)	62,93,113	1.93	13 (20%)
12	CLA	B	1210	2	53,57,73	1.21	6 (11%)	62,93,113	1.93	13 (20%)
12	CLA	B	1238	-	53,57,73	1.23	7 (13%)	62,93,113	1.93	13 (20%)
12	CLA	B	1228	2	53,57,73	1.22	6 (11%)	62,93,113	1.89	12 (19%)
12	CLA	A	1131	1	53,57,73	1.21	6 (11%)	62,93,113	1.86	12 (19%)
12	CLA	B	1220	2	53,57,73	1.22	7 (13%)	62,93,113	1.93	14 (22%)
12	CLA	A	1132	10	59,63,73	1.17	6 (10%)	71,101,113	1.78	13 (18%)
14	SF4	C	3002	-	0,12,12	-	-	-		
15	BCR	B	4010	-	41,41,41	1.91	4 (9%)	56,56,56	4.49	18 (32%)
12	CLA	A	1101	-	53,57,73	1.21	6 (11%)	62,93,113	2.02	16 (25%)
12	CLA	A	1114	-	53,57,73	1.21	6 (11%)	62,93,113	1.90	12 (19%)
12	CLA	B	1215	2	53,57,73	1.21	7 (13%)	62,93,113	1.90	11 (17%)
14	SF4	C	3003	-	0,12,12	-	-	-		
12	CLA	B	1231	-	53,57,73	1.22	6 (11%)	62,93,113	1.93	13 (20%)
12	CLA	B	1225	2	53,57,73	1.21	6 (11%)	62,93,113	1.82	11 (17%)
12	CLA	A	1111	-	53,57,73	1.22	6 (11%)	62,93,113	1.82	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.04	4 (7%)
12	CLA	A	1125	1	53,57,73	1.24	6 (11%)	62,93,113	1.95	13 (20%)
12	CLA	B	1235	2	69,73,73	1.08	6 (8%)	83,113,113	1.74	13 (15%)
12	CLA	B	1236	2	53,57,73	1.22	6 (11%)	62,93,113	1.88	11 (17%)
13	PQN	A	2001	-	34,34,34	0.43	0	42,45,45	1.09	3 (7%)
12	CLA	A	1138	1	69,73,73	1.08	6 (8%)	83,113,113	1.73	13 (15%)
12	CLA	B	1214	-	64,68,73	1.10	6 (9%)	77,107,113	1.70	13 (16%)
12	CLA	A	1013	-	69,73,73	1.07	6 (8%)	83,113,113	1.68	15 (18%)
16	LHG	A	5003	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
12	CLA	B	1227	-	53,57,73	1.20	6 (11%)	62,93,113	1.98	13 (20%)
12	CLA	A	1134	1	53,57,73	1.21	6 (11%)	62,93,113	1.91	13 (20%)
12	CLA	A	1141	-	49,53,73	1.25	7 (14%)	59,89,113	1.79	10 (16%)
12	CLA	A	1126	-	64,68,73	1.10	7 (10%)	77,107,113	1.72	13 (16%)
12	CLA	B	1216	-	53,57,73	1.21	6 (11%)	62,93,113	1.88	12 (19%)
12	CLA	B	1212	-	53,57,73	1.20	6 (11%)	62,93,113	1.92	12 (19%)
12	CLA	F	1302	10	53,57,73	1.21	6 (11%)	62,93,113	1.94	13 (20%)
12	CLA	B	1206	-	53,57,73	1.21	7 (13%)	62,93,113	1.88	12 (19%)
12	CLA	A	1122	1	53,57,73	1.21	7 (13%)	62,93,113	1.92	12 (19%)
12	CLA	B	1229	2	59,63,73	1.14	6 (10%)	71,101,113	1.92	15 (21%)
12	CLA	J	1303	10	53,57,73	1.21	6 (11%)	62,93,113	1.90	13 (20%)
12	CLA	B	1223	2	53,57,73	1.27	7 (13%)	62,93,113	1.93	12 (19%)
12	CLA	A	1107	1	54,58,73	1.53	8 (14%)	65,95,113	2.10	12 (18%)
24	LMT	F	6001	-	36,36,36	1.14	5 (13%)	47,47,47	1.03	2 (4%)
12	CLA	B	1237	-	53,57,73	1.20	6 (11%)	62,93,113	1.90	12 (19%)
12	CLA	B	1207	-	53,57,73	1.23	6 (11%)	62,93,113	1.95	13 (20%)
12	CLA	B	1023	-	53,57,73	1.21	7 (13%)	62,93,113	1.89	12 (19%)
12	CLA	B	1219	2	53,57,73	1.20	6 (11%)	62,93,113	1.89	12 (19%)
15	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.47	15 (26%)
15	BCR	B	4018	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	17 (30%)
12	CLA	A	1135	-	53,57,73	1.22	6 (11%)	62,93,113	1.96	13 (20%)
12	CLA	A	1118	1	54,58,73	1.20	6 (11%)	65,95,113	1.86	12 (18%)
15	BCR	K	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.39	15 (26%)
12	CLA	B	1211	-	53,57,73	1.24	6 (11%)	62,93,113	1.90	13 (20%)
12	CLA	A	1012	-	53,57,73	1.23	7 (13%)	62,93,113	1.84	13 (20%)
12	CLA	A	1133	-	53,57,73	1.20	6 (11%)	62,93,113	1.88	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	CLA	A	1102	12	69,73,73	1.06	7 (10%)	83,113,113	1.74	17 (20%)
21	SQD	B	5008	-	53,54,54	0.78	0	62,65,65	0.91	2 (3%)
12	CLA	A	1123	-	64,68,73	1.11	7 (10%)	77,107,113	1.76	14 (18%)
12	CLA	A	1128	-	69,73,73	1.08	6 (8%)	83,113,113	1.69	15 (18%)
23	C7Z	F	4016	-	43,43,43	5.36	18 (41%)	58,60,60	5.24	32 (55%)
12	CLA	A	1119	-	50,54,73	1.27	6 (12%)	60,90,113	1.73	10 (16%)
12	CLA	A	1137	-	53,57,73	1.20	6 (11%)	62,93,113	1.90	12 (19%)
12	CLA	B	1209	2	53,57,73	1.20	7 (13%)	62,93,113	1.93	13 (20%)
12	CLA	B	1224	-	59,63,73	1.17	6 (10%)	71,101,113	1.83	13 (18%)
12	CLA	A	1139	-	59,63,73	1.16	6 (10%)	71,101,113	1.83	12 (16%)
15	BCR	A	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.36	18 (32%)
12	CLA	K	1401	-	49,53,73	1.25	6 (12%)	59,89,113	1.82	10 (16%)
12	CLA	B	1213	2	53,57,73	1.21	7 (13%)	62,93,113	1.97	14 (22%)
15	BCR	A	4012	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	14 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1120	-	-	11/20/96/115	-
12	CLA	A	1104	-	-	10/20/96/115	-
12	CLA	A	1124	-	-	9/20/96/115	-
12	CLA	A	1105	1	-	11/39/115/115	-
12	CLA	B	1240	-	-	14/20/96/115	-
12	CLA	B	1217	2	-	9/20/96/115	-
12	CLA	B	1230	-	-	12/20/96/115	-
12	CLA	B	1204	-	-	9/20/96/115	-
12	CLA	A	1115	1	-	7/29/105/115	-
12	CLA	B	1232	-	-	10/20/96/115	-
12	CLA	J	1302	8	-	9/20/96/115	-
12	CLA	B	1021	-	-	27/39/115/115	-
16	LHG	B	5004	-	-	23/53/53/53	-
12	CLA	A	1106	-	-	19/39/115/115	-
12	CLA	A	1121	-	-	11/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1127	-	-	9/20/96/115	-
12	CLA	B	1202	-	-	16/39/115/115	-
12	CLA	B	1218	2	-	11/20/96/115	-
23	C7Z	J	4015	-	-	14/29/67/67	0/2/2/2
16	LHG	B	5006	2	-	11/23/23/53	-
20	LMG	B	5005	-	-	17/50/70/70	0/1/1/1
15	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
12	CLA	B	1203	2	-	8/20/96/115	-
19	ECH	M	4021	-	-	12/29/66/66	0/2/2/2
12	CLA	A	1113	-	-	16/20/96/115	-
17	45D	B	4011	-	-	11/29/69/69	0/2/2/2
12	CLA	B	1222	-	-	8/21/97/115	-
12	CLA	B	1234	2	-	16/33/109/115	-
12	CLA	B	1201	2	-	9/20/96/115	-
12	CLA	B	1022	-	-	13/33/109/115	-
15	BCR	B	4005	-	-	12/29/63/63	0/2/2/2
12	CLA	A	1112	-	-	12/20/96/115	-
13	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
15	BCR	J	4013	-	-	14/29/63/63	0/2/2/2
21	SQD	F	5001	-	-	17/49/69/69	0/1/1/1
12	CLA	A	1110	-	-	11/20/96/115	-
12	CLA	A	1011	1	-	11/27/103/115	-
12	CLA	A	1109	12	-	18/39/115/115	-
12	CLA	A	1129	-	-	7/20/96/115	-
15	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
25	EQ3	I	4020	-	-	15/29/68/68	0/2/2/2
12	CLA	A	1130	-	-	9/20/96/115	-
15	BCR	B	4017	-	-	8/29/63/63	0/2/2/2
12	CLA	A	1116	-	-	10/20/96/115	-
12	CLA	B	1239	-	-	13/20/96/115	-
15	BCR	A	4007	-	-	11/29/63/63	0/2/2/2
12	CLA	F	1301	-	-	6/20/96/115	-
15	BCR	A	4003	-	-	15/29/63/63	0/2/2/2
12	CLA	B	1205	2	-	13/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	K	1402	-	-	12/20/96/115	-
15	BCR	F	4014	-	-	12/29/63/63	0/2/2/2
20	LMG	B	5002	-	-	10/50/70/70	0/1/1/1
12	CLA	A	1117	-	-	8/20/96/115	-
12	CLA	A	1108	-	-	11/20/96/115	-
12	CLA	B	1221	-	-	8/20/96/115	-
12	CLA	A	1136	-	-	13/20/96/115	-
14	SF4	A	3001	-	-	-	0/6/5/5
19	ECH	B	4006	-	-	8/29/66/66	0/2/2/2
12	CLA	B	1208	2	-	8/20/96/115	-
12	CLA	L	1502	-	-	12/20/96/115	-
12	CLA	A	1140	1	-	20/39/115/115	-
12	CLA	B	1226	-	-	9/20/96/115	-
12	CLA	A	1103	1	-	13/20/96/115	-
12	CLA	B	1210	2	-	13/20/96/115	-
12	CLA	B	1238	-	-	10/20/96/115	-
12	CLA	B	1228	2	-	10/20/96/115	-
12	CLA	A	1131	1	-	7/20/96/115	-
12	CLA	B	1220	2	-	10/20/96/115	-
12	CLA	A	1132	10	-	16/27/103/115	-
14	SF4	C	3002	-	-	-	0/6/5/5
15	BCR	B	4010	-	-	11/29/63/63	0/2/2/2
12	CLA	A	1101	-	-	10/20/96/115	-
12	CLA	A	1114	-	-	9/20/96/115	-
12	CLA	B	1215	2	-	10/20/96/115	-
14	SF4	C	3003	-	-	-	0/6/5/5
12	CLA	B	1231	-	-	8/20/96/115	-
12	CLA	B	1225	2	-	9/20/96/115	-
12	CLA	A	1111	-	-	15/20/96/115	-
16	LHG	A	5001	-	-	35/53/53/53	-
12	CLA	A	1125	1	-	11/20/96/115	-
12	CLA	B	1235	2	-	20/39/115/115	-
12	CLA	B	1236	2	-	7/20/96/115	-
13	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
12	CLA	A	1138	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	1214	-	-	22/33/109/115	-
12	CLA	A	1013	-	-	15/39/115/115	-
16	LHG	A	5003	-	-	30/53/53/53	-
12	CLA	B	1227	-	-	13/20/96/115	-
12	CLA	A	1134	1	-	12/20/96/115	-
12	CLA	A	1141	-	-	11/15/91/115	-
12	CLA	A	1126	-	-	12/33/109/115	-
12	CLA	B	1216	-	-	14/20/96/115	-
12	CLA	B	1212	-	-	11/20/96/115	-
12	CLA	F	1302	10	-	13/20/96/115	-
12	CLA	B	1206	-	-	9/20/96/115	-
12	CLA	A	1122	1	-	10/20/96/115	-
12	CLA	B	1229	2	-	14/27/103/115	-
12	CLA	J	1303	10	-	11/20/96/115	-
12	CLA	B	1223	2	-	11/20/96/115	-
12	CLA	A	1107	1	-	7/21/97/115	-
24	LMT	F	6001	-	-	8/21/61/61	0/2/2/2
12	CLA	B	1237	-	-	9/20/96/115	-
12	CLA	B	1207	-	-	15/20/96/115	-
12	CLA	B	1023	-	-	9/20/96/115	-
12	CLA	B	1219	2	-	11/20/96/115	-
15	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
15	BCR	B	4018	-	-	9/29/63/63	0/2/2/2
12	CLA	A	1135	-	-	11/20/96/115	-
12	CLA	A	1118	1	-	9/21/97/115	-
15	BCR	K	4001	-	-	11/29/63/63	0/2/2/2
12	CLA	B	1211	-	-	9/20/96/115	-
12	CLA	A	1012	-	-	13/20/96/115	-
12	CLA	A	1133	-	-	13/20/96/115	-
12	CLA	A	1102	12	-	14/39/115/115	-
21	SQD	B	5008	-	-	10/49/69/69	0/1/1/1
12	CLA	A	1123	-	-	14/33/109/115	-
12	CLA	A	1128	-	-	19/39/115/115	-
23	C7Z	F	4016	-	-	17/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	1119	-	-	7/17/93/115	-
12	CLA	A	1137	-	-	8/20/96/115	-
12	CLA	B	1209	2	-	12/20/96/115	-
12	CLA	B	1224	-	-	15/27/103/115	-
12	CLA	A	1139	-	-	9/27/103/115	-
15	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
12	CLA	K	1401	-	-	10/15/91/115	-
12	CLA	B	1213	2	-	8/20/96/115	-
15	BCR	A	4012	-	-	14/29/63/63	0/2/2/2

The worst 5 of 730 bond length outliers are listed below:

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

The worst 5 of 1566 bond angle outliers are listed below:

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

There are no chirality outliers.

5 of 1494 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1012	CLA	CAD-CBD-CGD-O1D
12	A	1012	CLA	CAD-CBD-CGD-O2D
12	A	1013	CLA	C2-C1-O2A-CGA
12	A	1013	CLA	CHA-CBD-CGD-O1D
12	A	1013	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

113 monomers are involved in 336 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1124	CLA	2	0
12	A	1105	CLA	4	0
12	B	1240	CLA	1	0
12	B	1230	CLA	3	0
12	B	1204	CLA	3	0
12	A	1115	CLA	6	0
12	B	1232	CLA	2	0
12	J	1302	CLA	2	0
12	B	1021	CLA	12	0
16	B	5004	LHG	9	0
12	A	1106	CLA	8	0
12	A	1121	CLA	1	0
12	B	1202	CLA	5	0
12	B	1218	CLA	1	0
20	B	5005	LMG	3	0
15	I	4018	BCR	5	0
12	B	1203	CLA	4	0
19	M	4021	ECH	5	0
17	B	4011	45D	5	0
12	B	1222	CLA	8	0
12	B	1234	CLA	8	0
12	B	1201	CLA	2	0
12	B	1022	CLA	3	0
15	B	4005	BCR	1	0
12	A	1112	CLA	5	0
13	B	2002	PQN	4	0
15	J	4013	BCR	9	0
21	F	5001	SQD	3	0
12	A	1110	CLA	1	0
12	A	1011	CLA	8	0
12	A	1109	CLA	11	0
12	A	1129	CLA	2	0
15	A	4008	BCR	5	0
25	I	4020	EQ3	1	0
12	A	1130	CLA	2	0
15	B	4017	BCR	1	0
12	A	1116	CLA	5	0
12	B	1239	CLA	2	0
15	A	4007	BCR	2	0
12	F	1301	CLA	3	0
15	A	4003	BCR	1	0
12	B	1205	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	4014	BCR	10	0
20	B	5002	LMG	4	0
12	A	1117	CLA	2	0
12	A	1108	CLA	1	0
12	B	1221	CLA	4	0
12	A	1136	CLA	1	0
14	A	3001	SF4	1	0
19	B	4006	ECH	4	0
12	B	1208	CLA	2	0
12	L	1502	CLA	4	0
12	A	1140	CLA	3	0
12	B	1226	CLA	1	0
12	A	1103	CLA	6	0
12	B	1210	CLA	5	0
12	B	1238	CLA	4	0
12	B	1228	CLA	2	0
12	A	1131	CLA	1	0
12	B	1220	CLA	4	0
12	A	1132	CLA	7	0
14	C	3002	SF4	1	0
15	B	4010	BCR	3	0
12	A	1101	CLA	3	0
12	A	1114	CLA	2	0
12	B	1215	CLA	2	0
12	B	1231	CLA	4	0
12	B	1225	CLA	3	0
12	A	1111	CLA	2	0
16	A	5001	LHG	2	0
12	A	1125	CLA	4	0
12	B	1235	CLA	6	0
12	B	1236	CLA	4	0
13	A	2001	PQN	2	0
12	A	1138	CLA	9	0
12	B	1214	CLA	5	0
12	A	1013	CLA	6	0
16	A	5003	LHG	3	0
12	B	1227	CLA	3	0
12	A	1134	CLA	3	0
12	A	1141	CLA	1	0
12	A	1126	CLA	10	0
12	B	1216	CLA	3	0
12	B	1212	CLA	1	0

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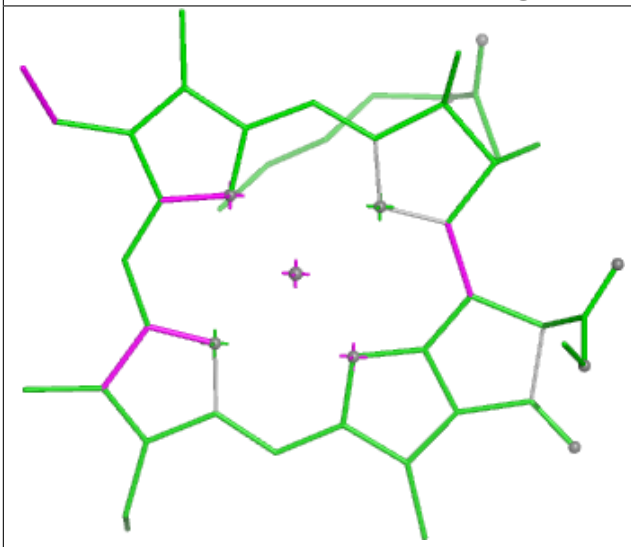
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	1206	CLA	4	0
12	A	1122	CLA	4	0
12	B	1229	CLA	5	0
12	B	1223	CLA	3	0
12	A	1107	CLA	8	0
24	F	6001	LMT	1	0
12	B	1207	CLA	5	0
12	B	1023	CLA	6	0
12	B	1219	CLA	1	0
15	B	4004	BCR	2	0
15	B	4018	BCR	3	0
12	A	1135	CLA	4	0
12	A	1118	CLA	2	0
15	K	4001	BCR	6	0
12	B	1211	CLA	3	0
12	A	1012	CLA	4	0
12	A	1133	CLA	3	0
12	A	1102	CLA	6	0
12	A	1123	CLA	3	0
12	A	1128	CLA	6	0
23	F	4016	C7Z	1	0
12	A	1119	CLA	4	0
12	A	1137	CLA	1	0
12	B	1224	CLA	7	0
12	A	1139	CLA	4	0
15	A	4001	BCR	5	0
12	K	1401	CLA	1	0
12	B	1213	CLA	1	0
15	A	4012	BCR	8	0

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

Ligand CLA A 1120



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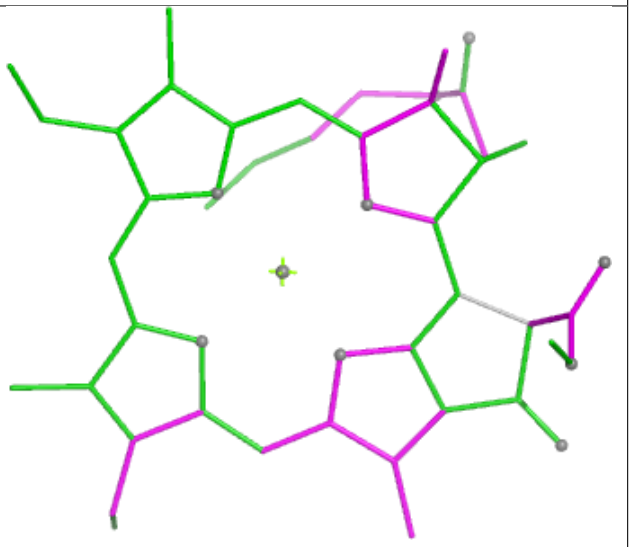
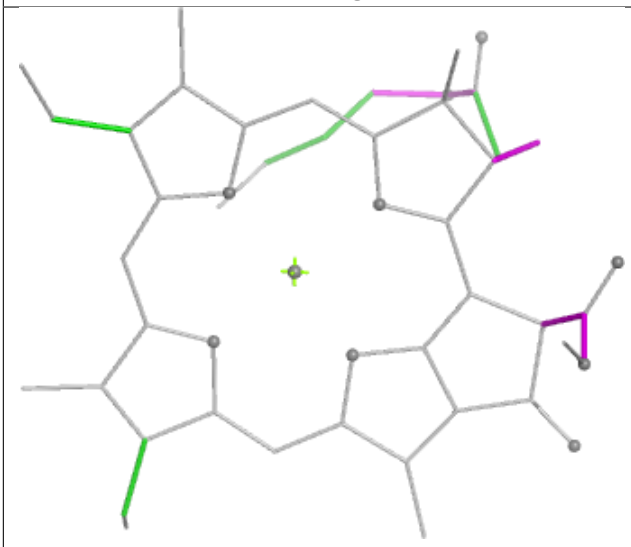
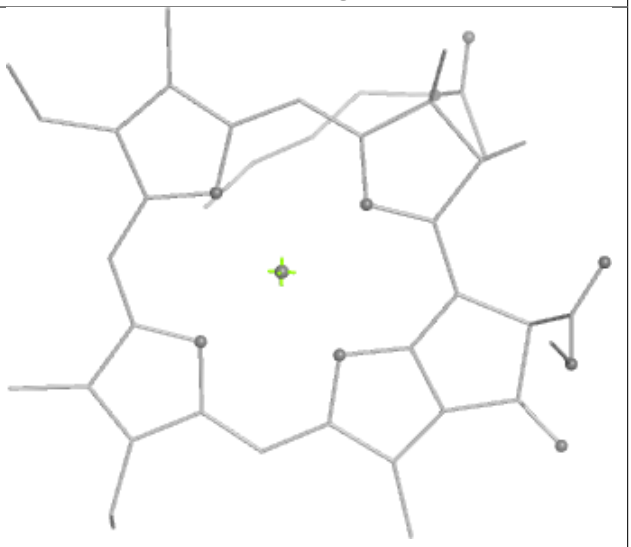


Bond angles

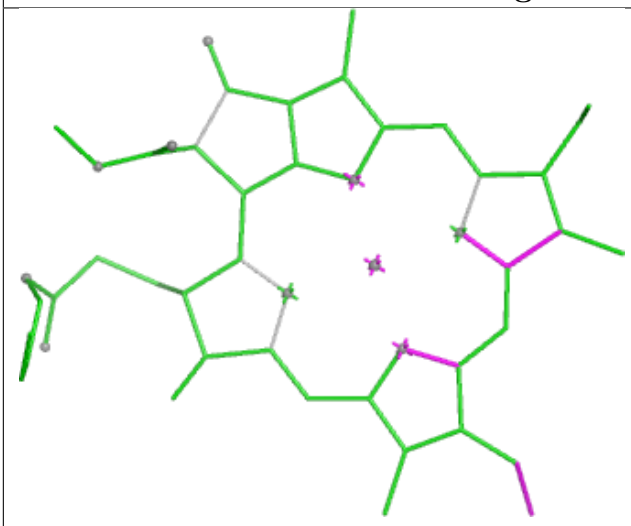


Torsions

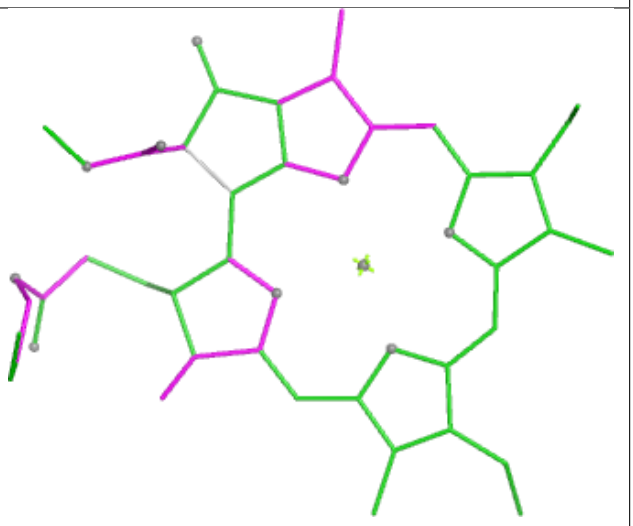


Rings

Ligand CLA A 1104



Bond lengths



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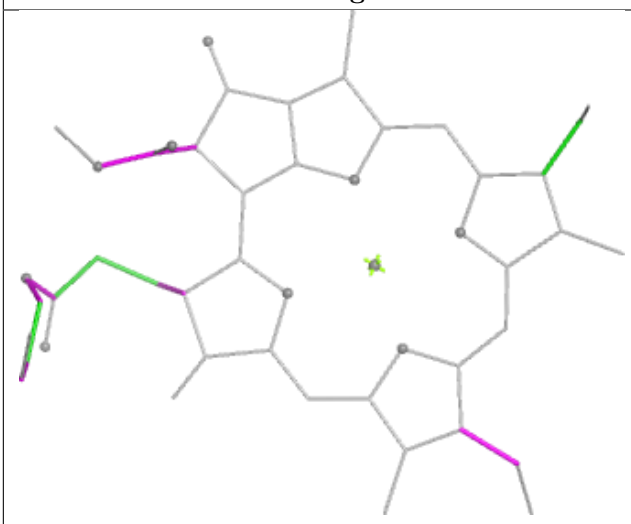

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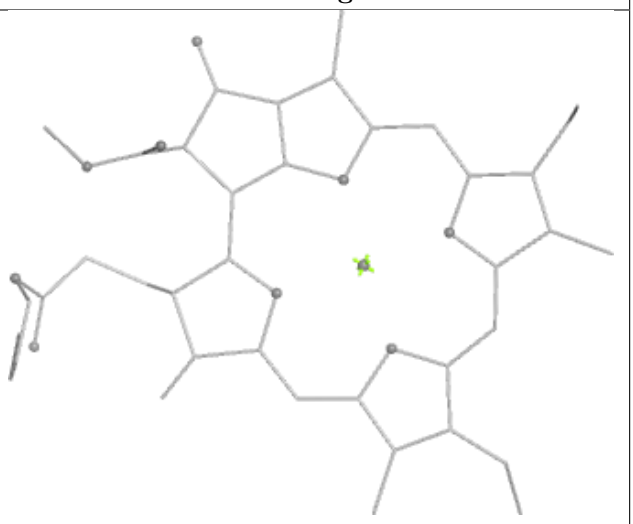
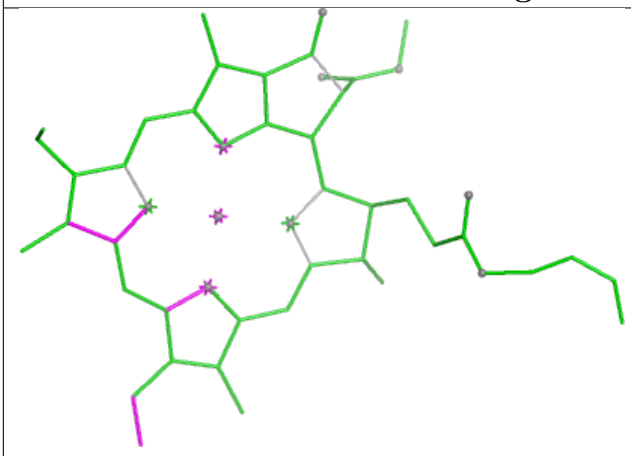


Rings

Ligand CLA A 1124



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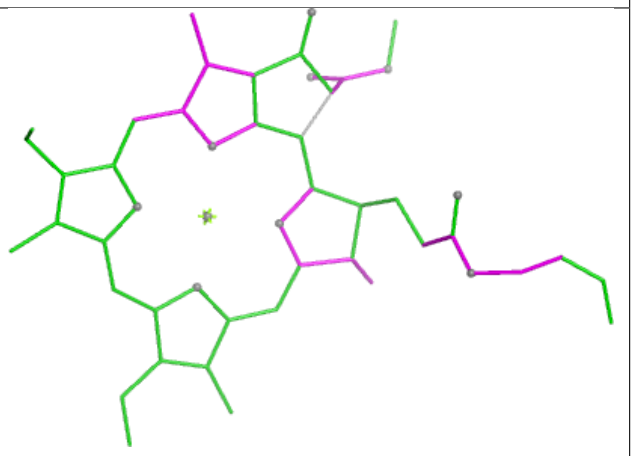
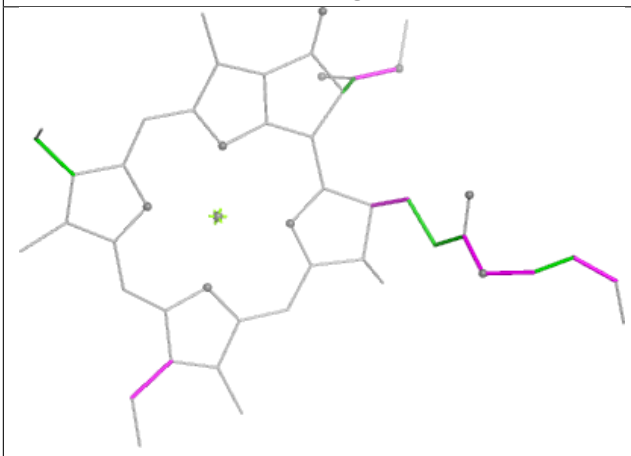
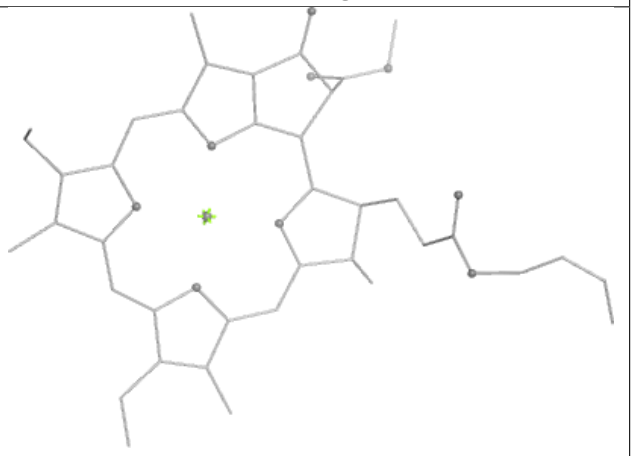


Bond angles

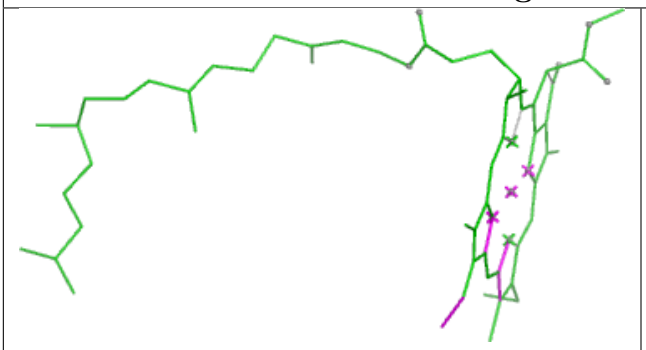


Torsions



Rings

Ligand CLA A 1105



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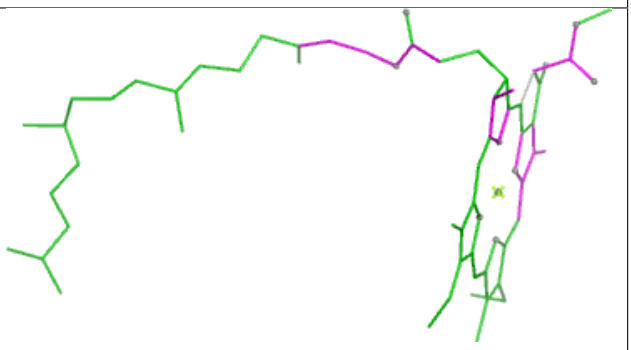

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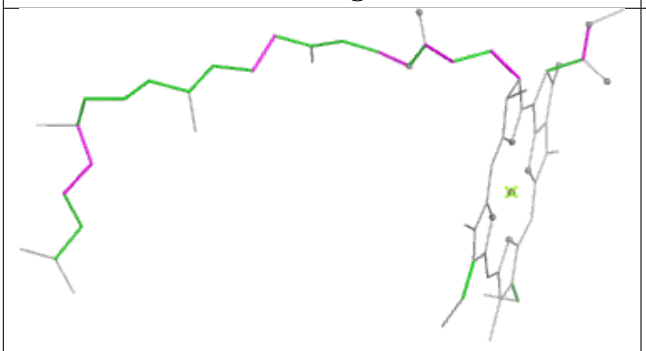
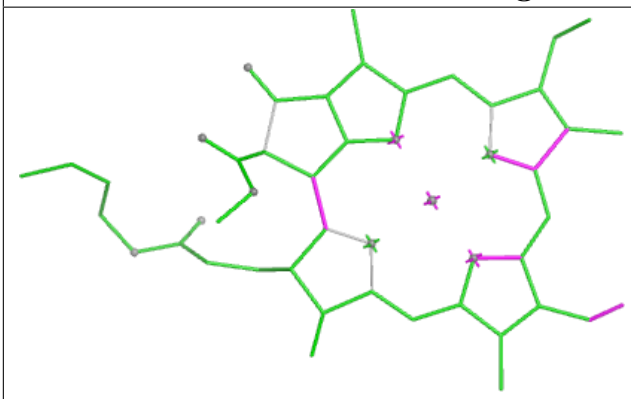


Torsions



Rings

Ligand CLA B 1240



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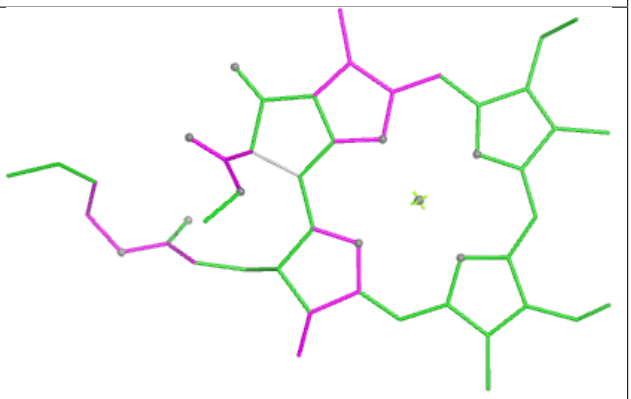

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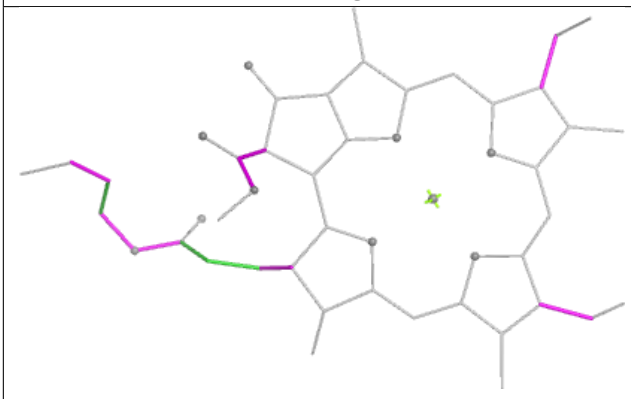
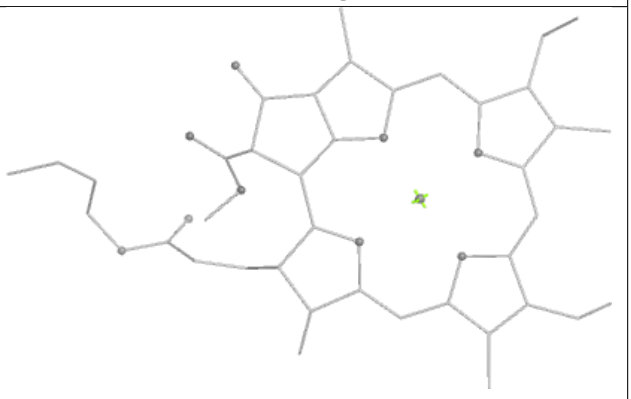
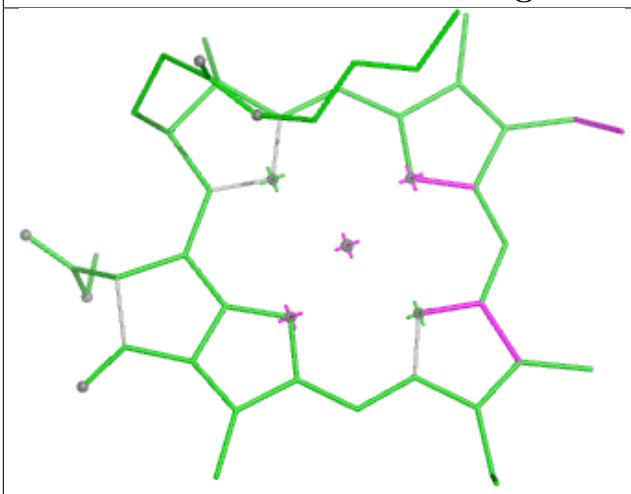


Torsions



Rings

Ligand CLA B 1217



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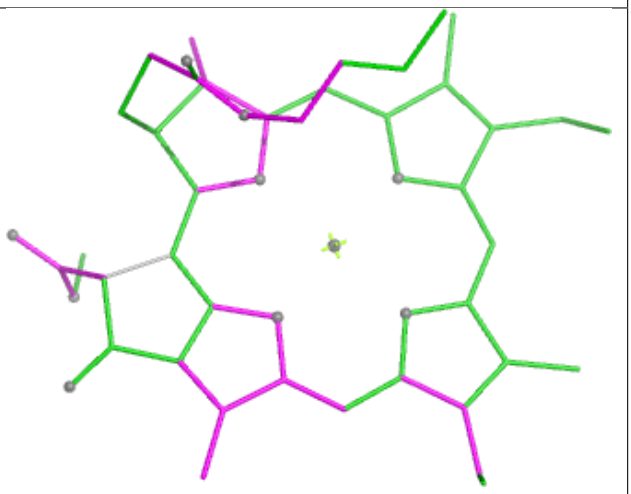

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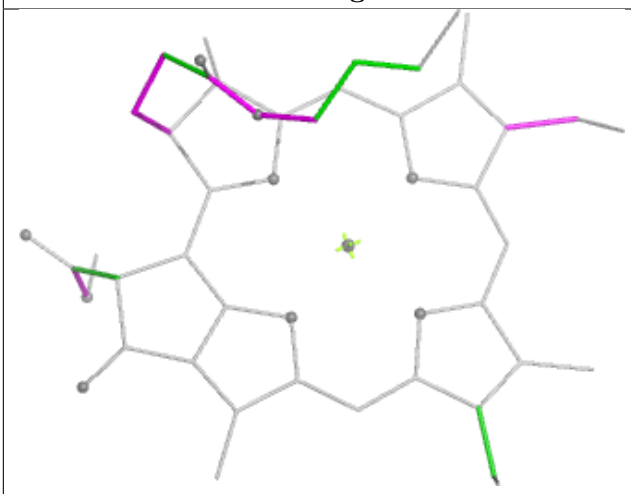

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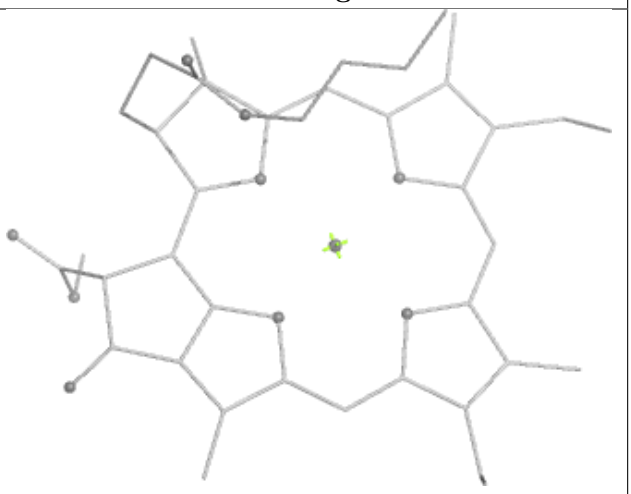
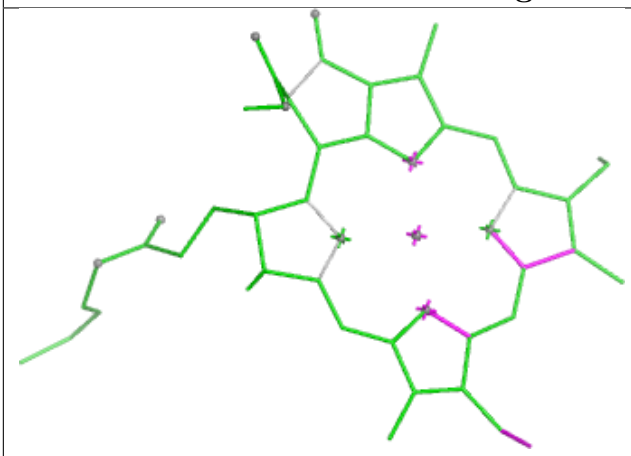


Rings

Ligand CLA B 1230



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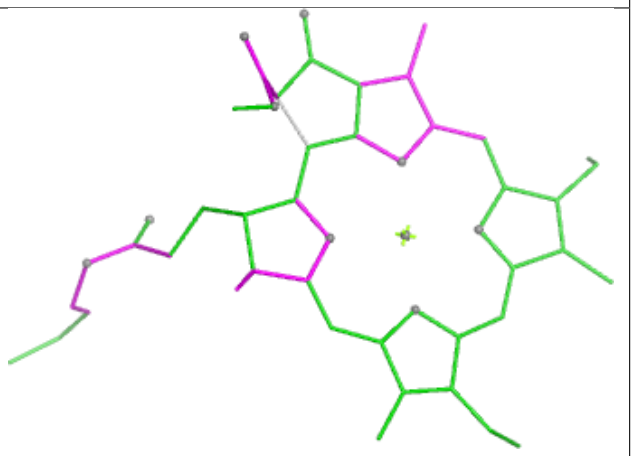

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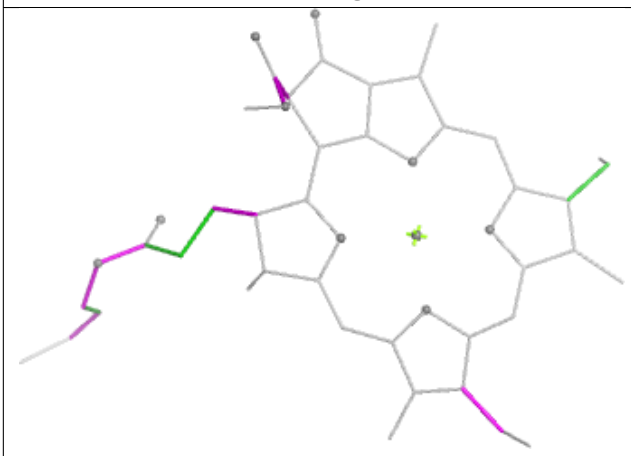

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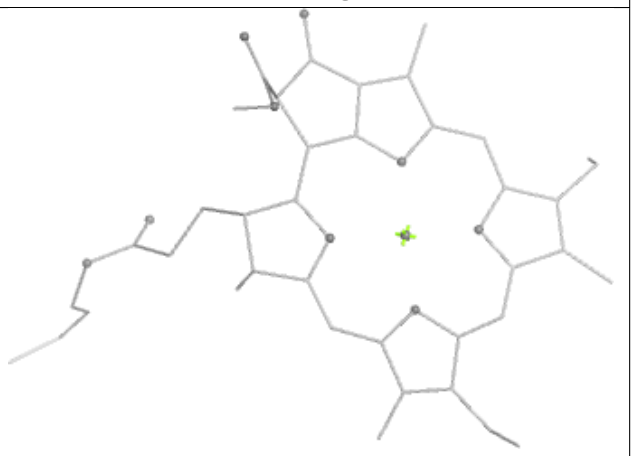
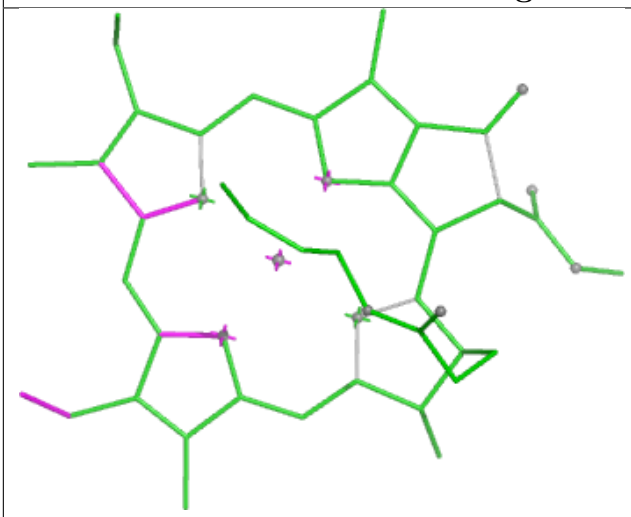


Rings

Ligand CLA B 1204



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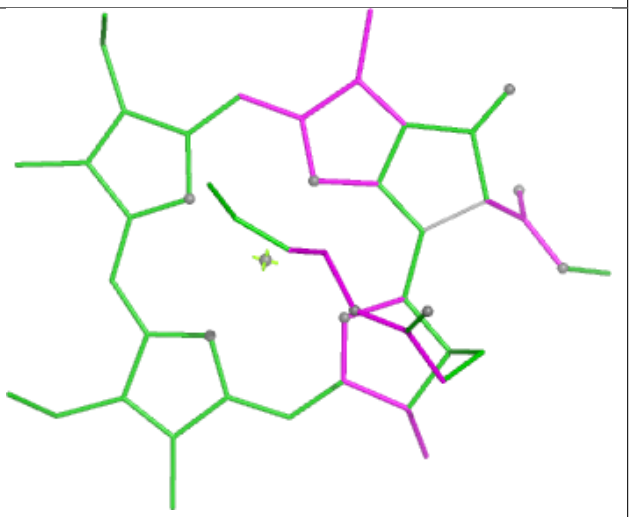
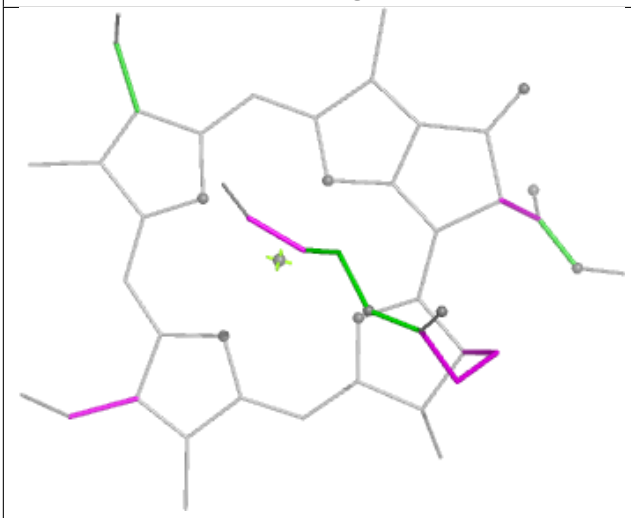


Bond angles



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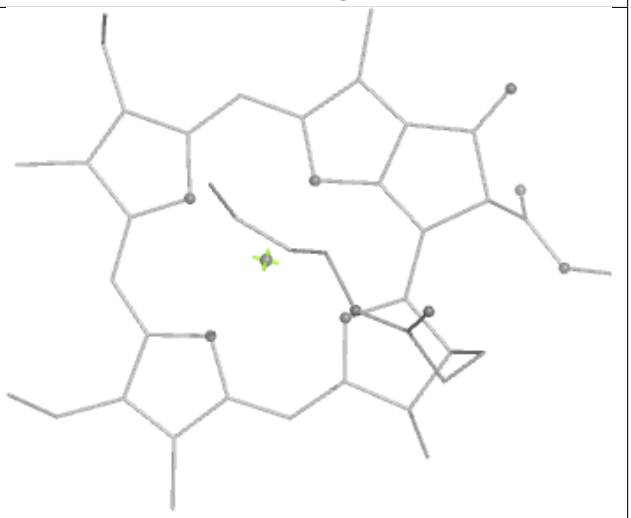
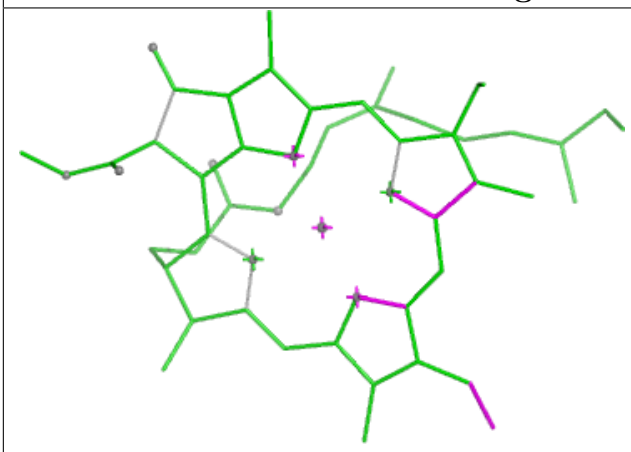


Rings

Ligand CLA A 1115



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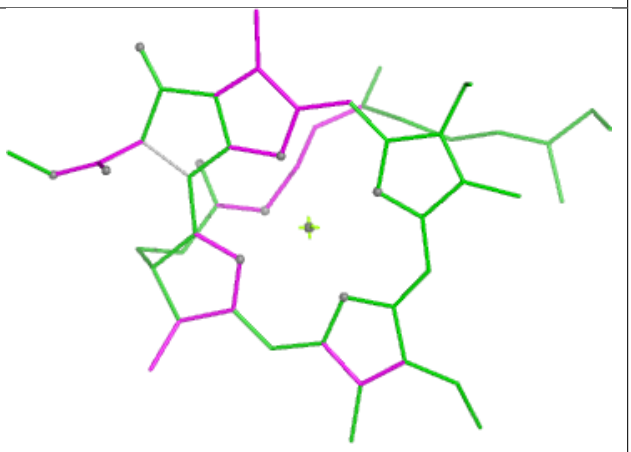
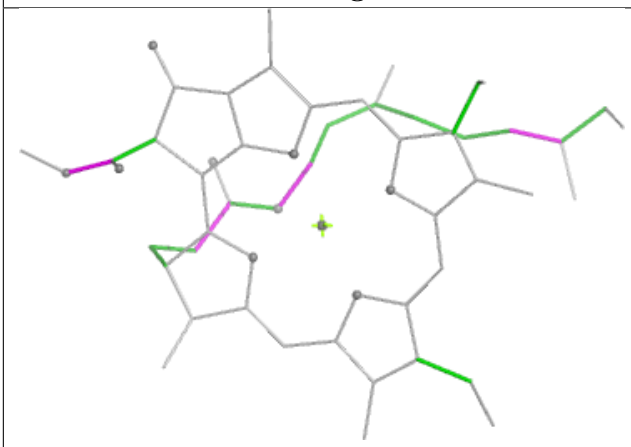


Bond angles



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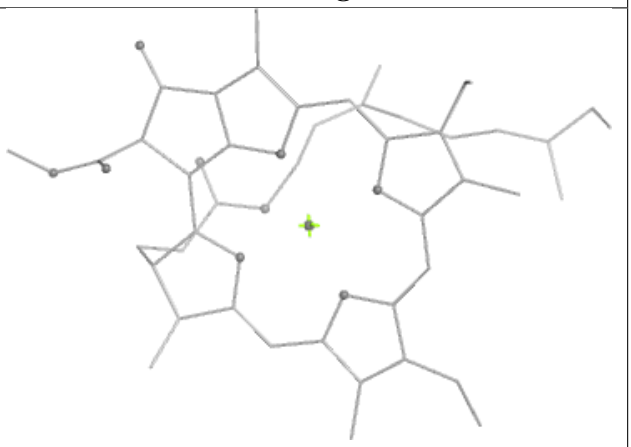
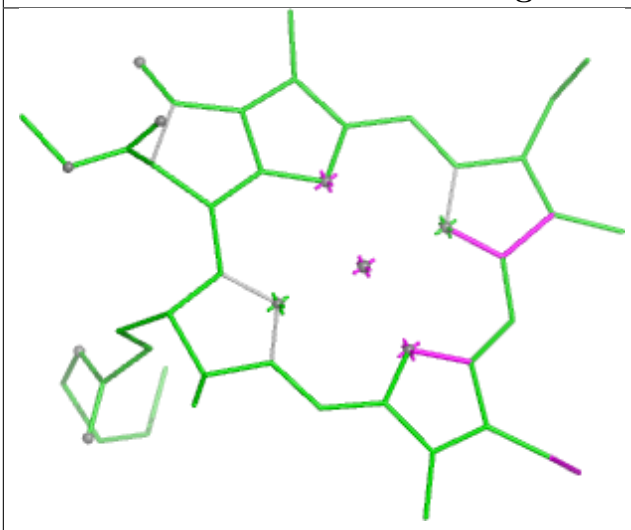


Rings

Ligand CLA B 1232



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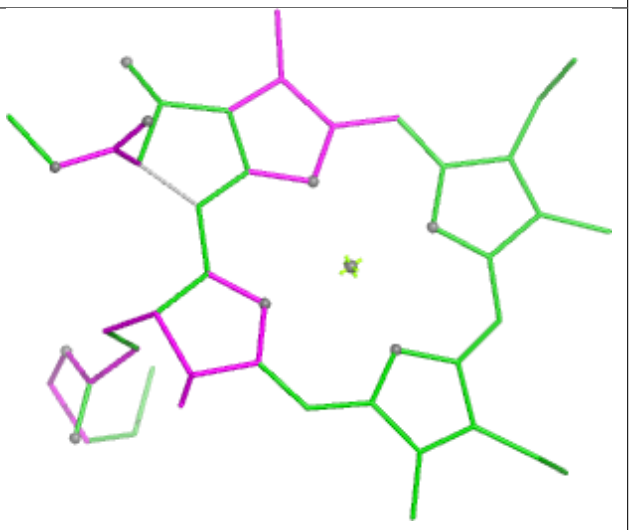
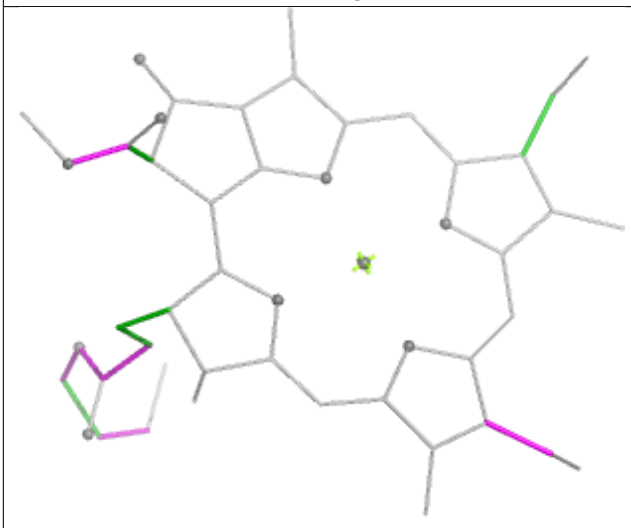


Bond angles



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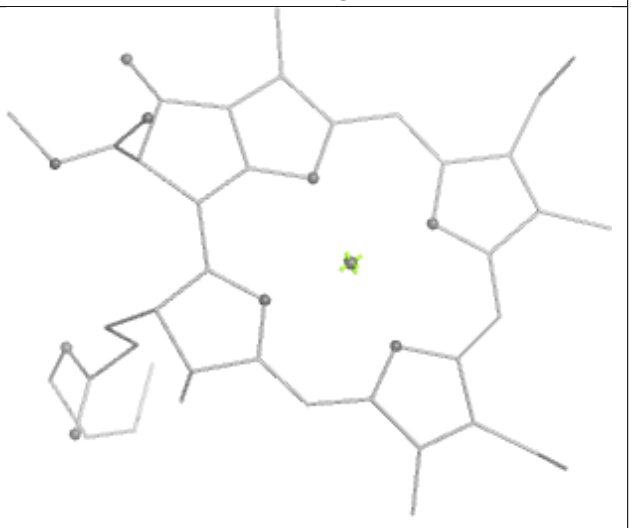
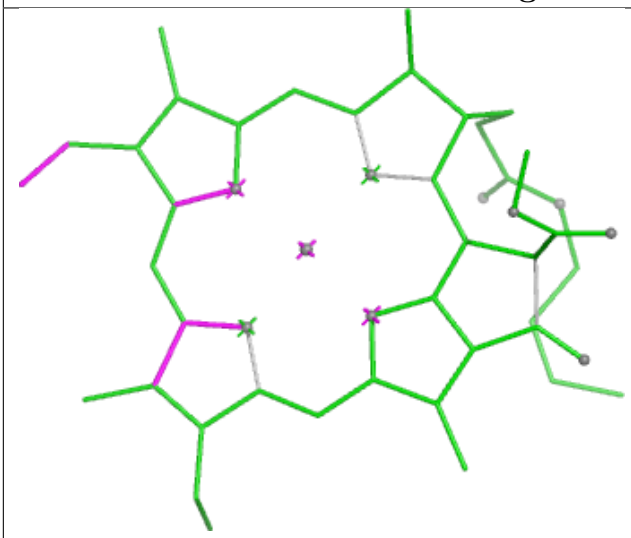
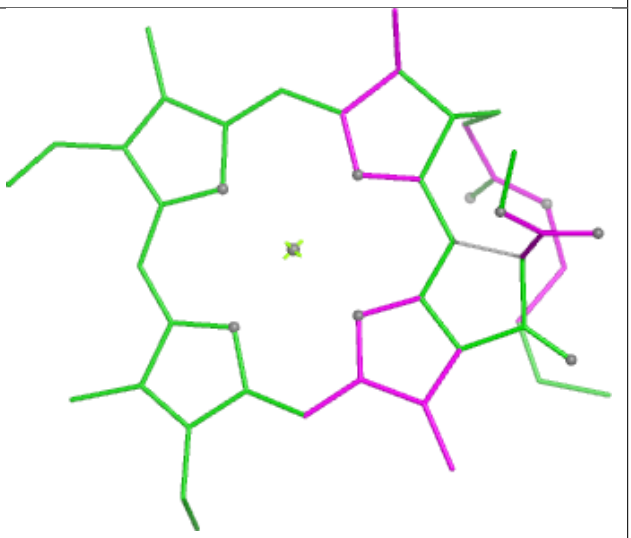


Rings

Ligand CLA J 1302



Bond lengths



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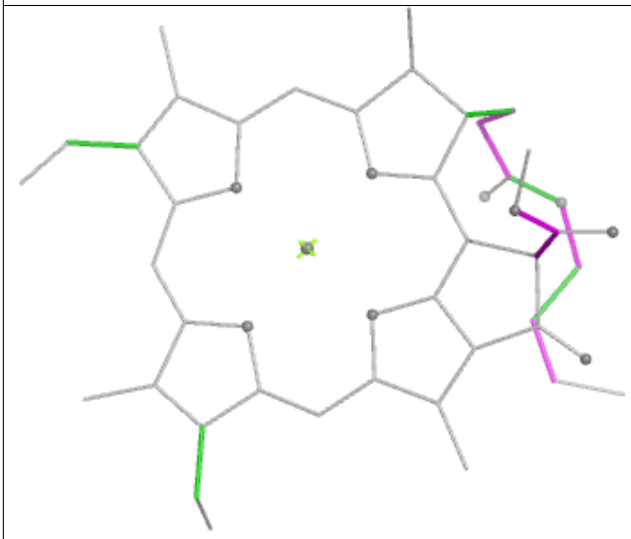

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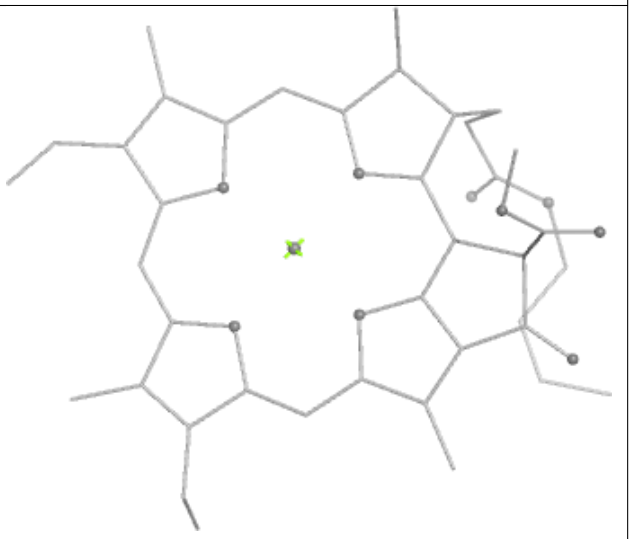
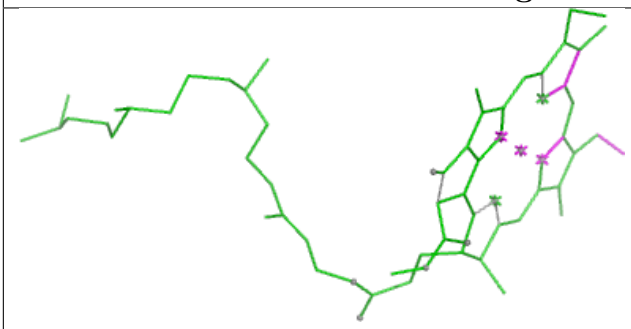
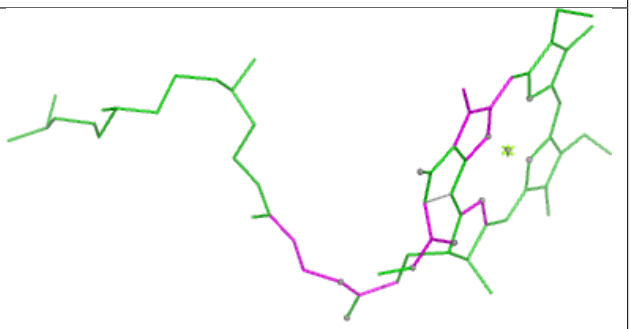


Rings

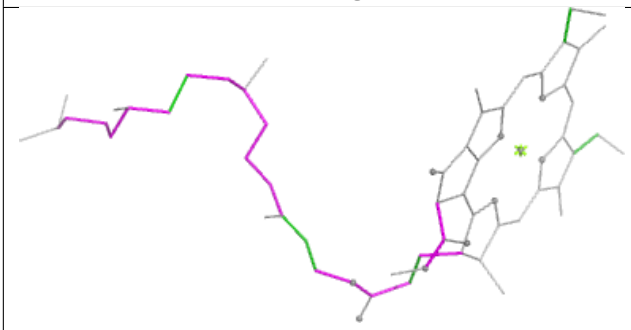
Ligand CLA B 1021



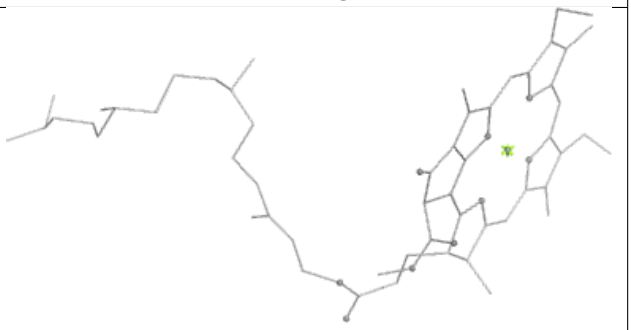
Bond lengths



Bond angles

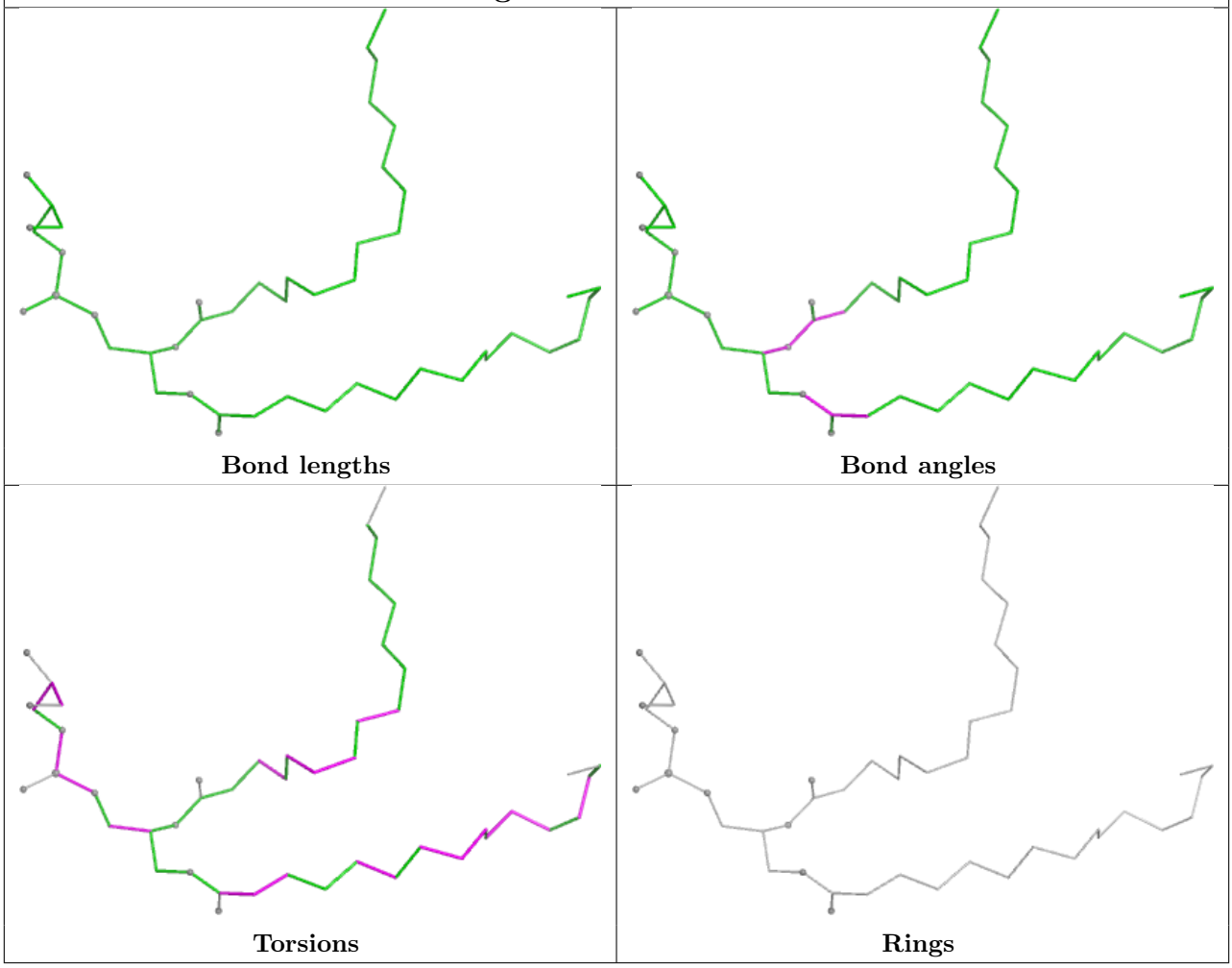


Torsions

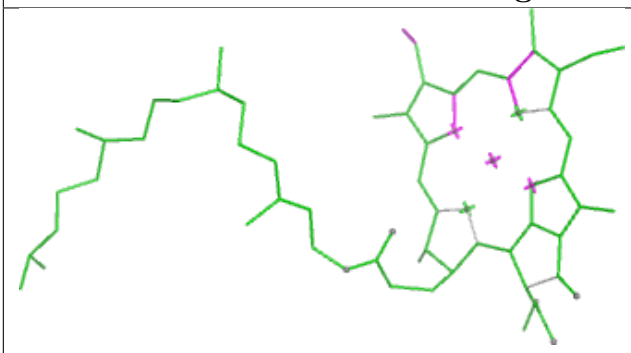


Rings

Ligand LHG B 5004



Ligand CLA A 1106



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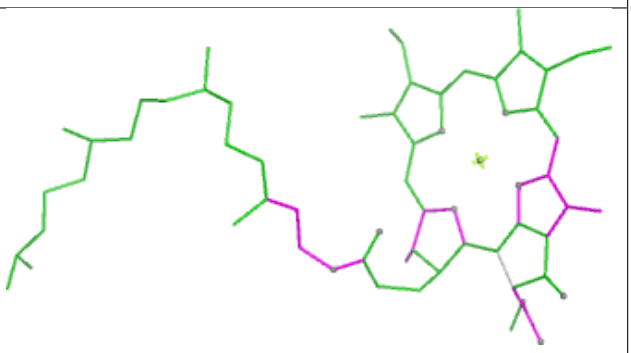
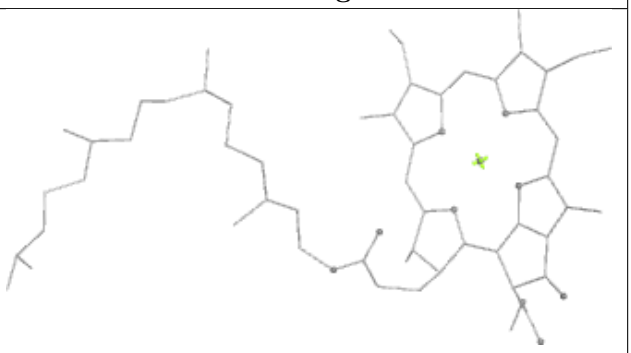


Bond angles

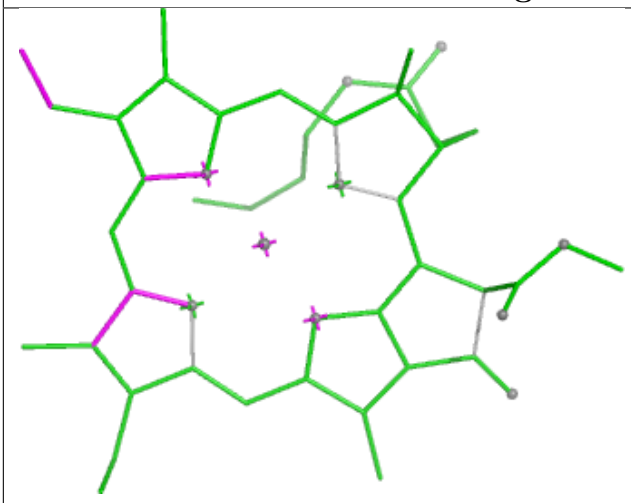


Torsions

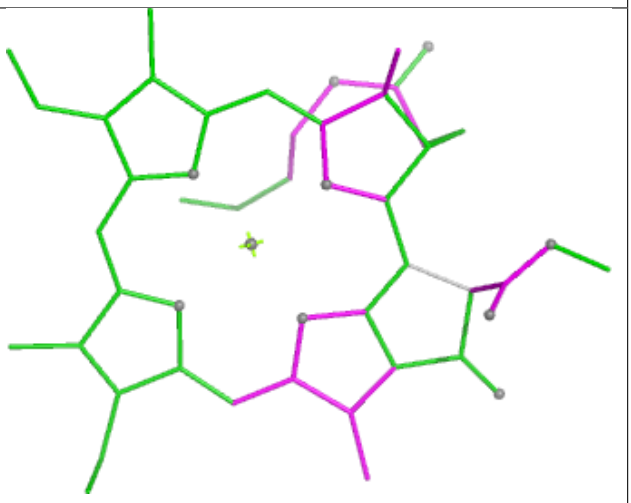


Rings

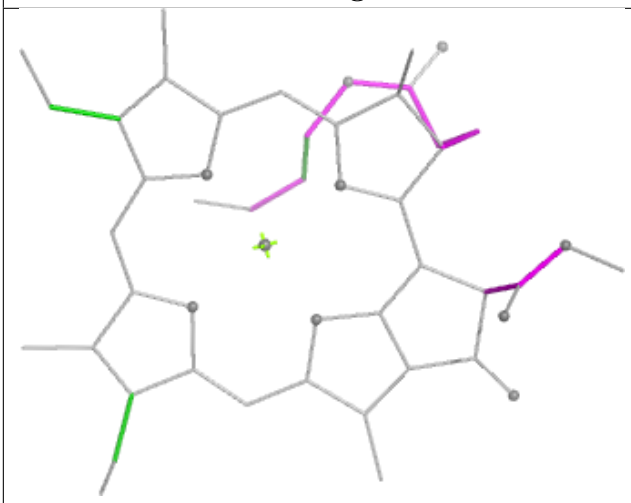
Ligand CLA A 1121



Bond lengths



Bond angles



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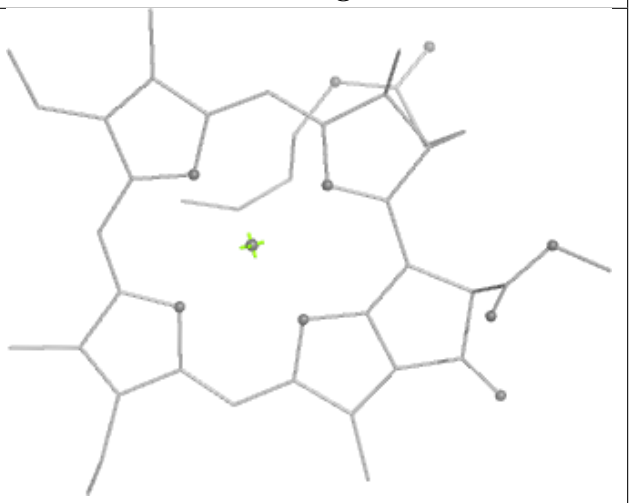
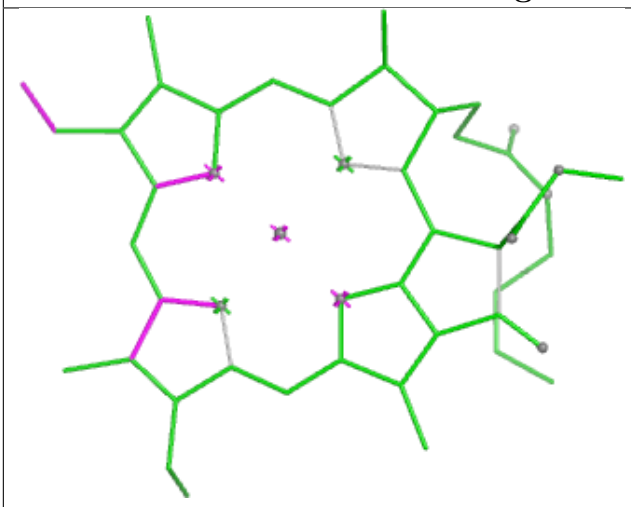


Rings

Ligand CLA A 1127



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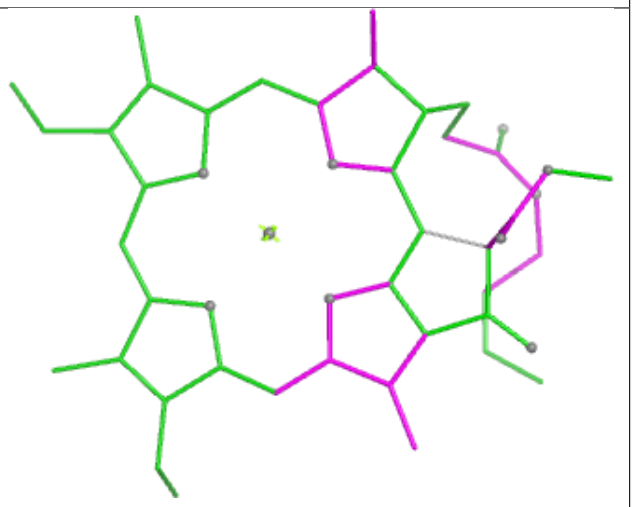
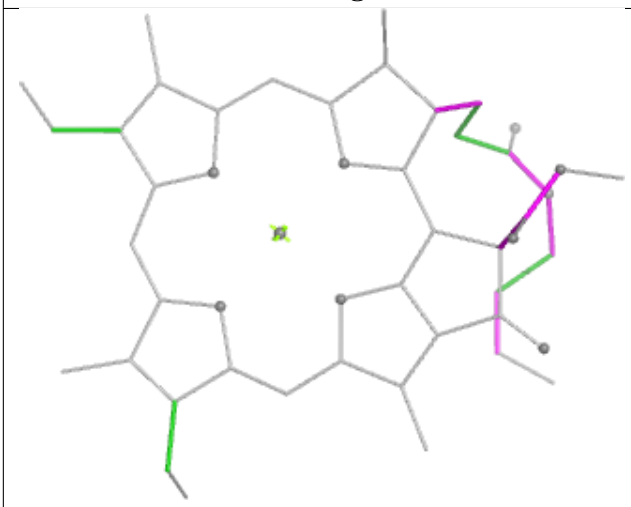


Bond angles



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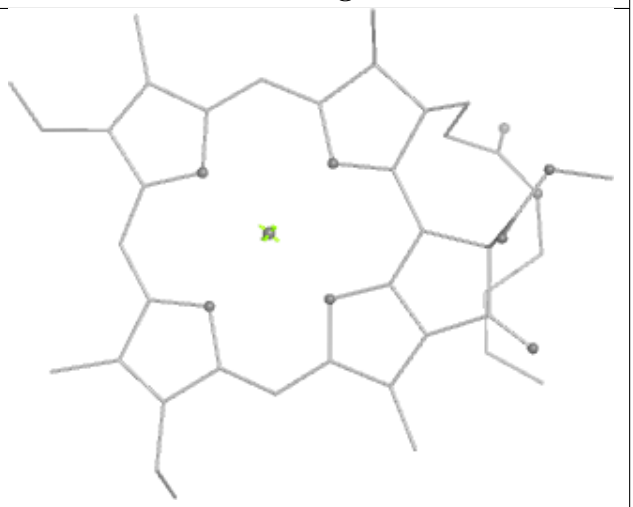
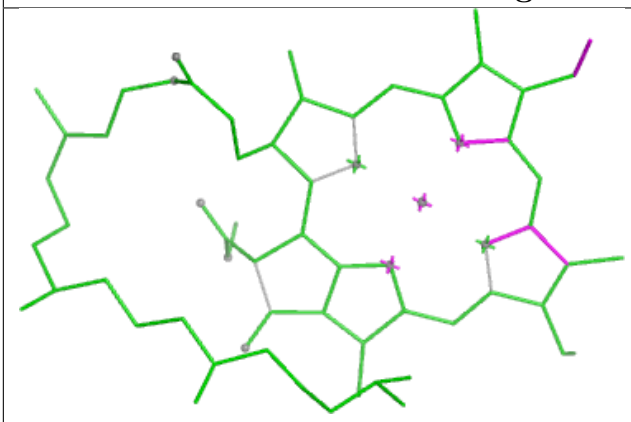
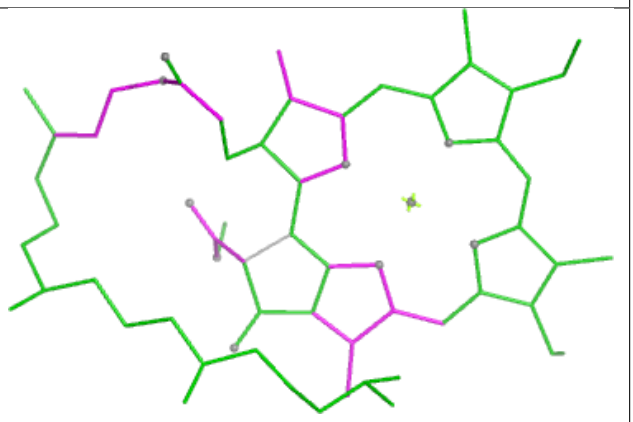


Rings

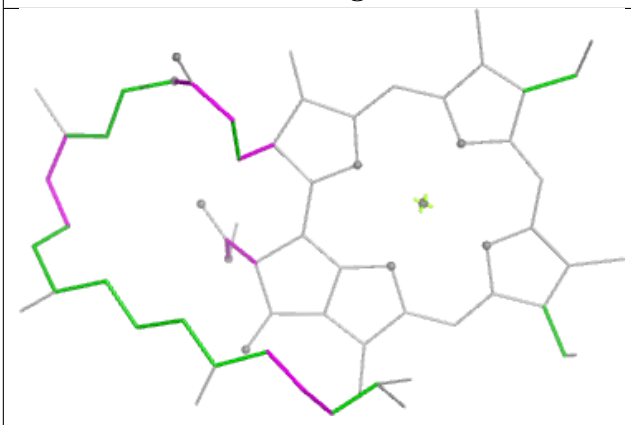
Ligand CLA B 1202



Bond lengths



Bond angles



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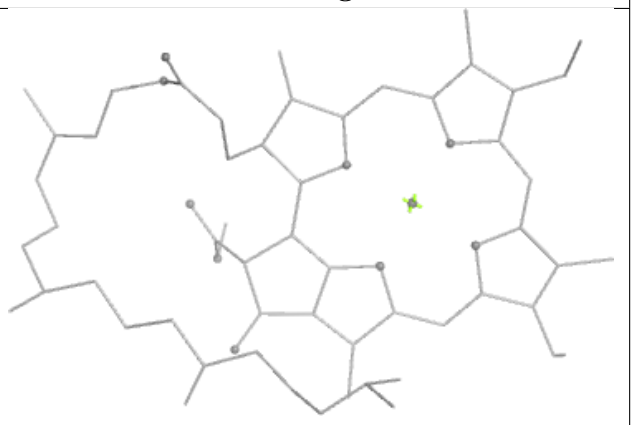
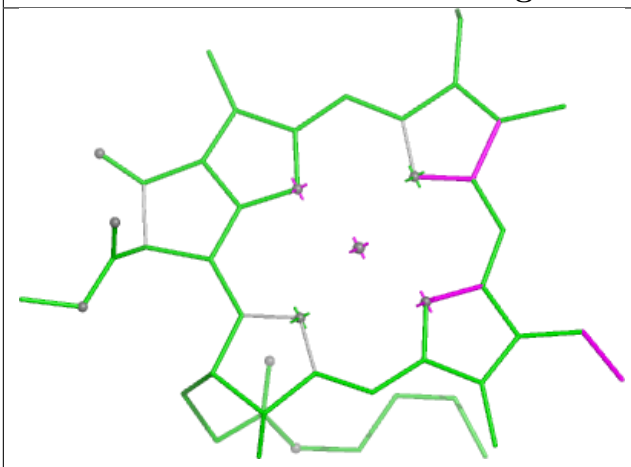


Rings

Ligand CLA B 1218



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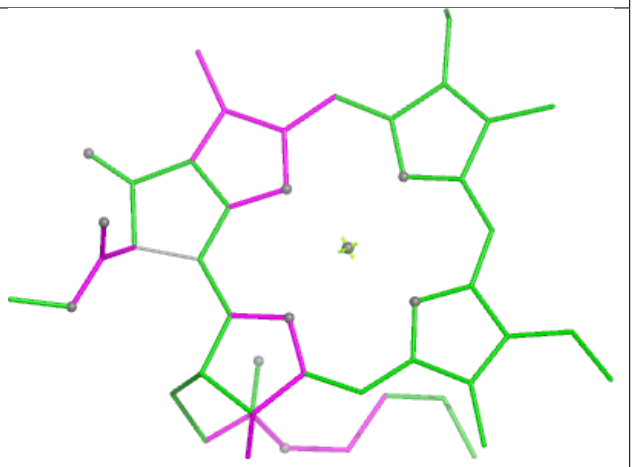
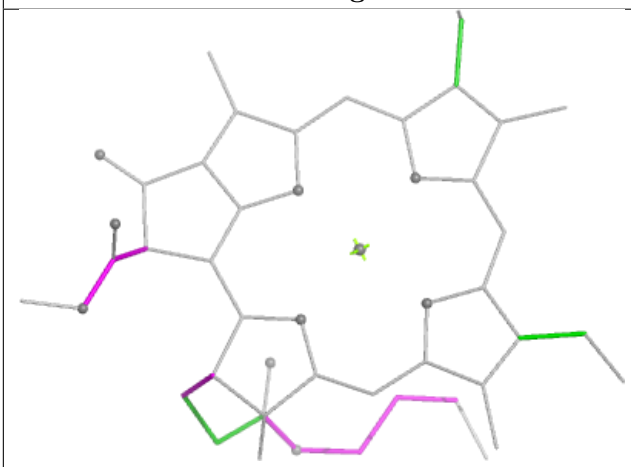


Bond angles



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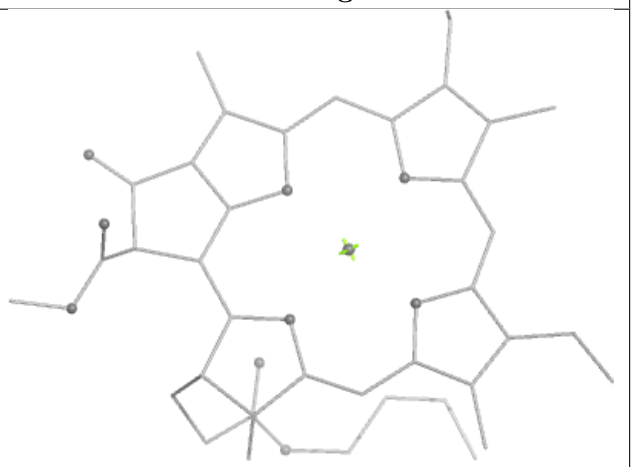
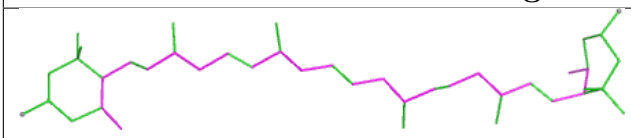


Rings

Ligand C7Z J 4015



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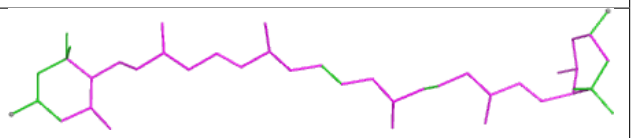
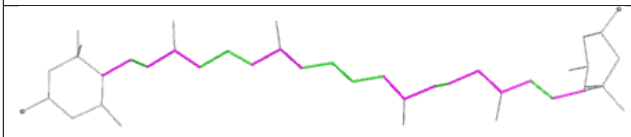


Bond angles



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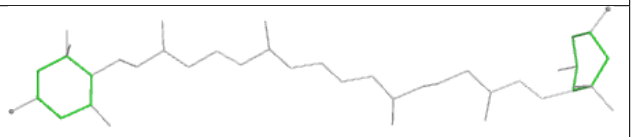
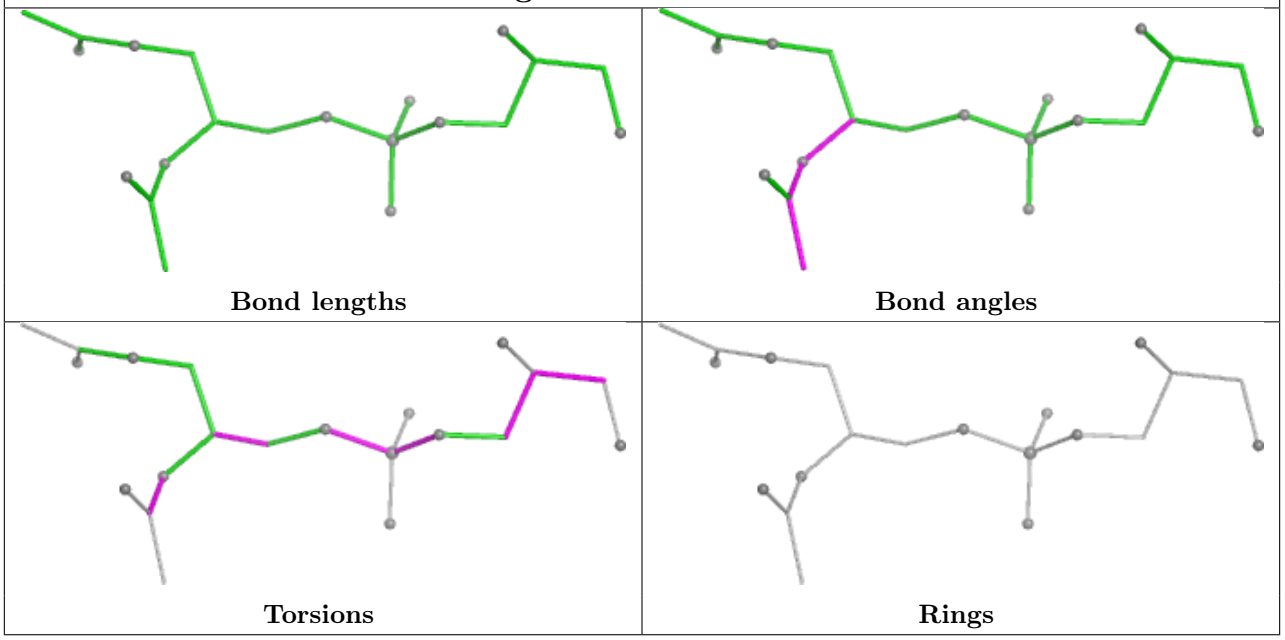
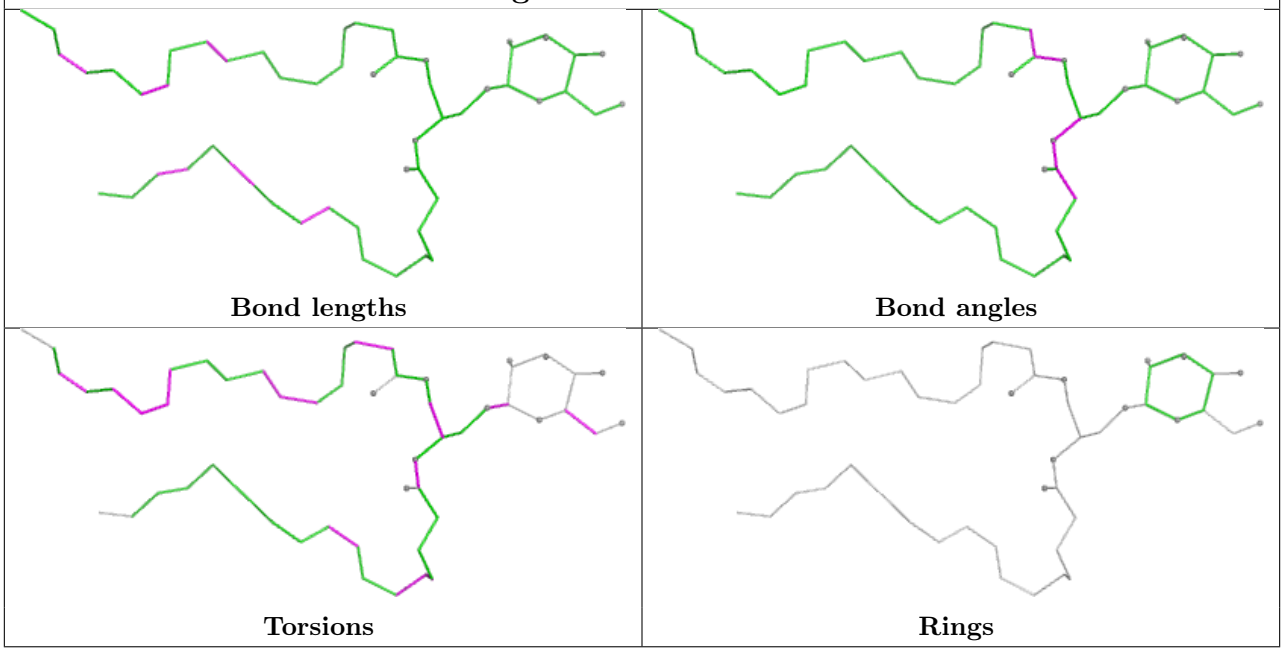


Rings

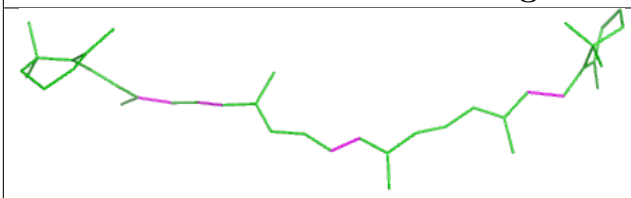
Ligand LHG B 5006



Ligand LMG B 5005



Ligand BCR I 4018



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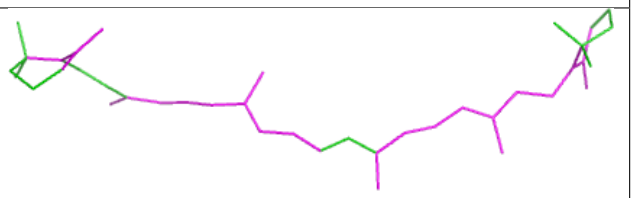
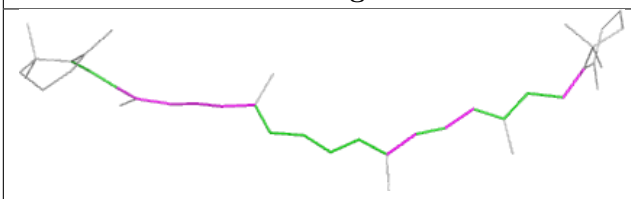


Bond angles



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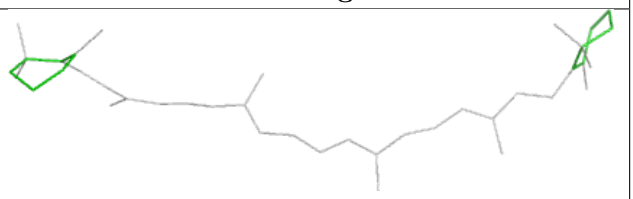
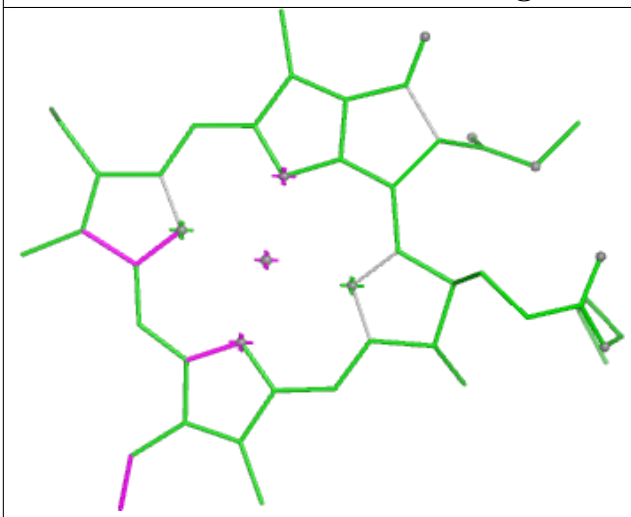
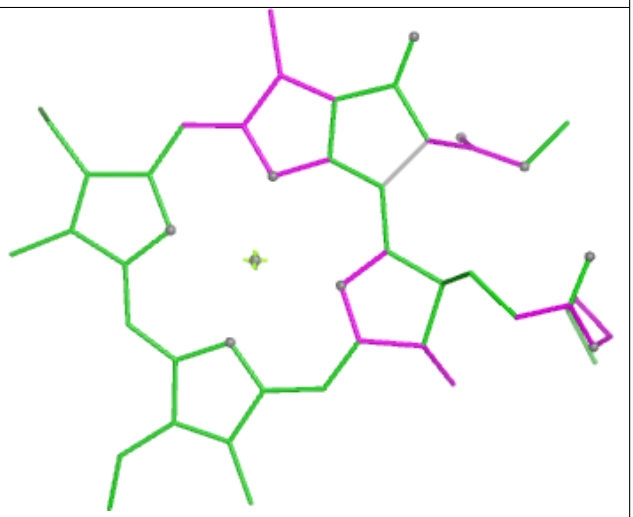


Rings

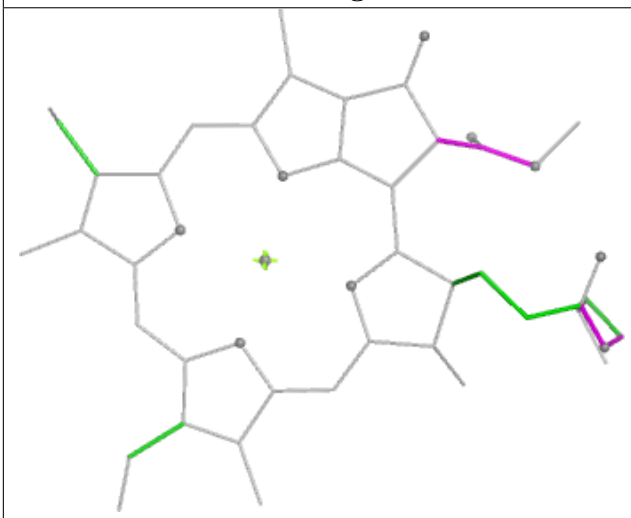
Ligand CLA B 1203



Bond lengths



Bond angles



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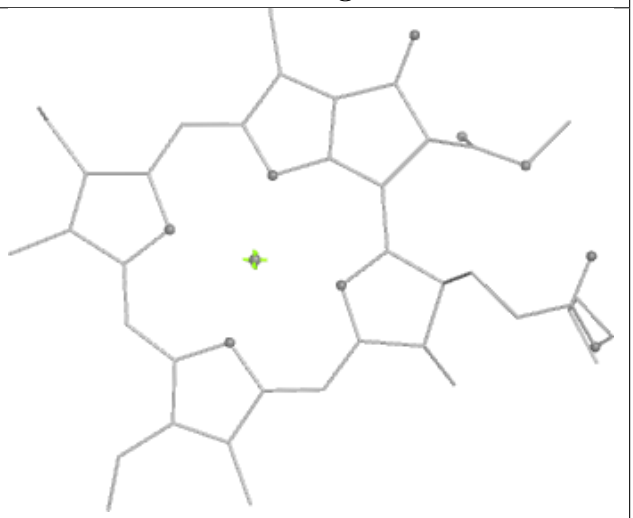
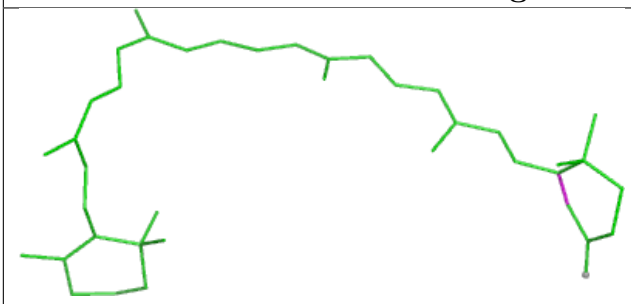


Rings

Ligand ECH M 4021



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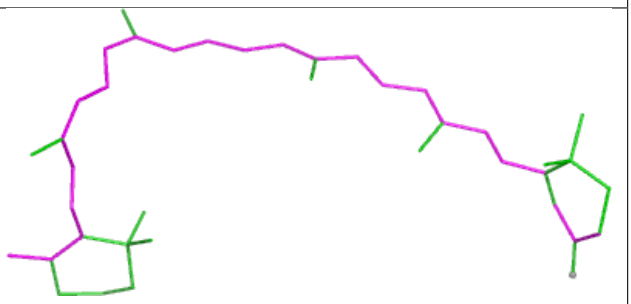
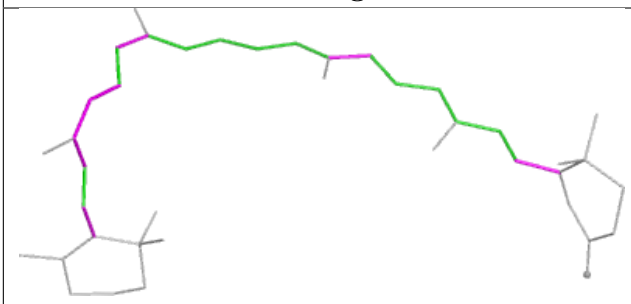


Bond angles



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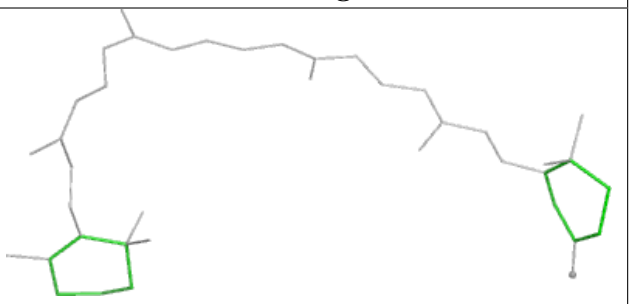
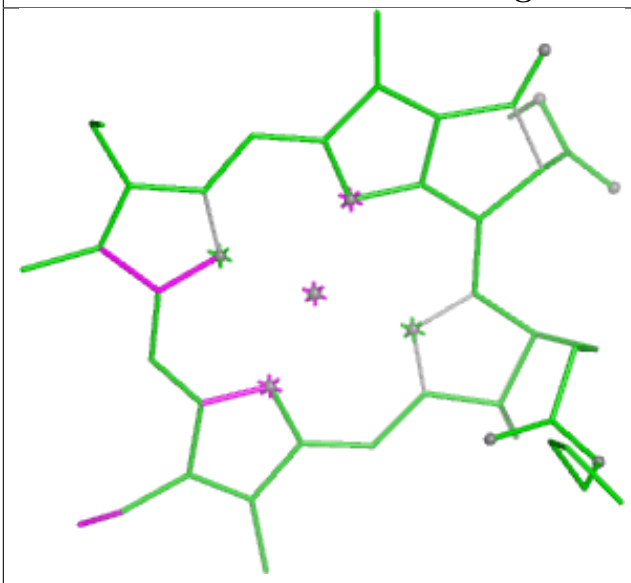


Rings

Ligand CLA A 1113



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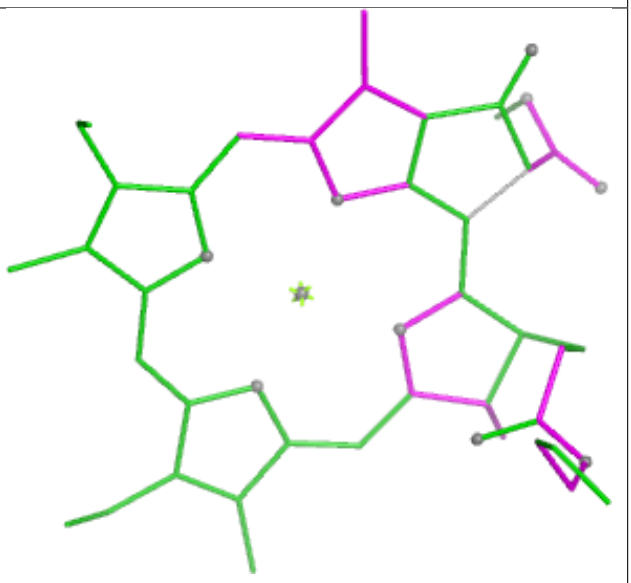
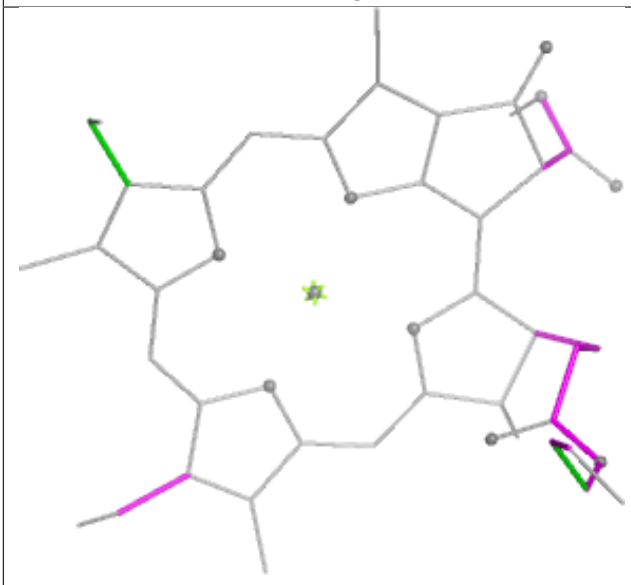


Bond angles



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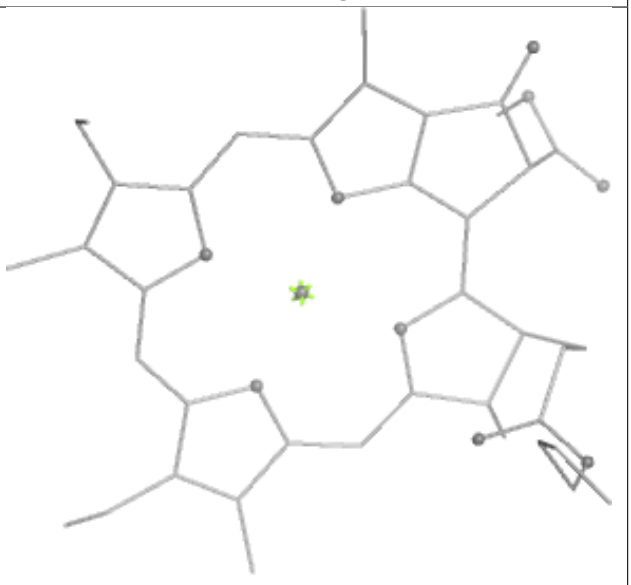
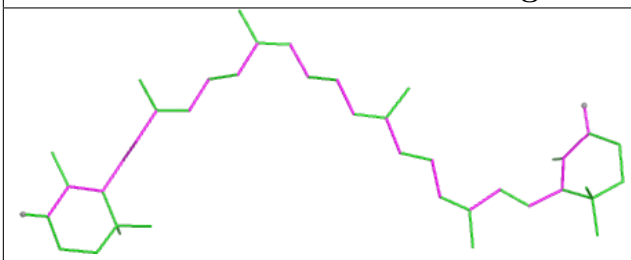


Rings

Ligand 45D B 4011



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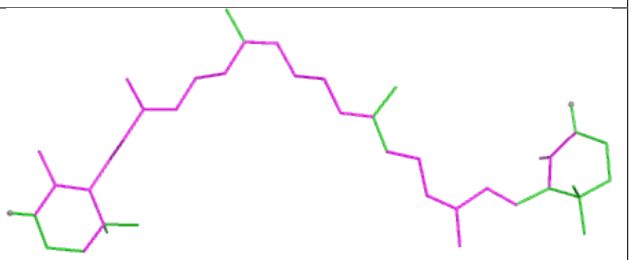
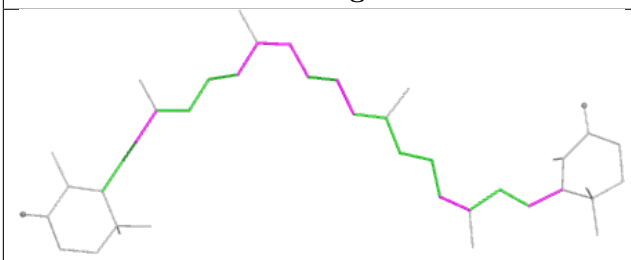


Bond angles



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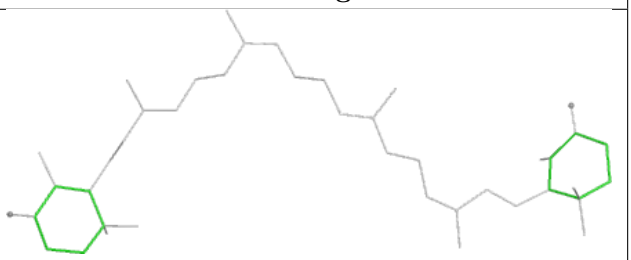
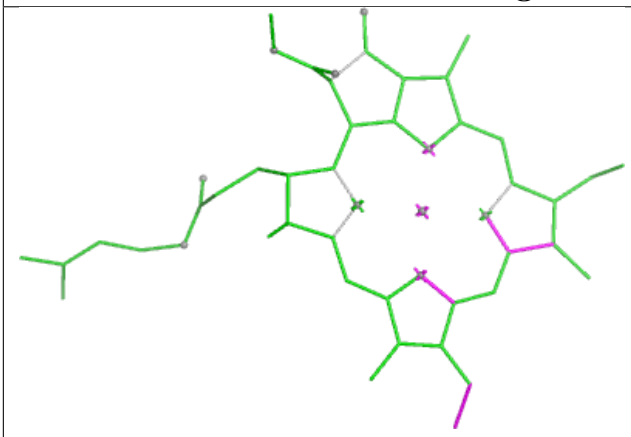
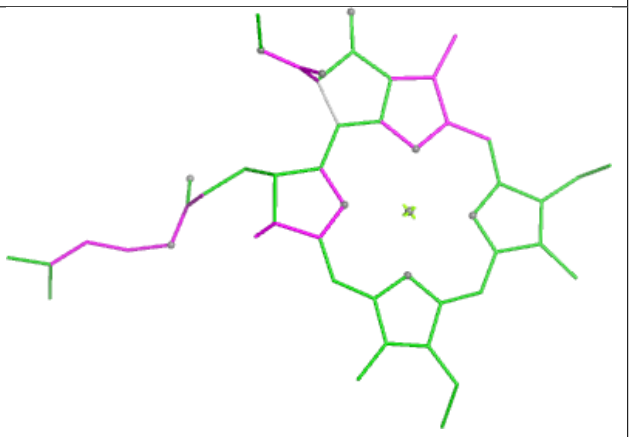


Rings

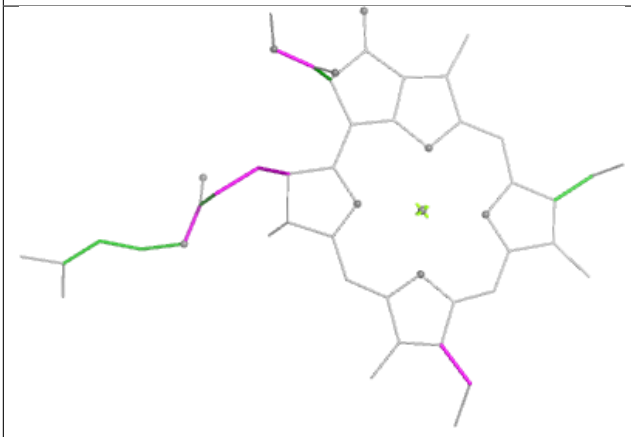
Ligand CLA B 1222



Bond lengths



Bond angles



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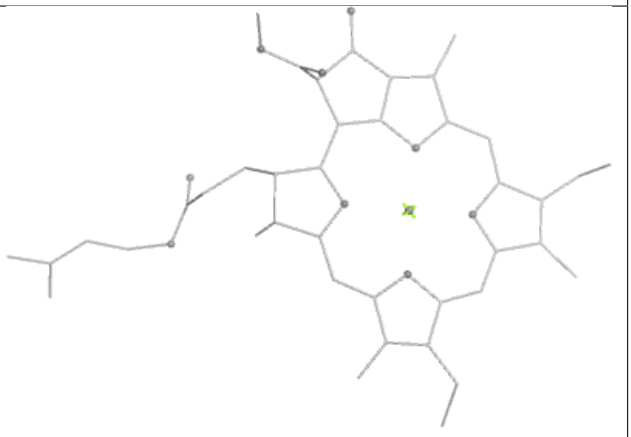
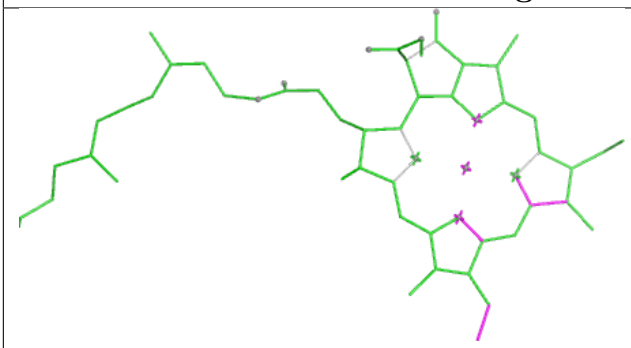
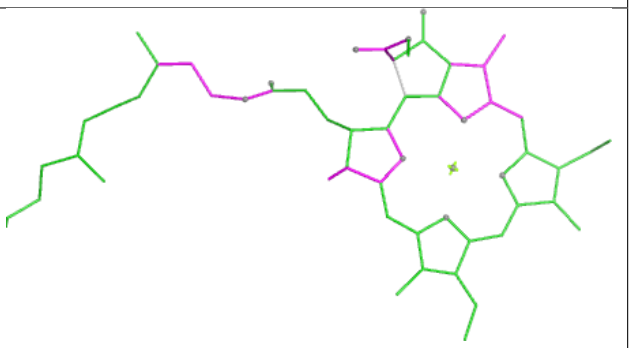


Rings

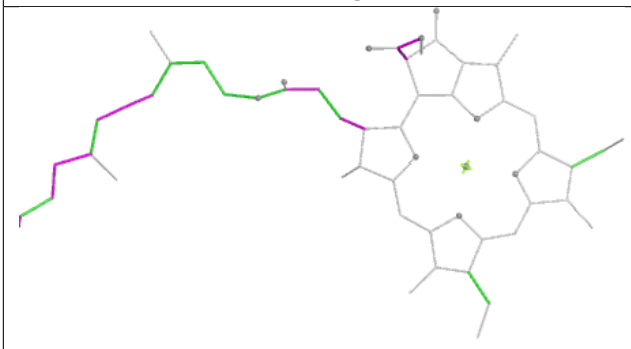
Ligand CLA B 1234



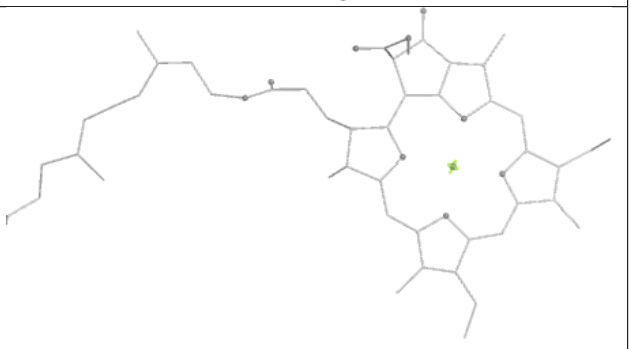
Bond lengths



Bond angles

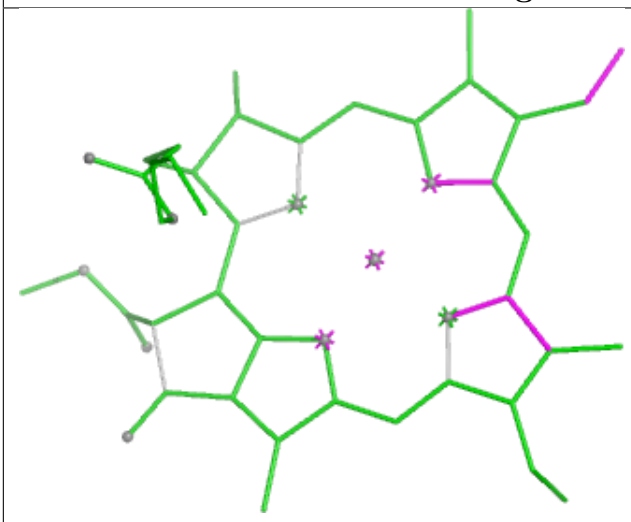


Torsions

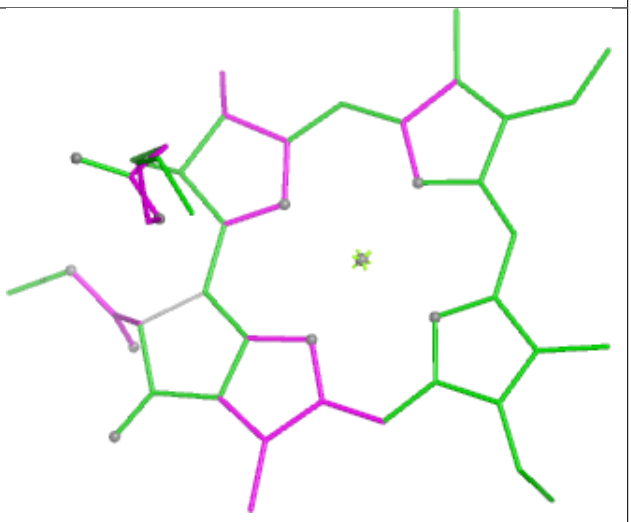


Rings

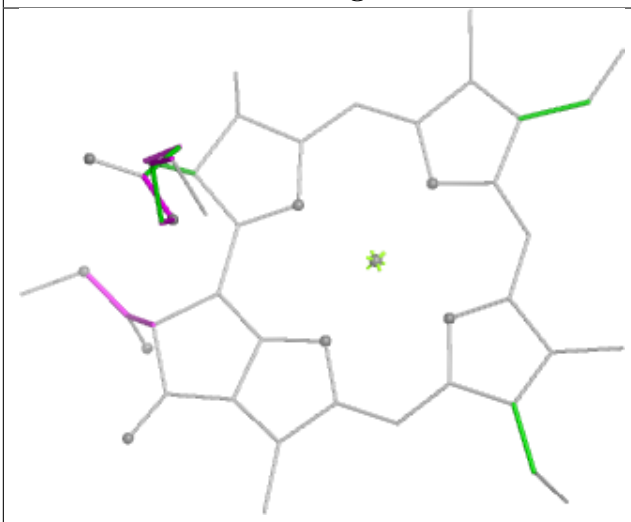
Ligand CLA B 1201



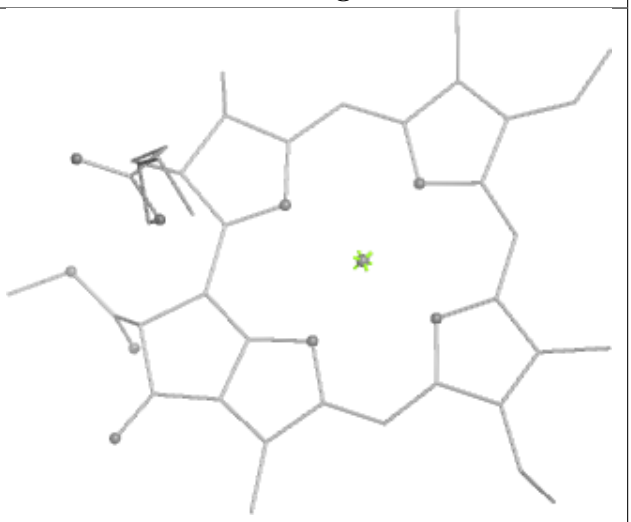
Bond lengths



Bond angles

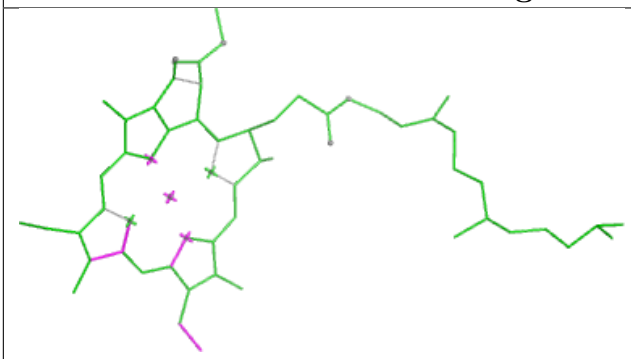


Torsions

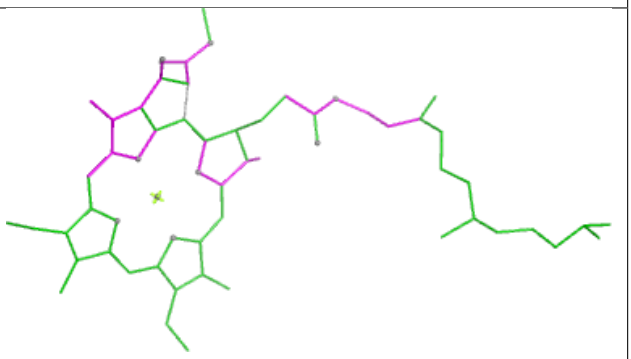


Rings

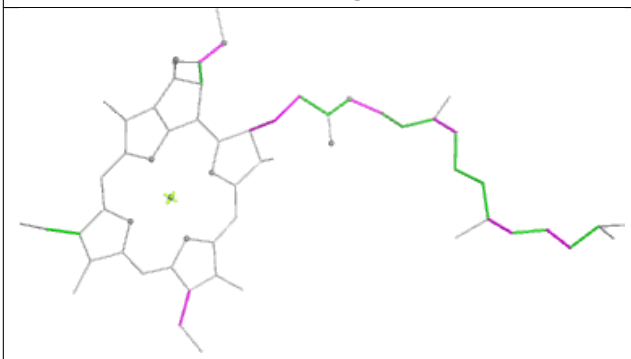
Ligand CLA B 1022



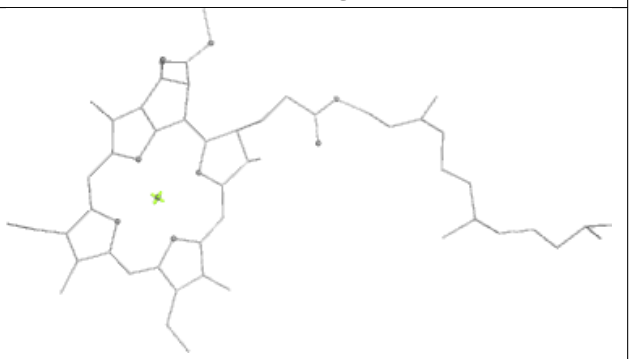
Bond lengths



Bond angles

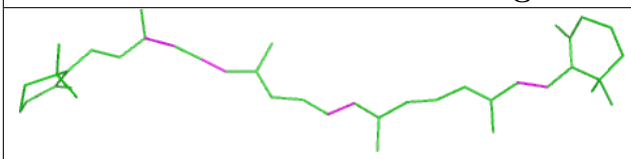


Torsions



Rings

Ligand BCR B 4005



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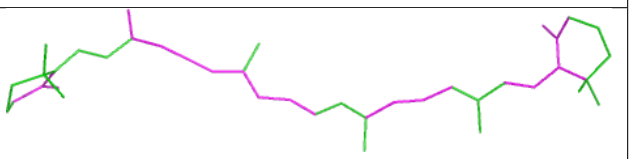
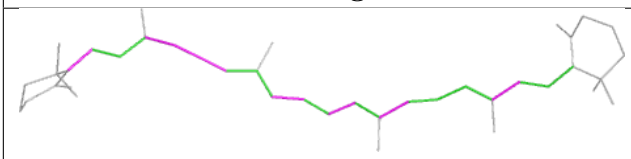
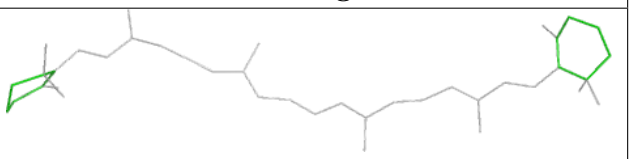


Bond angles

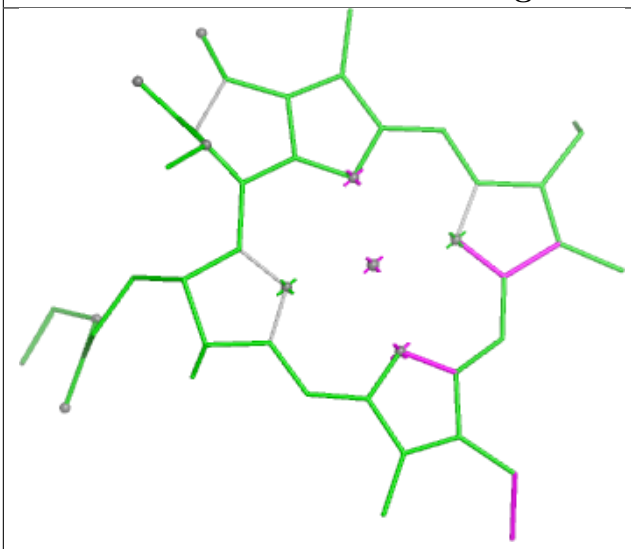


Torsions



Rings

Ligand CLA A 1112



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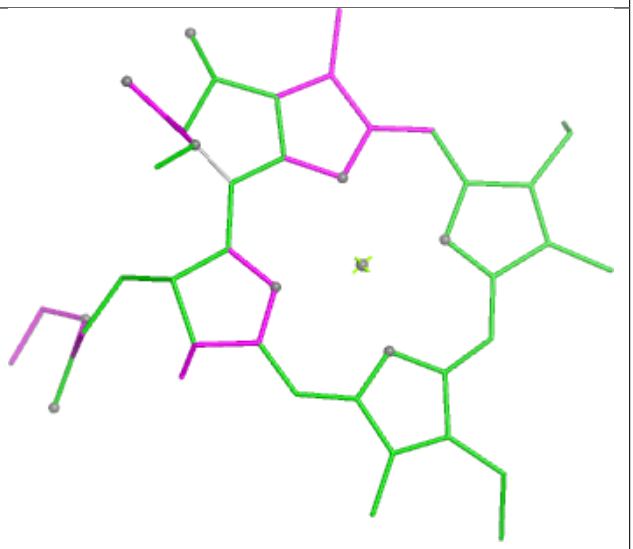
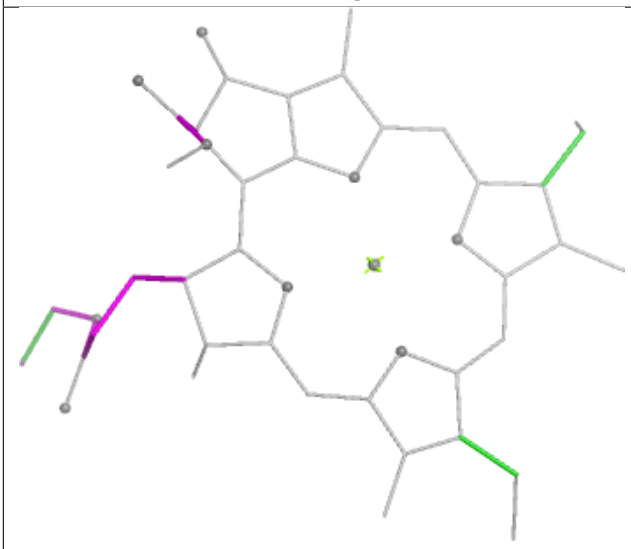
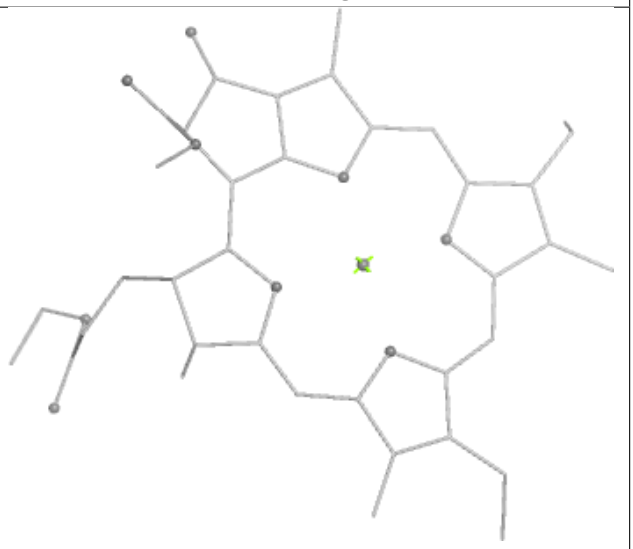


Bond angles

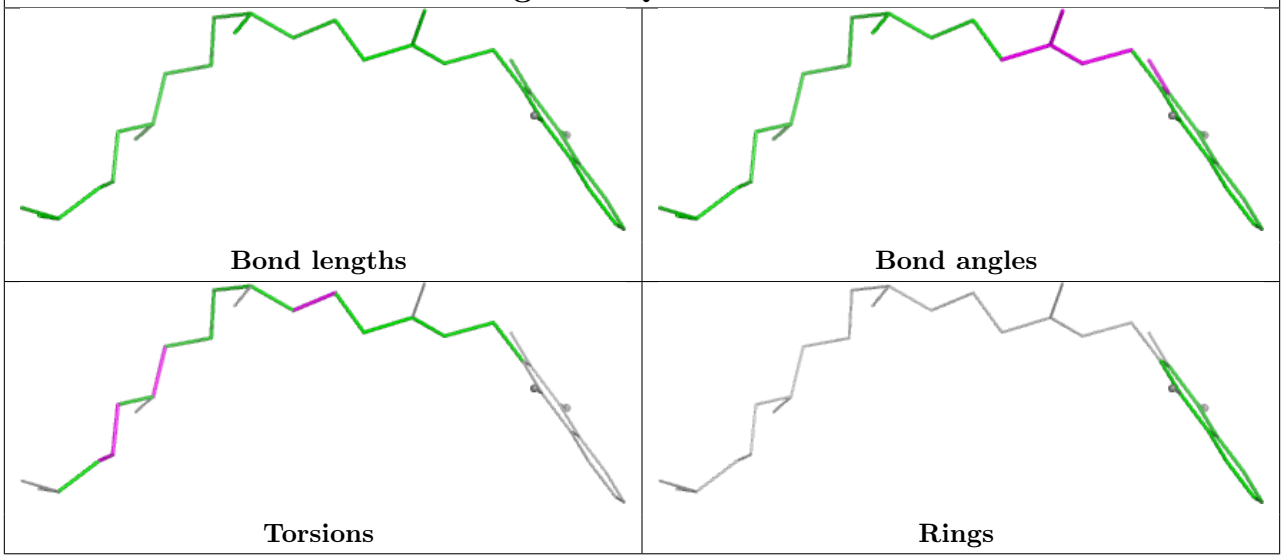


Torsions

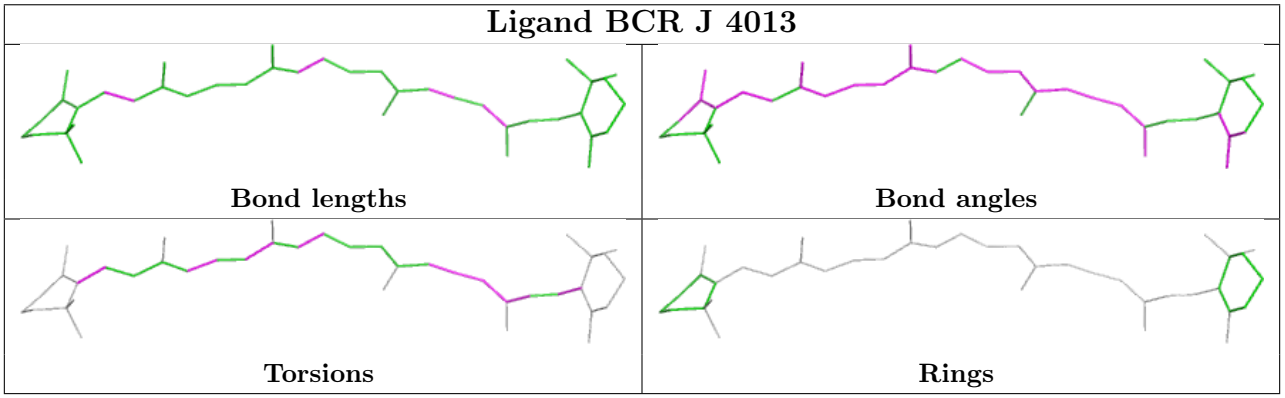


Rings

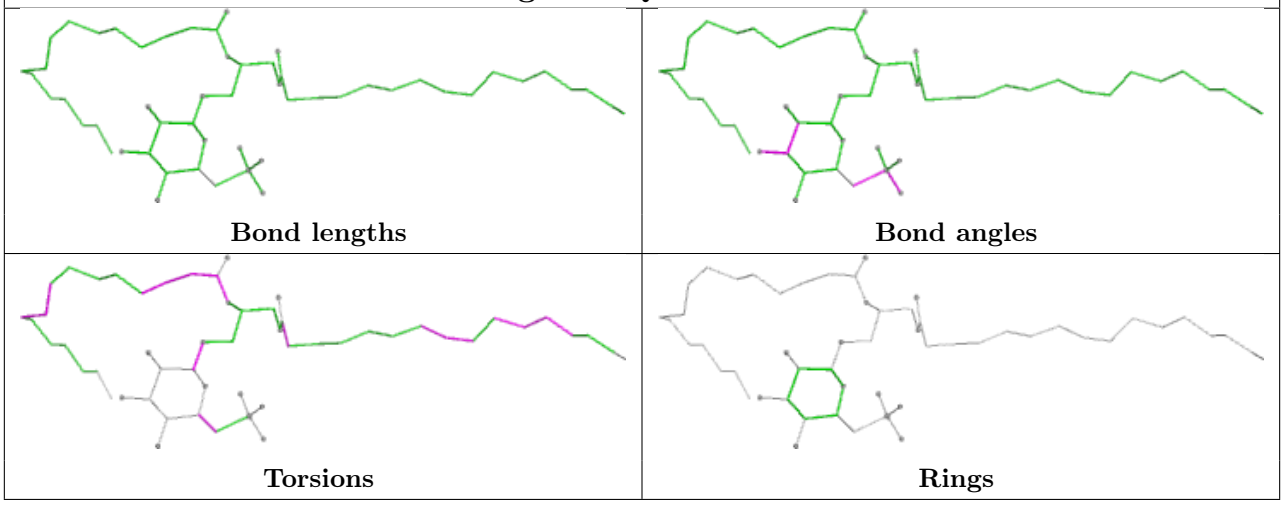
Ligand PQN B 2002



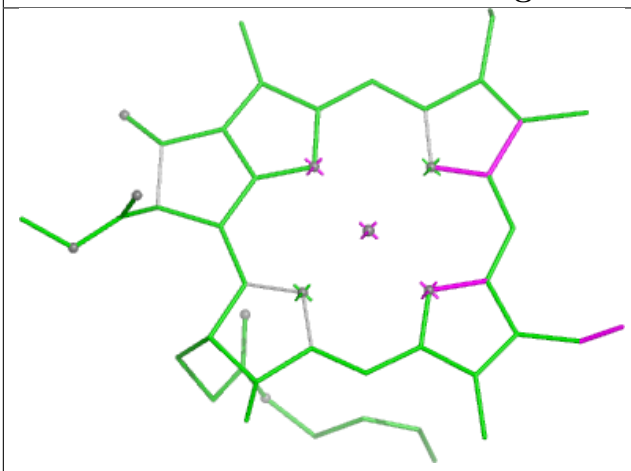
Ligand BCR J 4013



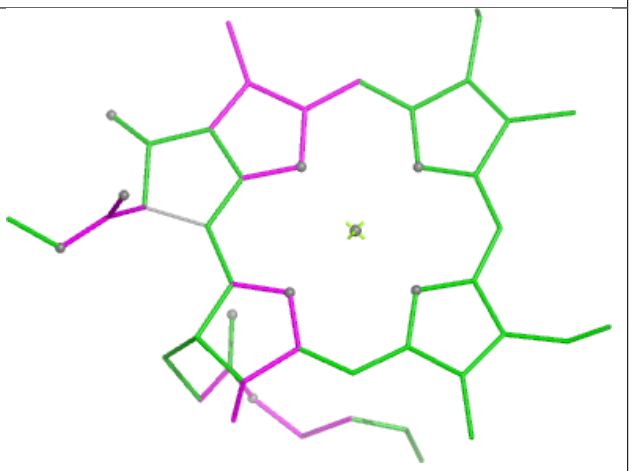
Ligand SQD F 5001



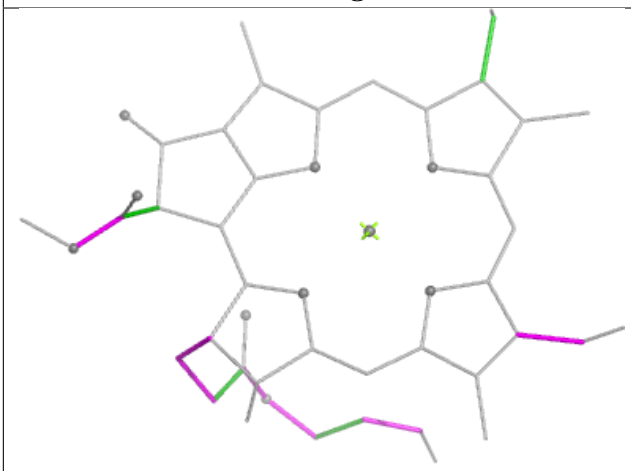
Ligand CLA A 1110



Bond lengths



Bond angles



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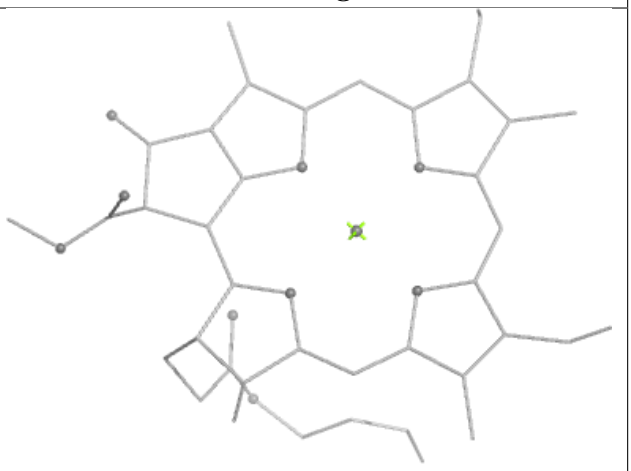
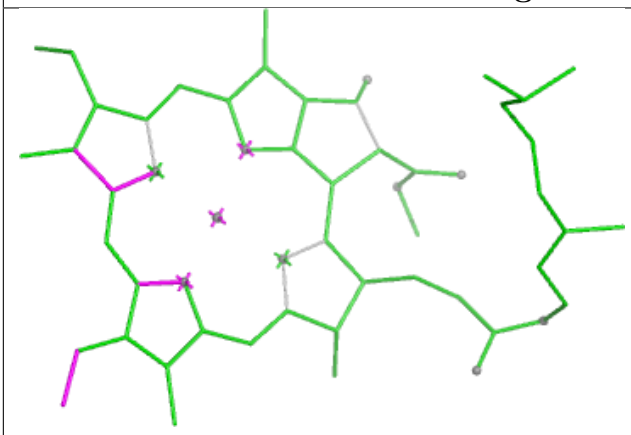


Rings

Ligand CLA A 1011



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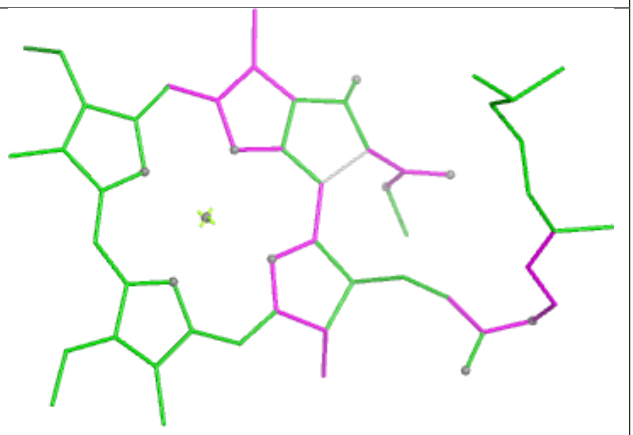
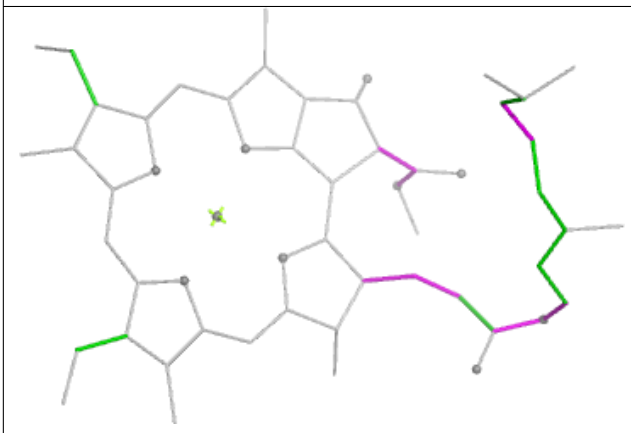


Bond angles



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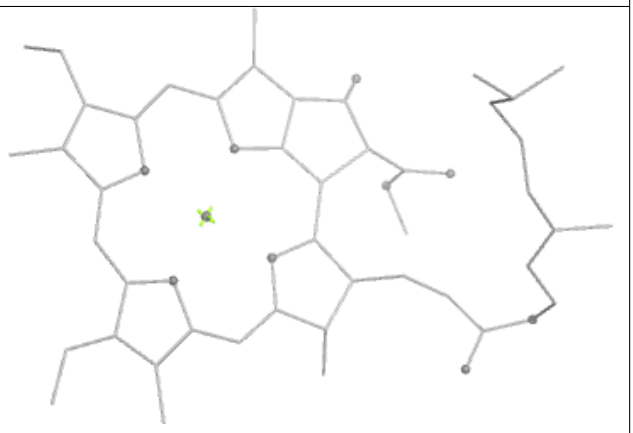
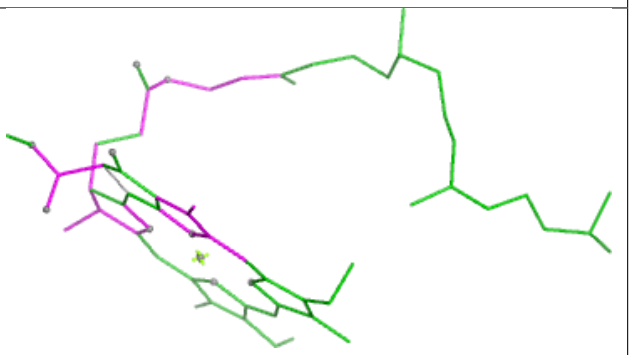


Rings

Ligand CLA A 1109



Bond lengths



Bond angles

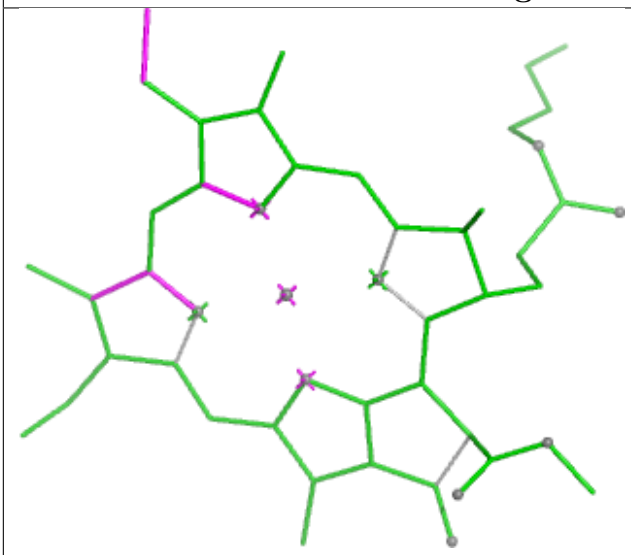


Torsions



Rings

Ligand CLA A 1129



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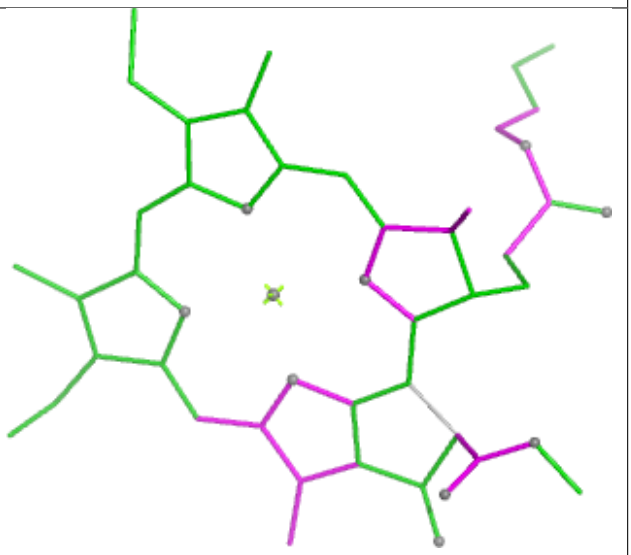
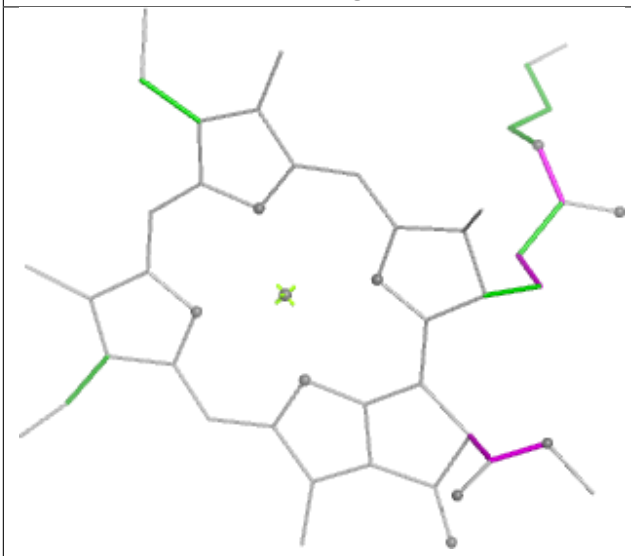


Bond angles

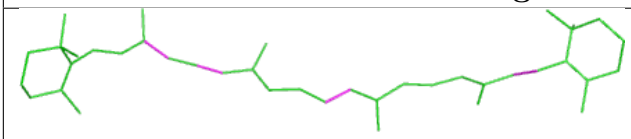


Torsions



Rings

Ligand BCR A 4008



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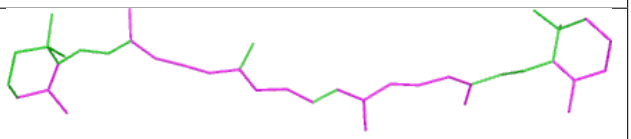
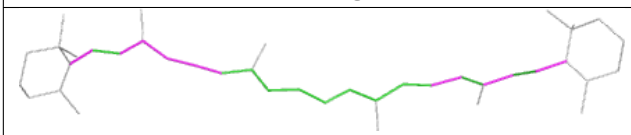
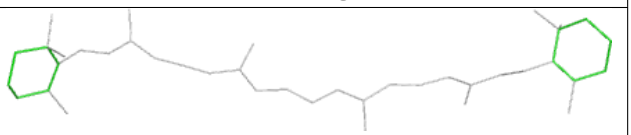


Bond angles

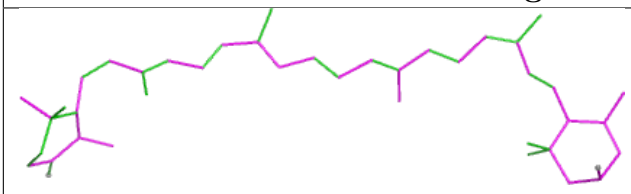


Torsions



Rings

Ligand EQ3 I 4020



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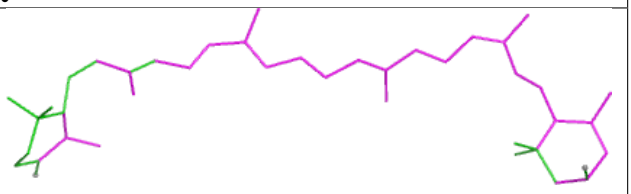
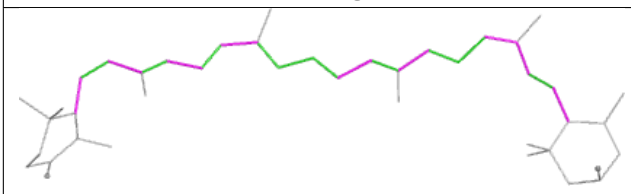
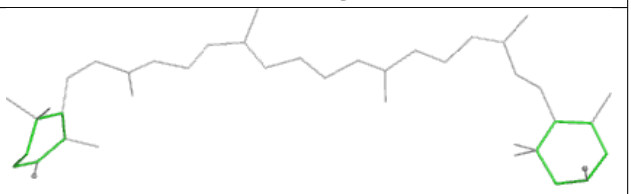


Bond angles

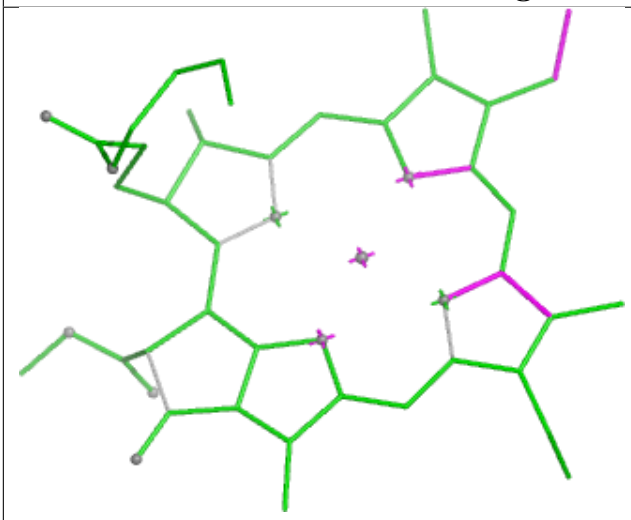


Torsions



Rings

Ligand CLA A 1130



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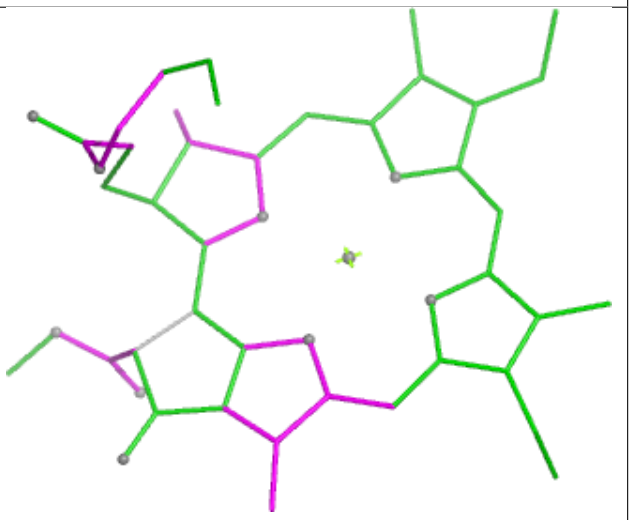
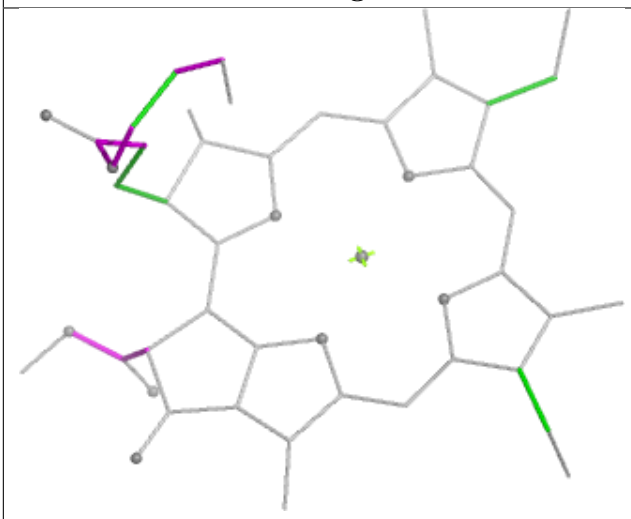
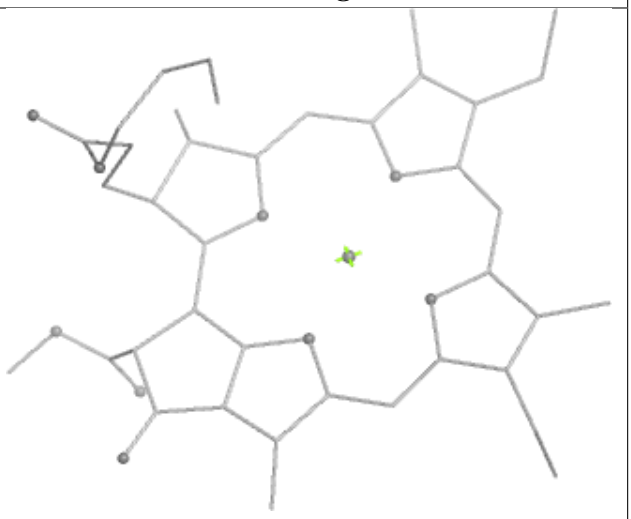


Bond angles

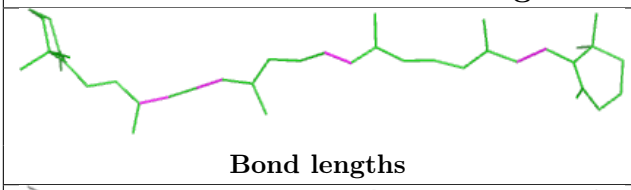


Torsions



Rings

Ligand BCR B 4017



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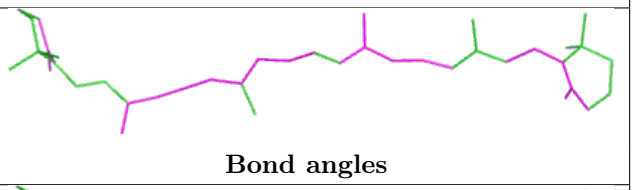
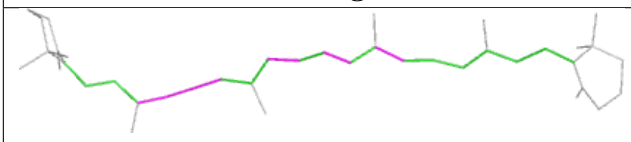


Bond angles



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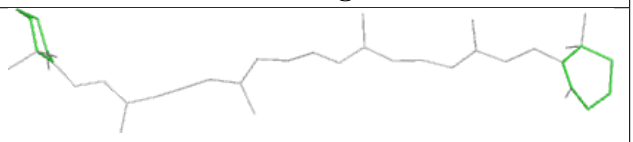
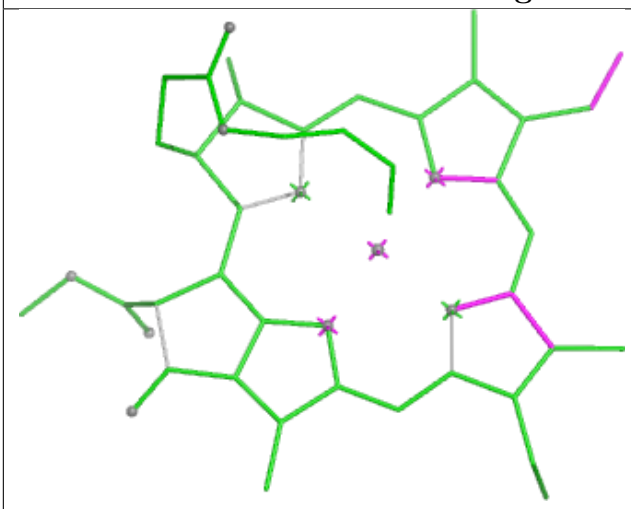


Rings

Ligand CLA A 1116



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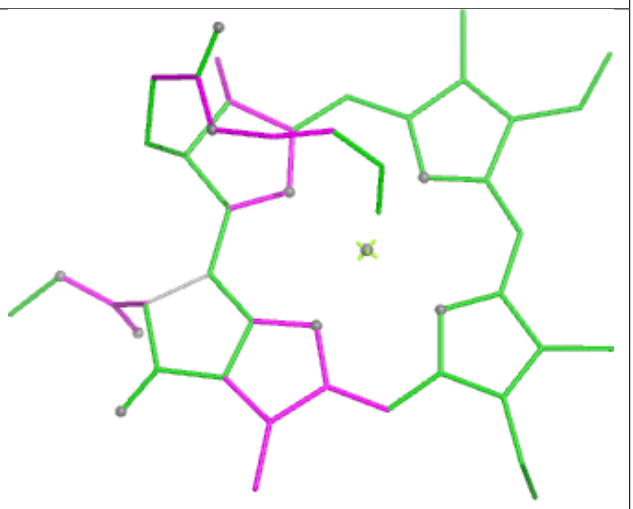
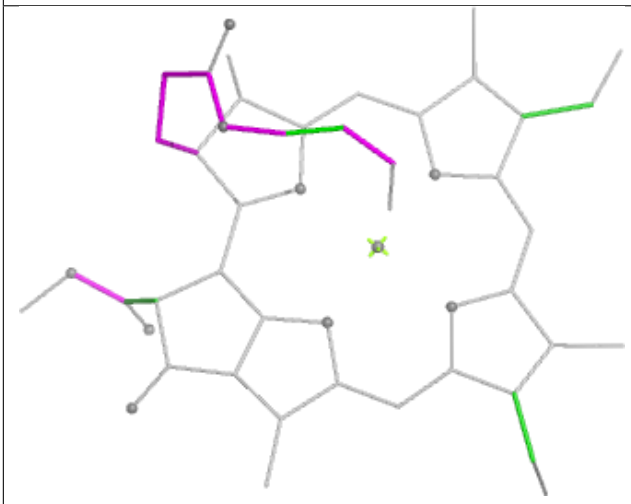


Bond angles



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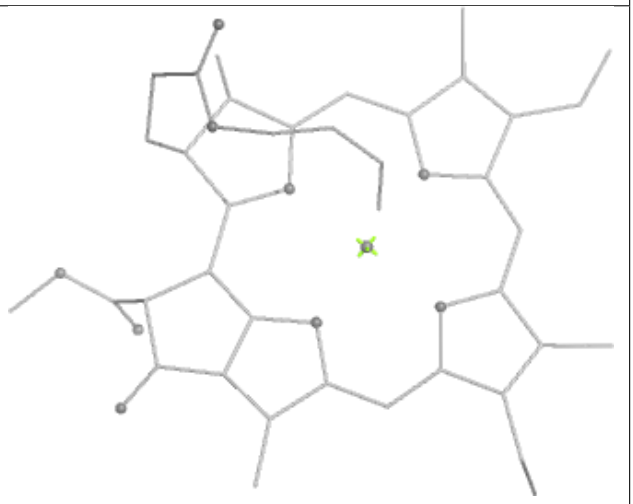
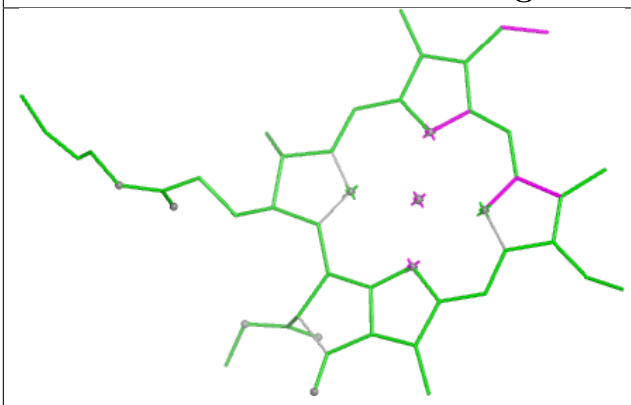


Rings

Ligand CLA B 1239



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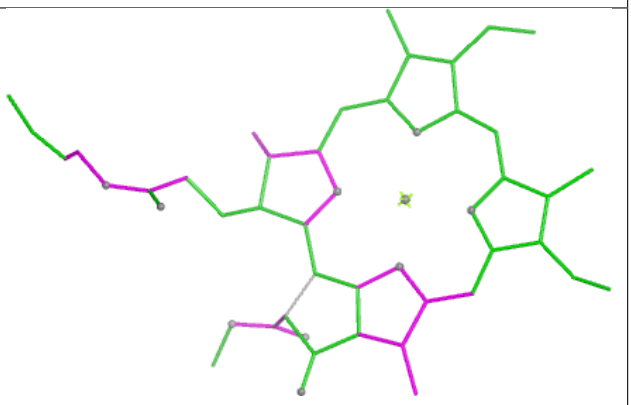
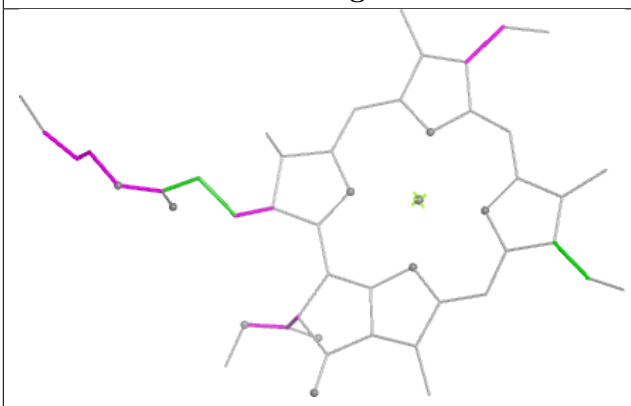


Bond angles



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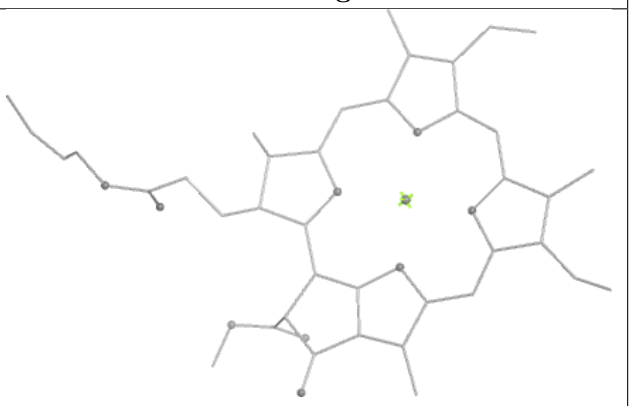
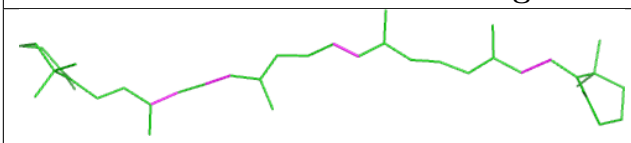
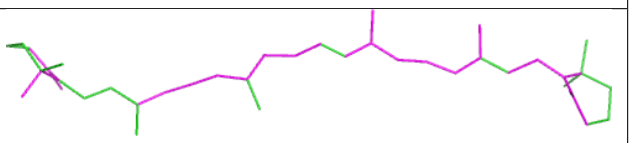


Rings

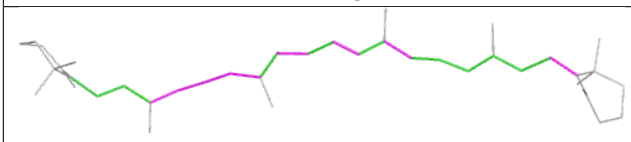
Ligand BCR A 4007



Bond lengths



Bond angles



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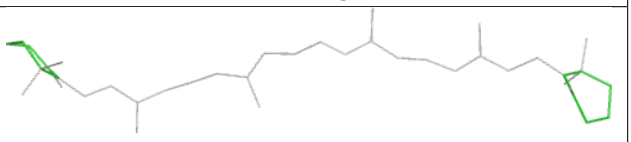
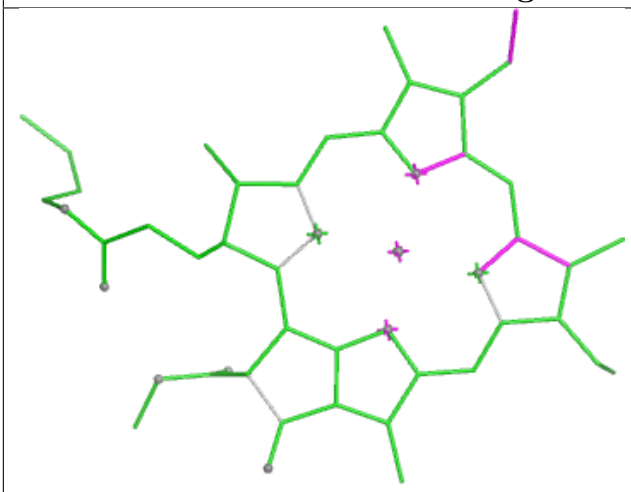
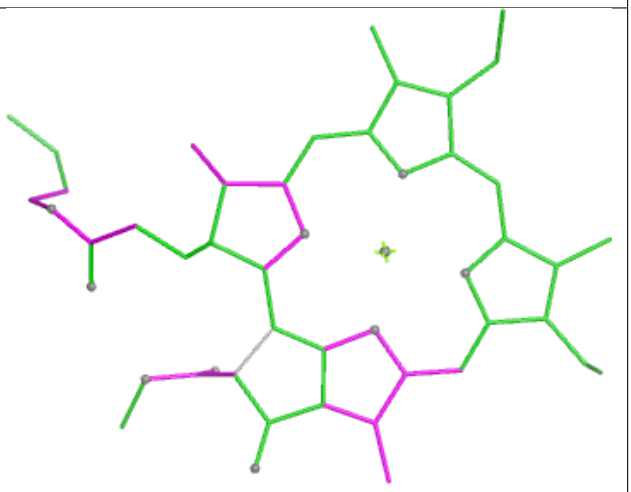


Rings

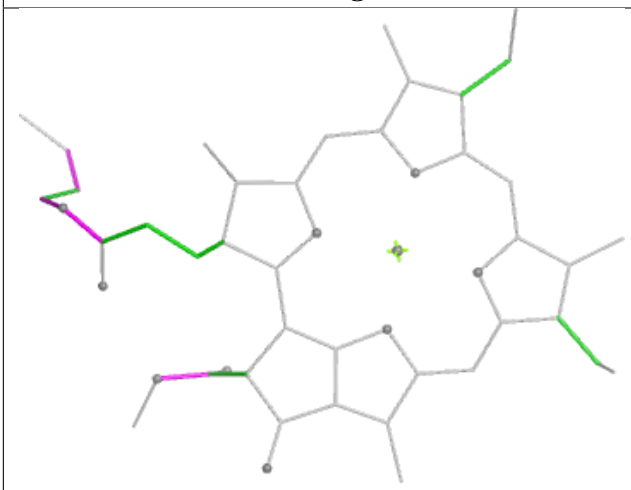
Ligand CLA F 1301



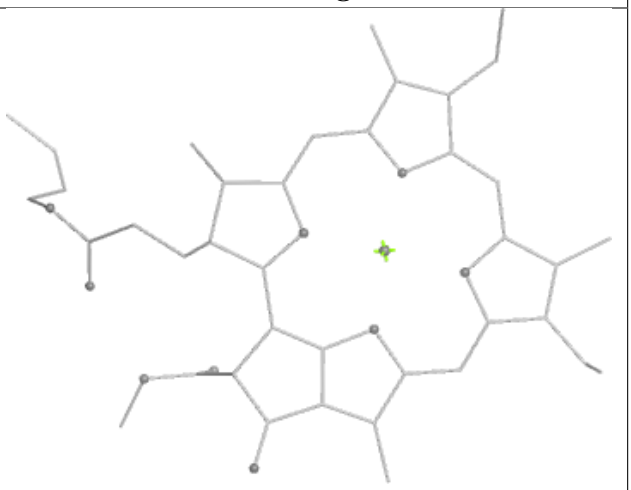
Bond lengths



Bond angles

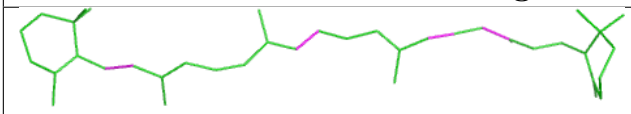


Torsions



Rings

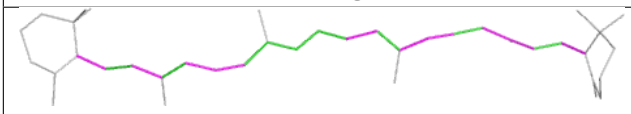
Ligand BCR A 4003



Bond lengths



Bond angles

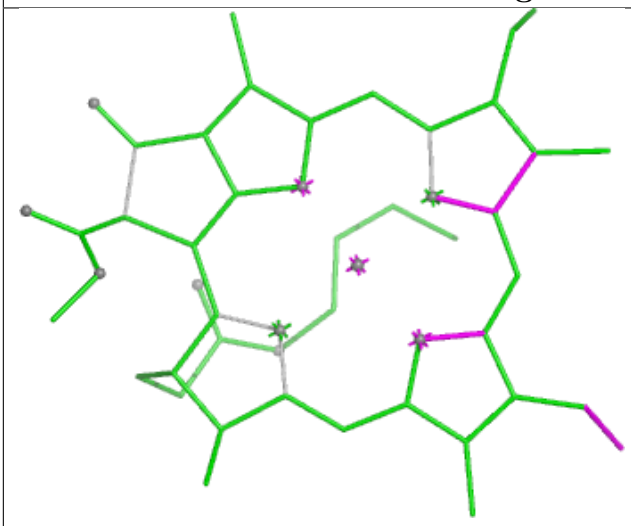


Torsions

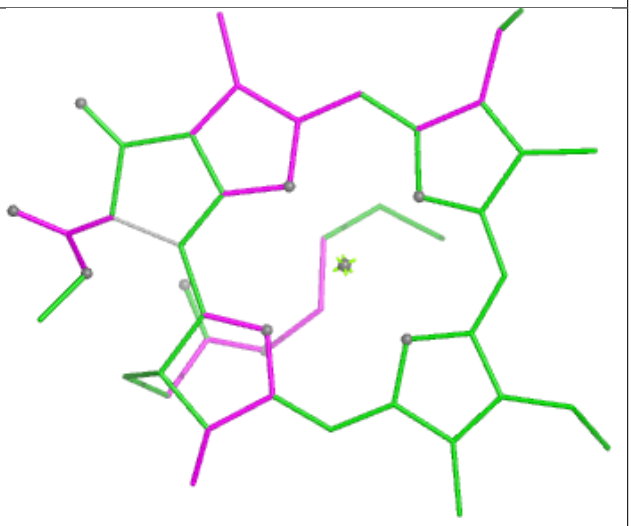


Rings

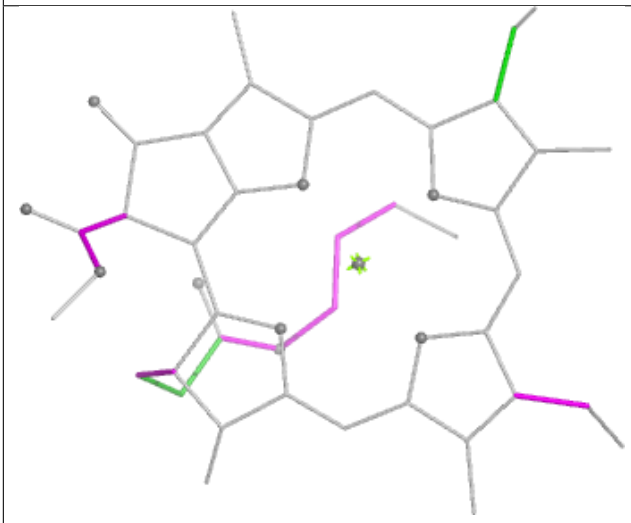
Ligand CLA B 1205



Bond lengths



Bond angles



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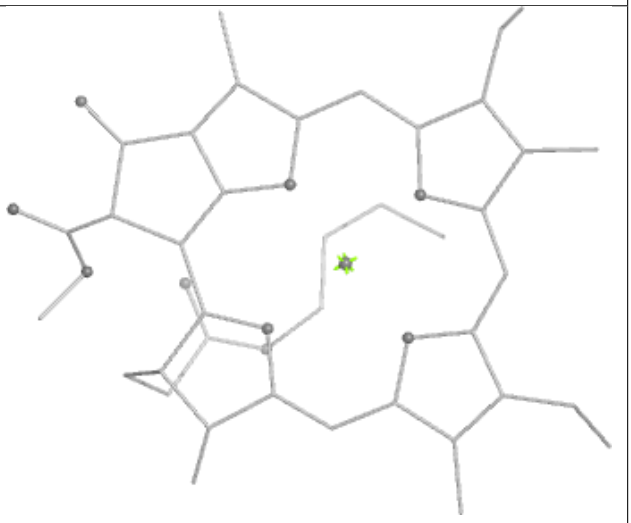
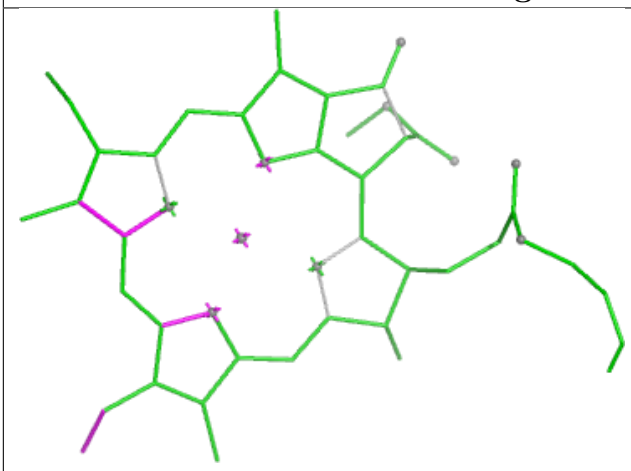


Rings

Ligand CLA K 1402



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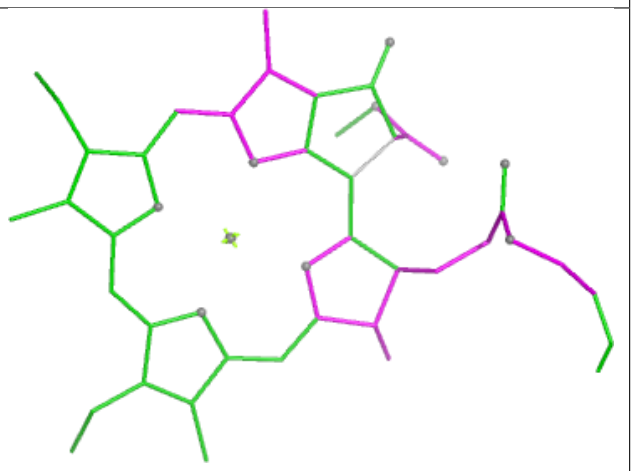
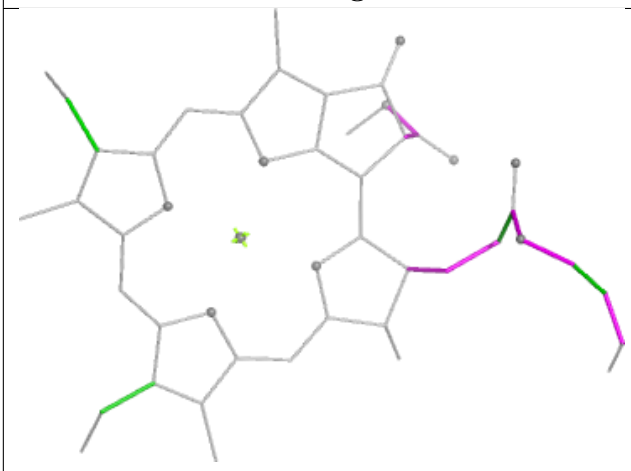


Bond angles



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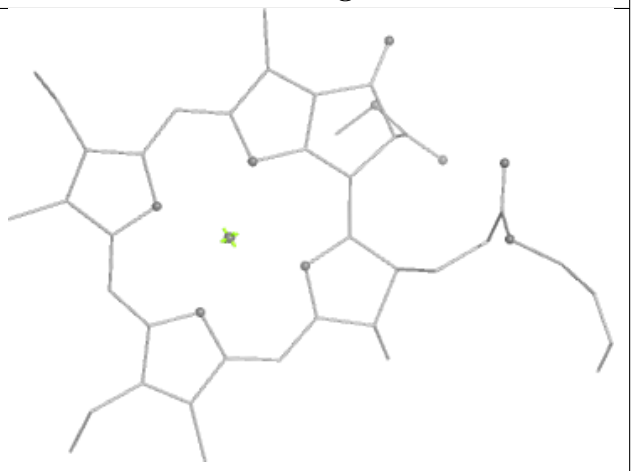
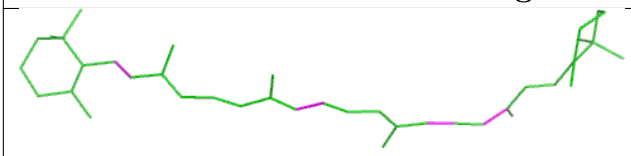


Rings

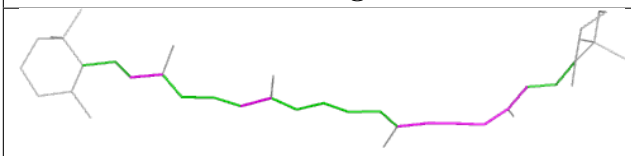
Ligand BCR F 4014



Bond lengths



Bond angles



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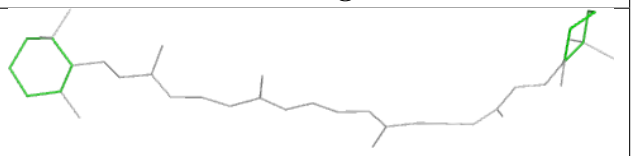
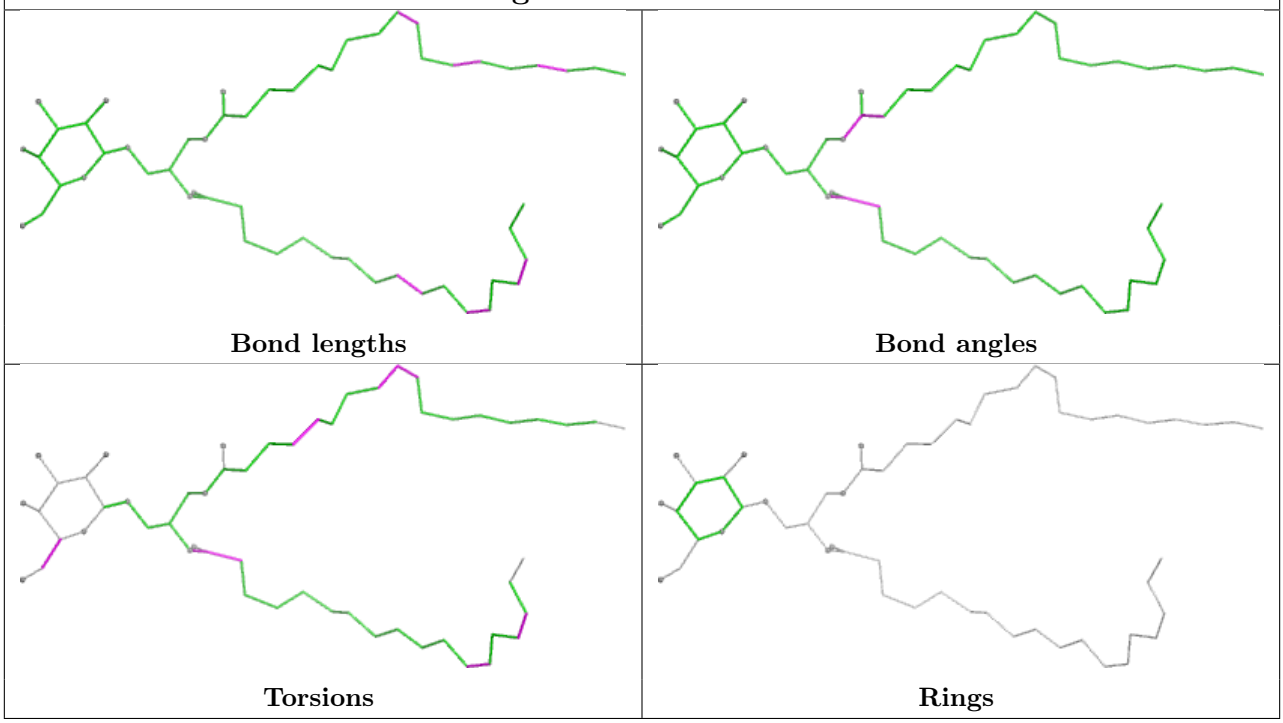
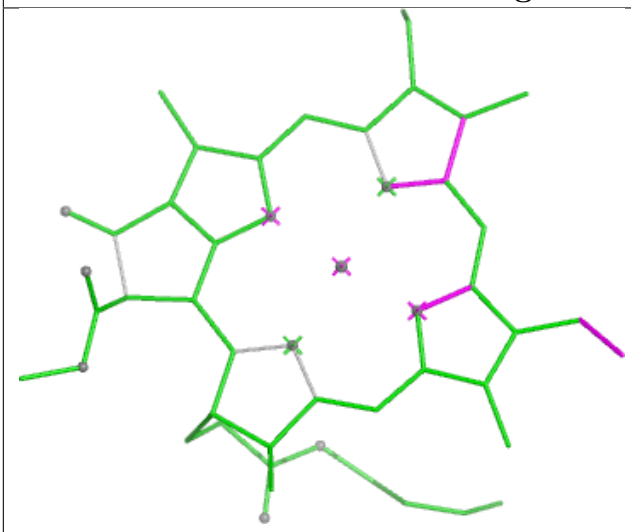


Rings

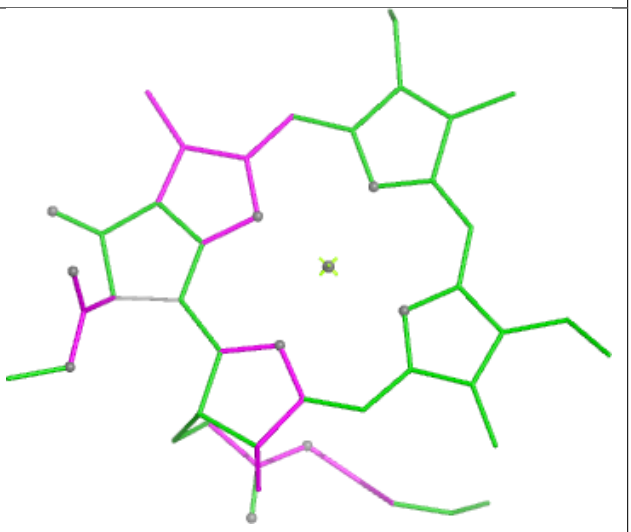
Ligand LMG B 5002



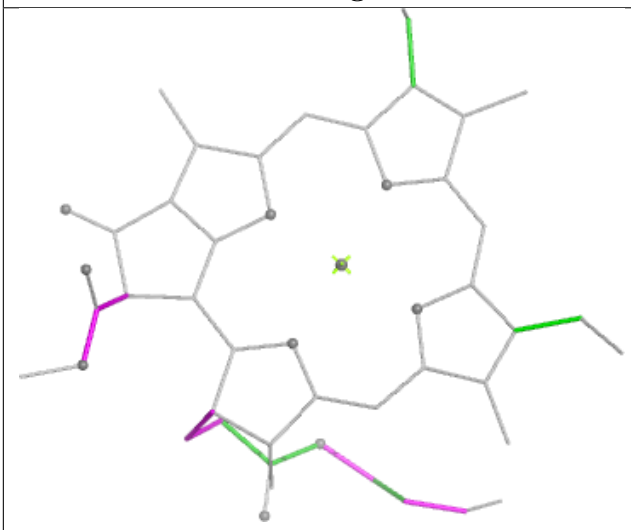
Ligand CLA A 1117



Bond lengths



Bond angles



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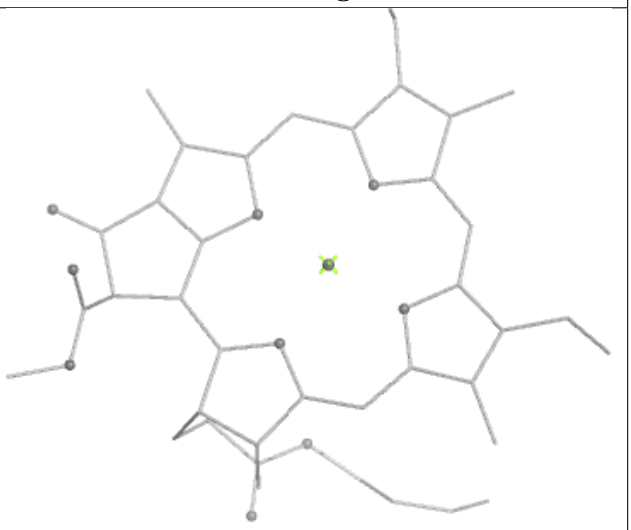
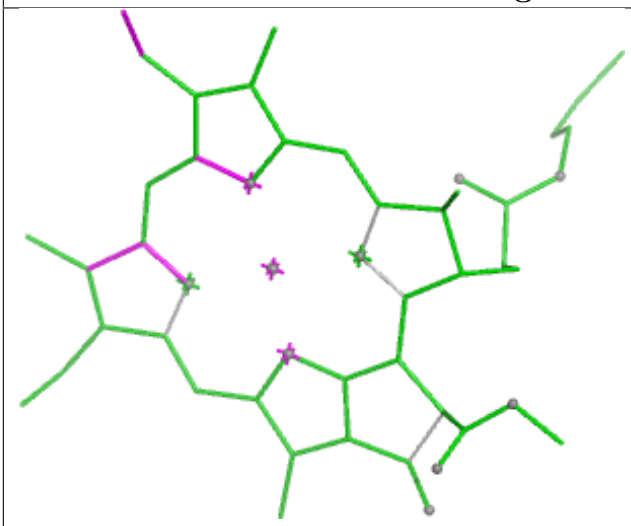


Rings

Ligand CLA A 1108



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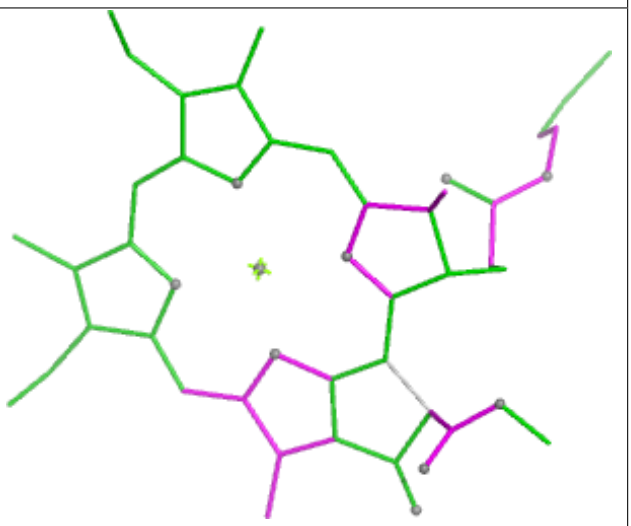
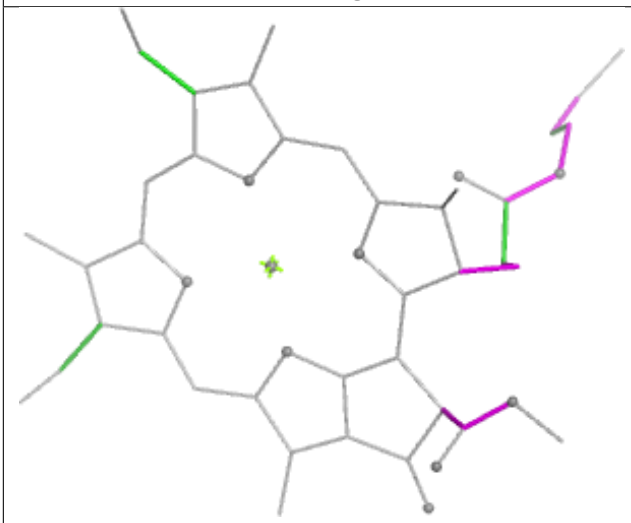


Bond angles



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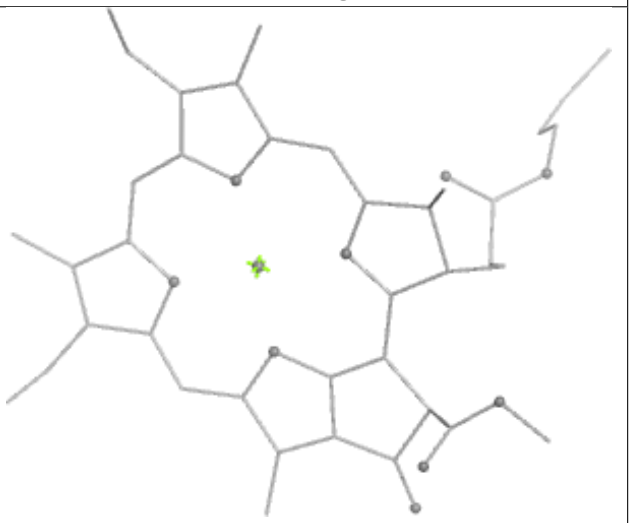
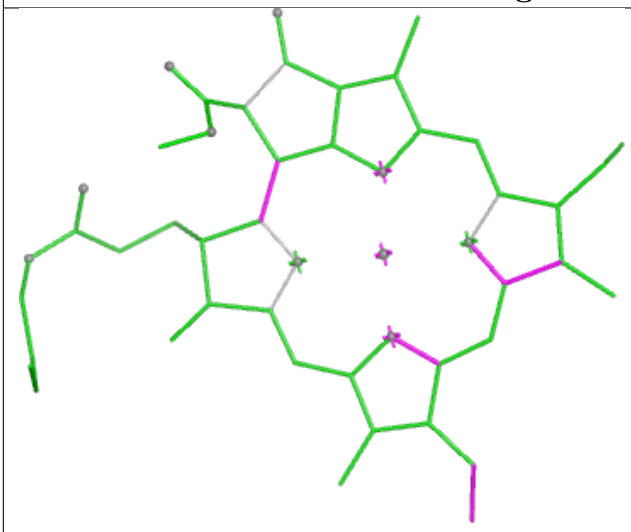


Rings

Ligand CLA B 1221



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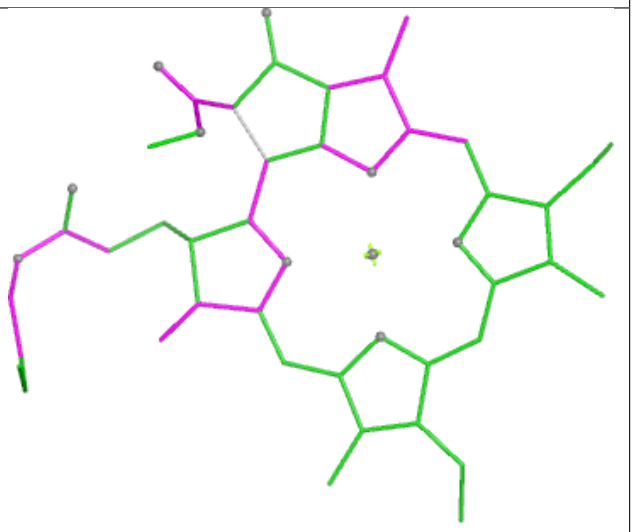
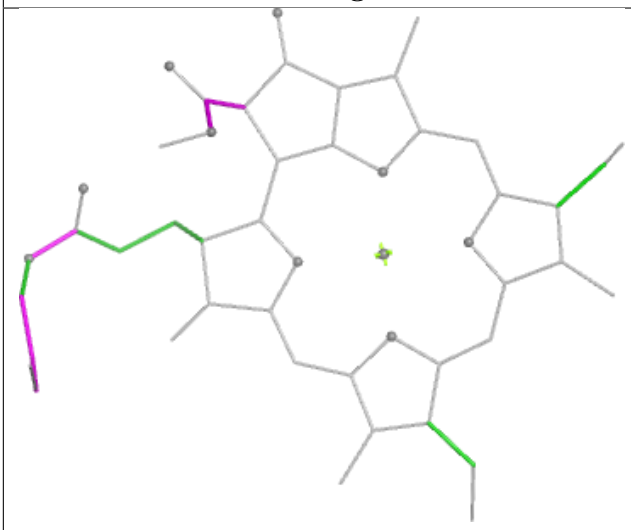


Bond angles



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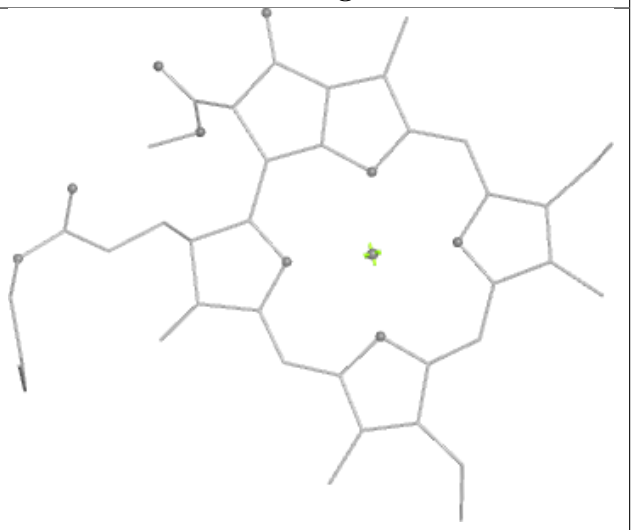
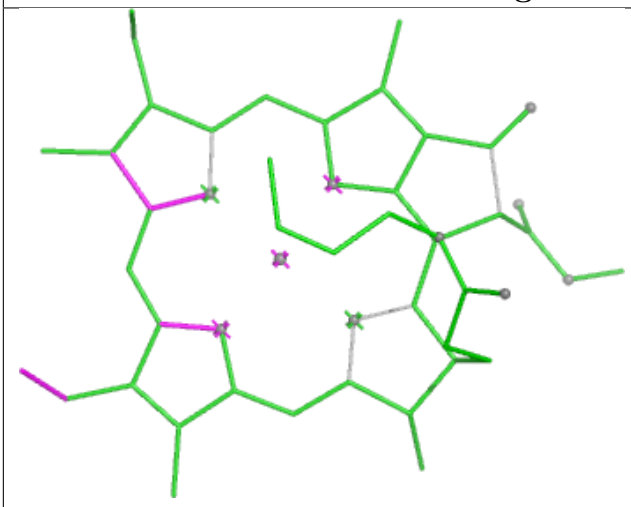


Rings

Ligand CLA A 1136



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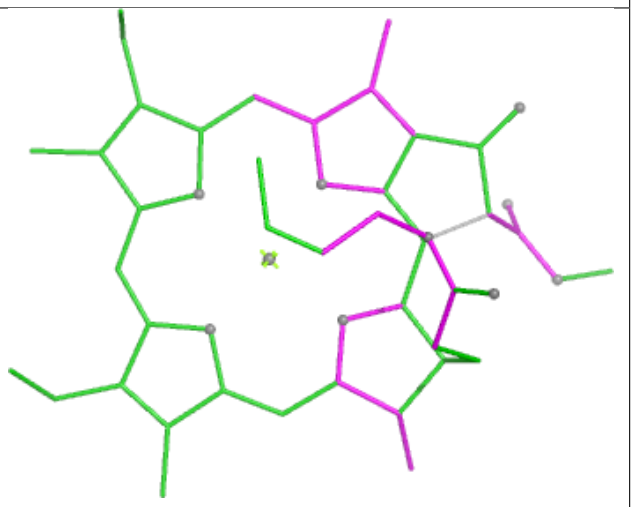
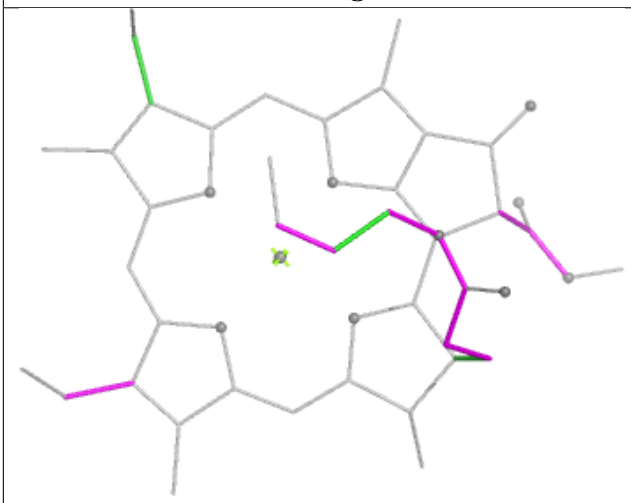


Bond angles



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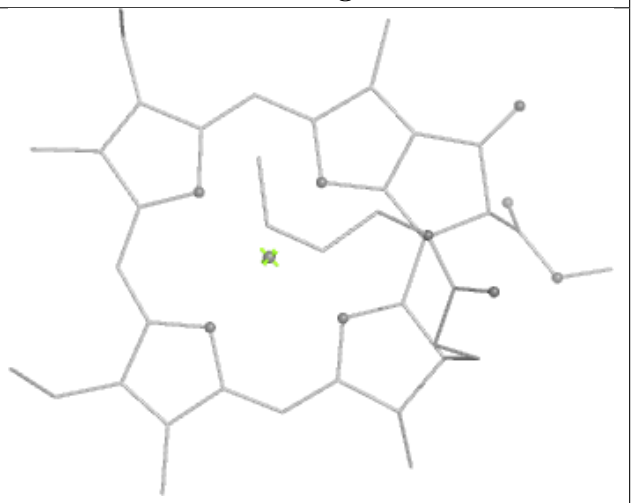


Rings

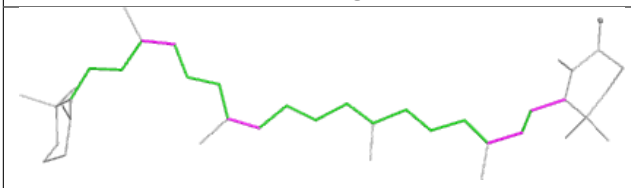
Ligand ECH B 4006



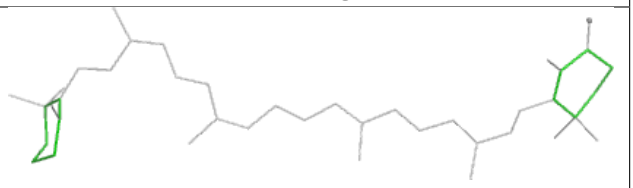
Bond lengths



Bond angles

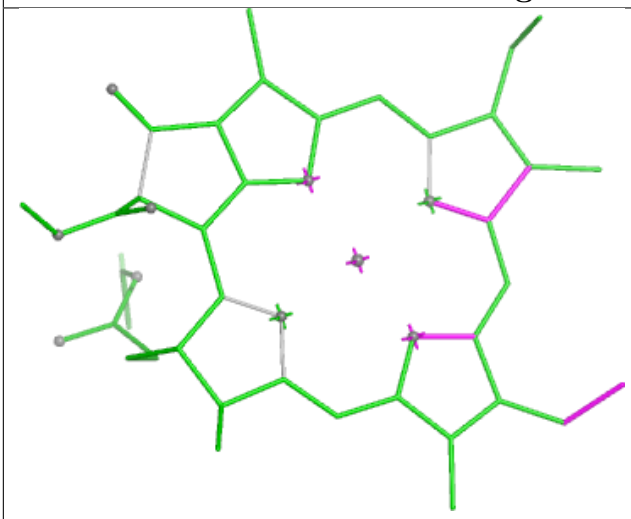


Torsions



Rings

Ligand CLA B 1208



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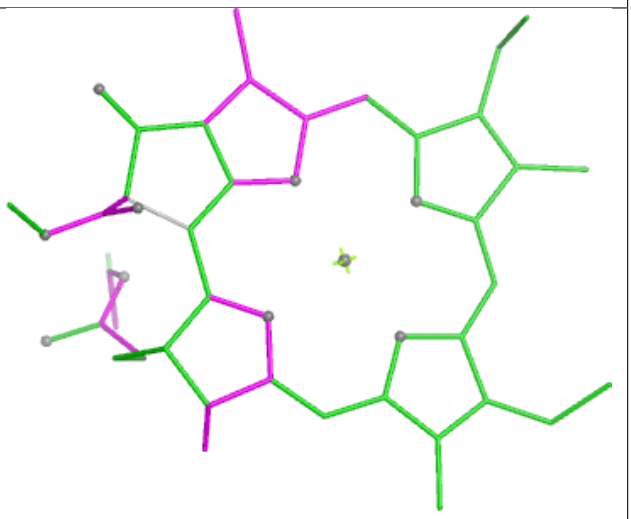
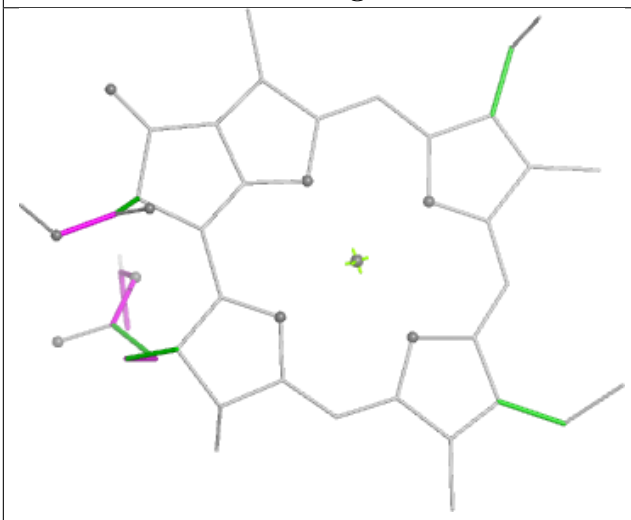


Bond angles



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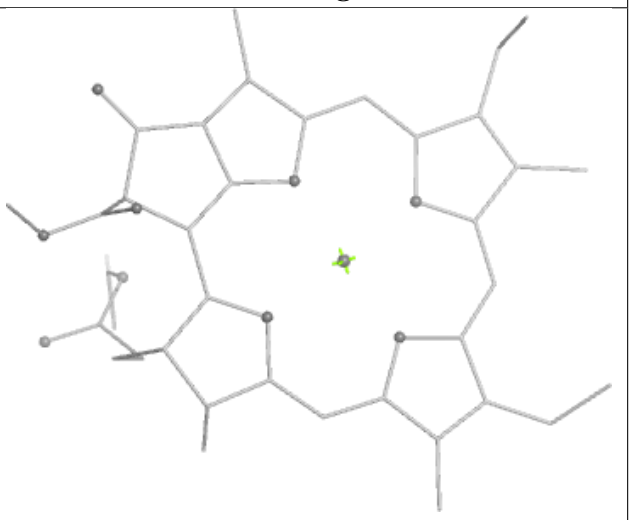
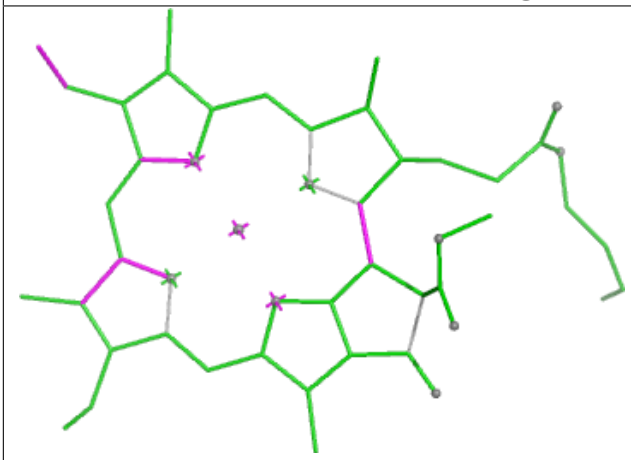


Rings

Ligand CLA L 1502



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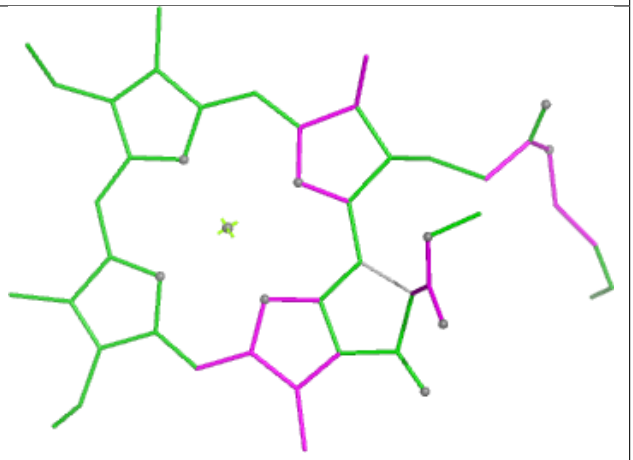
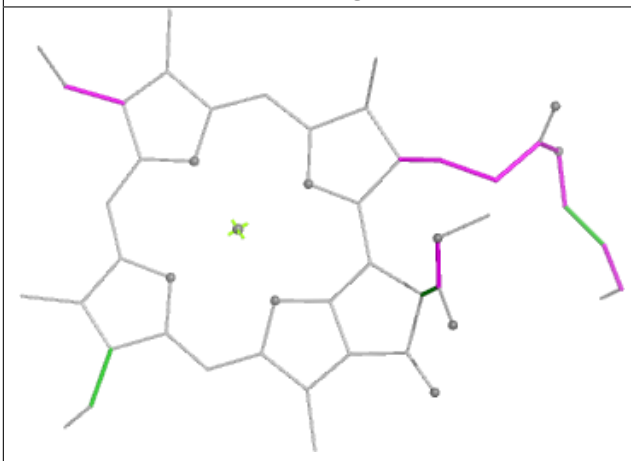


Bond angles



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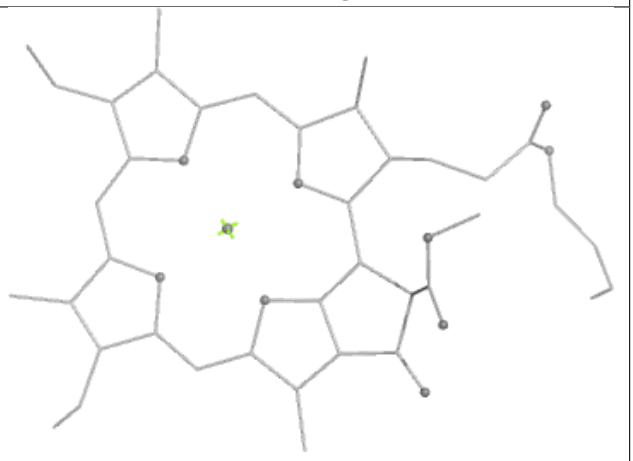
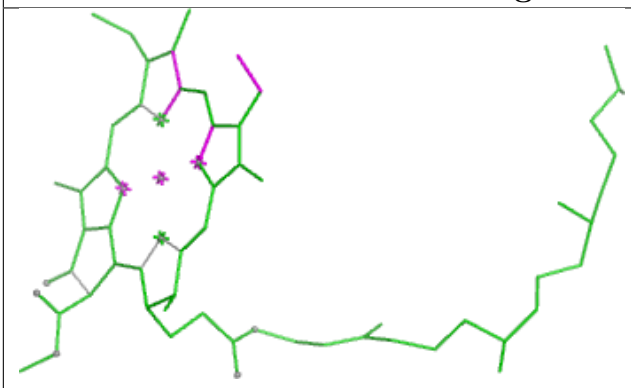
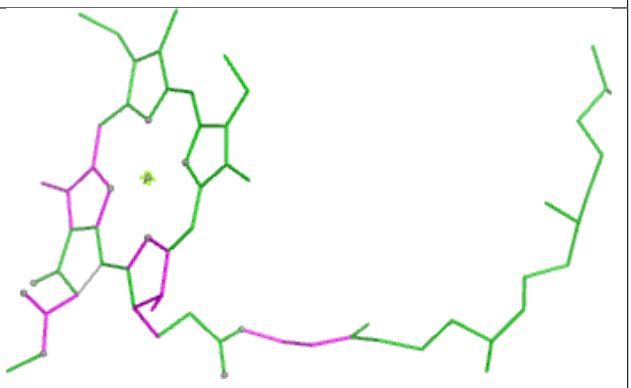


Rings

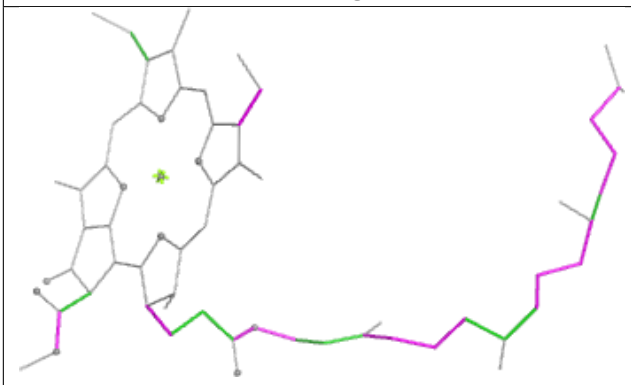
Ligand CLA A 1140



Bond lengths



Bond angles



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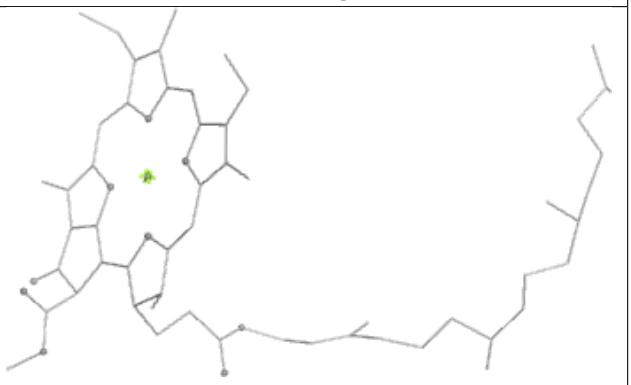
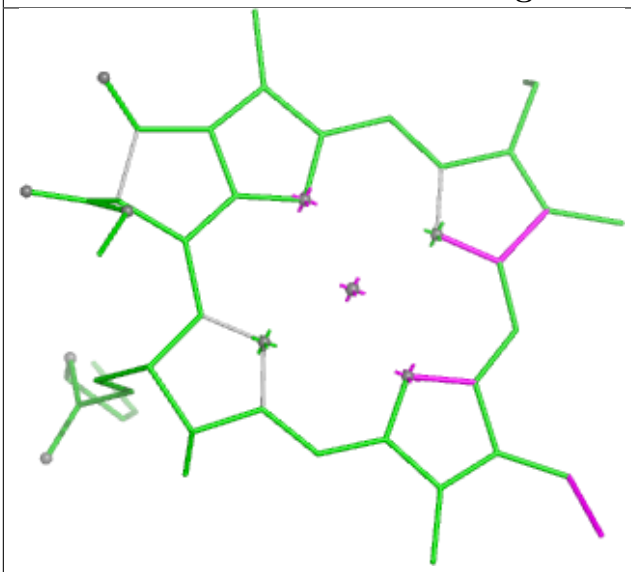
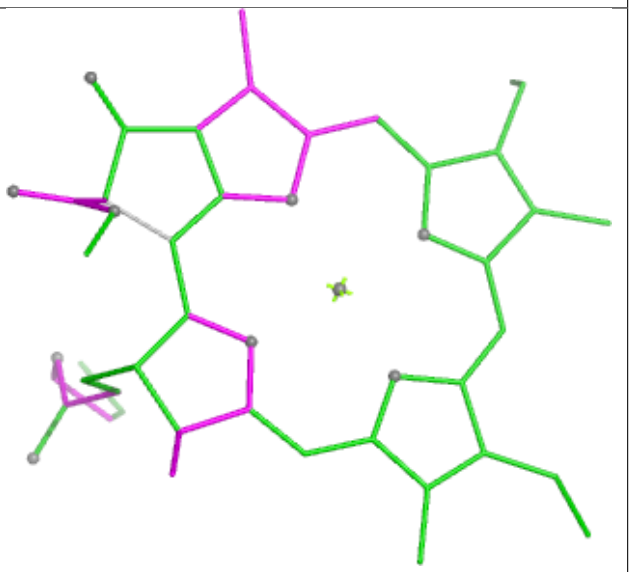


Rings

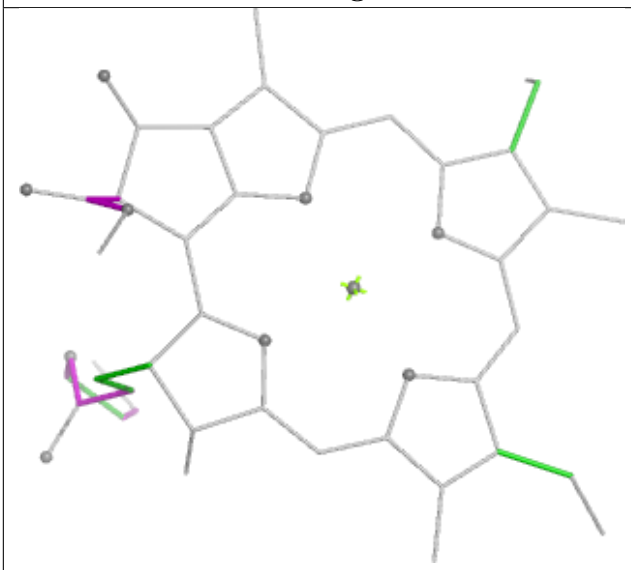
Ligand CLA B 1226



Bond lengths



Bond angles



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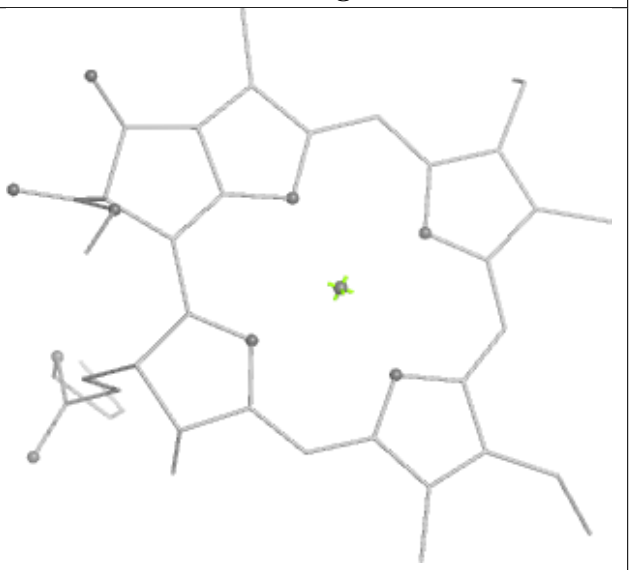
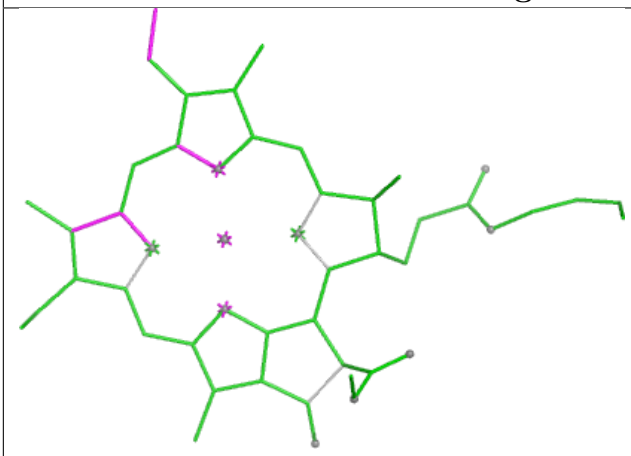
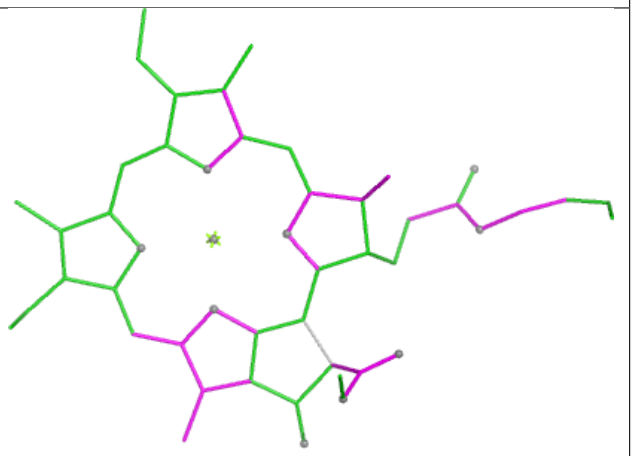


Rings

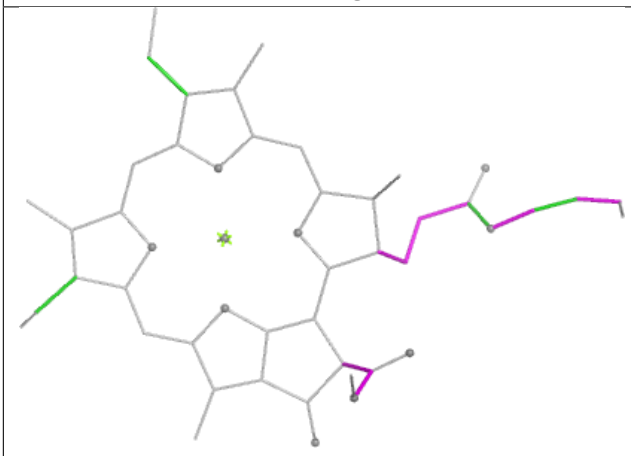
Ligand CLA A 1103



Bond lengths



Bond angles



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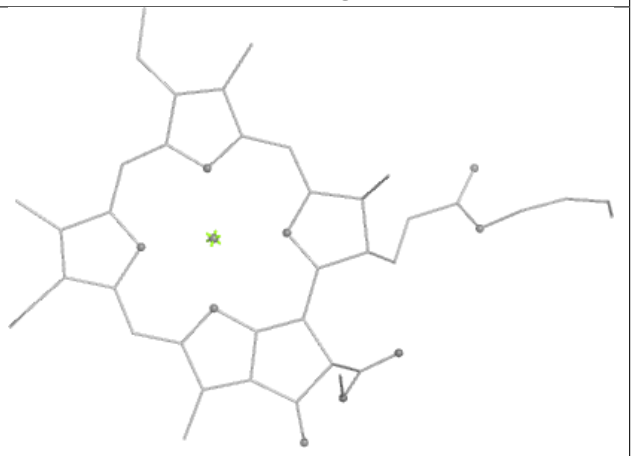
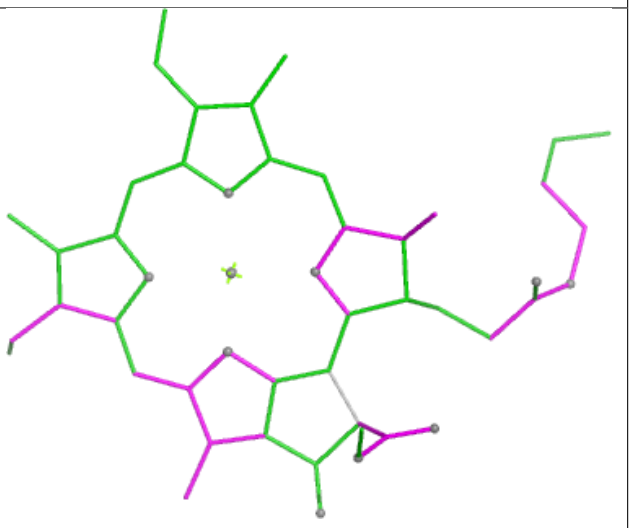


Rings

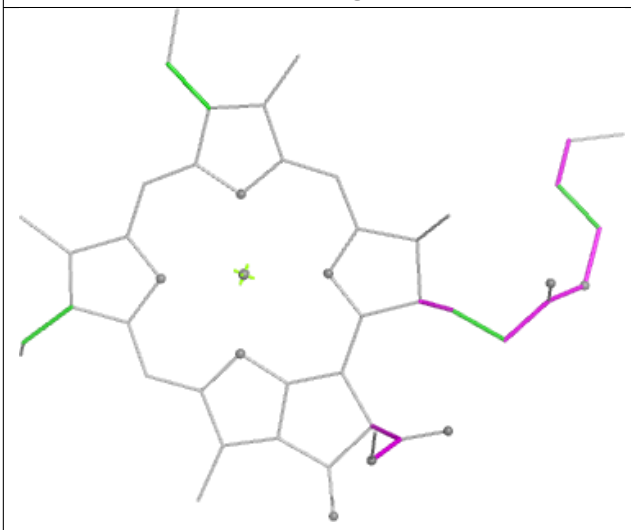
Ligand CLA B 1210



Bond lengths



Bond angles



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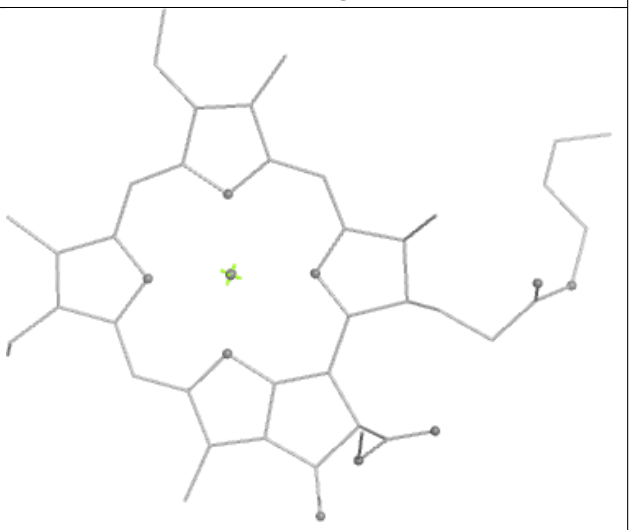
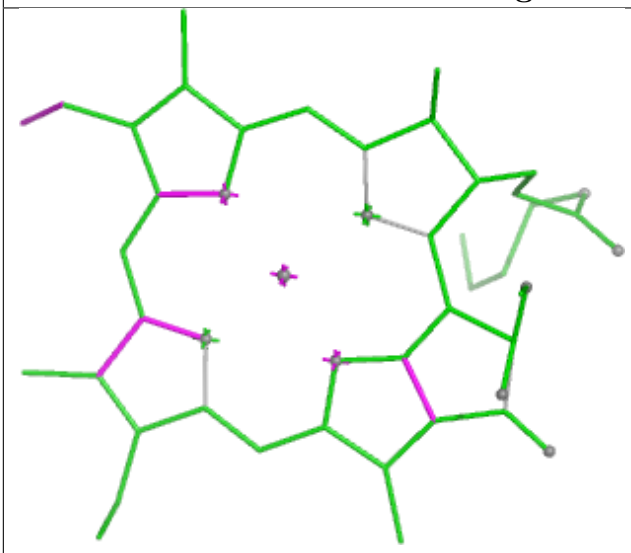
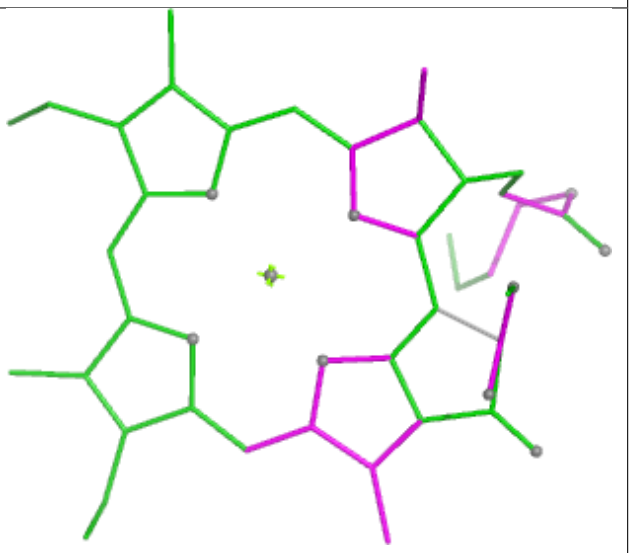


Rings

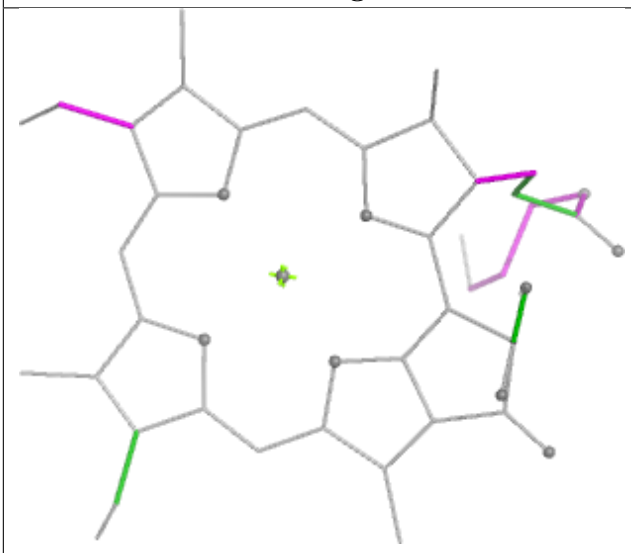
Ligand CLA B 1238



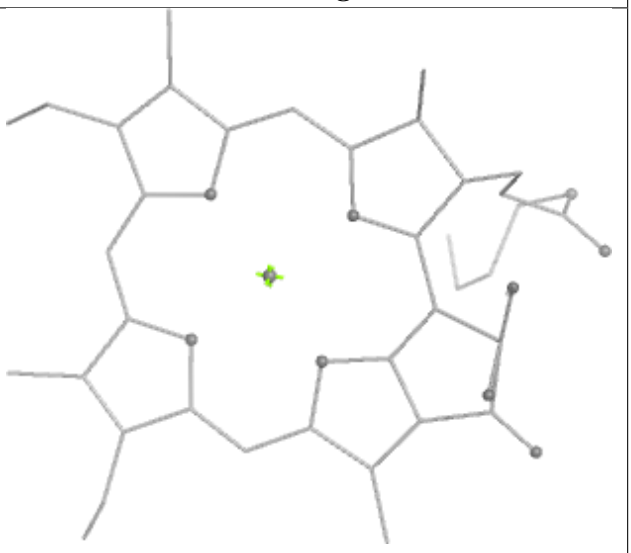
Bond lengths



Bond angles

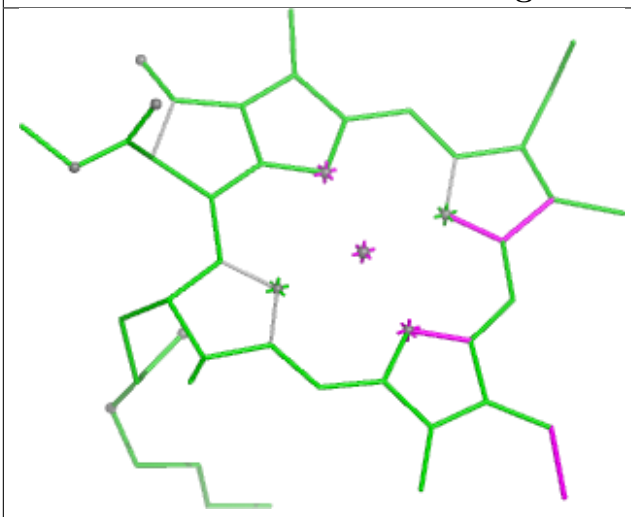


Torsions



Rings

Ligand CLA B 1228



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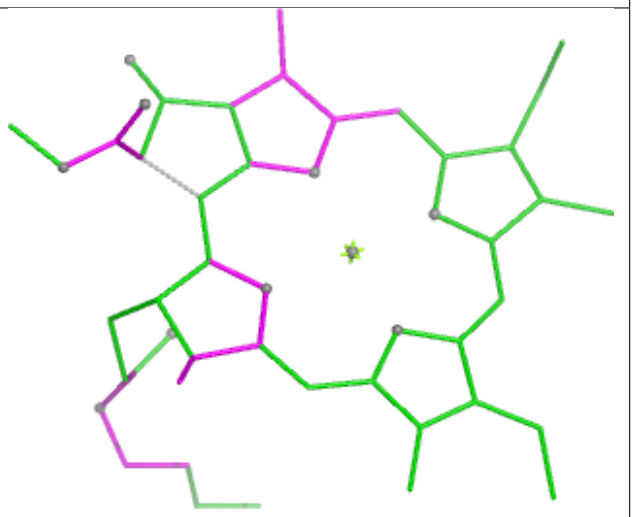

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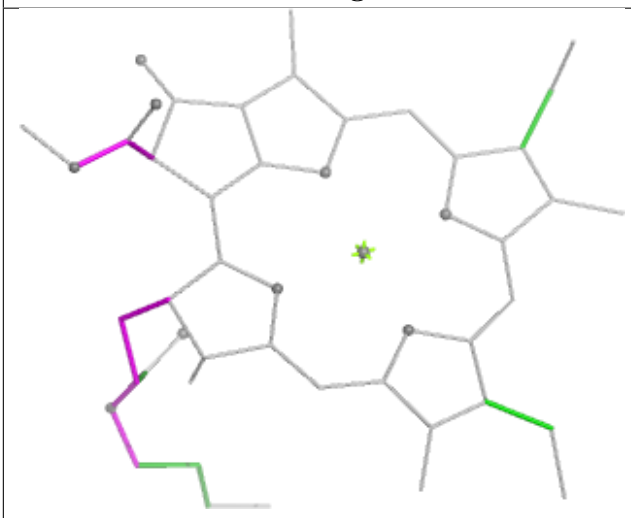

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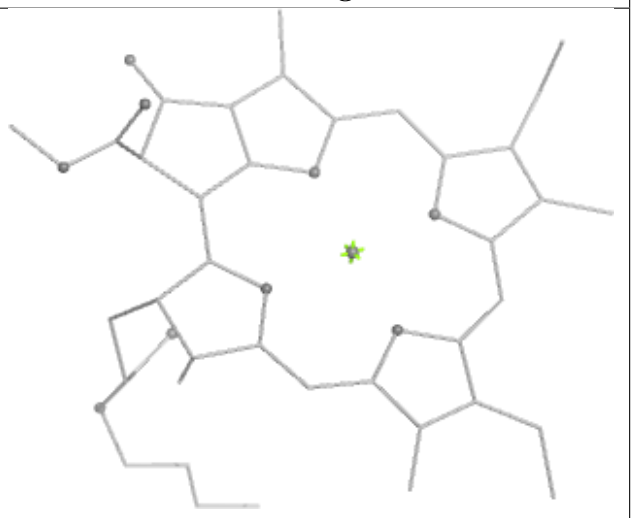
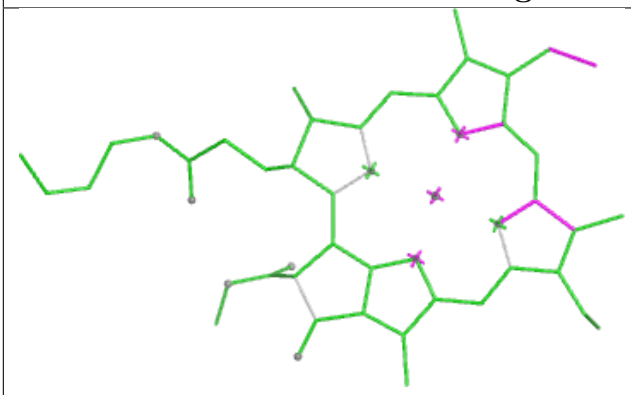


Rings

Ligand CLA A 1131



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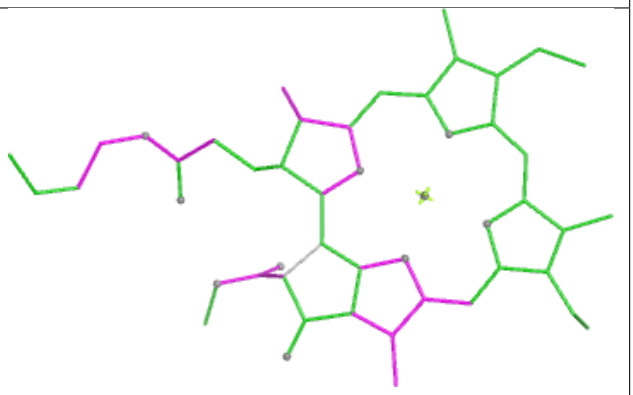
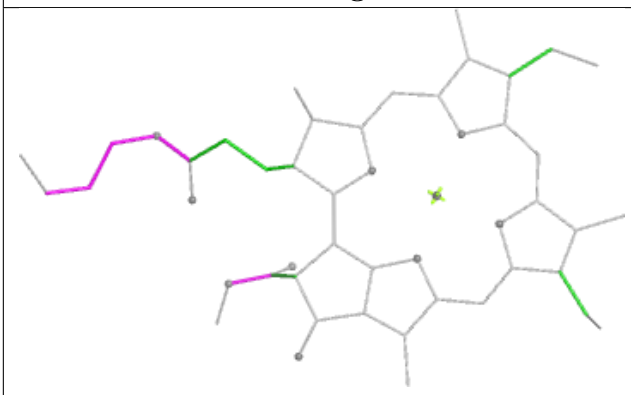


Bond angles



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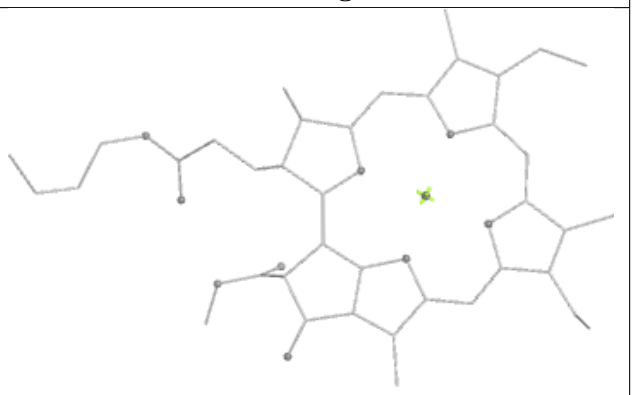
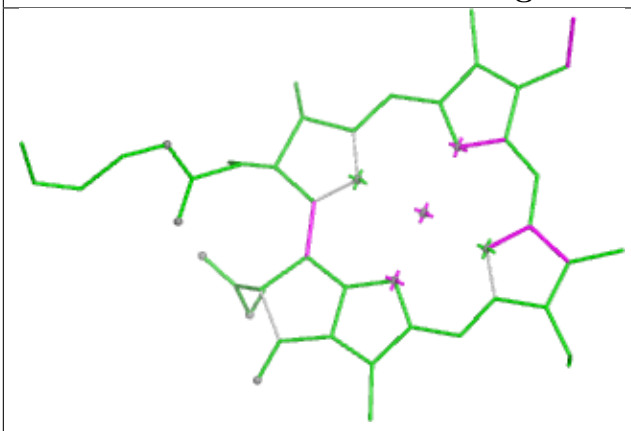


Rings

Ligand CLA B 1220



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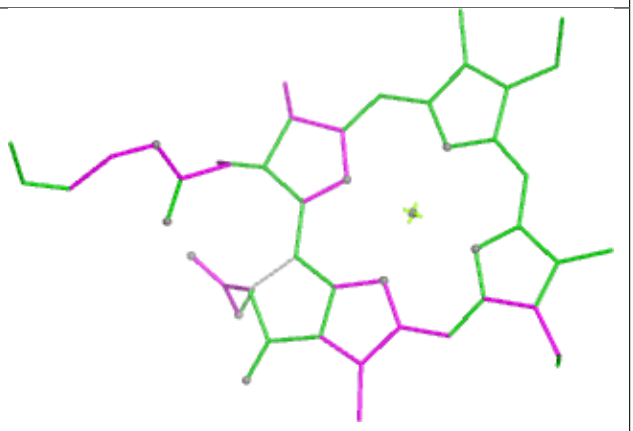
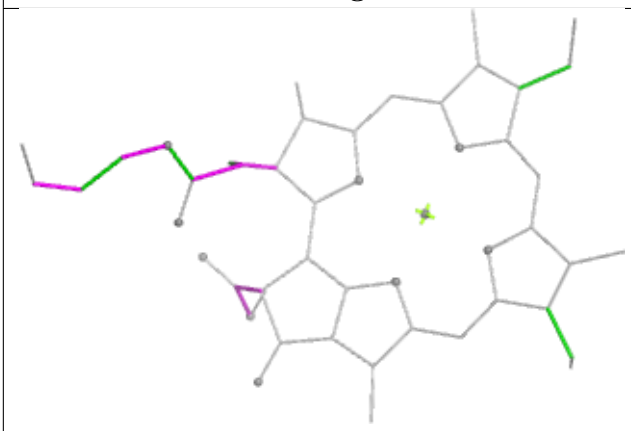


Bond angles

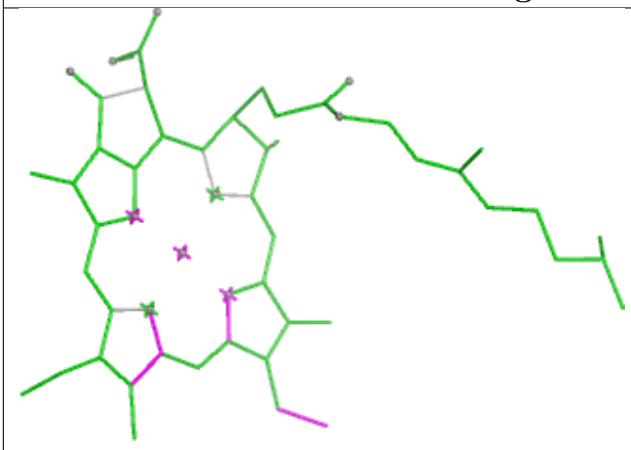


Torsions



Rings

Ligand CLA A 1132



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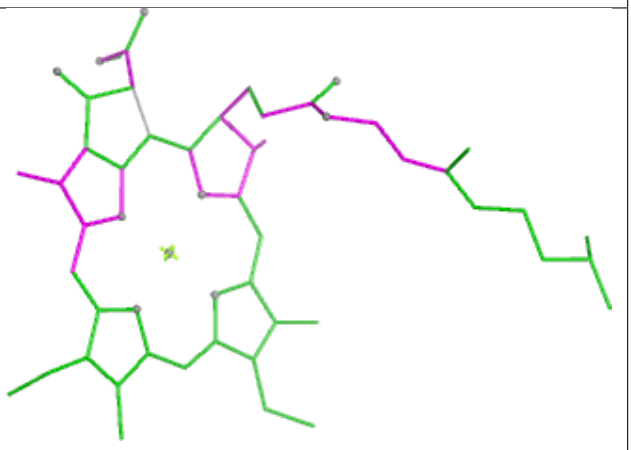

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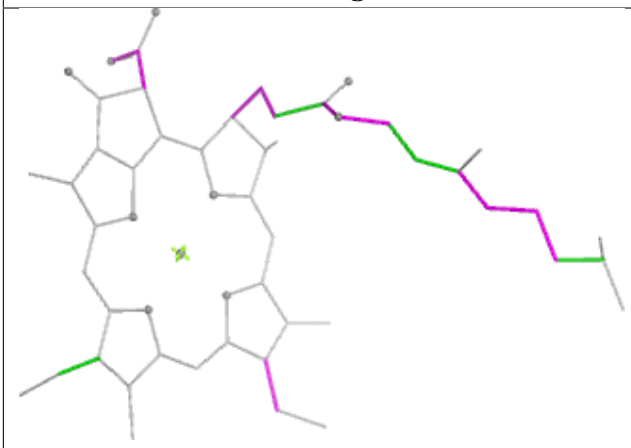
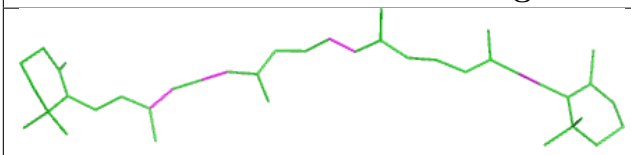


Torsions



Rings

Ligand BCR B 4010



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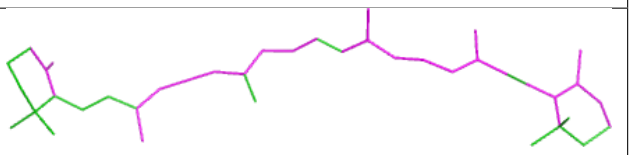
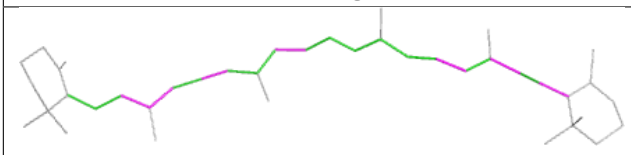


Bond angles



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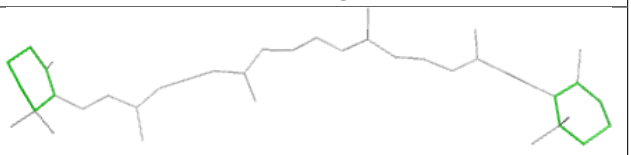
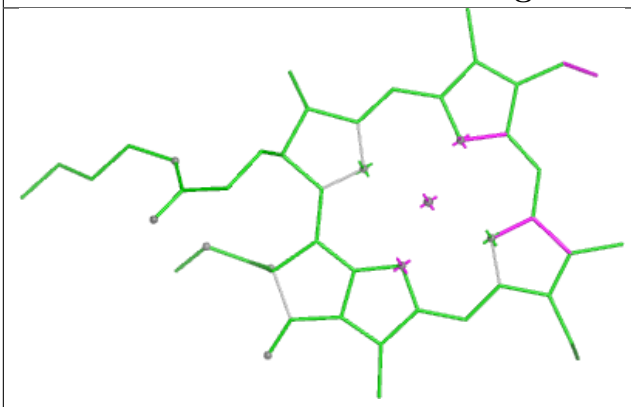


Rings

Ligand CLA A 1101



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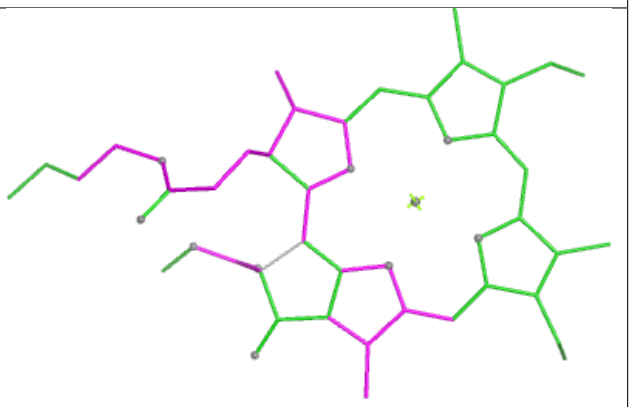
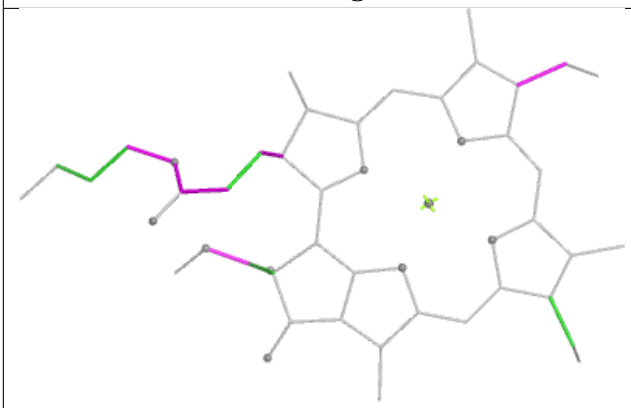


Bond angles



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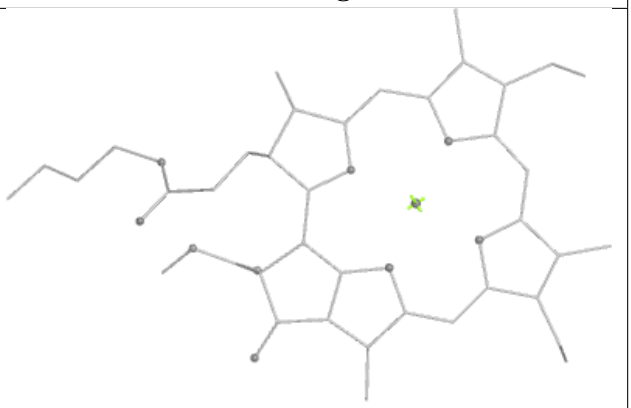
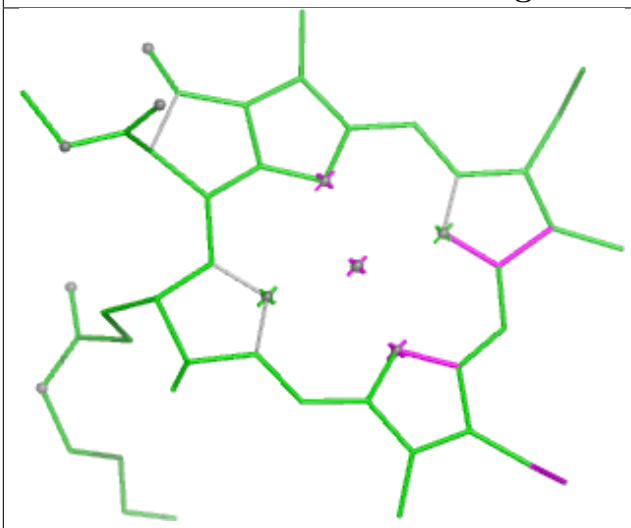


Rings

Ligand CLA A 1114



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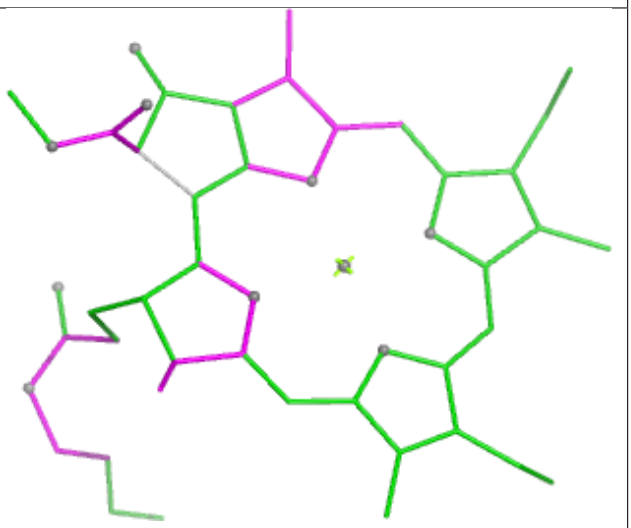
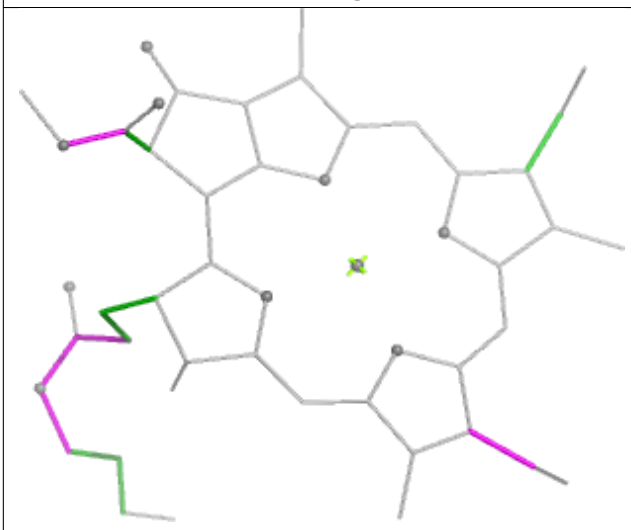


Bond angles



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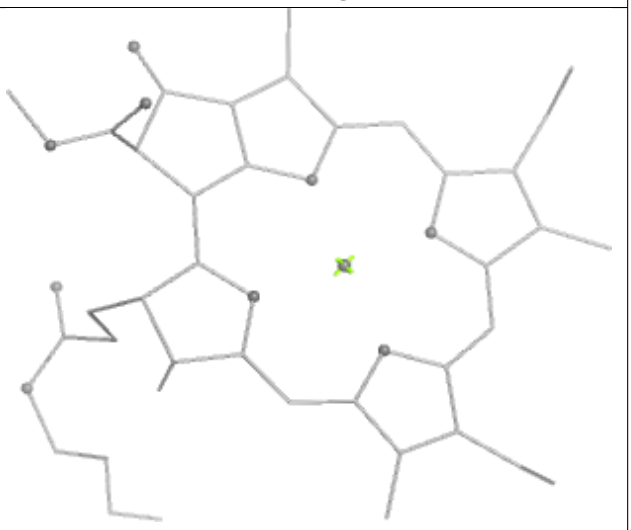
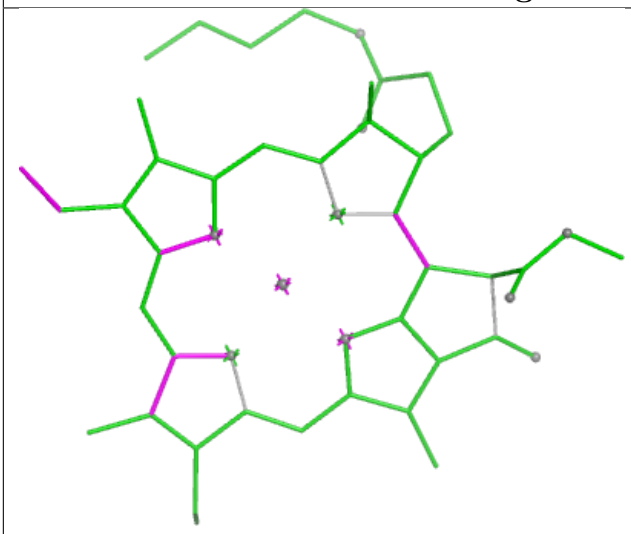


Rings

Ligand CLA B 1215



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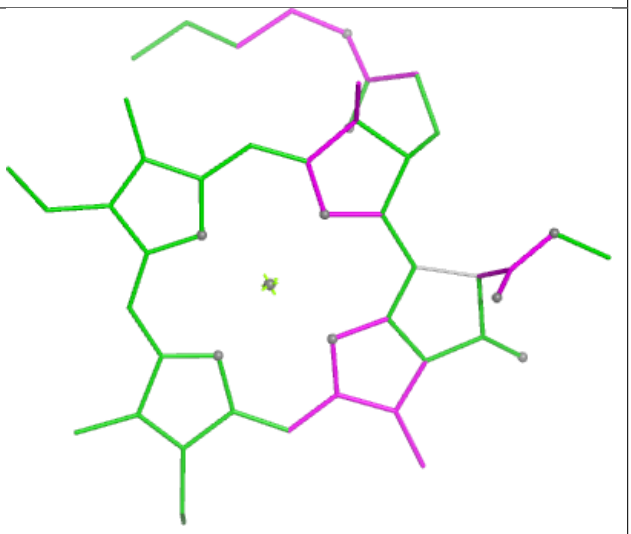
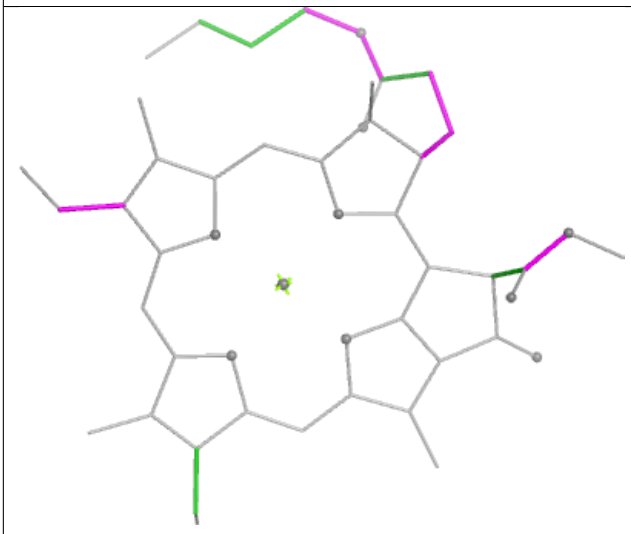


Bond angles



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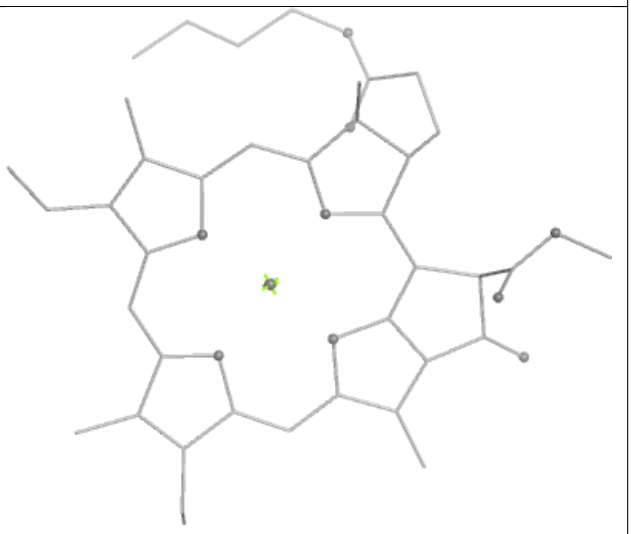
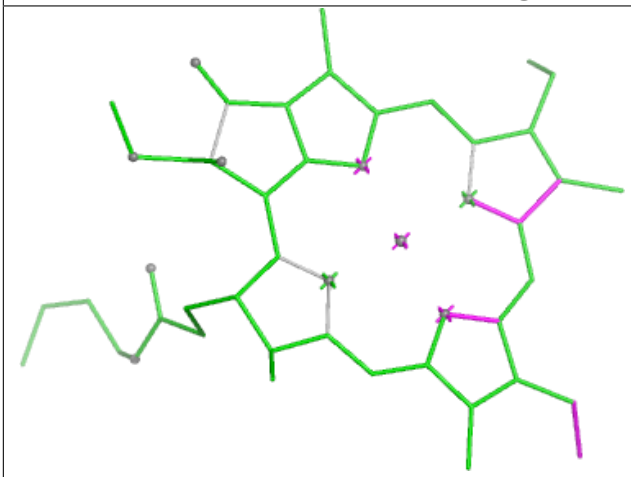


Rings

Ligand CLA B 1231



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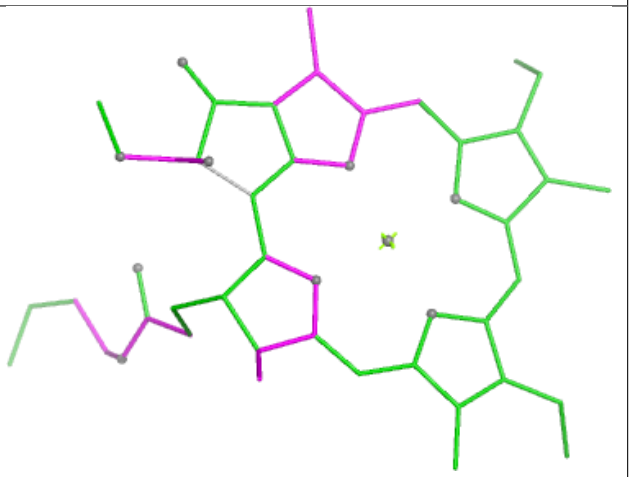
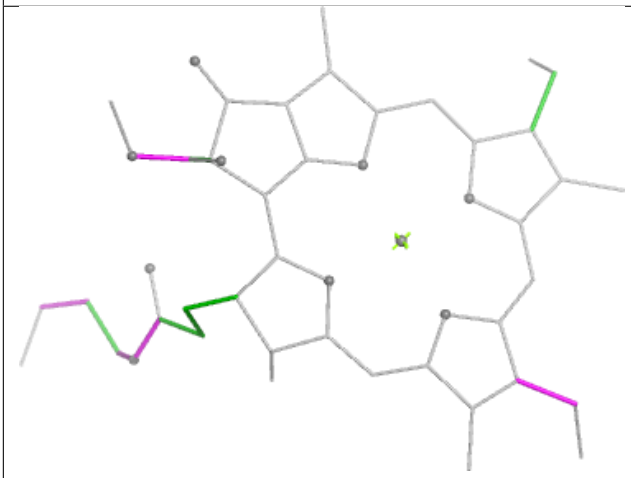


Bond angles



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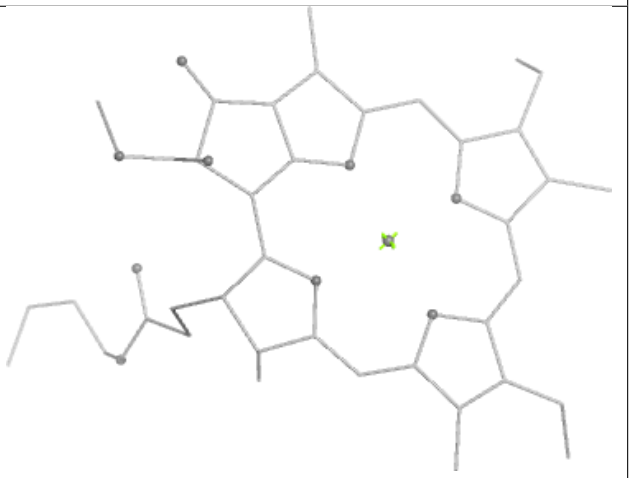
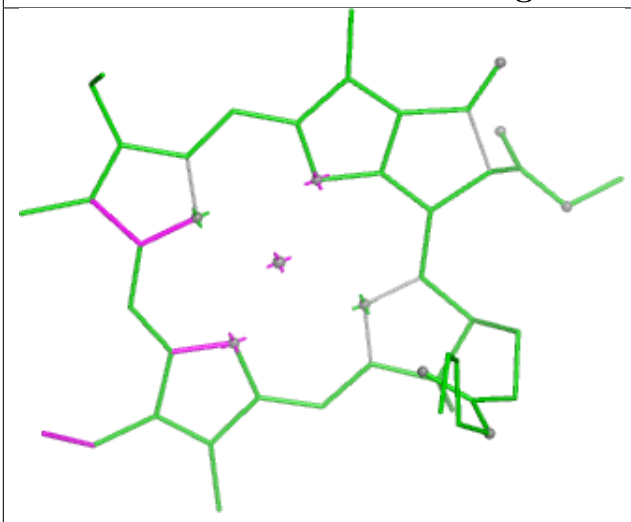


Rings

Ligand CLA B 1225



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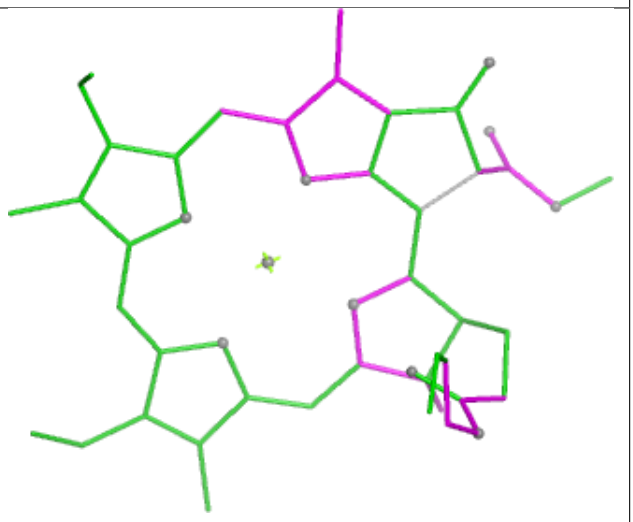
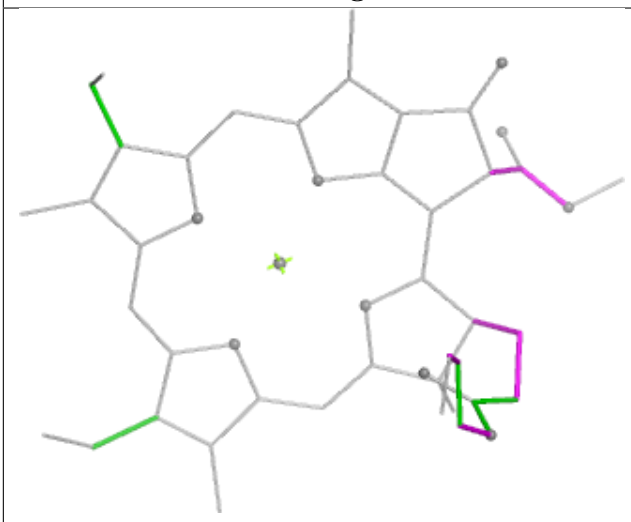


Bond angles



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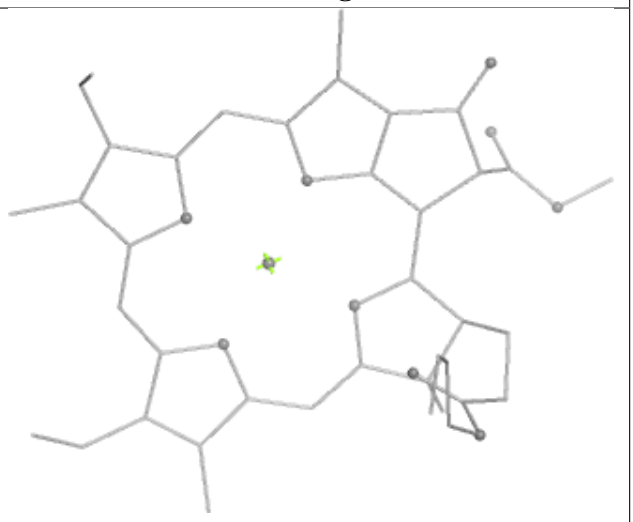
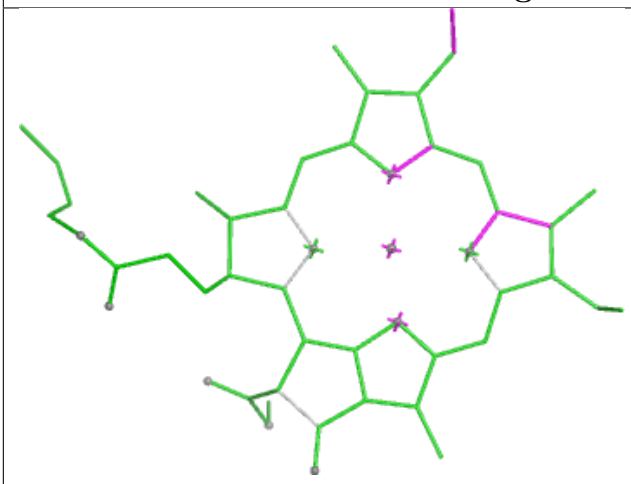


Rings

Ligand CLA A 1111



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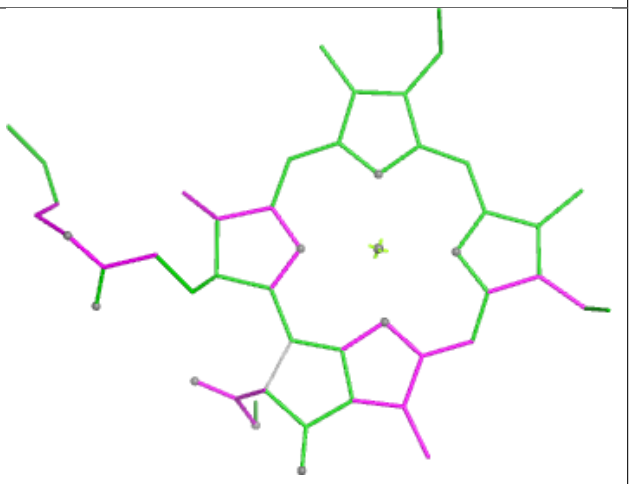
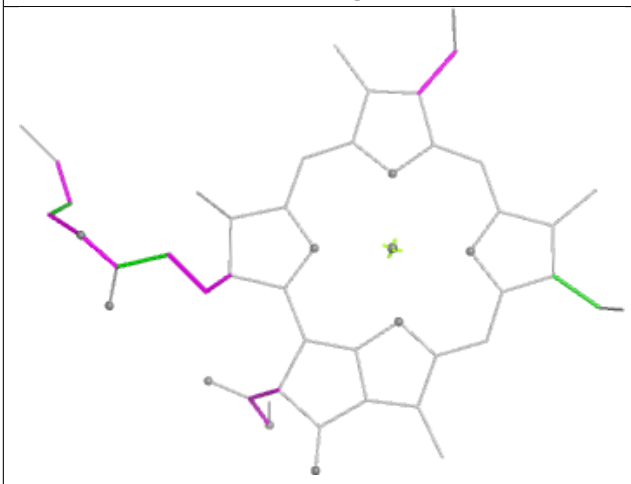


Bond angles



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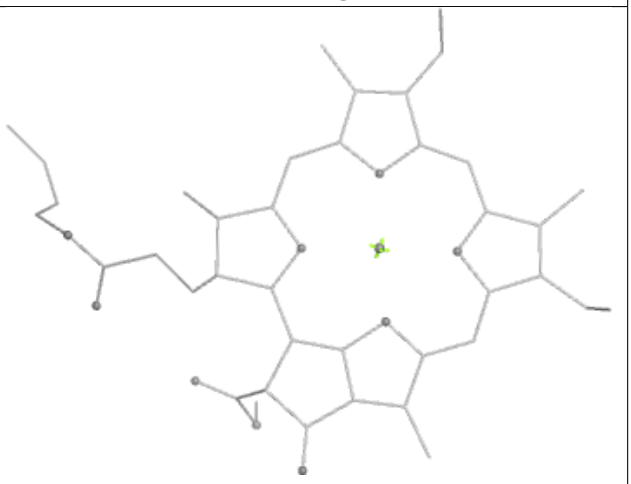
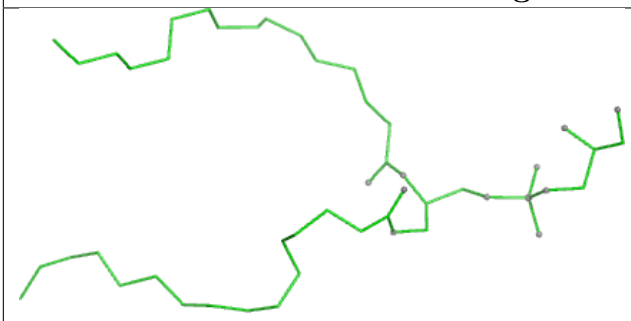


Rings

Ligand LHG A 5001



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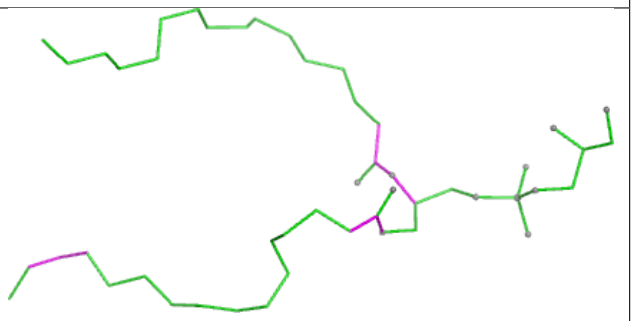
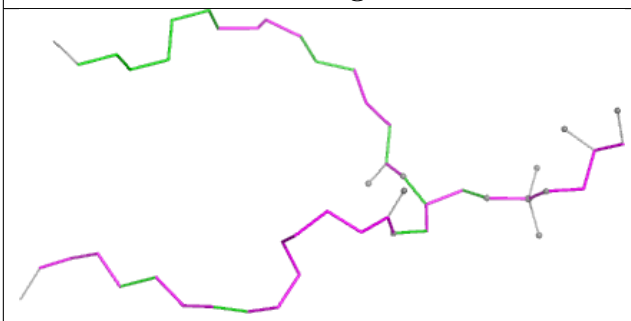


Bond angles

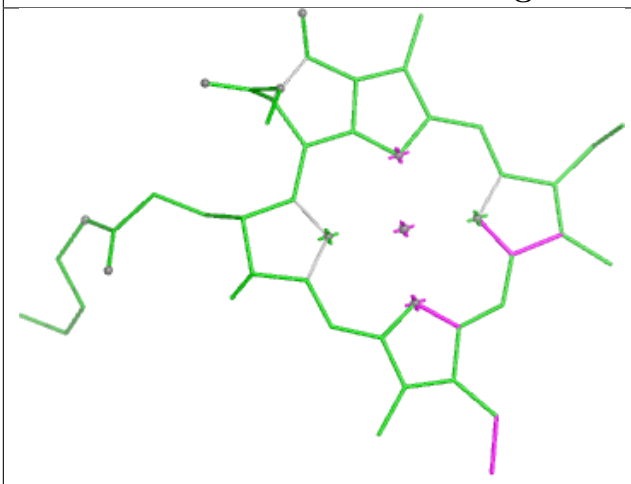


Torsions



Rings

Ligand CLA A 1125



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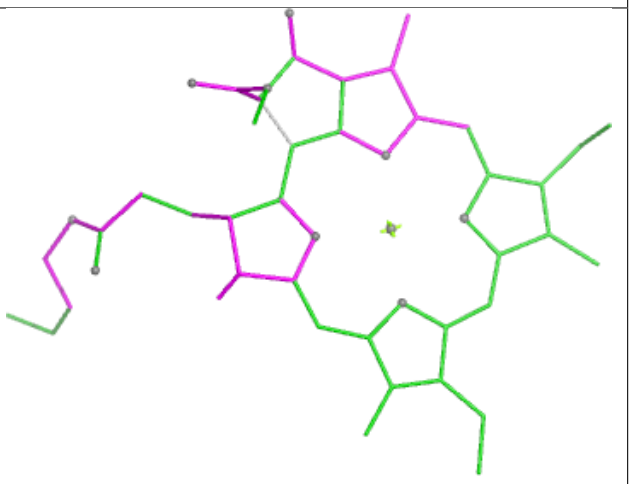
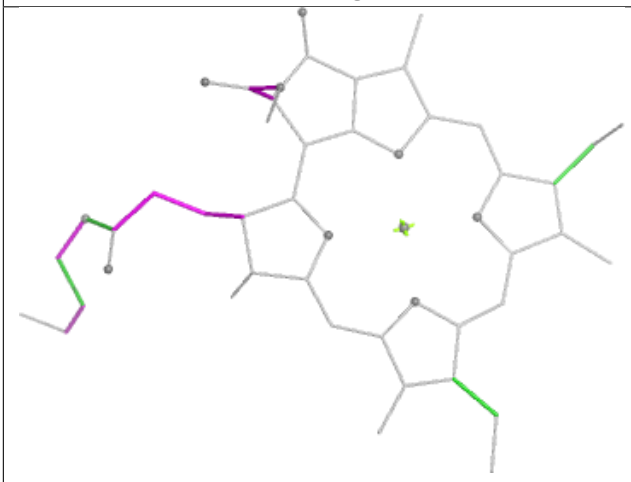


Bond angles



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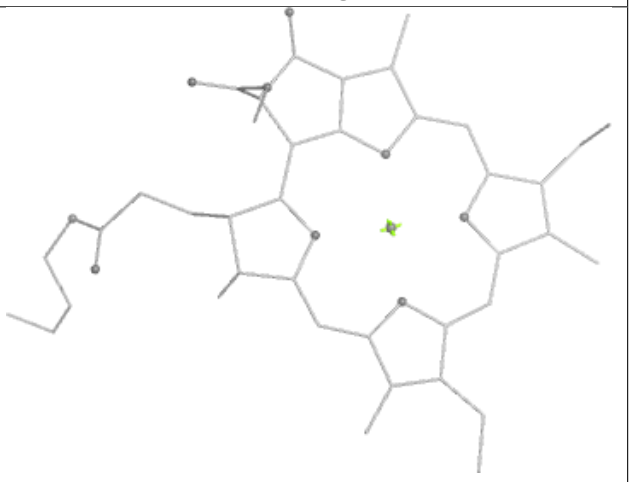
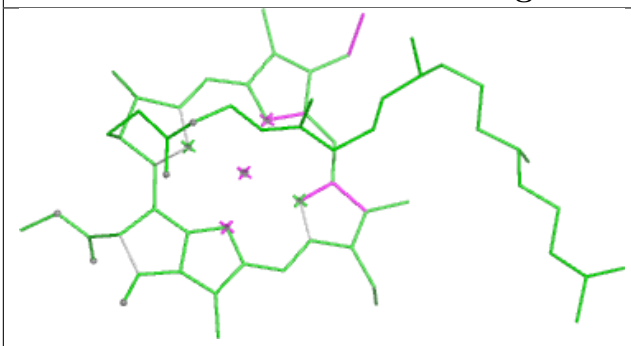


Rings

Ligand CLA B 1235



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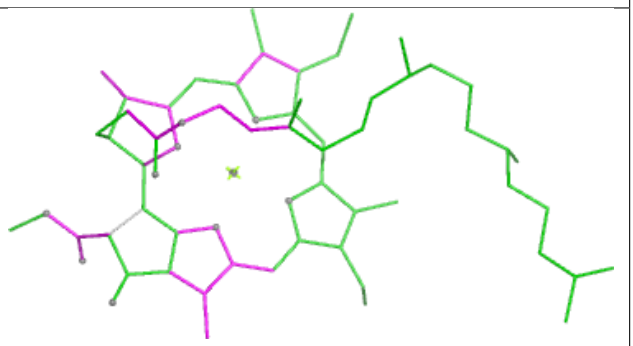
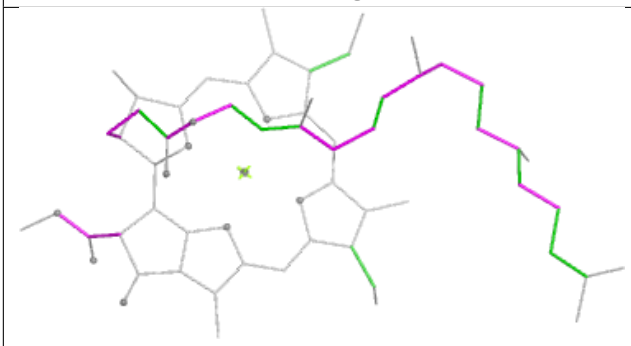


Bond angles

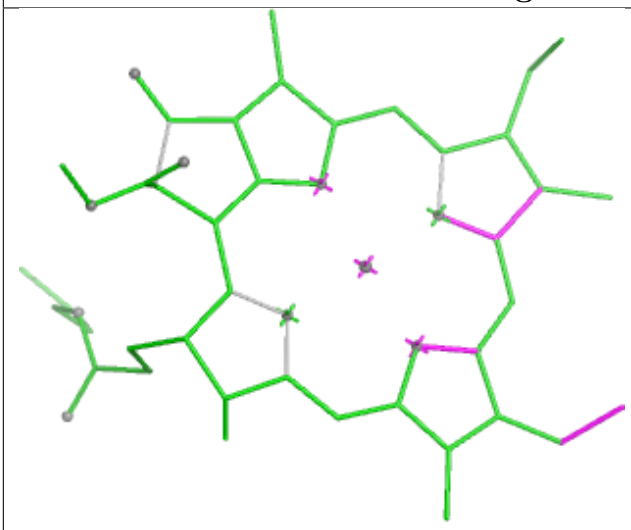


Torsions

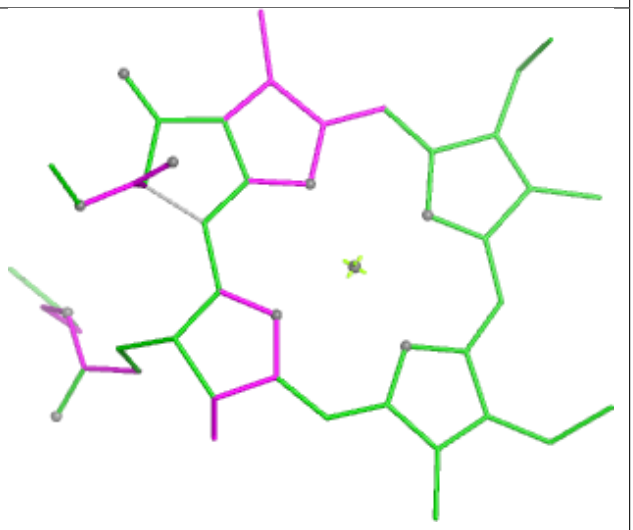


Rings

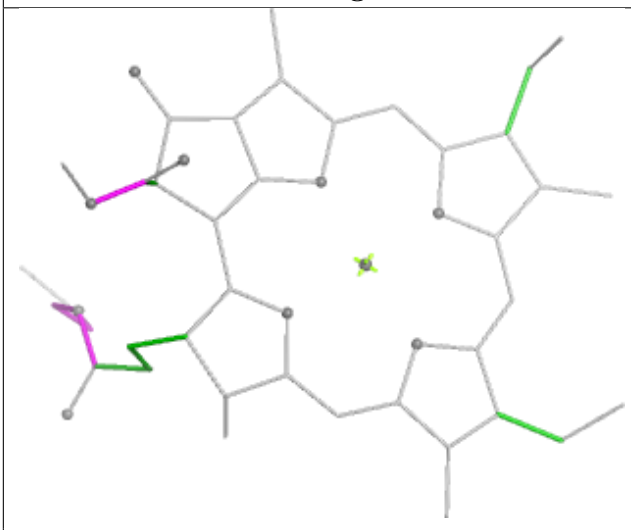
Ligand CLA B 1236



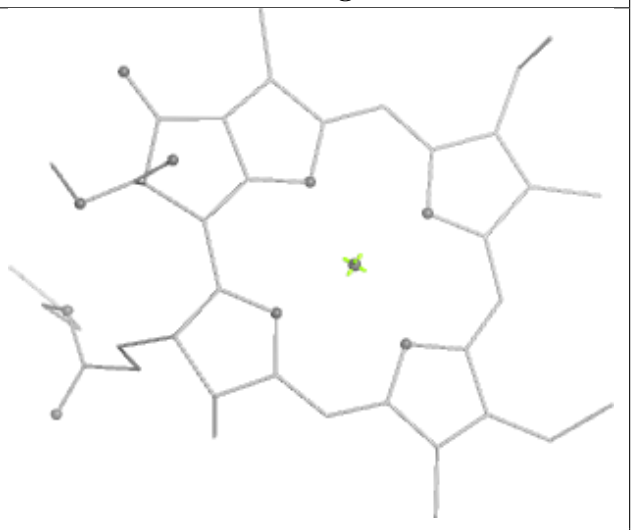
Bond lengths



Bond angles

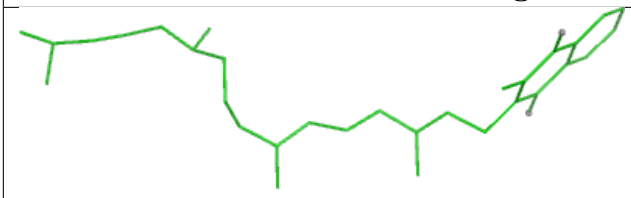


Torsions

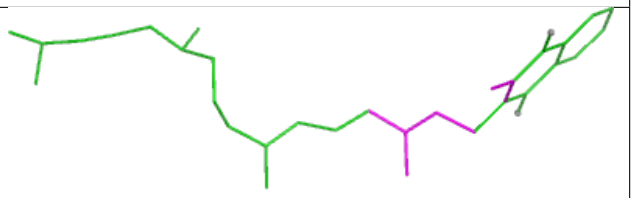


Rings

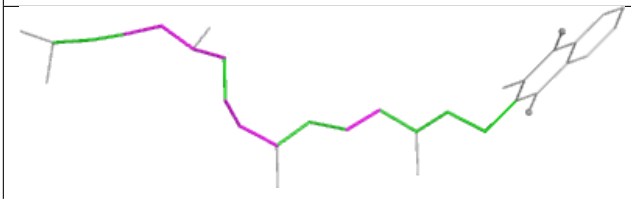
Ligand PQN A 2001



Bond lengths



Bond angles



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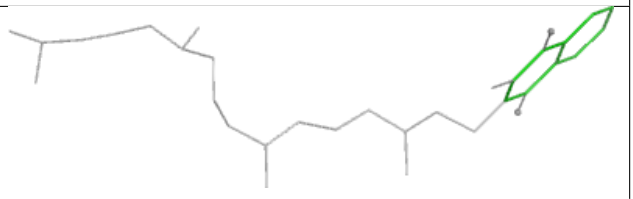
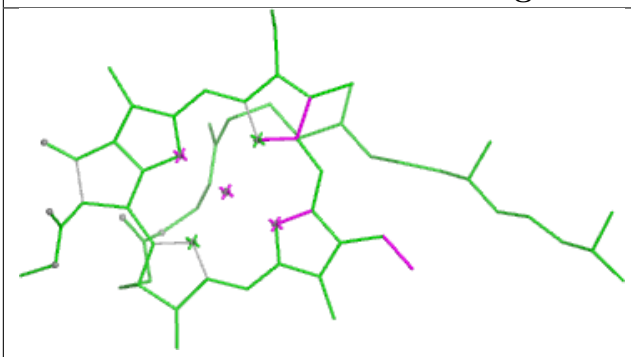


Rings

Ligand CLA A 1138



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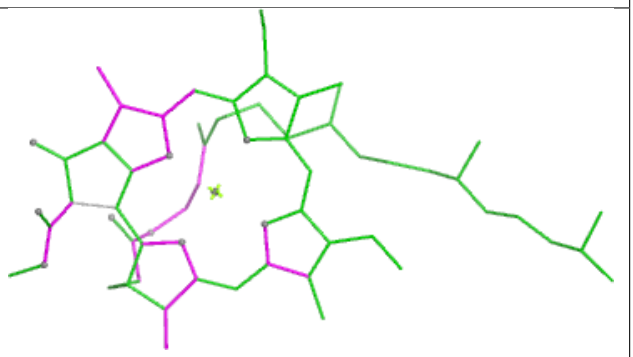

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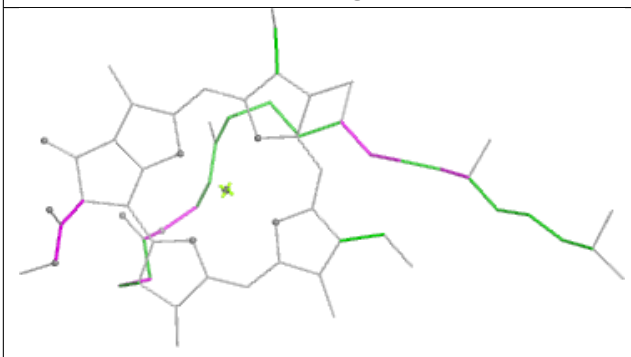

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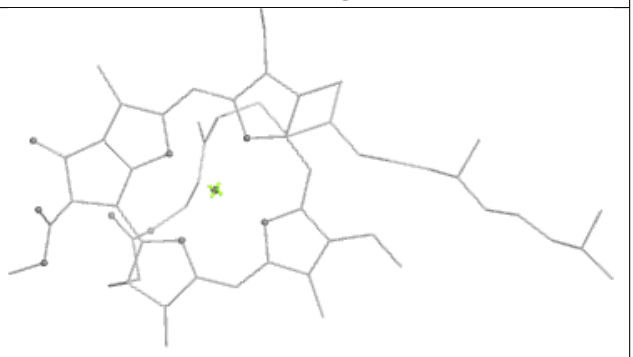
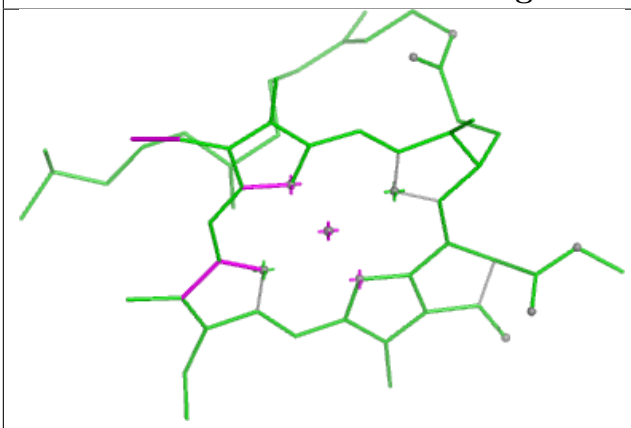


Rings

Ligand CLA B 1214



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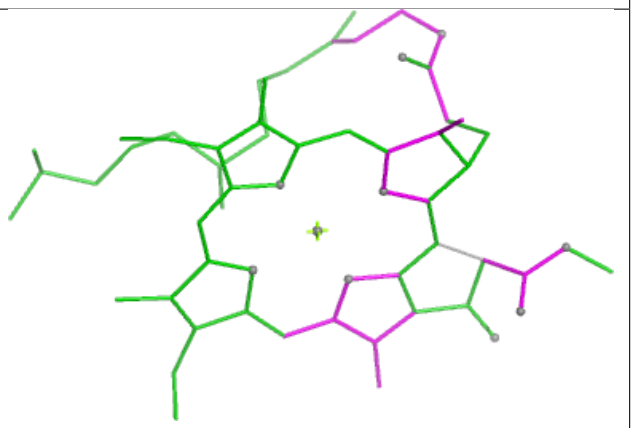

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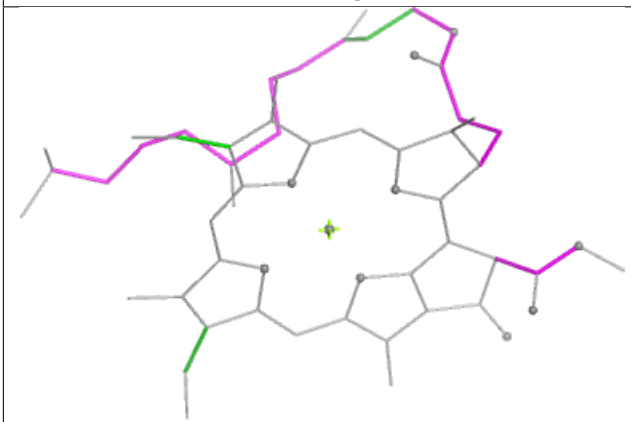

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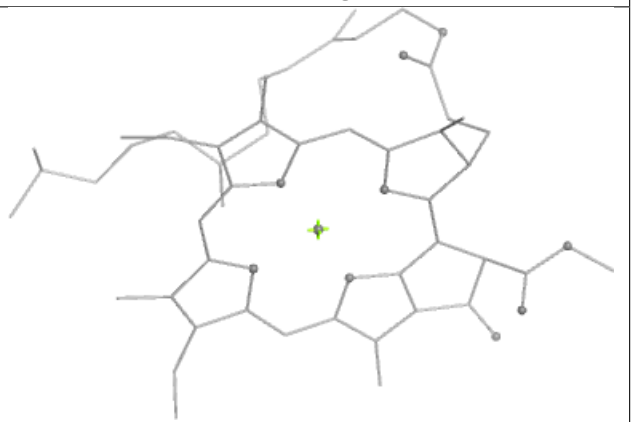
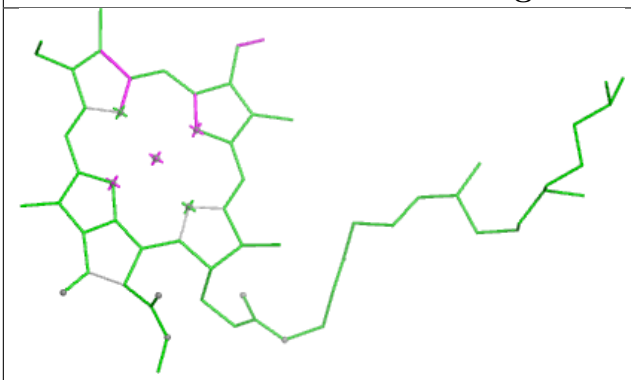


Rings

Ligand CLA A 1013



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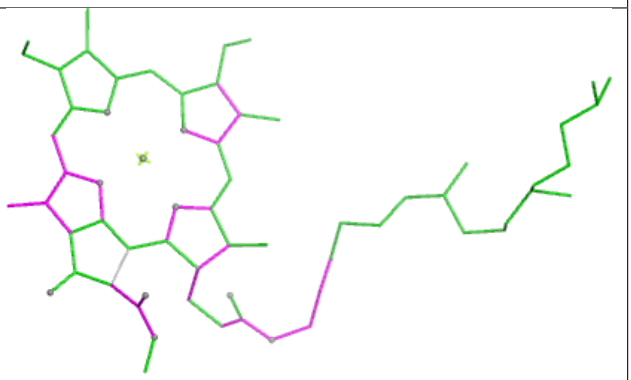
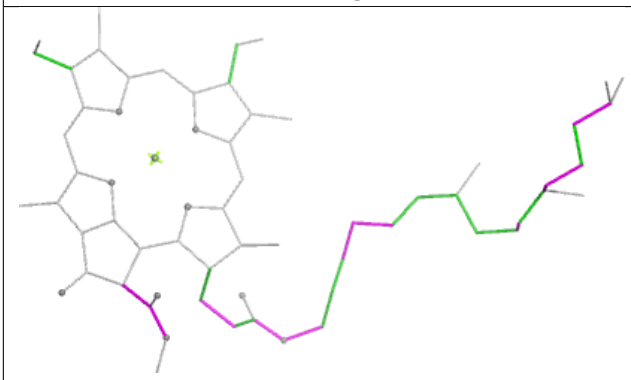


Bond angles



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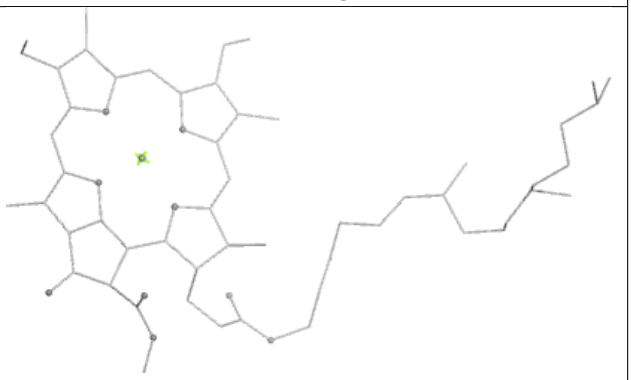
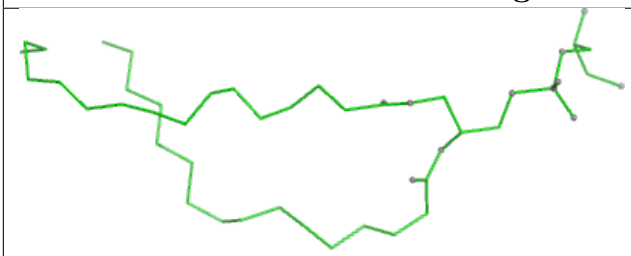


Rings

Ligand LHG A 5003



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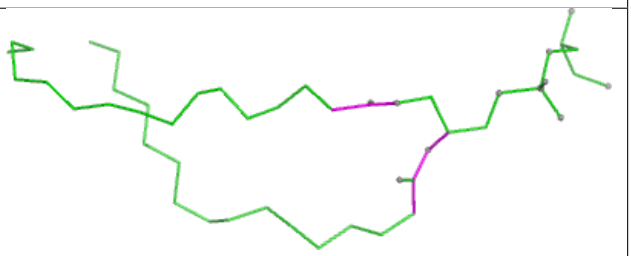

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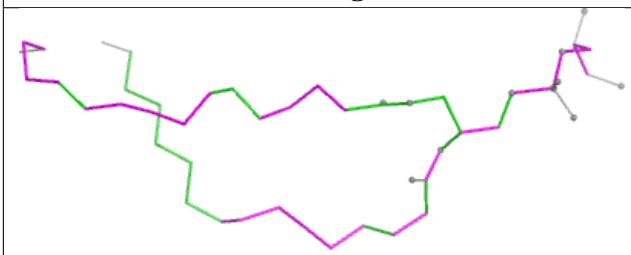

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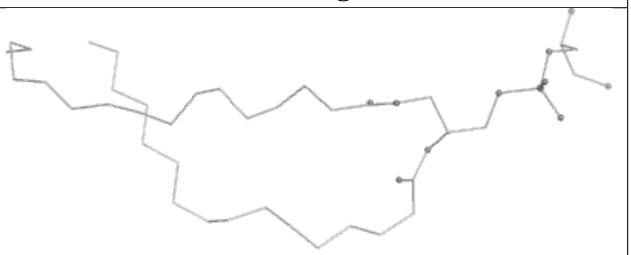
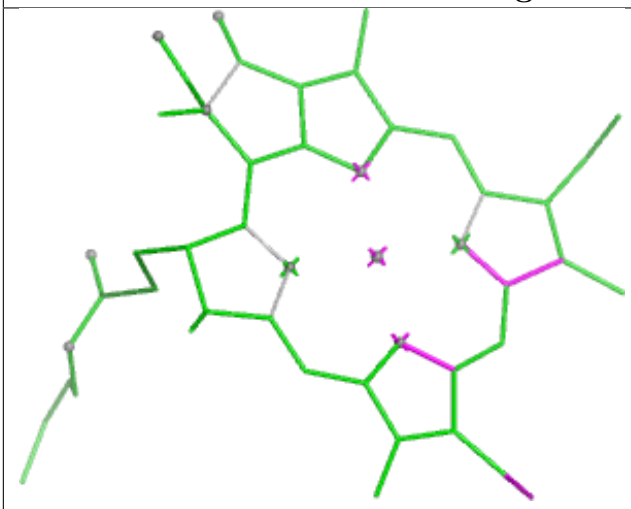


Rings

Ligand CLA B 1227



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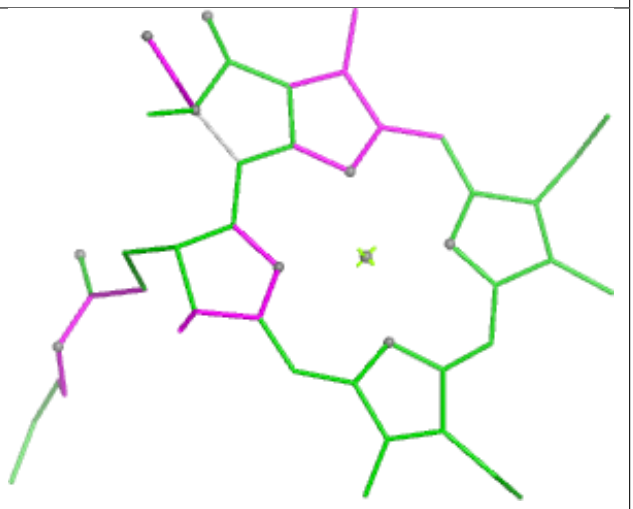
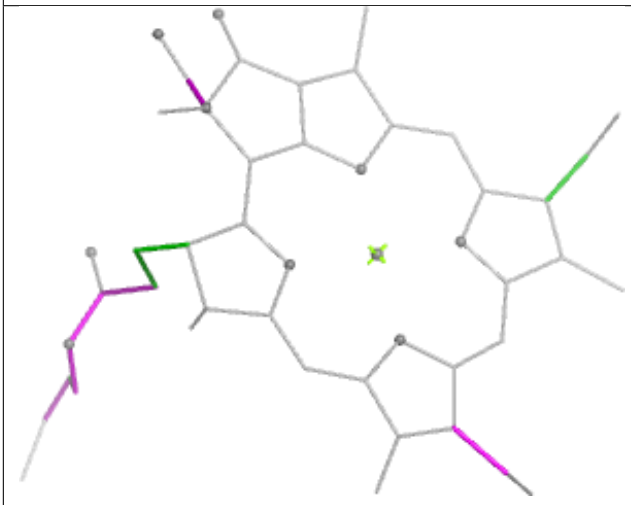


Bond angles



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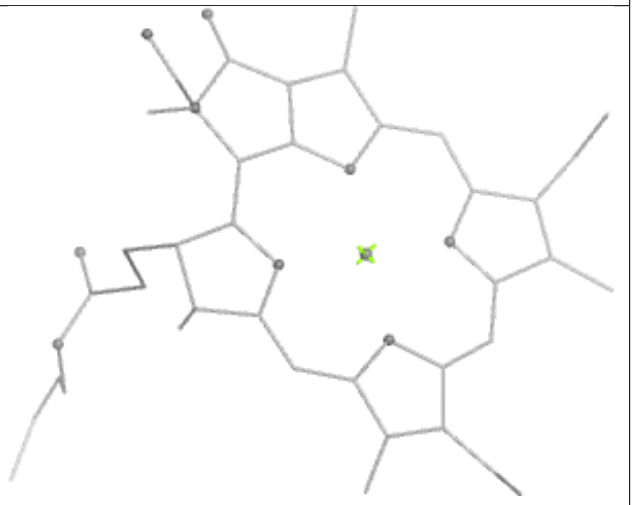
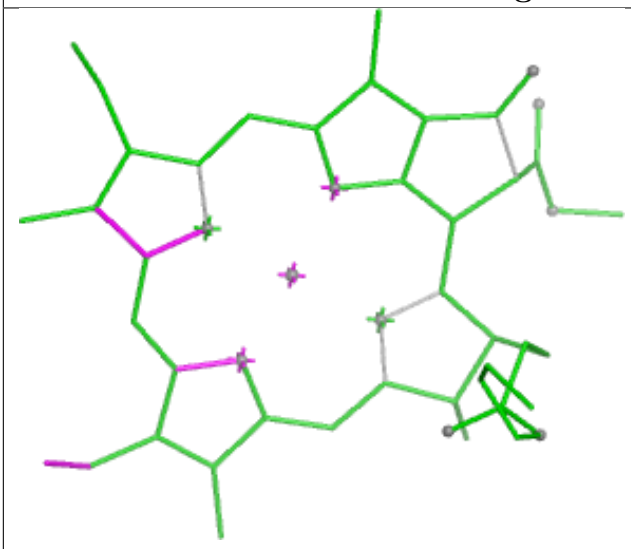


Rings

Ligand CLA A 1134



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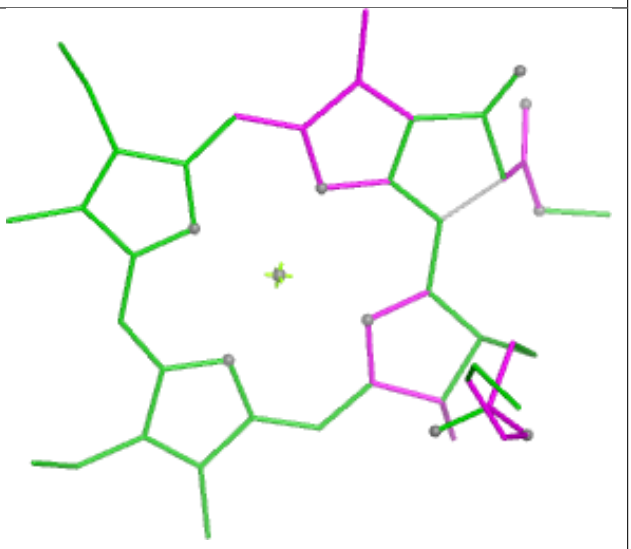

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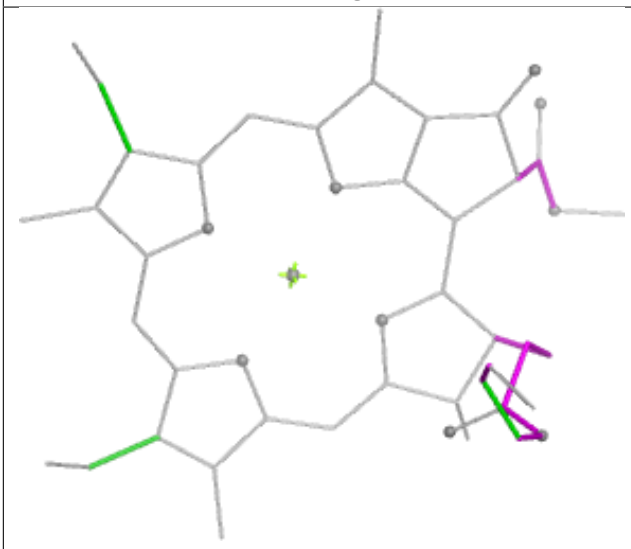

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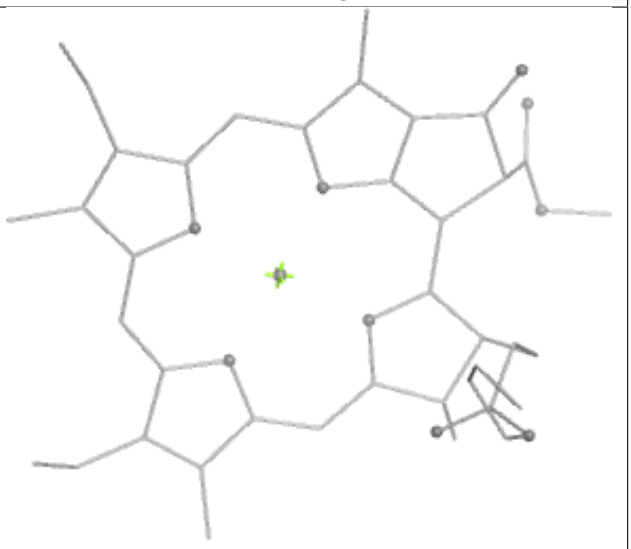
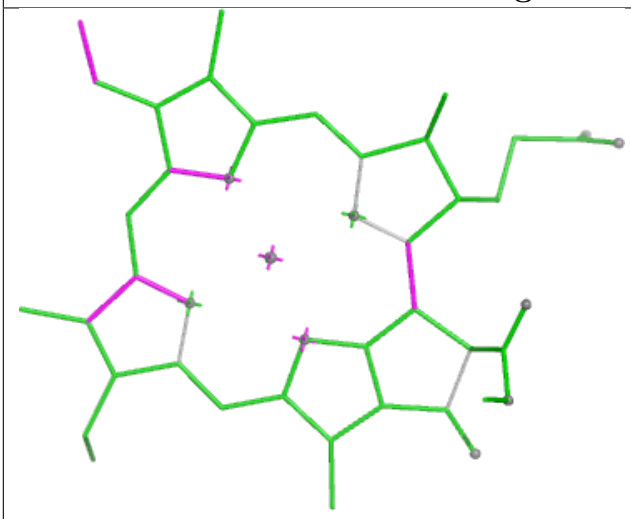


Rings

Ligand CLA A 1141



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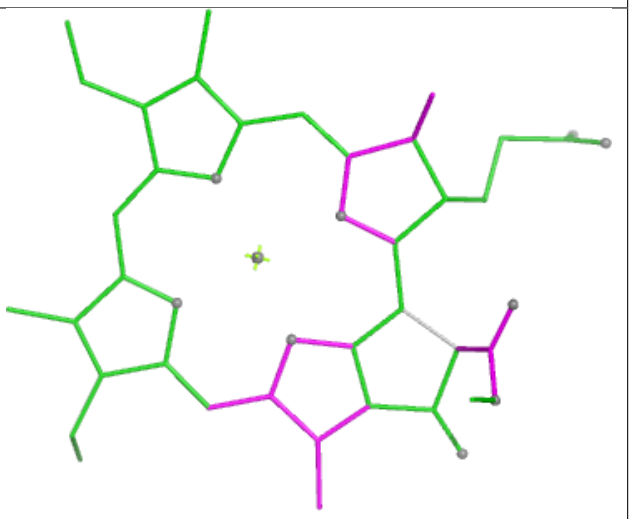
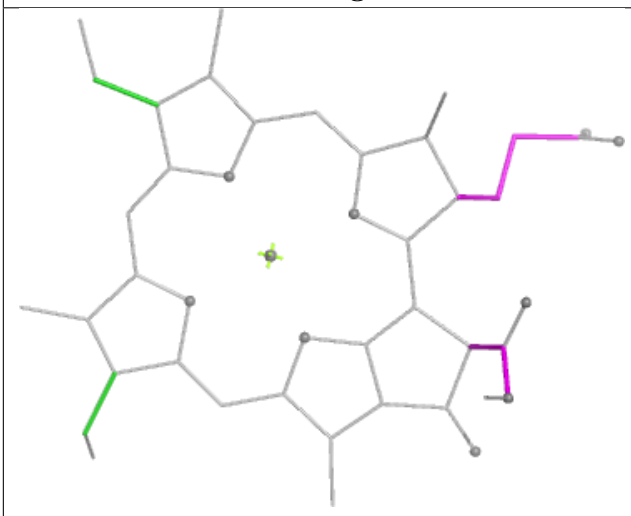


Bond angles



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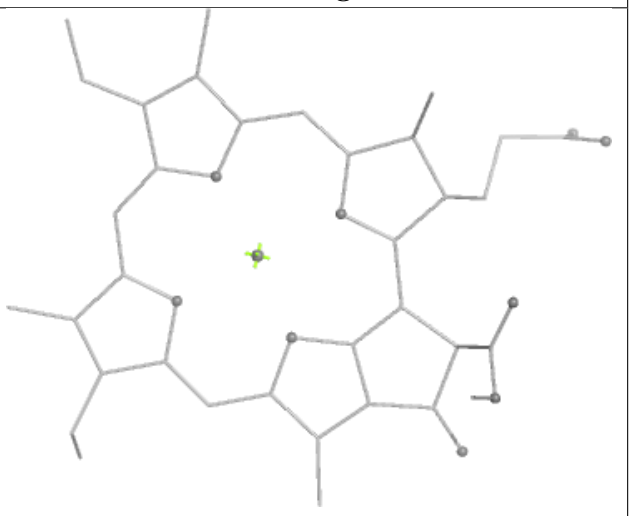
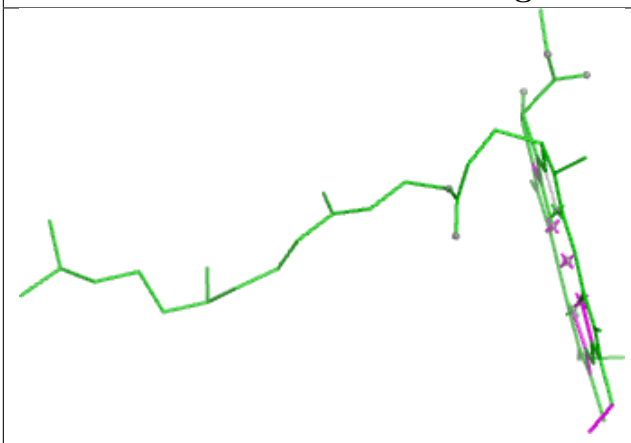


Rings

Ligand CLA A 1126



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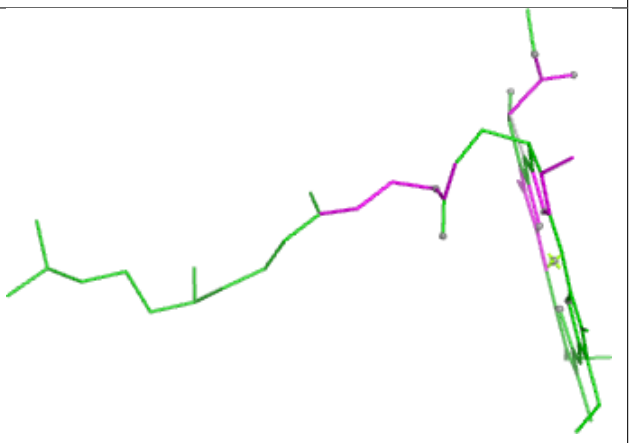
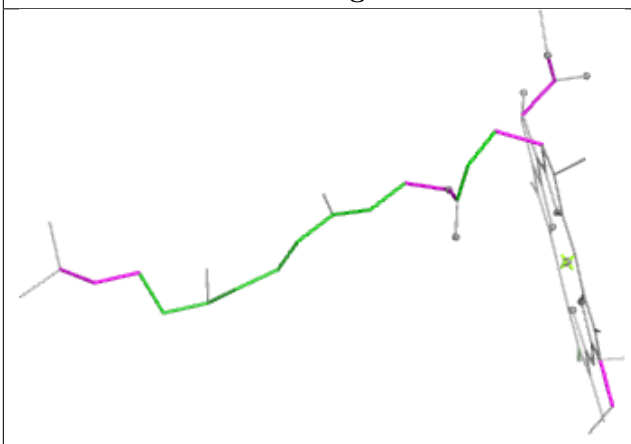


Bond angles



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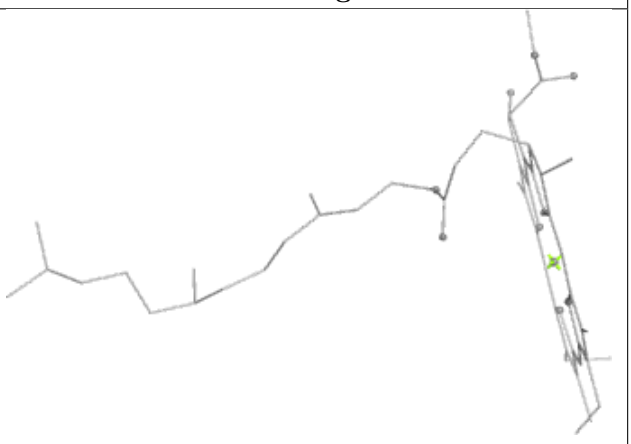
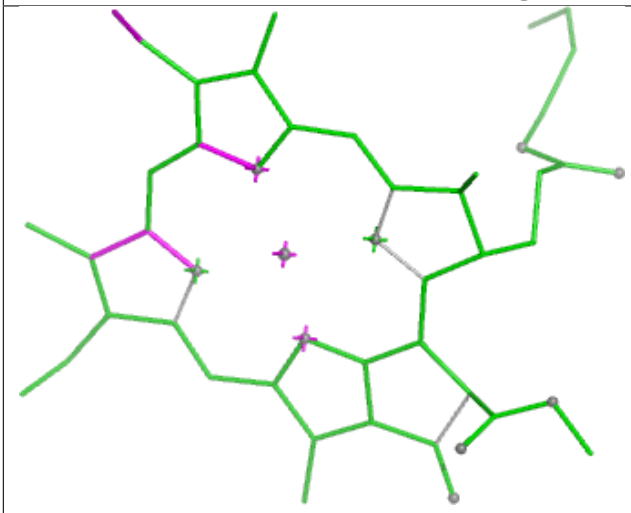


Rings

Ligand CLA B 1216



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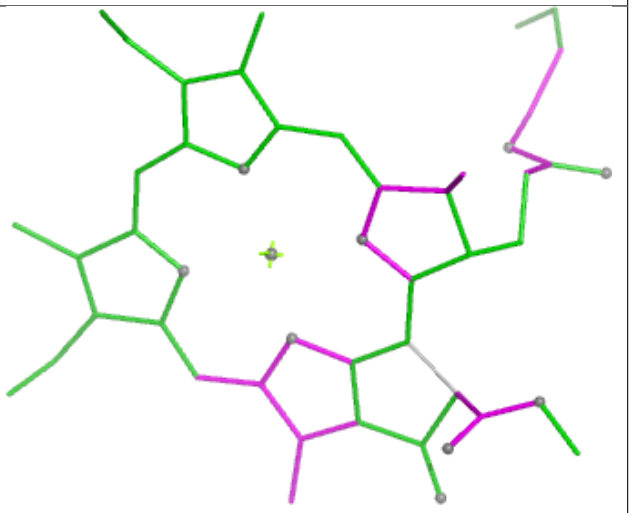
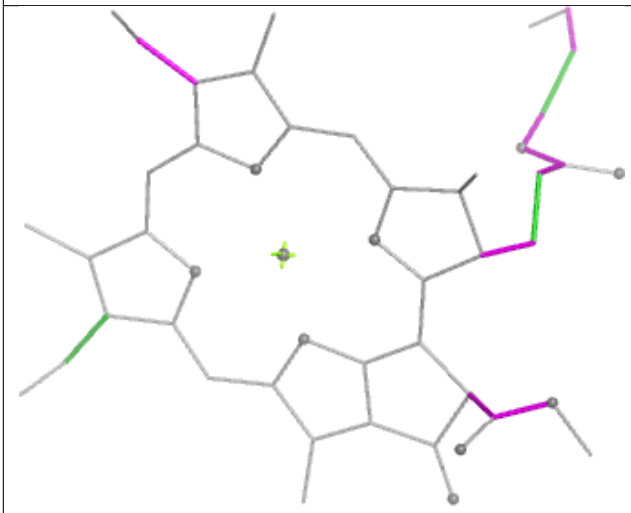


Bond angles



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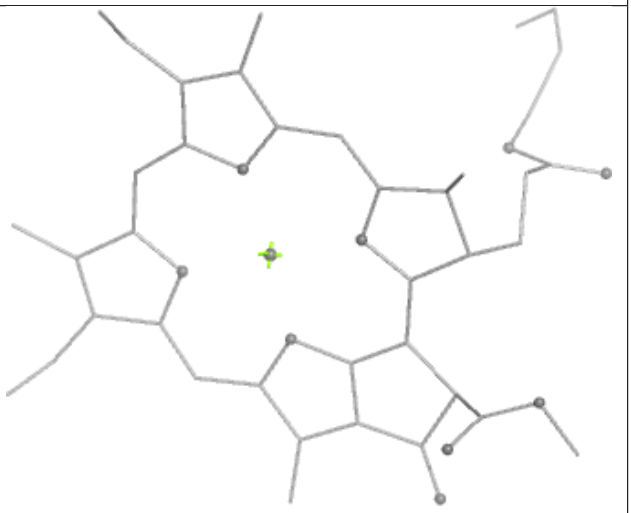
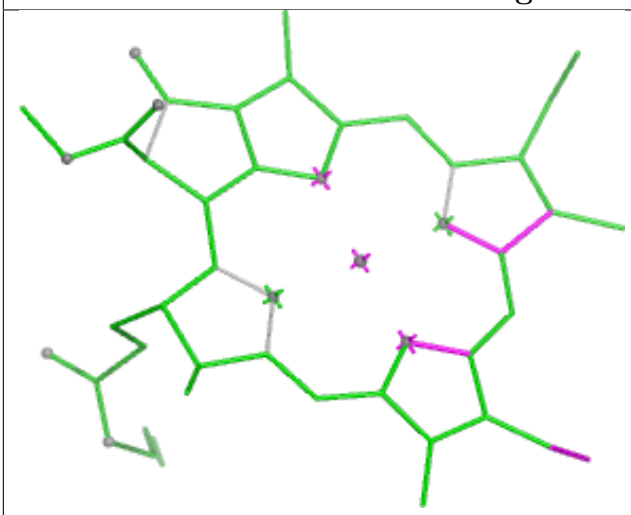


Rings

Ligand CLA B 1212



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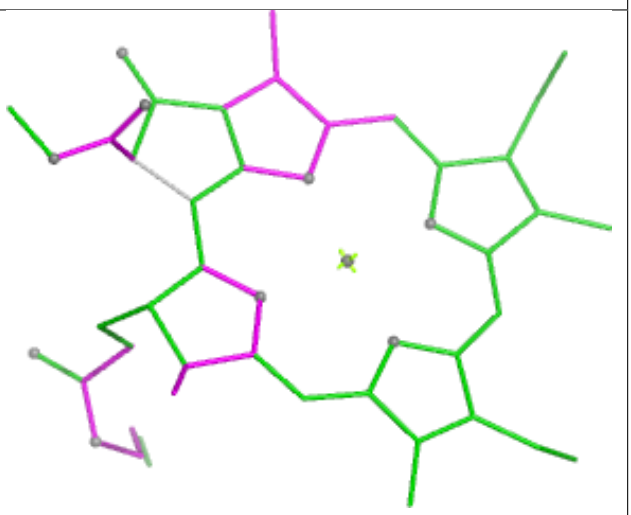
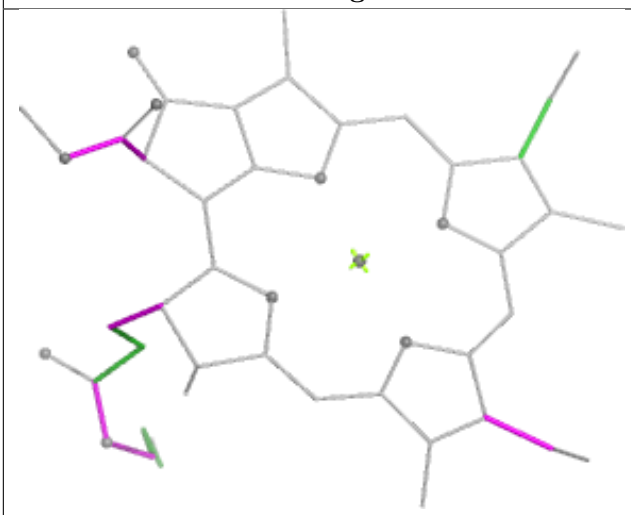


Bond angles



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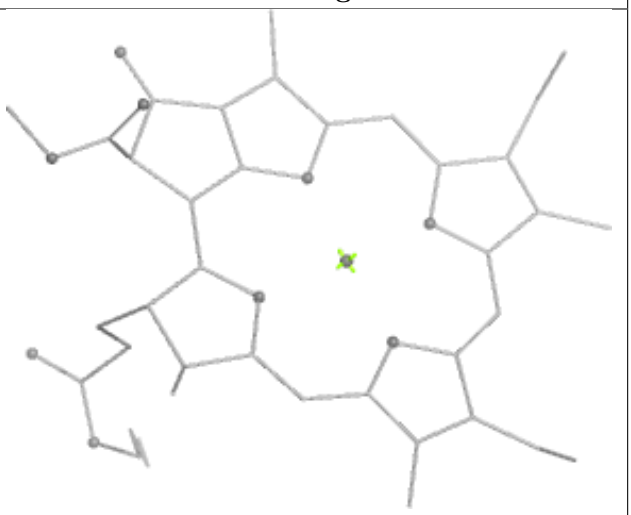
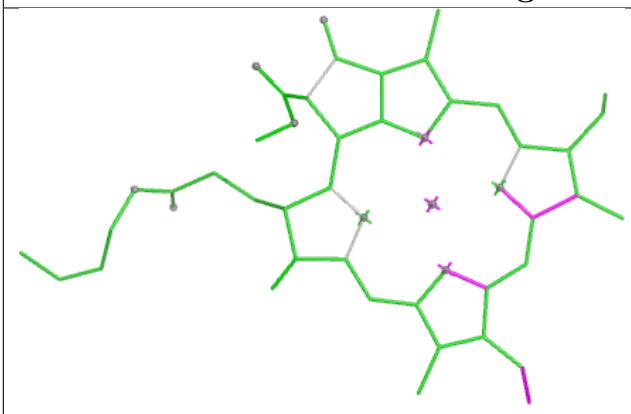


Rings

Ligand CLA F 1302



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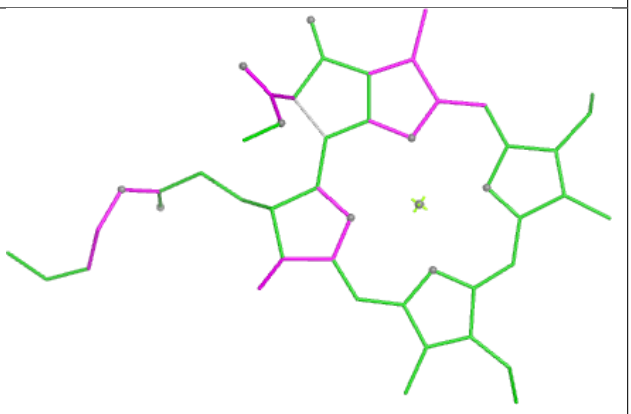
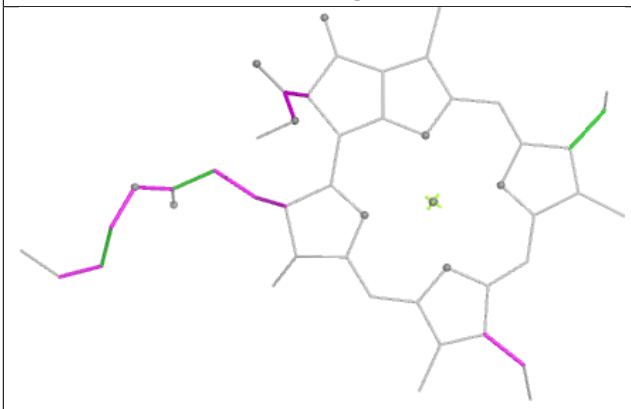


Bond angles



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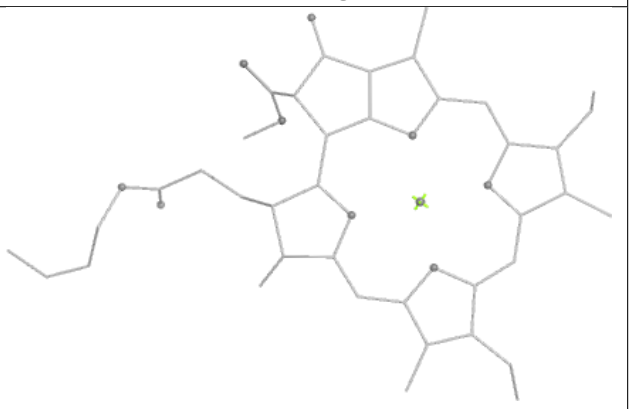
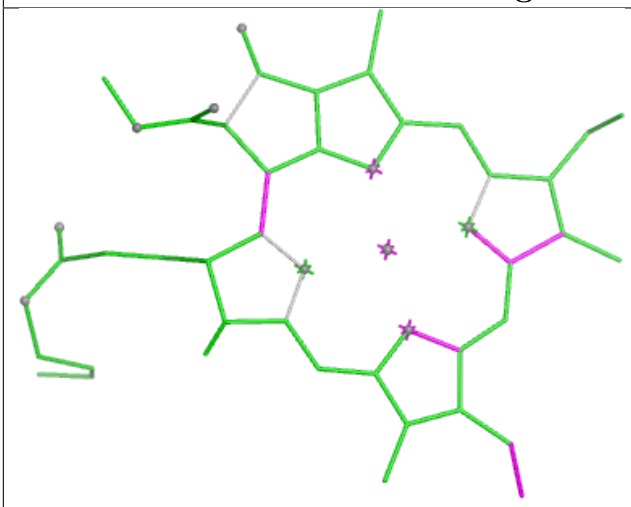
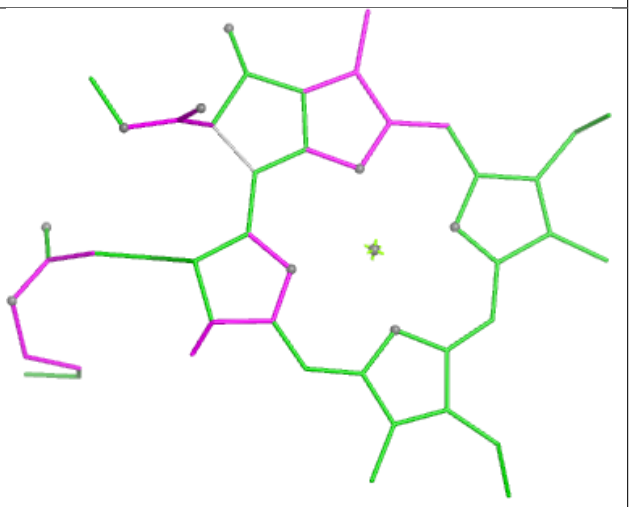


Rings

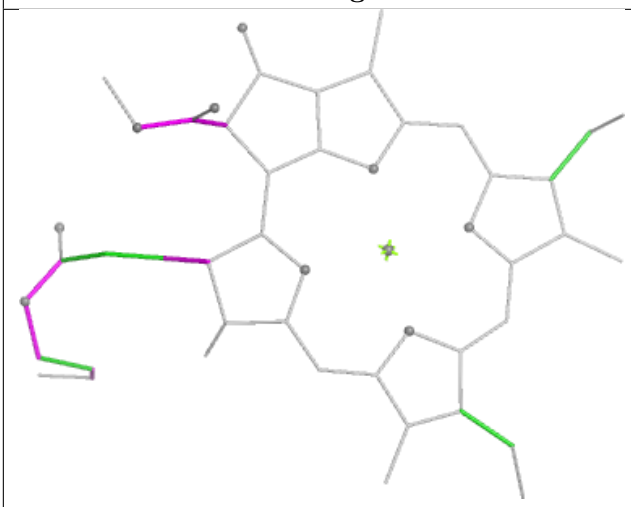
Ligand CLA B 1206



Bond lengths



Bond angles



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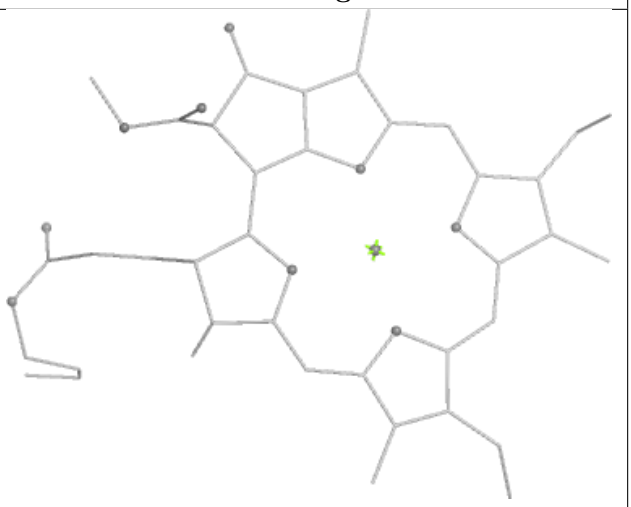
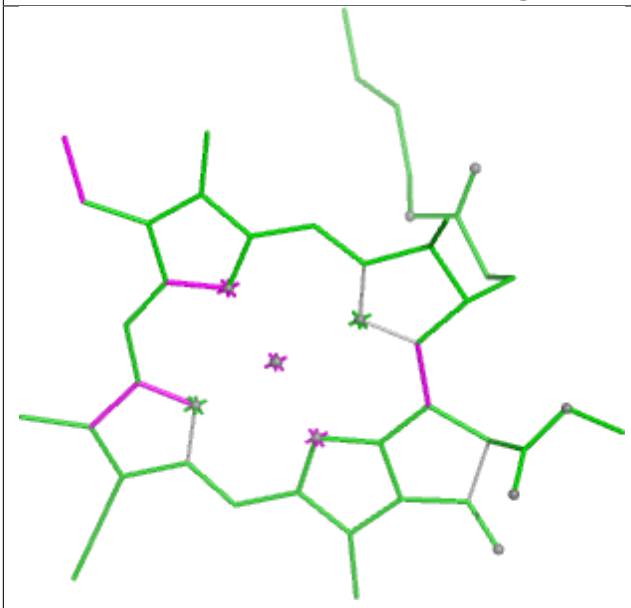


Rings

Ligand CLA A 1122



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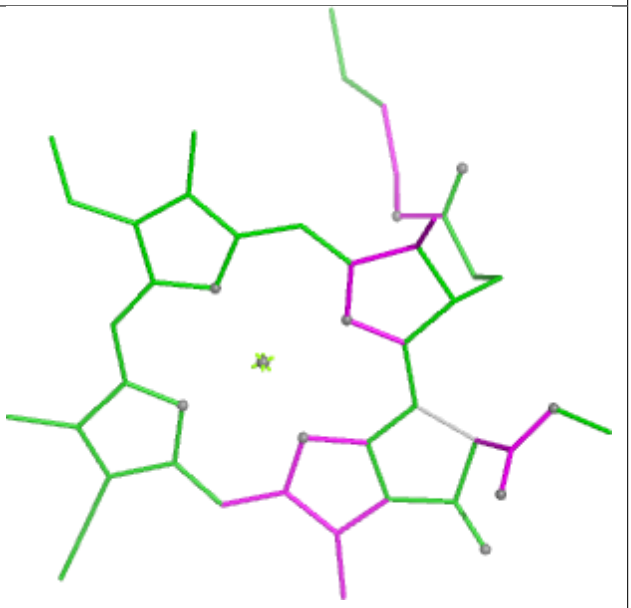
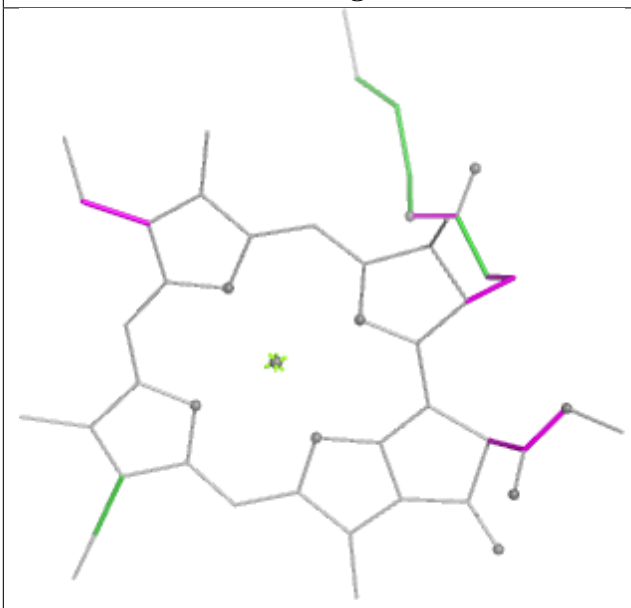


Bond angles



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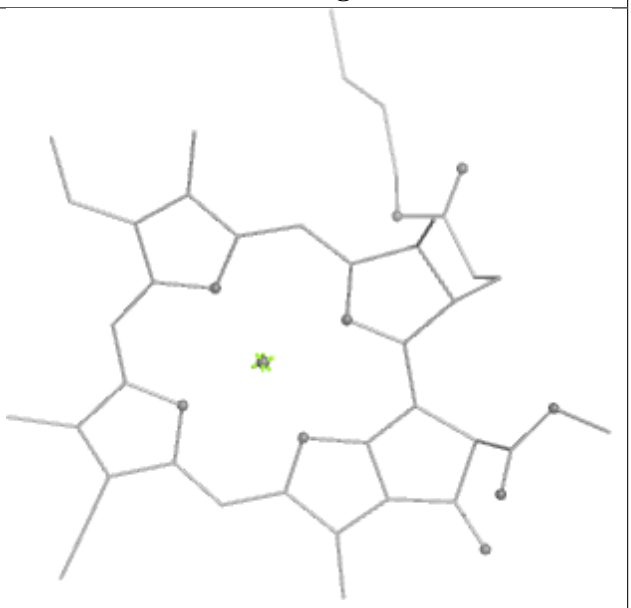
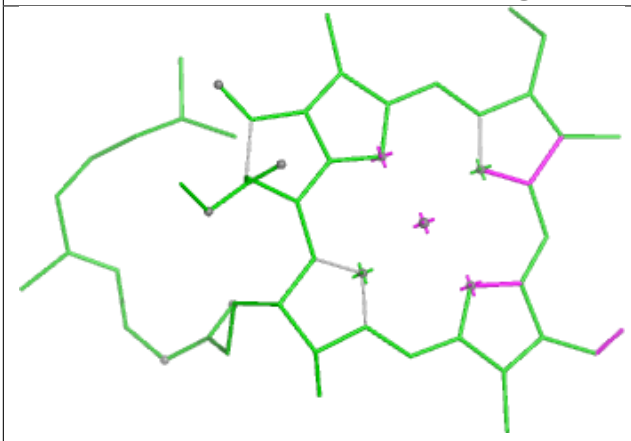
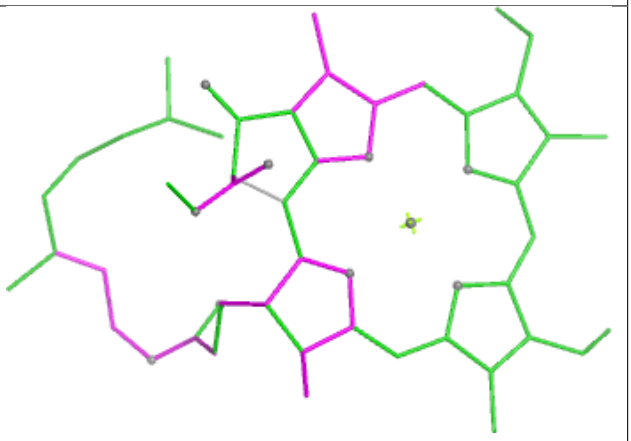


Rings

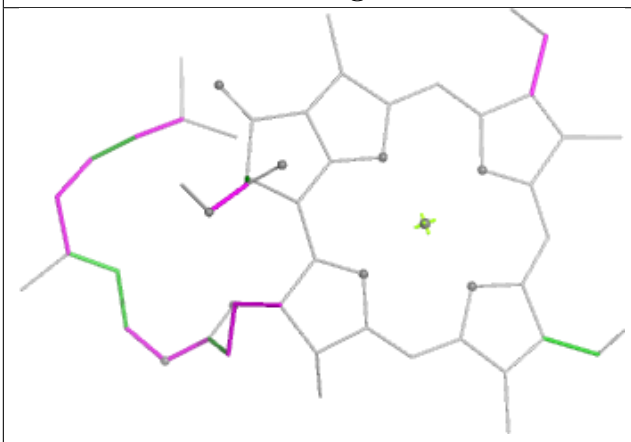
Ligand CLA B 1229



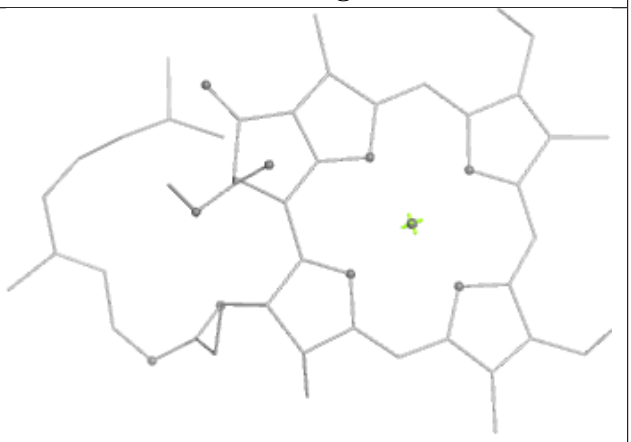
Bond lengths



Bond angles

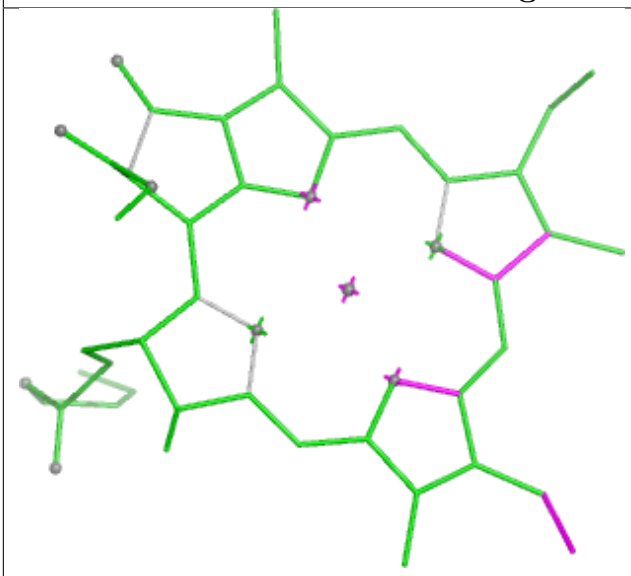


Torsions



Rings

Ligand CLA J 1303



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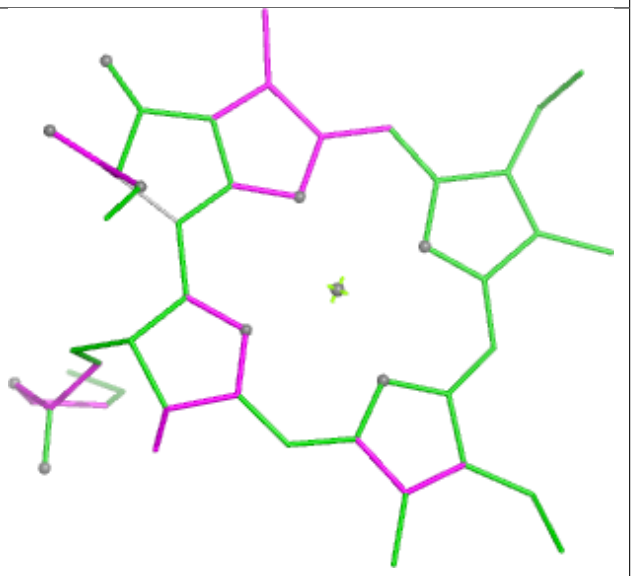
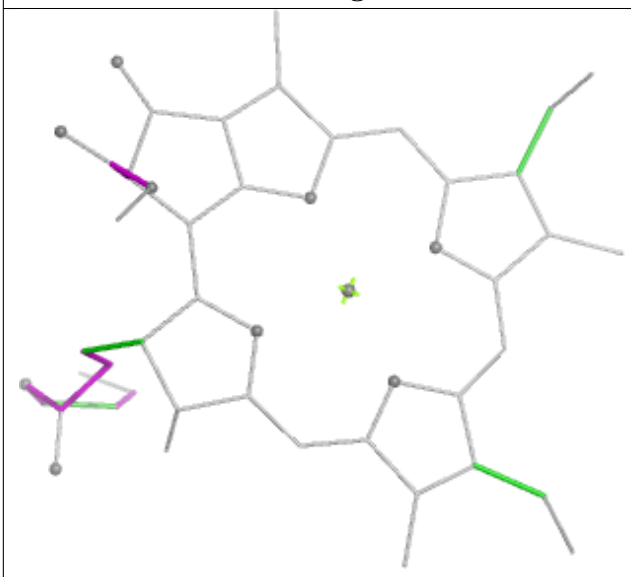


Bond angles



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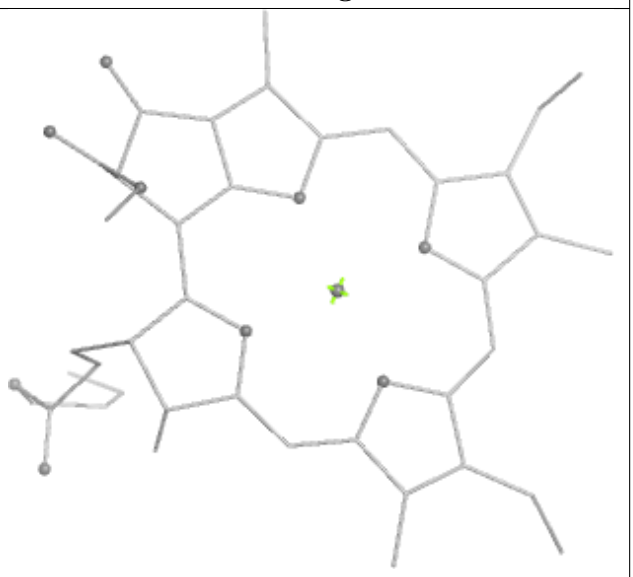
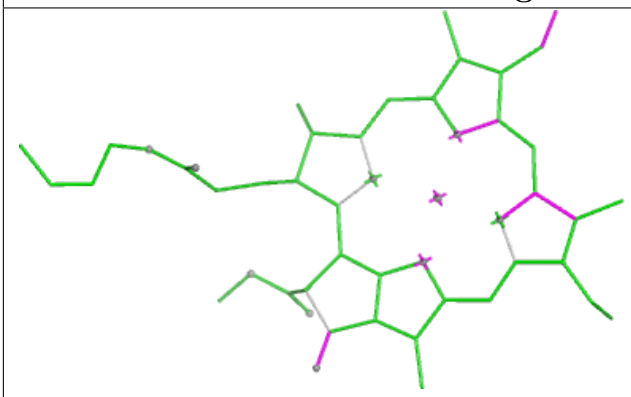


Rings

Ligand CLA B 1223



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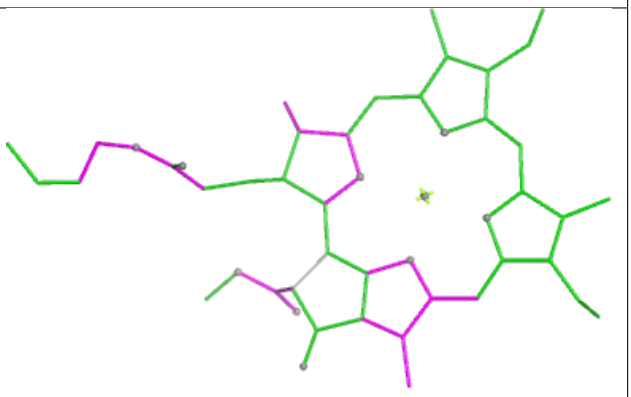
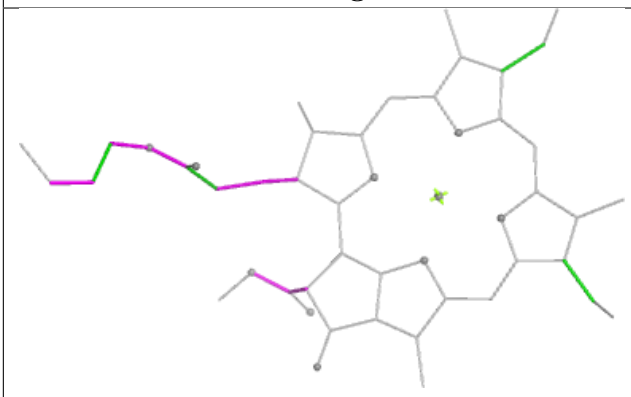


Bond angles



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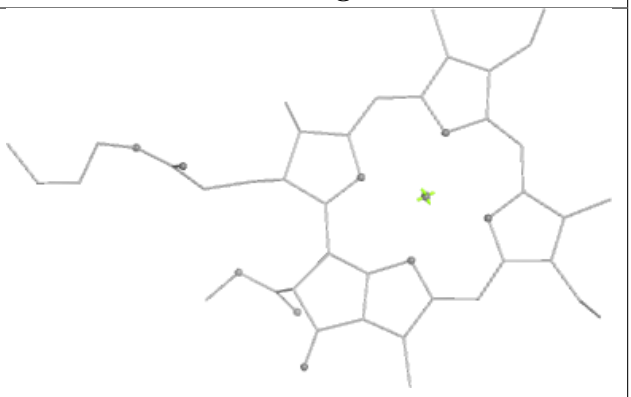
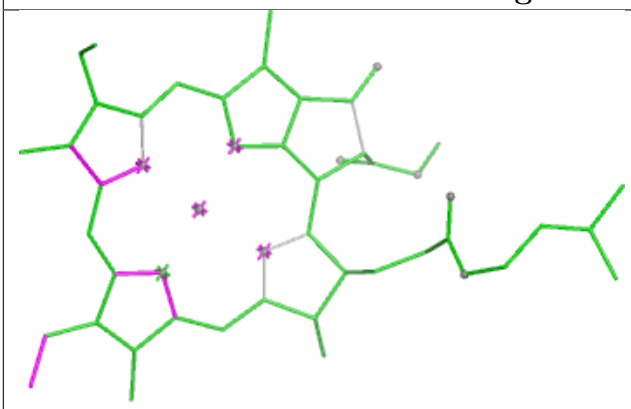


Rings

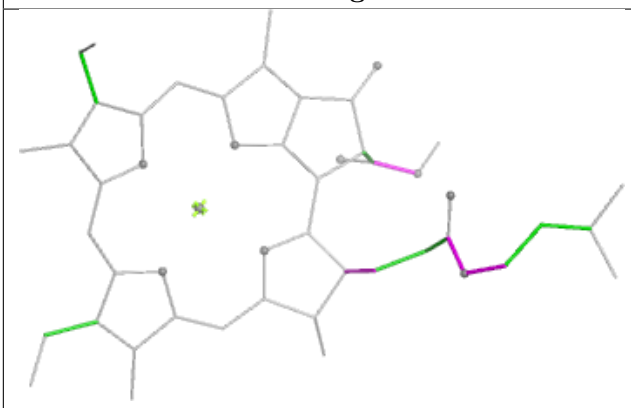
Ligand CLA A 1107



Bond lengths



Bond angles



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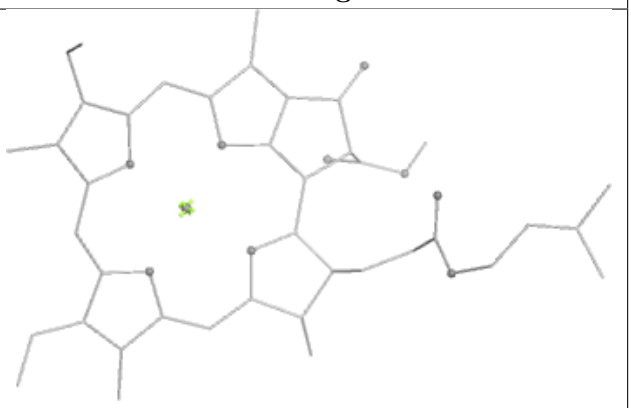
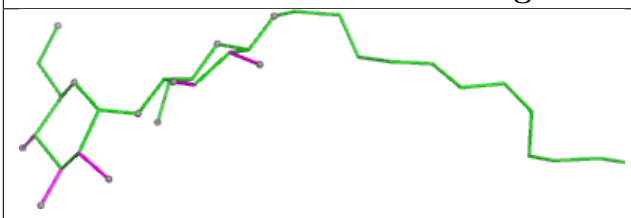


Rings

Ligand LMT F 6001



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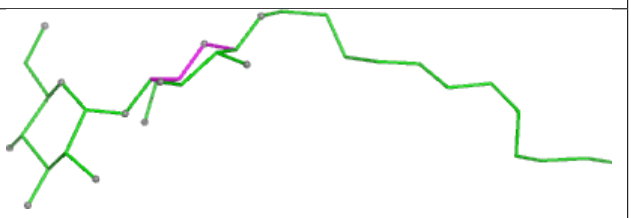
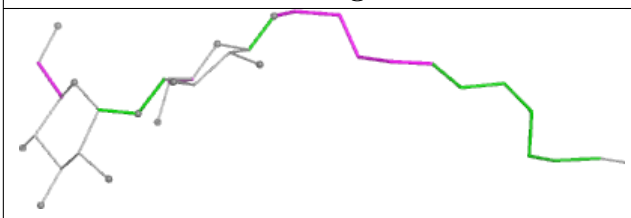


Bond angles



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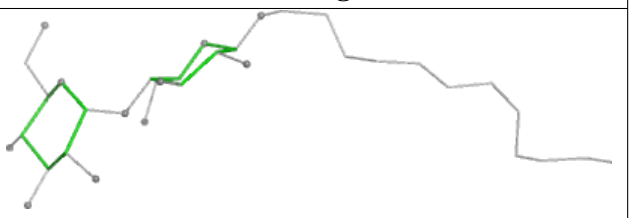
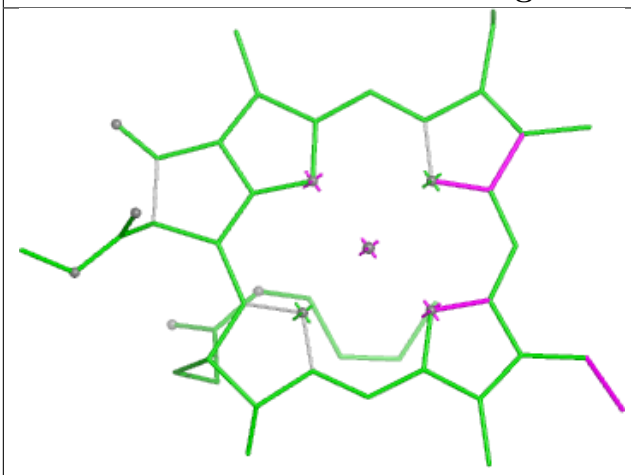


Rings

Ligand CLA B 1237



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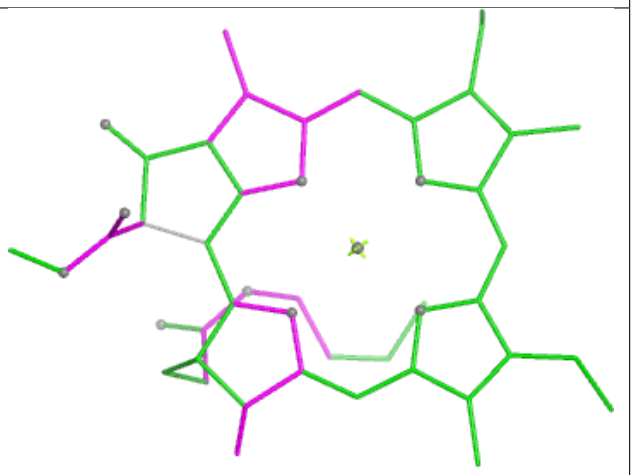
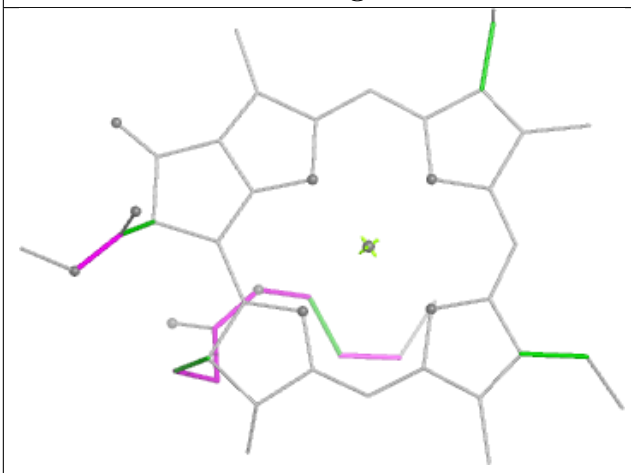


Bond angles



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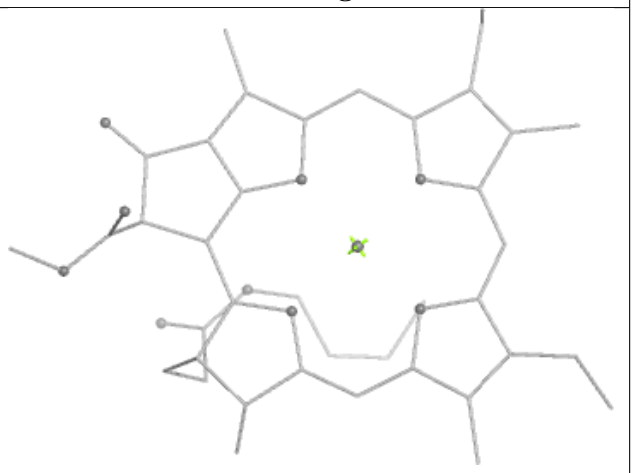
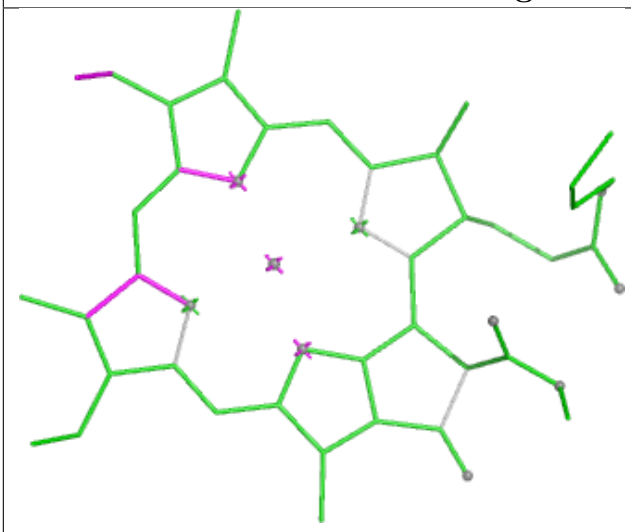


Rings

Ligand CLA B 1207



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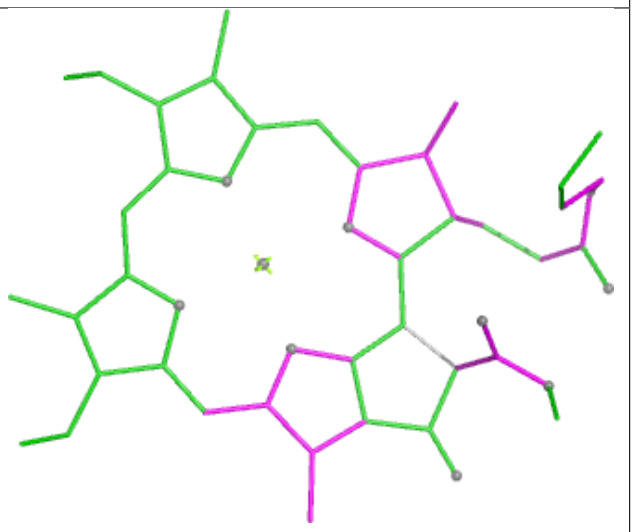
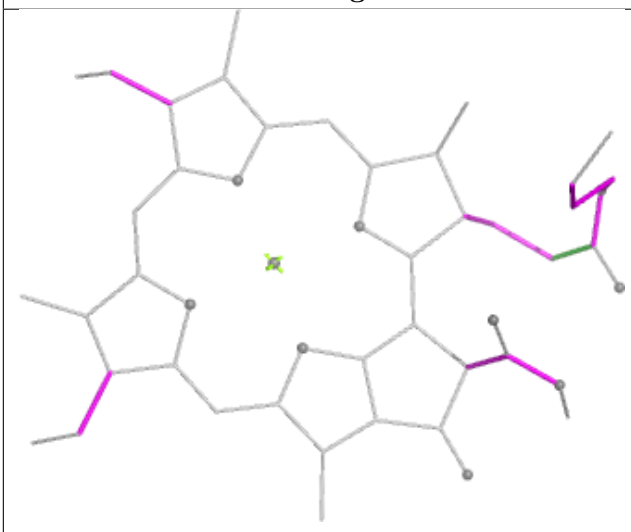


Bond angles



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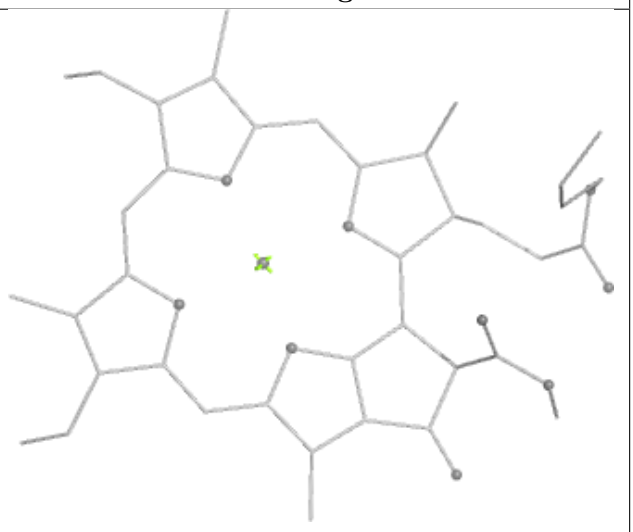
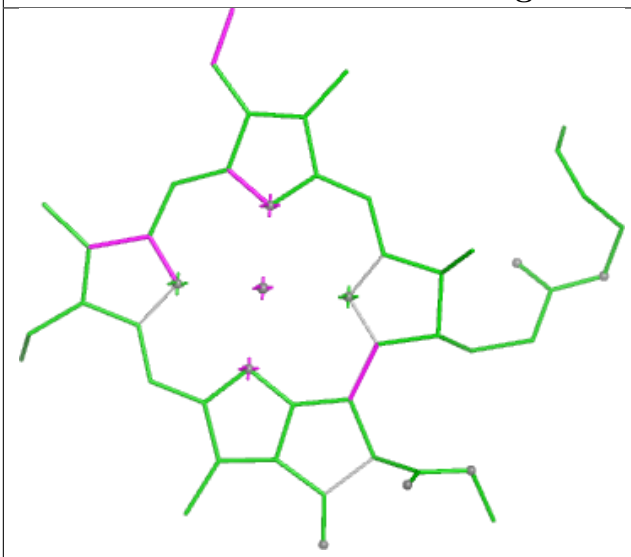


Rings

Ligand CLA B 1023



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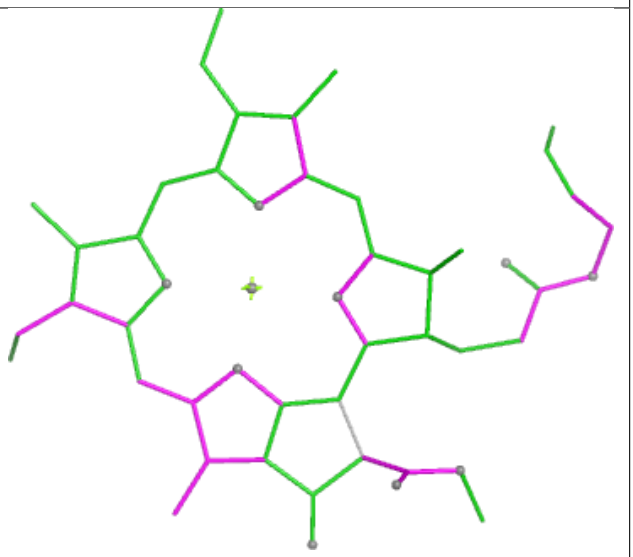
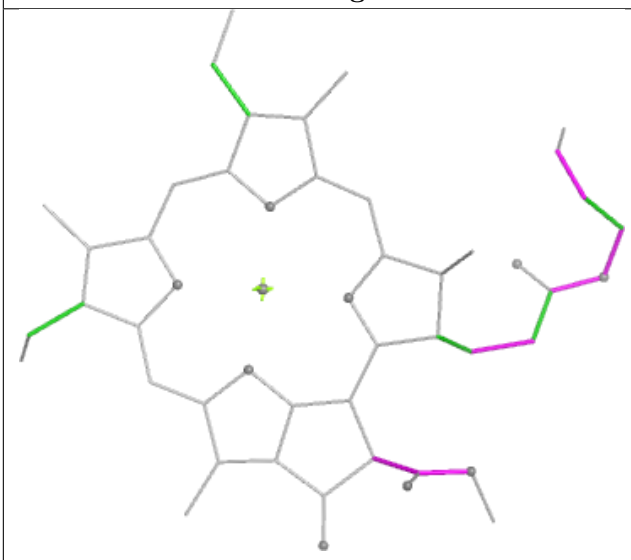


Bond angles



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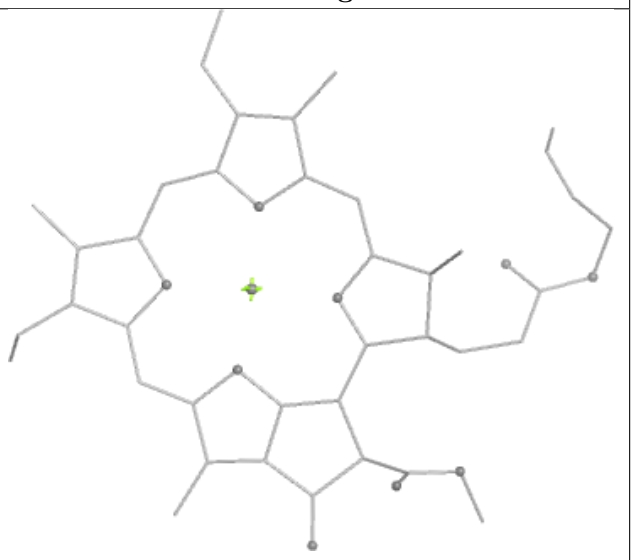
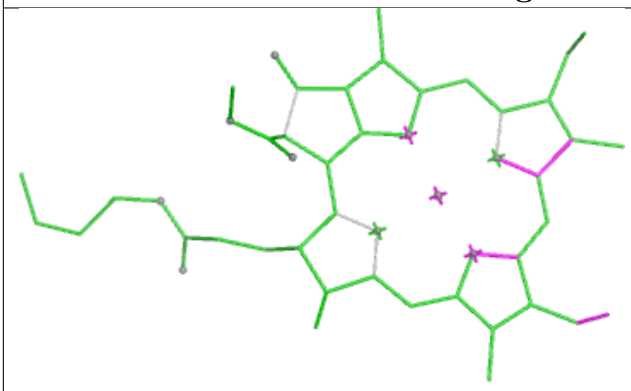


Rings

Ligand CLA B 1219



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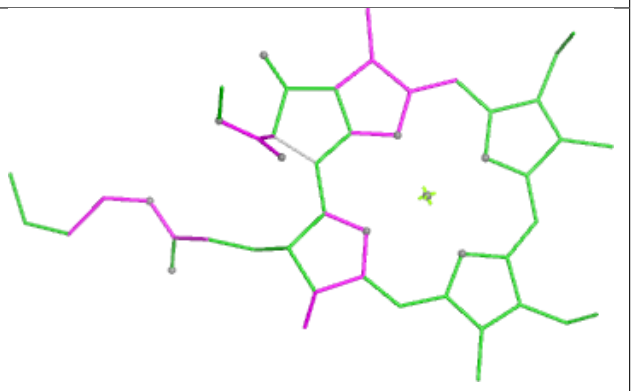
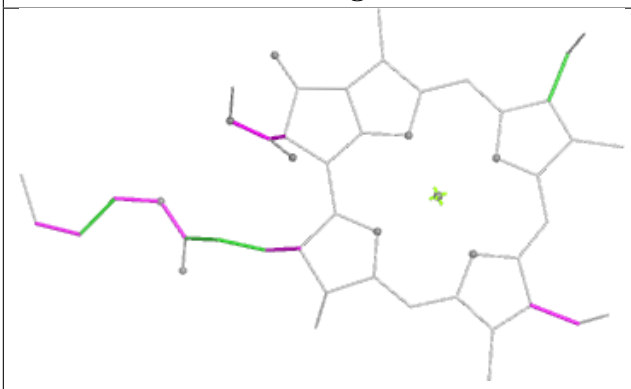


Bond angles



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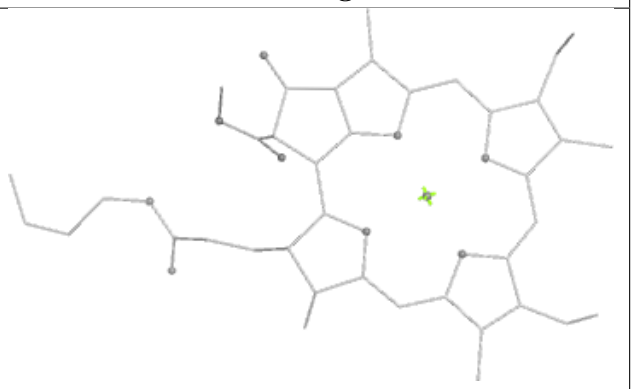
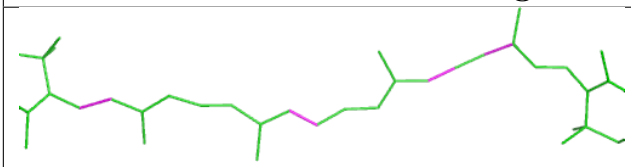


Rings

Ligand BCR B 4004



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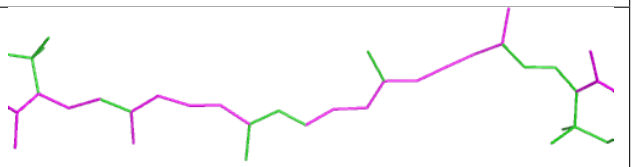
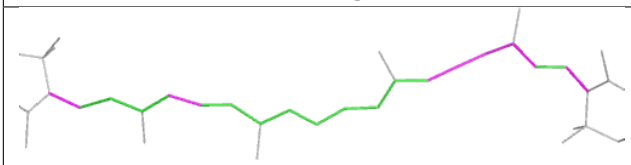


Bond angles



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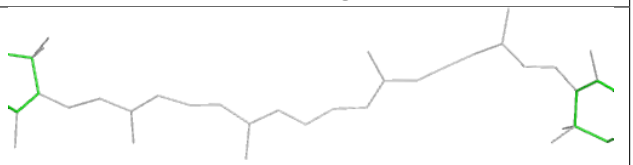
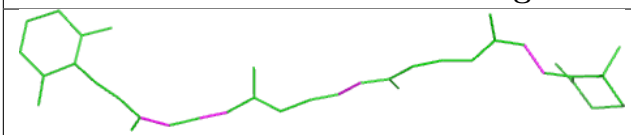


Rings

Ligand BCR B 4018



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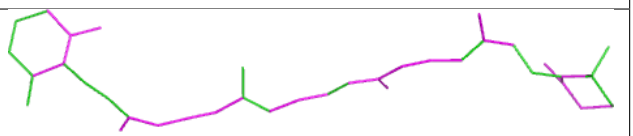
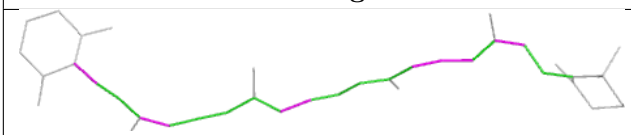


Bond angles

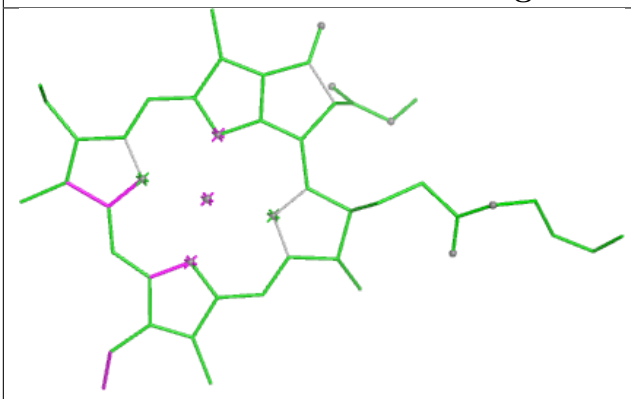


Torsions



Rings

Ligand CLA A 1135



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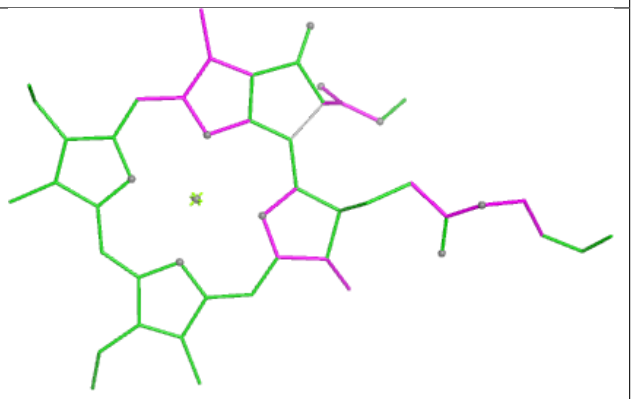
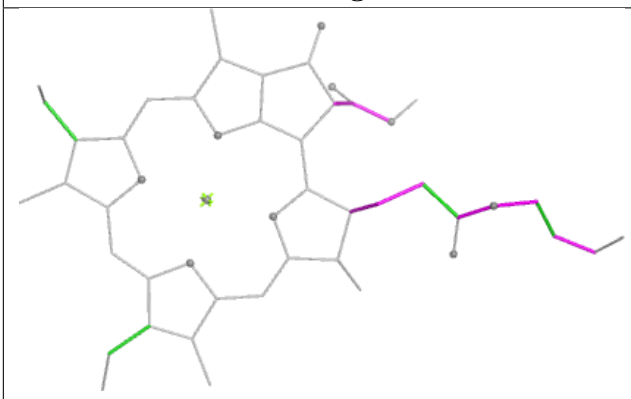


Bond angles



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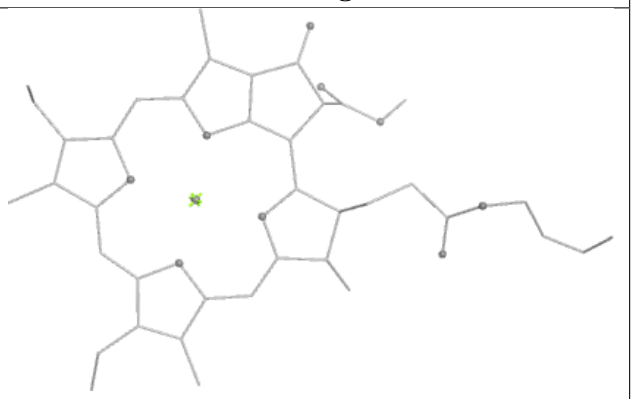
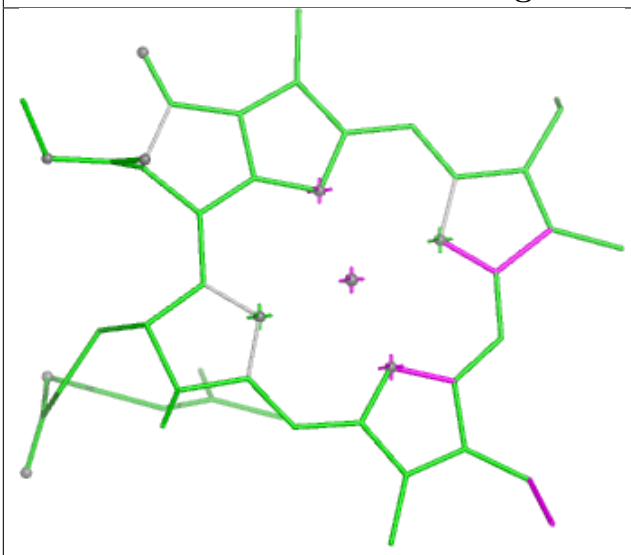


Rings

Ligand CLA A 1118



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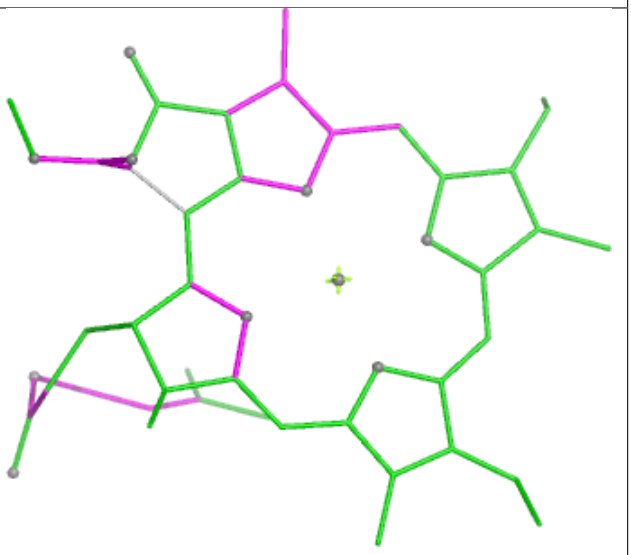
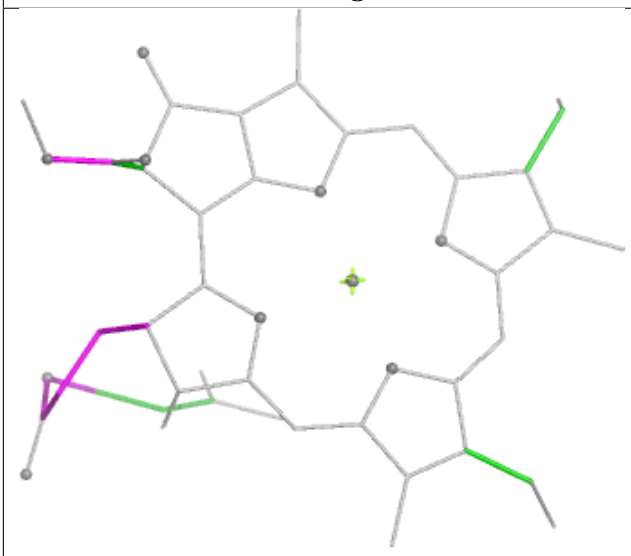


Bond angles



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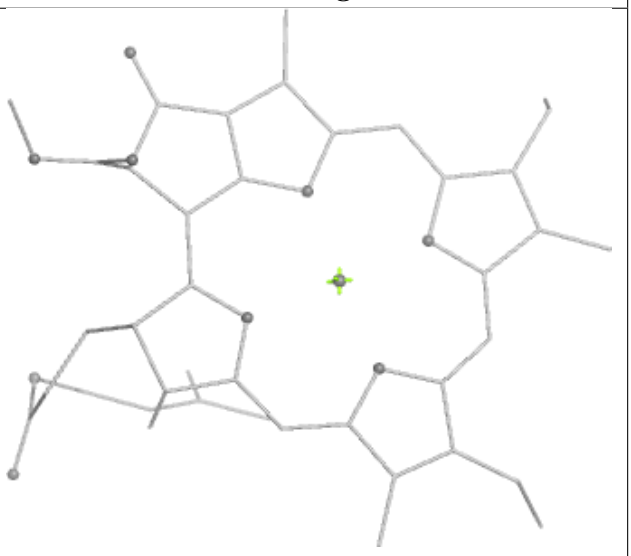
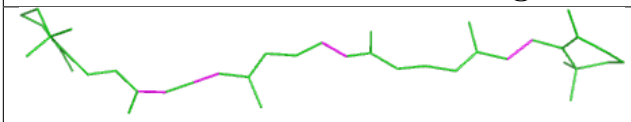


Rings

Ligand BCR K 4001



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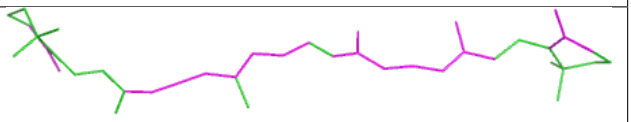
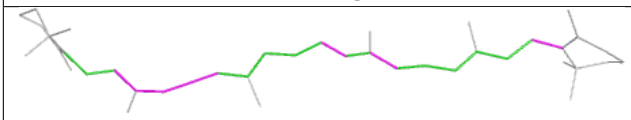


Bond angles



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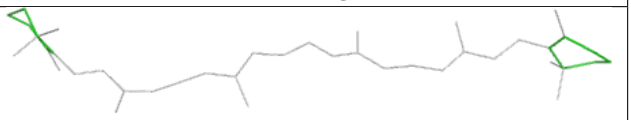
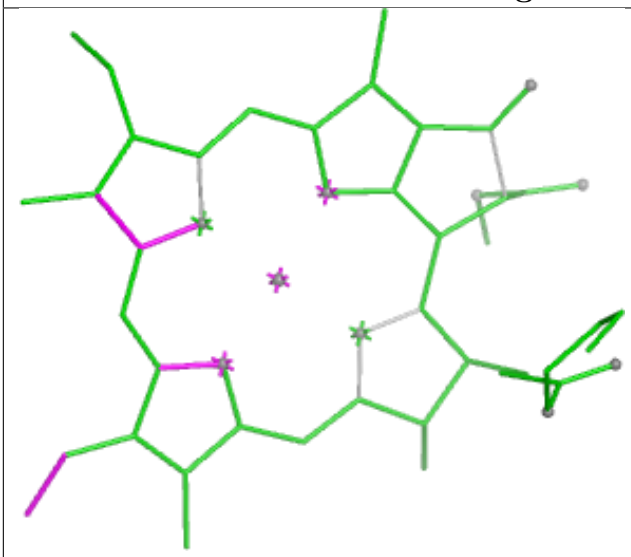
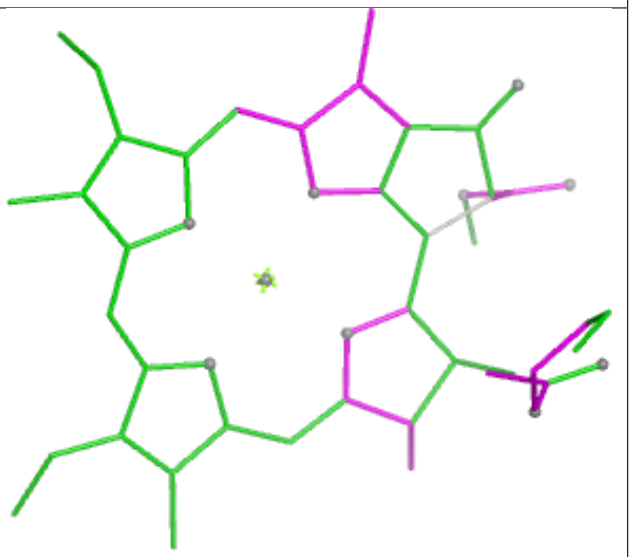


Rings

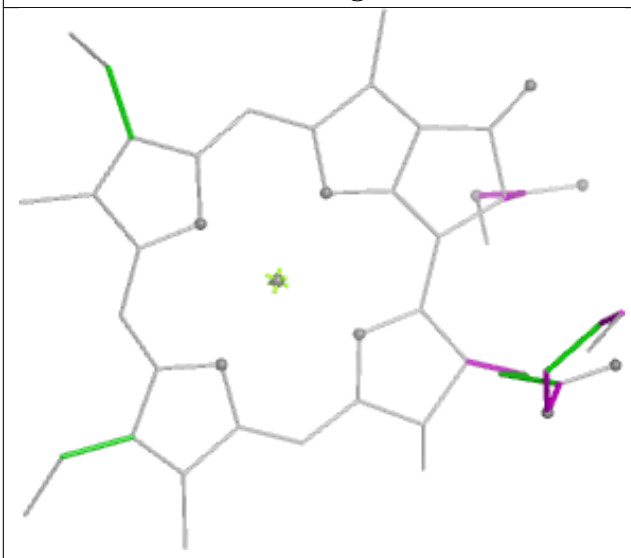
Ligand CLA B 1211



Bond lengths



Bond angles



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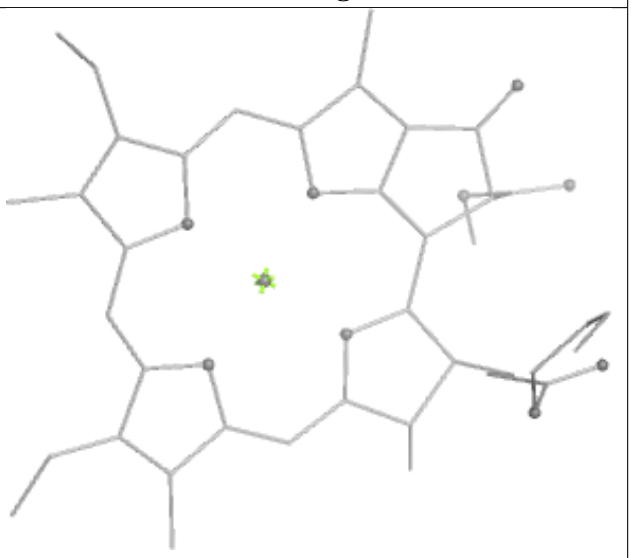
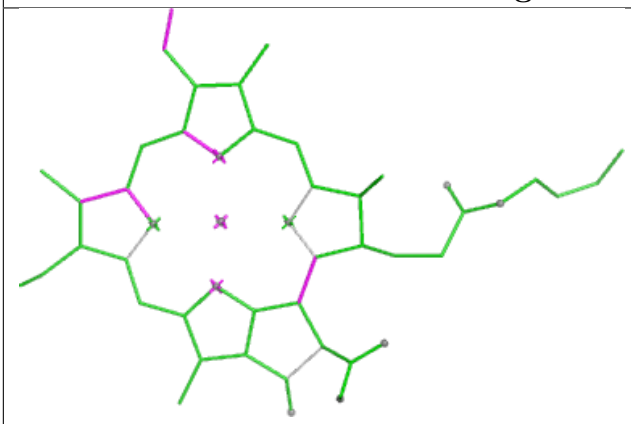
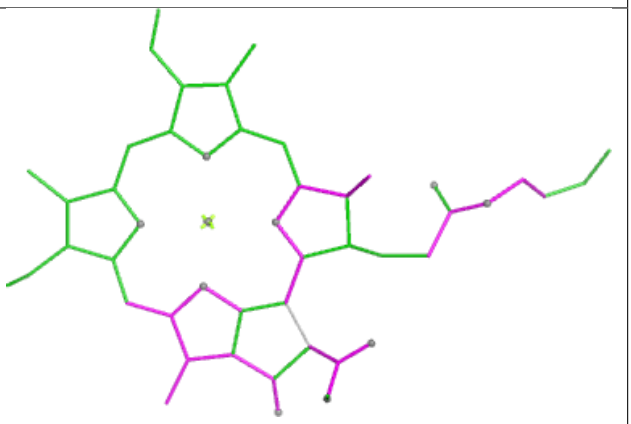


Rings

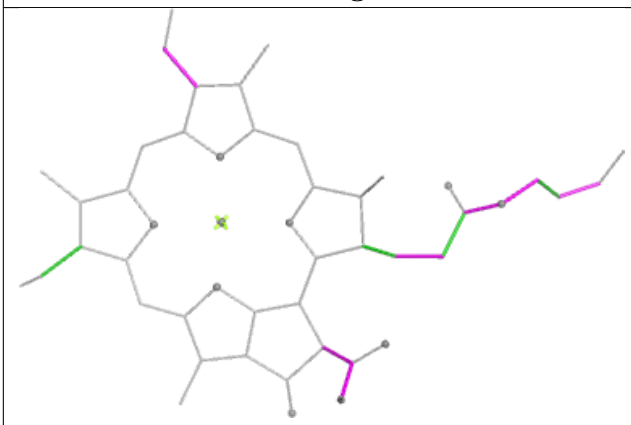
Ligand CLA A 1012



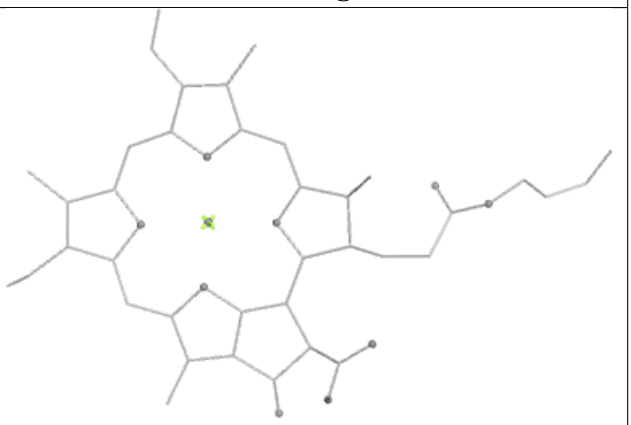
Bond lengths



Bond angles

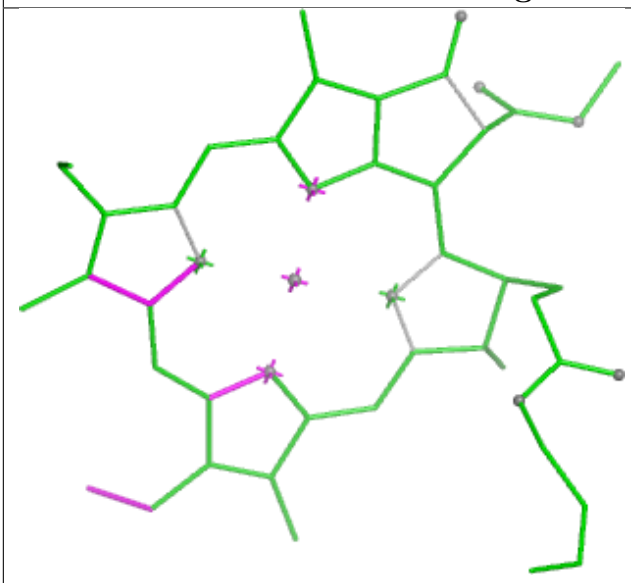


Torsions



Rings

Ligand CLA A 1133



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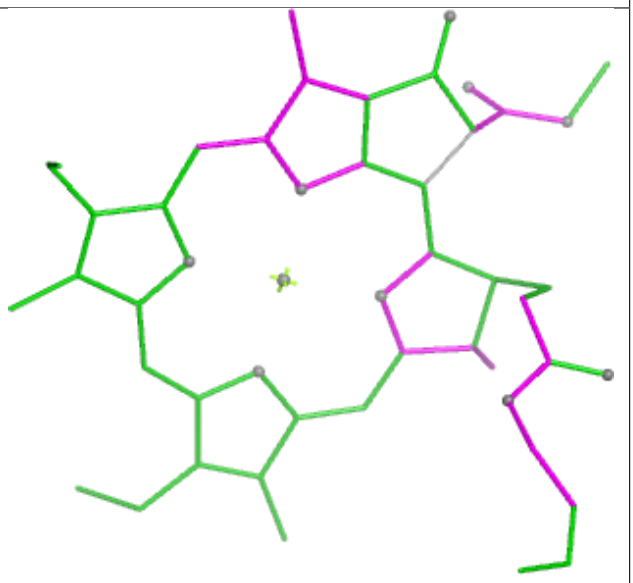
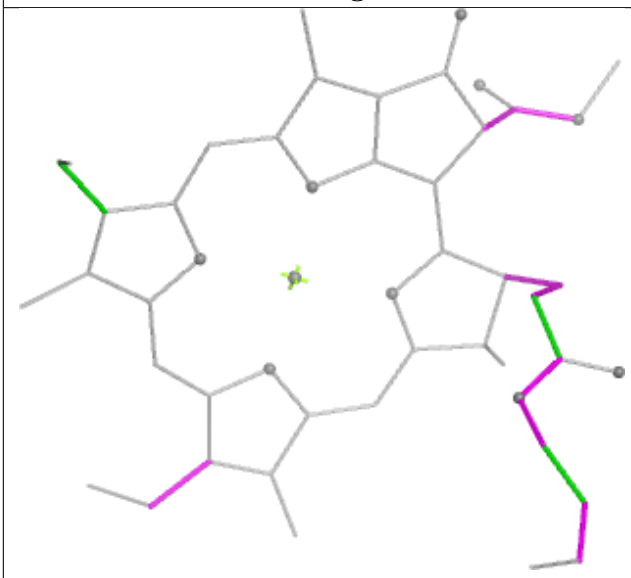


Bond angles



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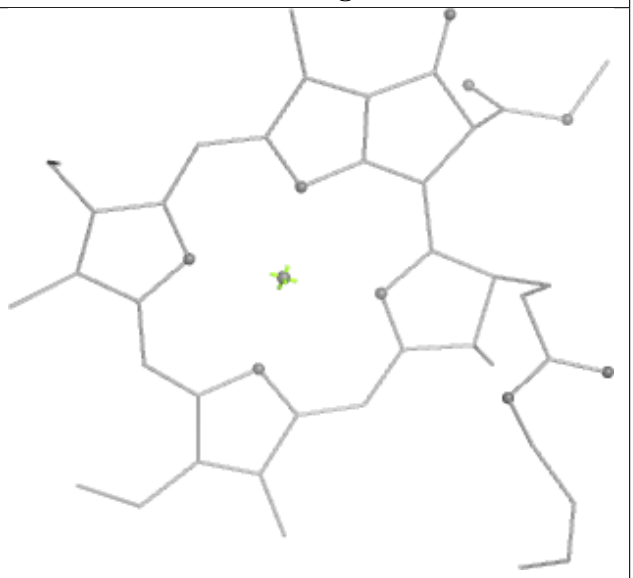
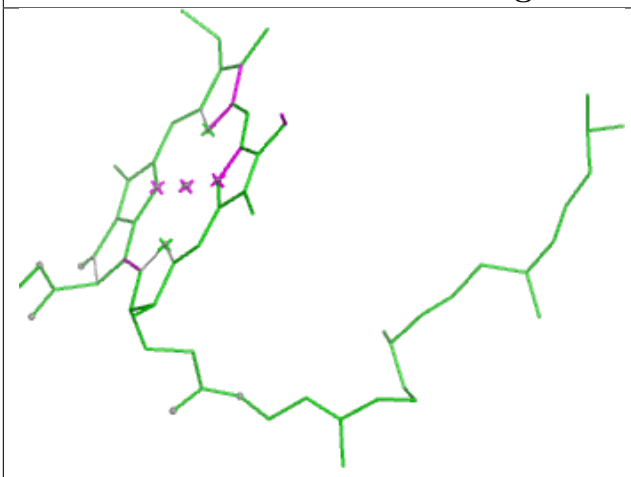


Rings

Ligand CLA A 1102



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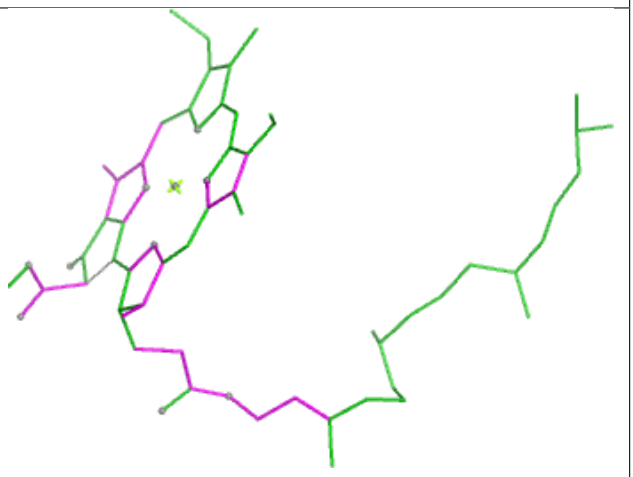
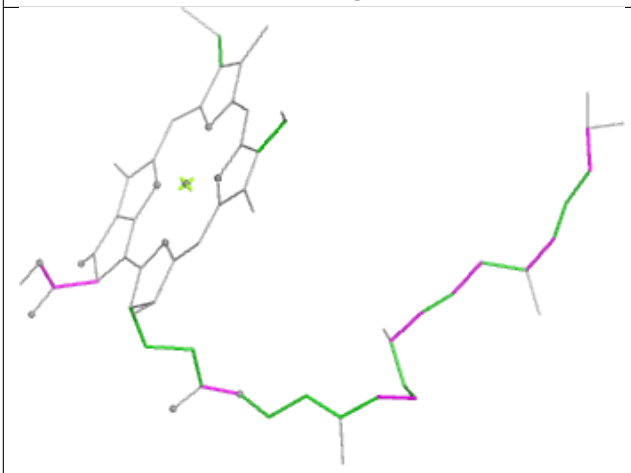


Bond angles



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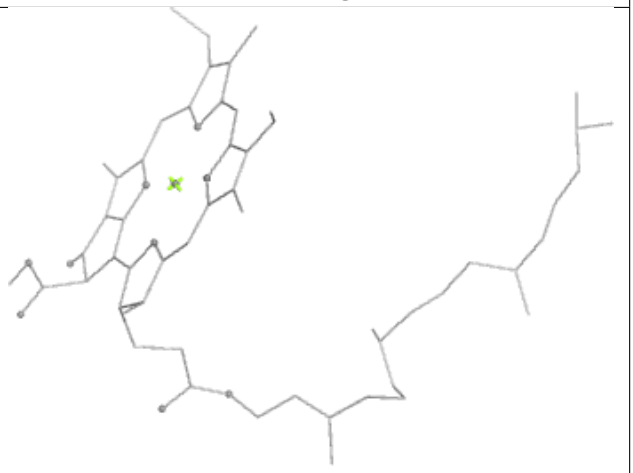
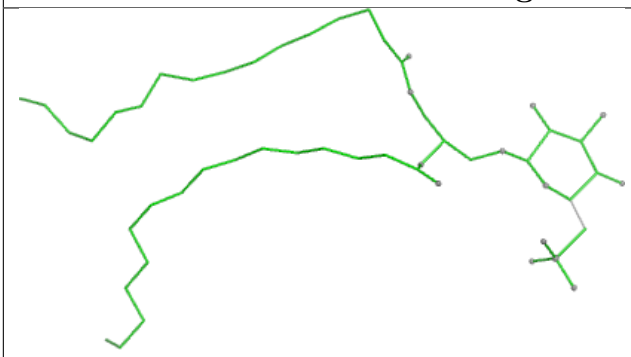


Rings

Ligand SQD B 5008



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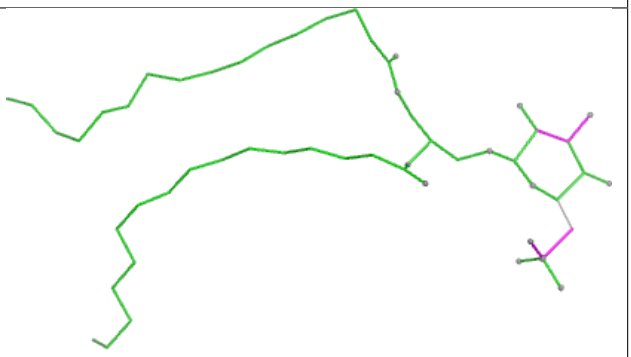
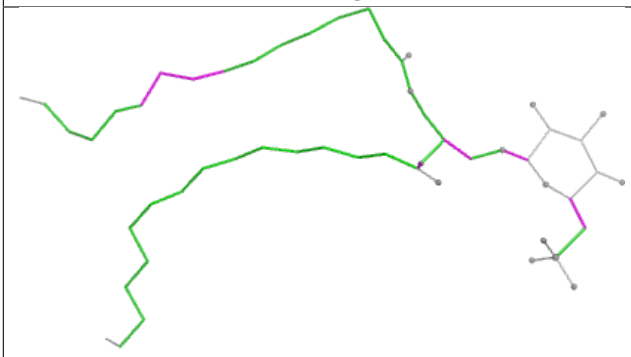


Bond angles



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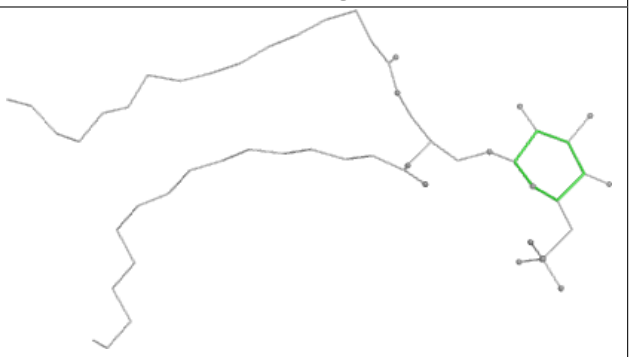
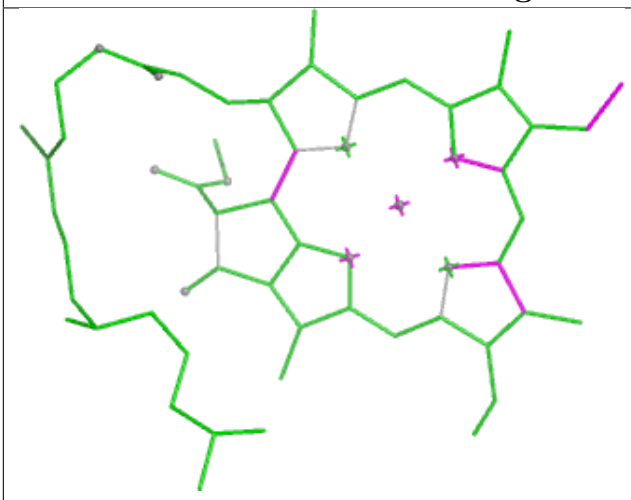


Rings

Ligand CLA A 1123



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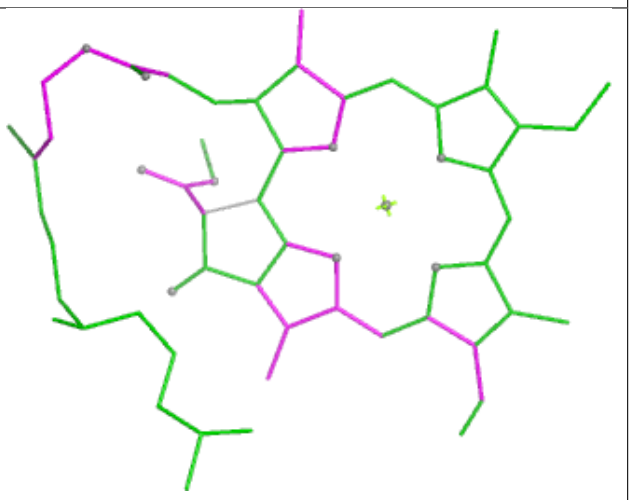
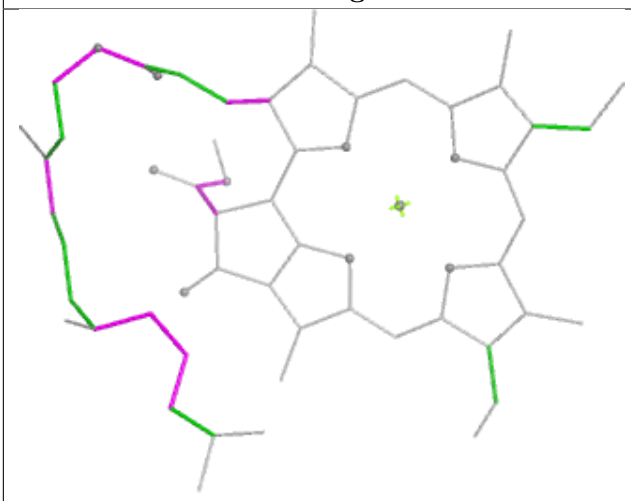


Bond angles



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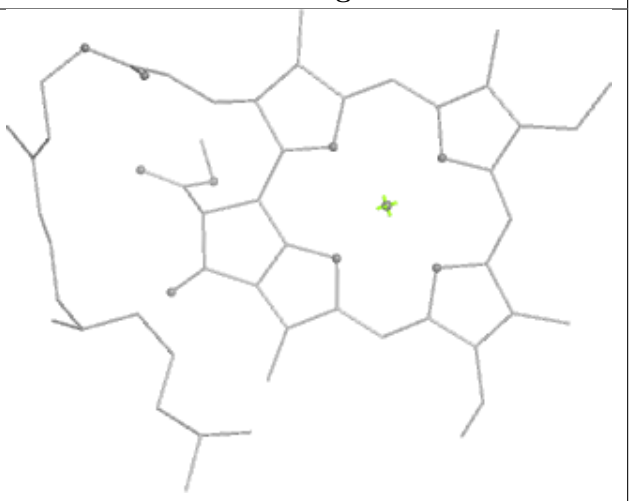
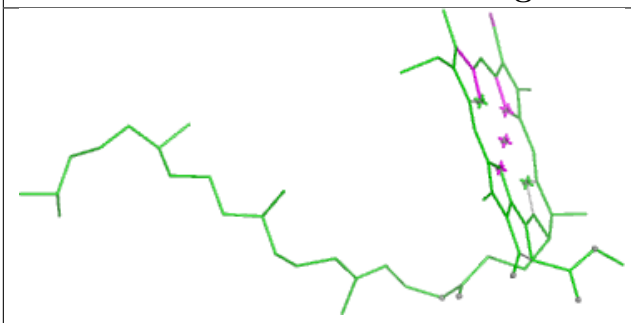


Rings

Ligand CLA A 1128



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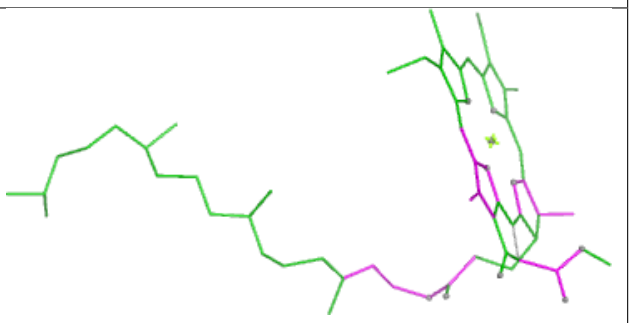
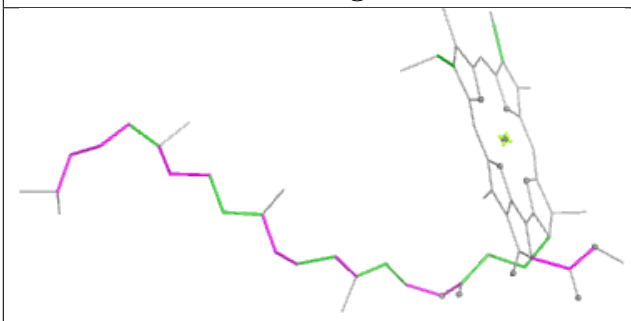


Bond angles

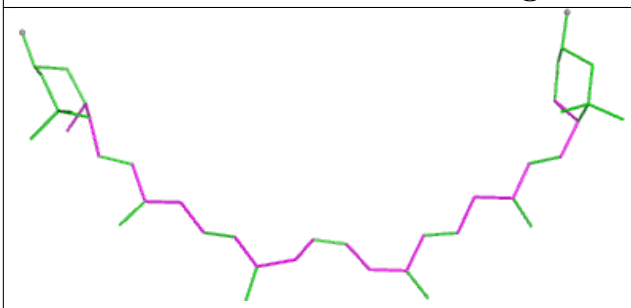


Torsions



Rings

Ligand C7Z F 4016



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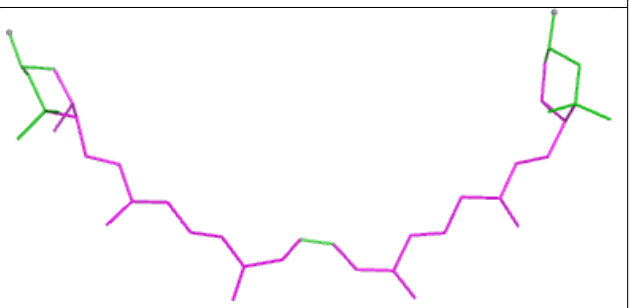
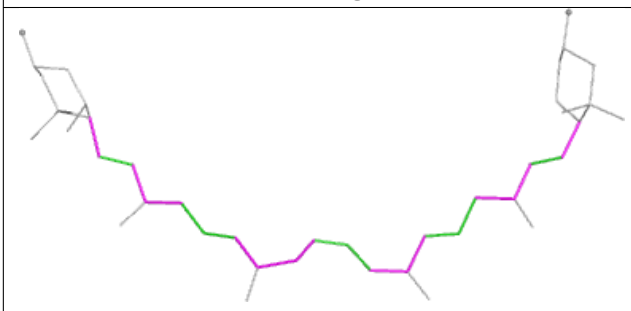


Bond angles



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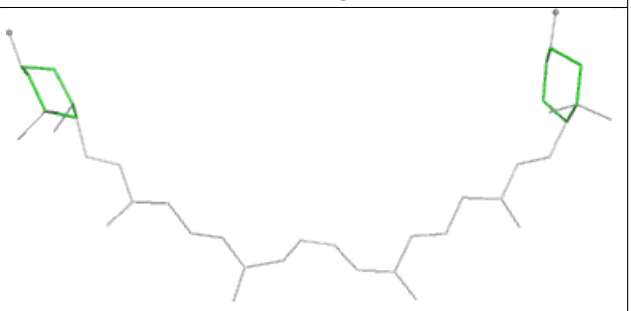
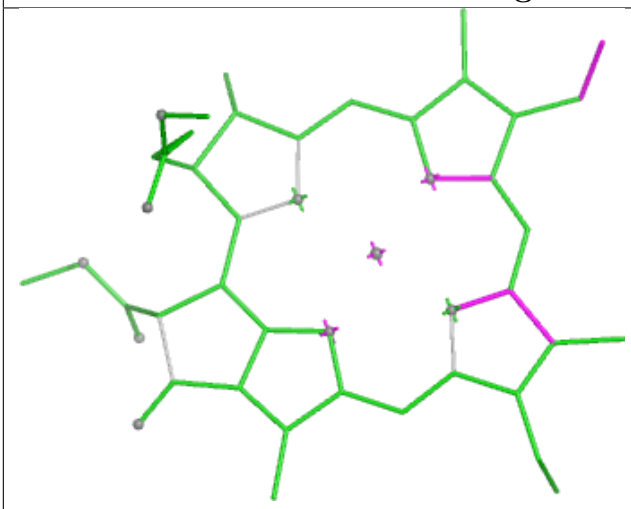


Rings

Ligand CLA A 1119



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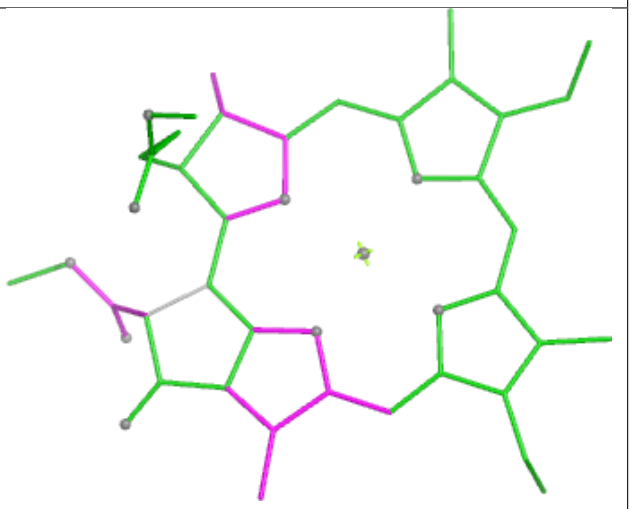
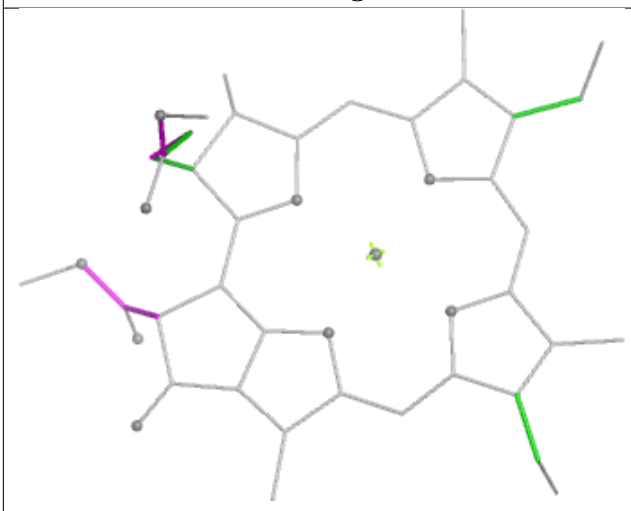


Bond angles



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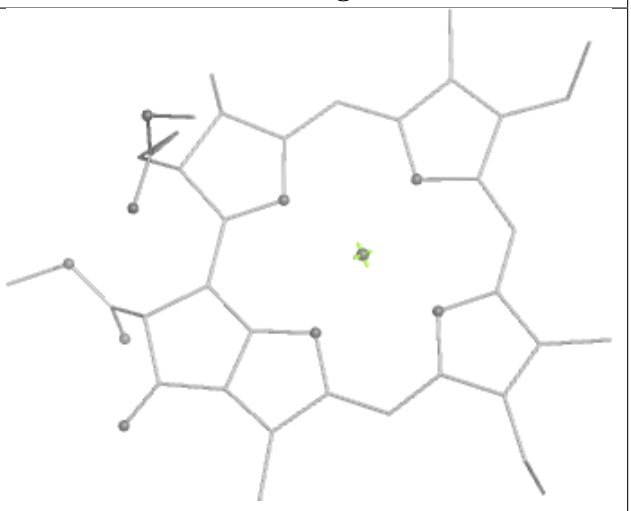
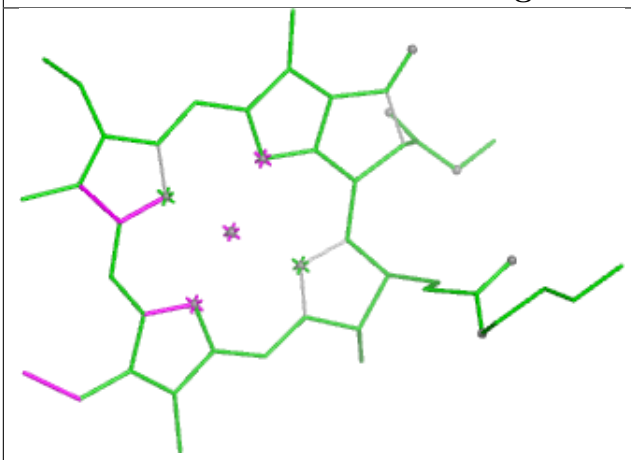


Rings

Ligand CLA A 1137



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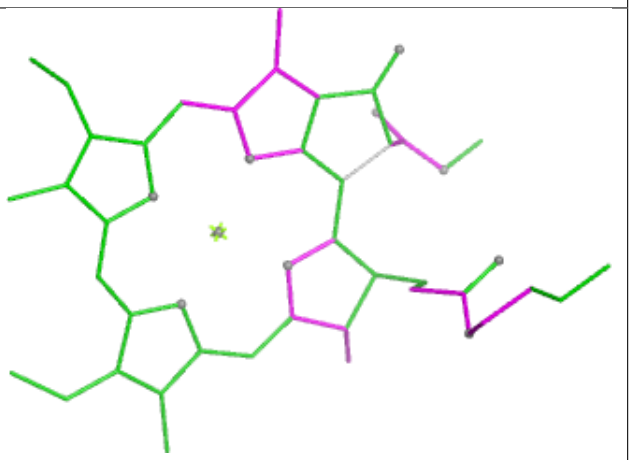
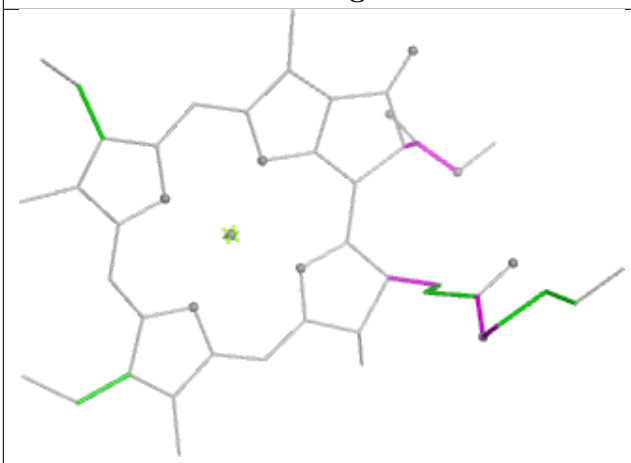


Bond angles



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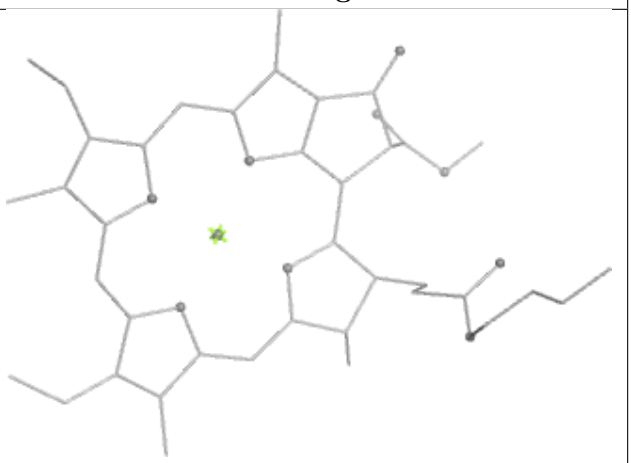
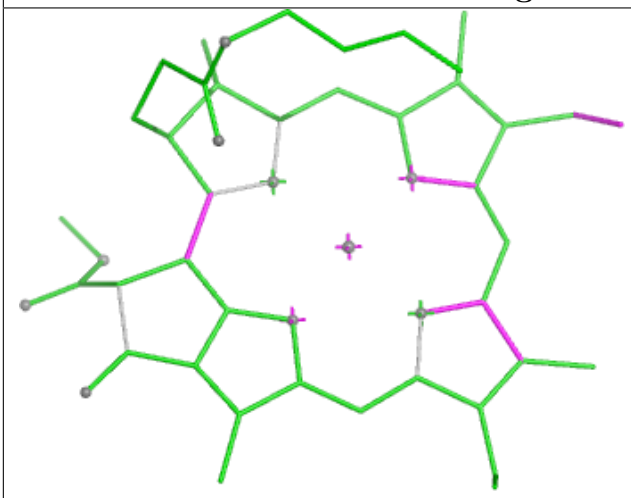


Rings

Ligand CLA B 1209



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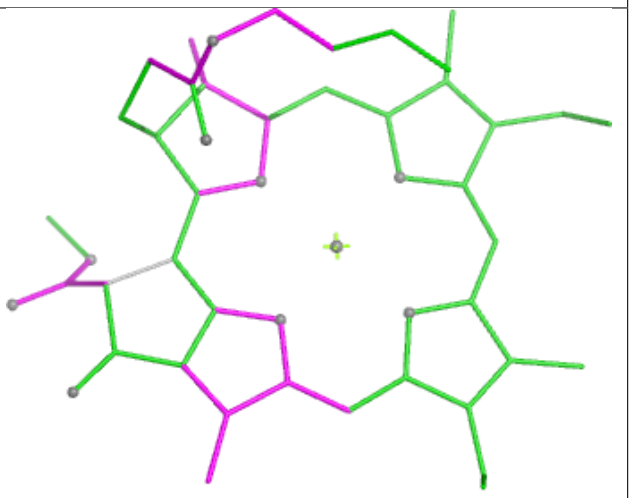
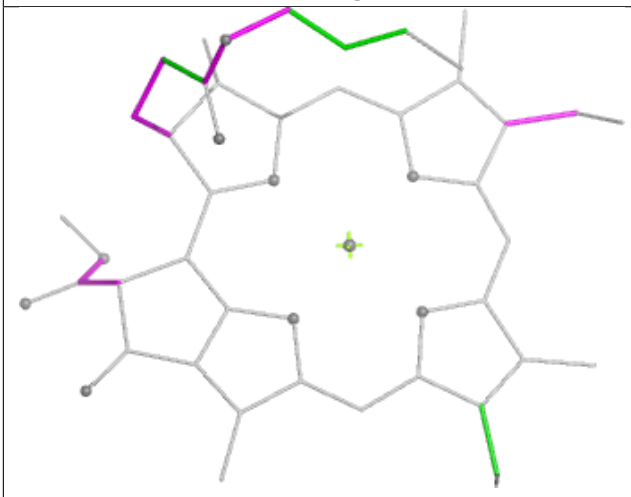


Bond angles



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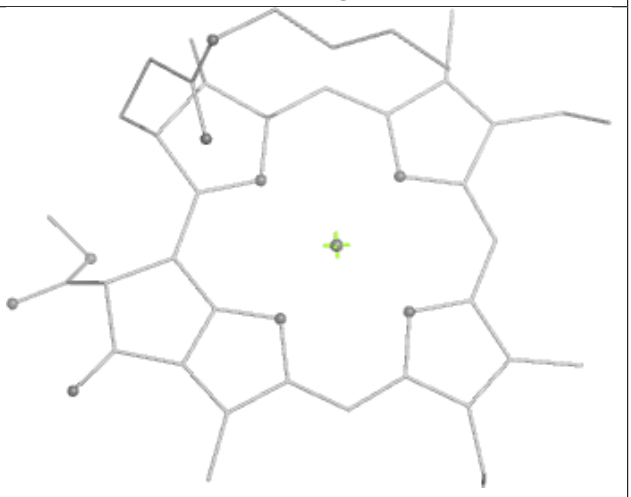
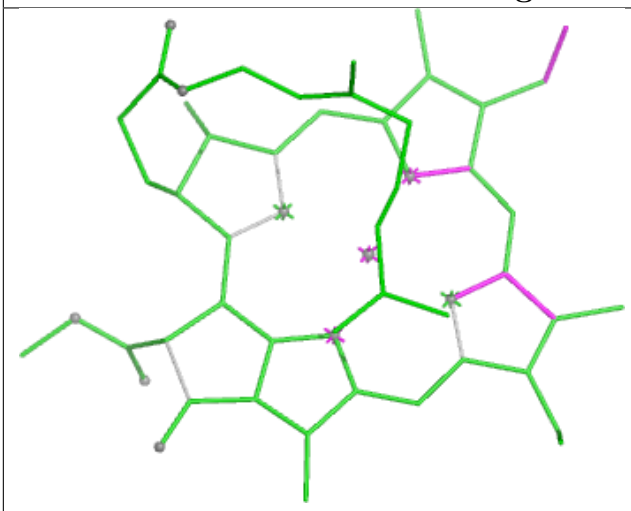


Rings

Ligand CLA B 1224



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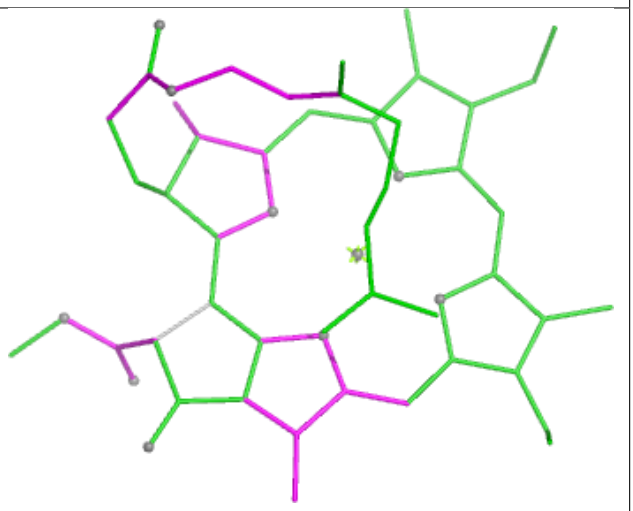
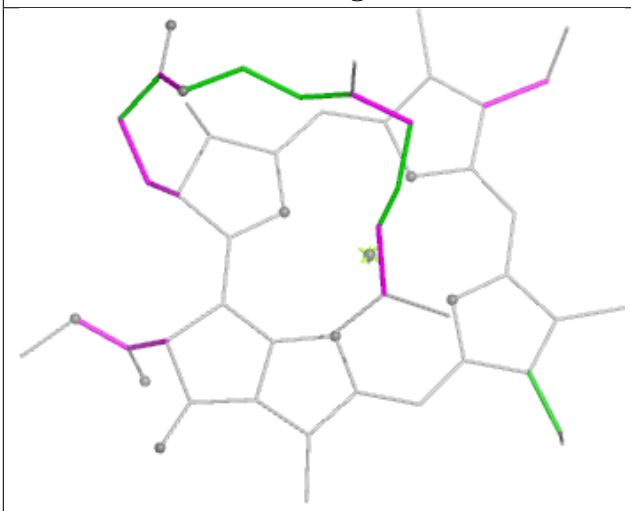


Bond angles



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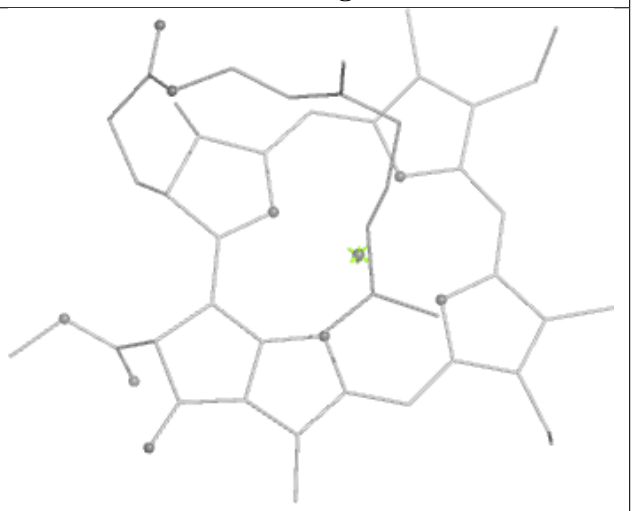
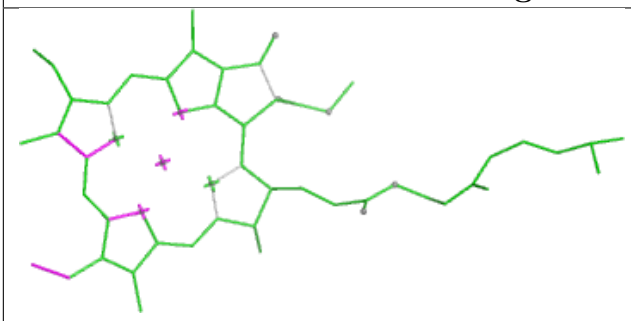


Rings

Ligand CLA A 1139



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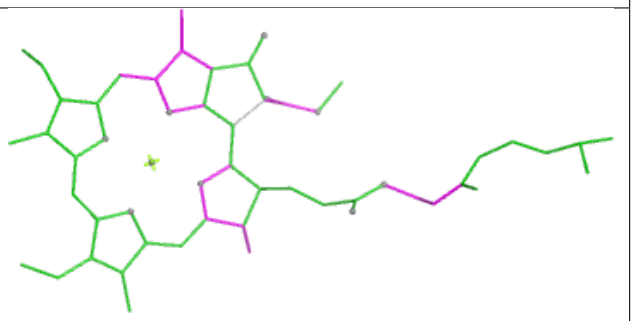
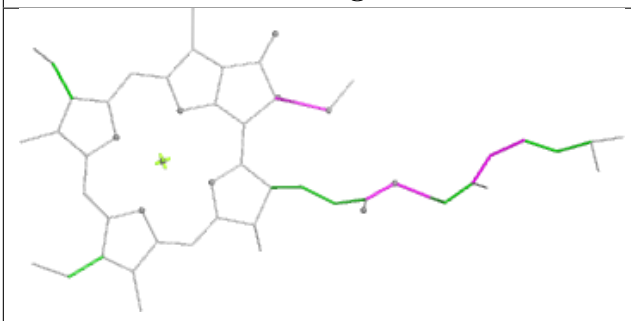


Bond angles



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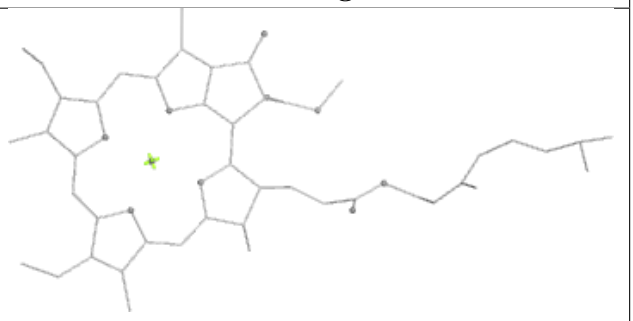
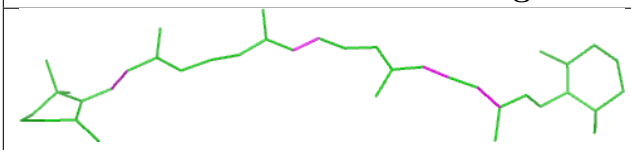
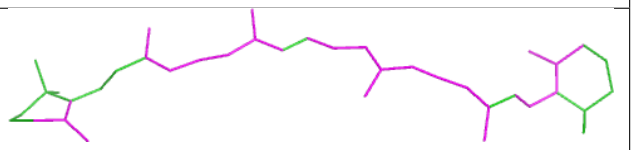


Rings

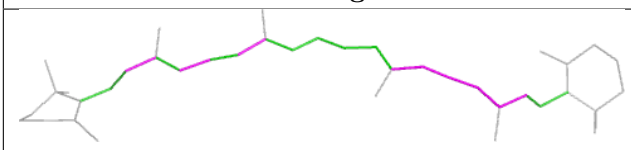
Ligand BCR A 4001



Bond lengths



Bond angles



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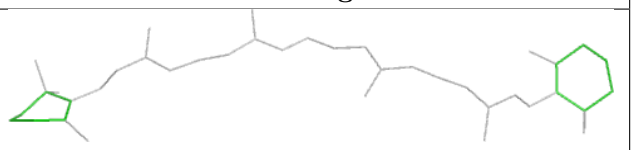
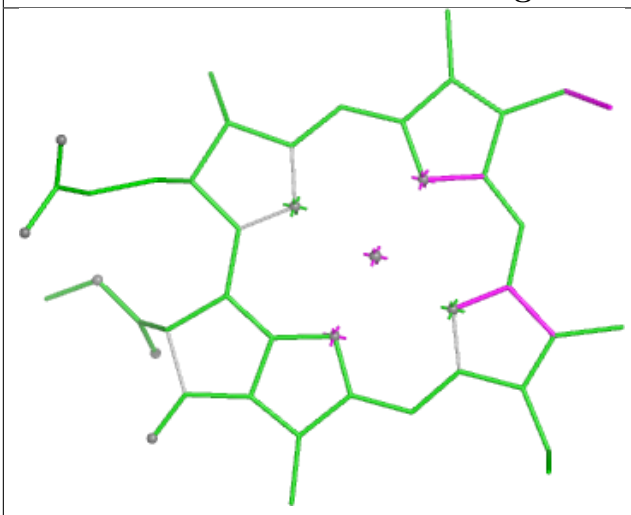
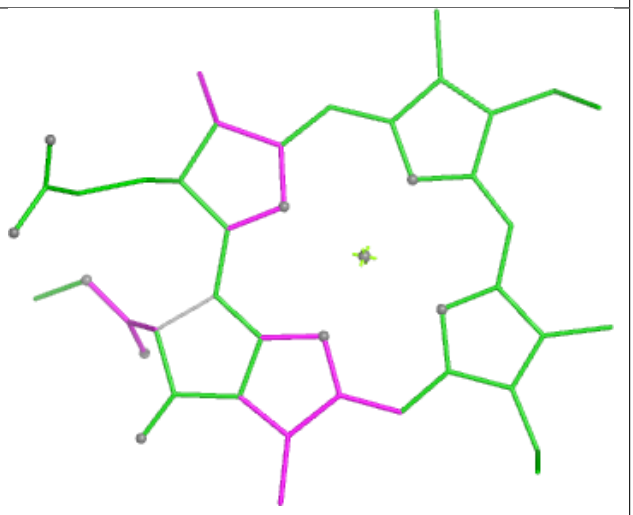


Rings

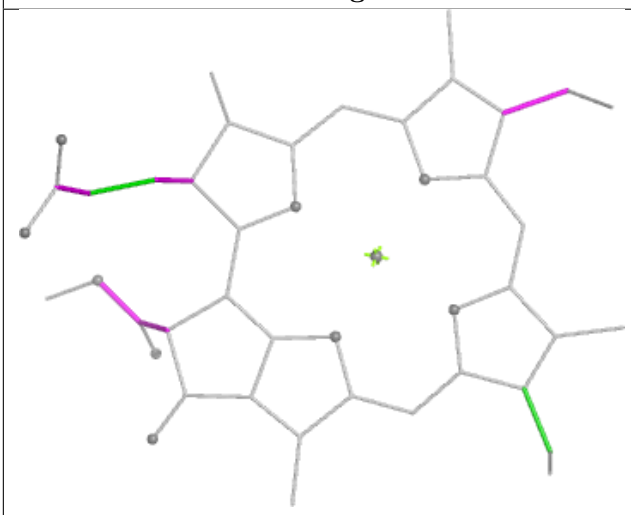
Ligand CLA K 1401



Bond lengths



Bond angles



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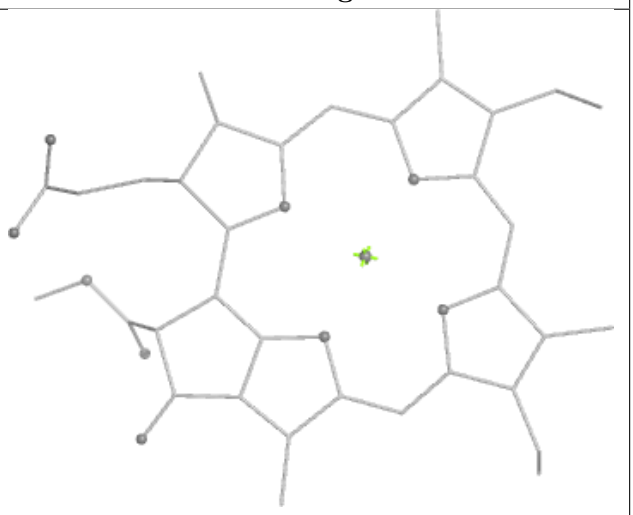
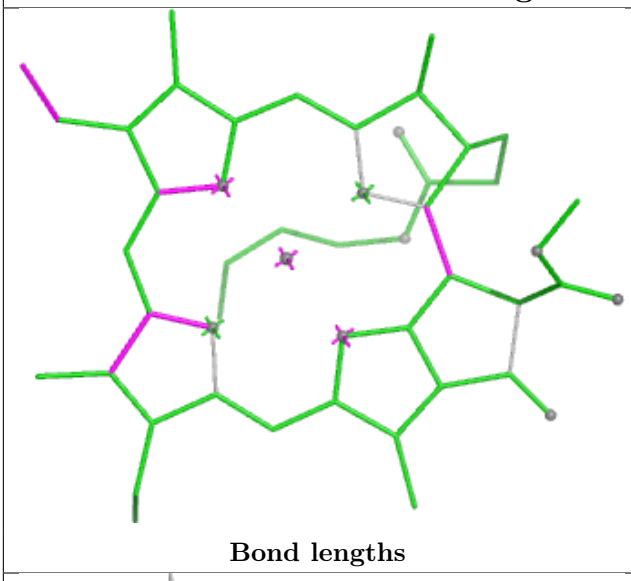
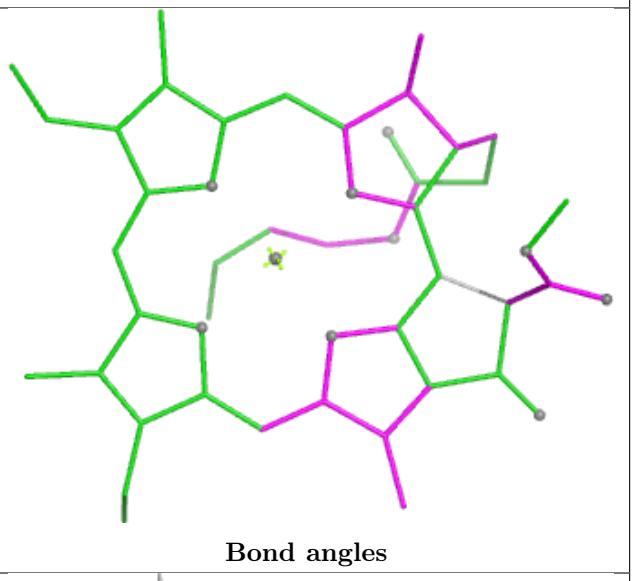


Rings

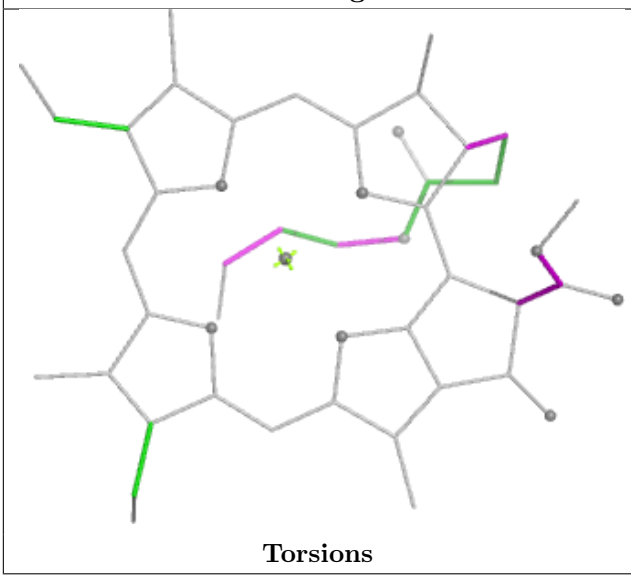
Ligand CLA B 1213



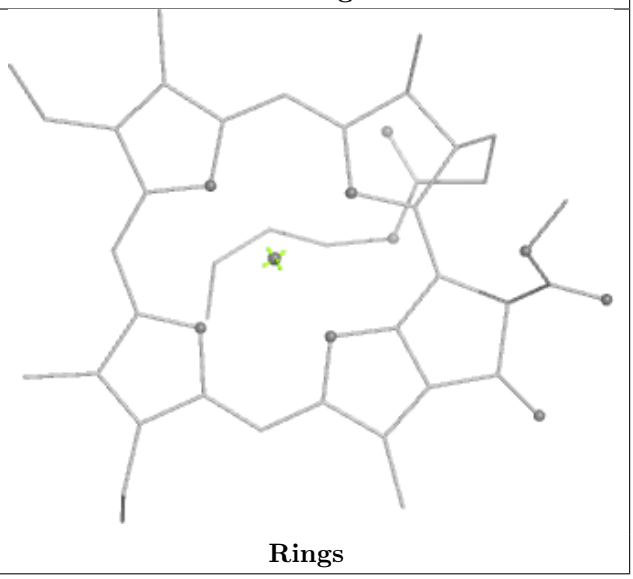
Bond lengths



Bond angles



Torsions

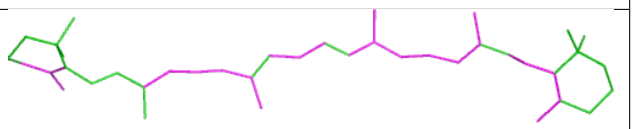


Rings

Ligand BCR A 4012



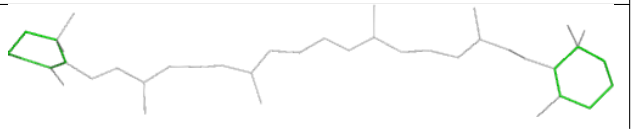
Bond lengths



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	751/751 (100%)	0.76	70 (9%) 14 16	27, 117, 229, 322	0
2	B	731/731 (100%)	0.65	63 (8%) 16 17	18, 95, 176, 428	0
3	C	80/80 (100%)	0.74	7 (8%) 15 17	30, 87, 122, 144	0
4	D	141/141 (100%)	0.77	16 (11%) 10 13	67, 112, 187, 399	0
5	E	69/69 (100%)	0.47	2 (2%) 53 39	45, 81, 154, 170	0
6	F	143/143 (100%)	0.64	12 (8%) 17 18	28, 98, 148, 186	0
7	I	40/40 (100%)	2.23	21 (52%) 0 1	228, 290, 404, 432	0
8	J	40/40 (100%)	0.39	1 (2%) 58 43	73, 106, 144, 149	0
9	K	70/70 (100%)	0.71	7 (10%) 12 15	150, 241, 380, 499	0
10	L	137/137 (100%)	1.25	24 (17%) 4 7	231, 373, 583, 606	0
11	M	31/31 (100%)	1.13	8 (25%) 1 4	123, 149, 199, 221	0
All	All	2233/2233 (100%)	0.76	231 (10%) 12 14	18, 108, 335, 606	0

The worst 5 of 231 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	9.2
6	F	92	GLU	8.8
7	I	8	SER	7.5
1	A	238	LEU	7.1
7	I	2	ASP	6.5

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	L	1502	49/65	0.22	0.22	382,393,407,412	0
16	LHG	B	5006	21/49	0.39	0.20	154,179,195,201	0
20	LMG	B	5005	55/55	0.51	0.18	80,149,188,190	0
21	SQD	B	5008	54/54	0.53	0.21	92,154,193,201	0
25	EQ3	I	4020	42/42	0.53	0.27	224,232,241,245	0
24	LMT	F	6001	35/35	0.58	0.18	78,142,171,178	0
15	BCR	K	4001	40/40	0.68	0.17	129,194,221,223	0
19	ECH	M	4021	41/41	0.72	0.28	148,166,189,200	0
21	SQD	F	5001	54/54	0.72	0.26	149,164,176,178	0
15	BCR	A	4001	40/40	0.74	0.24	148,169,184,185	0
12	CLA	B	1207	49/65	0.77	0.19	131,157,223,227	0
12	CLA	K	1401	45/65	0.77	0.14	127,147,170,175	0
12	CLA	A	1113	49/65	0.77	0.16	135,160,184,192	0
12	CLA	B	1240	49/65	0.78	0.18	76,105,156,163	0
15	BCR	I	4018	40/40	0.79	0.30	161,194,217,223	0
12	CLA	B	1219	49/65	0.79	0.15	64,91,133,135	0
15	BCR	A	4003	40/40	0.79	0.35	124,164,188,189	0
12	CLA	B	1217	49/65	0.80	0.14	72,85,95,103	0
12	CLA	J	1303	49/65	0.80	0.15	145,167,176,202	0
12	CLA	A	1115	56/65	0.80	0.15	118,146,155,156	0
12	CLA	K	1402	49/65	0.80	0.16	168,189,213,218	0
16	LHG	A	5003	49/49	0.81	0.17	106,135,156,160	0
12	CLA	F	1302	49/65	0.81	0.15	63,82,106,112	0
22	CA	L	1001	1/1	0.81	0.08	156,156,156,156	0
12	CLA	B	1212	49/65	0.81	0.15	124,146,166,171	0
12	CLA	B	1204	49/65	0.81	0.17	94,111,127,139	0
12	CLA	A	1114	49/65	0.82	0.15	142,154,173,178	0
19	ECH	B	4006	41/41	0.82	0.27	111,135,146,150	0
12	CLA	J	1302	49/65	0.82	0.16	134,150,159,160	0
12	CLA	A	1133	49/65	0.83	0.17	98,115,131,133	0
15	BCR	B	4004	40/40	0.83	0.16	105,125,134,138	0
12	CLA	B	1209	49/65	0.84	0.15	107,131,139,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	A	1120	49/65	0.84	0.17	130,149,195,200	0
12	CLA	A	1108	49/65	0.85	0.14	89,101,135,142	0
12	CLA	B	1208	49/65	0.85	0.14	90,107,128,130	0
12	CLA	A	1130	49/65	0.85	0.15	77,95,130,133	0
12	CLA	A	1112	49/65	0.85	0.18	138,146,155,164	0
23	C7Z	F	4016	42/42	0.85	0.17	35,58,93,97	0
12	CLA	B	1213	49/65	0.85	0.14	105,121,132,141	0
12	CLA	B	1216	49/65	0.85	0.15	58,113,119,124	0
20	LMG	B	5002	55/55	0.86	0.20	37,69,102,118	0
12	CLA	A	1105	65/65	0.86	0.17	66,114,126,130	0
12	CLA	B	1201	49/65	0.86	0.14	77,89,106,110	0
12	CLA	A	1011	55/65	0.86	0.19	43,63,72,89	0
12	CLA	A	1111	49/65	0.86	0.20	70,113,131,146	0
12	CLA	A	1141	45/65	0.86	0.13	137,156,176,188	0
15	BCR	A	4007	40/40	0.86	0.16	66,82,134,137	0
15	BCR	A	4008	40/40	0.86	0.22	43,110,125,125	0
12	CLA	B	1211	49/65	0.87	0.18	100,120,130,134	0
12	CLA	A	1129	49/65	0.87	0.17	96,116,153,160	0
12	CLA	A	1119	46/65	0.87	0.19	106,126,144,154	0
15	BCR	A	4012	40/40	0.87	0.21	66,81,92,93	0
12	CLA	A	1134	49/65	0.87	0.13	109,140,149,156	0
15	BCR	B	4017	40/40	0.87	0.23	50,68,88,91	0
12	CLA	A	1118	50/65	0.87	0.18	120,151,195,209	0
12	CLA	B	1218	49/65	0.87	0.13	64,90,122,130	0
12	CLA	A	1121	49/65	0.87	0.13	90,117,137,142	0
12	CLA	B	1226	49/65	0.87	0.17	29,59,81,85	0
12	CLA	B	1234	60/65	0.88	0.18	55,77,106,112	0
12	CLA	A	1122	49/65	0.88	0.16	90,108,122,124	0
12	CLA	A	1110	49/65	0.88	0.19	130,154,173,179	0
22	CA	B	6001	1/1	0.88	0.12	171,171,171,171	0
12	CLA	A	1135	49/65	0.88	0.17	110,119,124,128	0
15	BCR	B	4005	40/40	0.88	0.18	31,63,141,143	0
12	CLA	B	1203	49/65	0.88	0.18	75,86,99,103	0
15	BCR	B	4018	40/40	0.88	0.20	61,121,136,140	0
15	BCR	B	4010	40/40	0.89	0.17	43,57,71,73	0
12	CLA	F	1301	49/65	0.89	0.17	80,98,136,138	0
12	CLA	A	1125	49/65	0.89	0.19	108,124,132,135	0
12	CLA	B	1205	49/65	0.89	0.19	57,73,97,106	0
15	BCR	J	4013	40/40	0.89	0.21	88,110,132,133	0
12	CLA	A	1132	55/65	0.89	0.17	107,148,273,351	0
12	CLA	B	1228	49/65	0.89	0.14	56,67,96,97	0
16	LHG	B	5004	49/49	0.89	0.18	57,80,128,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	A	1136	49/65	0.89	0.14	128,139,145,149	0
12	CLA	A	1131	49/65	0.89	0.16	111,130,156,163	0
12	CLA	A	1102	65/65	0.90	0.14	70,86,98,104	0
12	CLA	A	1109	65/65	0.90	0.14	64,113,123,126	0
12	CLA	B	1021	65/65	0.90	0.17	22,41,55,65	0
12	CLA	B	1022	60/65	0.90	0.17	31,89,94,102	0
12	CLA	B	1220	49/65	0.90	0.16	77,91,96,98	0
12	CLA	B	1221	49/65	0.90	0.17	60,105,115,122	0
12	CLA	A	1116	49/65	0.90	0.19	96,126,142,150	0
12	CLA	A	1137	49/65	0.90	0.15	92,112,121,126	0
13	PQN	B	2002	33/33	0.90	0.20	72,83,105,111	0
12	CLA	A	1107	50/65	0.90	0.13	42,53,69,94	0
12	CLA	B	1235	65/65	0.90	0.17	37,60,72,74	0
12	CLA	B	1239	49/65	0.90	0.16	36,61,108,114	0
12	CLA	B	1215	49/65	0.91	0.20	67,79,87,89	0
12	CLA	B	1238	49/65	0.91	0.18	82,108,125,127	0
17	45D	B	4011	42/42	0.91	0.18	45,59,68,68	0
12	CLA	B	1222	50/65	0.91	0.15	69,81,93,97	0
12	CLA	B	1224	55/65	0.91	0.17	13,49,70,75	0
12	CLA	B	1225	49/65	0.91	0.15	36,61,78,80	0
12	CLA	A	1101	49/65	0.91	0.15	52,74,79,86	0
12	CLA	B	1227	49/65	0.91	0.15	80,91,140,146	0
12	CLA	A	1140	65/65	0.91	0.16	16,65,78,88	0
15	BCR	F	4014	40/40	0.91	0.21	57,85,104,106	0
12	CLA	A	1013	65/65	0.91	0.17	19,57,67,79	0
12	CLA	B	1237	49/65	0.91	0.16	92,112,121,127	0
12	CLA	B	1236	49/65	0.91	0.16	49,63,76,77	0
12	CLA	B	1214	60/65	0.91	0.16	46,80,102,105	0
12	CLA	A	1117	49/65	0.92	0.18	78,99,110,116	0
12	CLA	A	1126	60/65	0.92	0.17	28,79,96,102	0
12	CLA	B	1206	49/65	0.92	0.14	75,86,127,132	0
12	CLA	A	1128	65/65	0.92	0.17	32,87,97,104	0
12	CLA	B	1202	65/65	0.92	0.13	12,70,77,79	0
12	CLA	B	1229	55/65	0.92	0.14	33,44,62,64	0
16	LHG	A	5001	49/49	0.92	0.17	38,59,91,113	0
12	CLA	B	1230	49/65	0.92	0.12	66,77,81,86	0
12	CLA	B	1232	49/65	0.92	0.10	70,82,98,101	0
23	C7Z	J	4015	42/42	0.92	0.16	60,87,96,101	0
12	CLA	A	1012	49/65	0.92	0.16	38,63,73,74	0
12	CLA	B	1223	49/65	0.92	0.20	81,96,110,113	0
12	CLA	B	1210	49/65	0.93	0.10	42,72,80,82	0
12	CLA	A	1123	60/65	0.93	0.17	67,85,100,104	0

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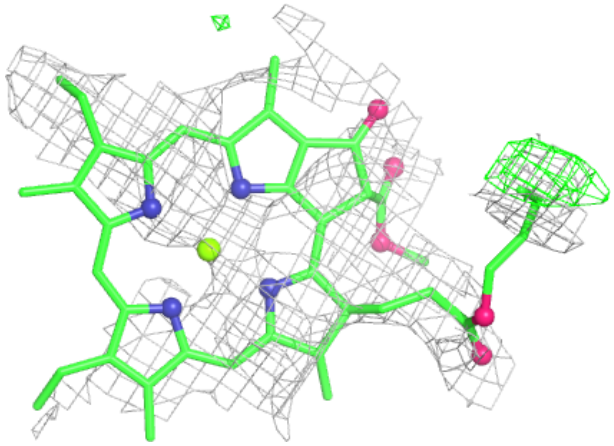
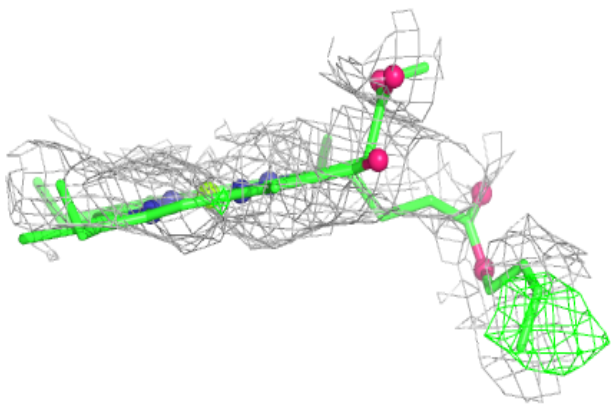
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	CLA	A	1127	49/65	0.93	0.17	72,86,97,103	0
18	CL	B	6000	1/1	0.93	0.08	89,89,89,89	0
12	CLA	B	1231	49/65	0.93	0.15	49,85,97,109	0
12	CLA	A	1139	55/65	0.93	0.19	43,59,110,117	0
12	CLA	A	1124	49/65	0.93	0.17	100,122,134,135	0
12	CLA	A	1103	49/65	0.93	0.16	75,90,108,114	0
12	CLA	A	1106	65/65	0.94	0.16	72,95,117,130	0
12	CLA	B	1023	49/65	0.94	0.14	65,80,89,93	0
13	PQN	A	2001	33/33	0.94	0.14	13,27,42,50	0
12	CLA	A	1104	49/65	0.94	0.12	60,85,96,101	0
12	CLA	A	1138	65/65	0.95	0.13	26,55,72,76	0
14	SF4	A	3001	8/8	0.98	0.08	36,63,86,101	0
14	SF4	C	3002	8/8	0.99	0.05	32,41,89,113	0
14	SF4	C	3003	8/8	0.99	0.11	32,57,177,197	0

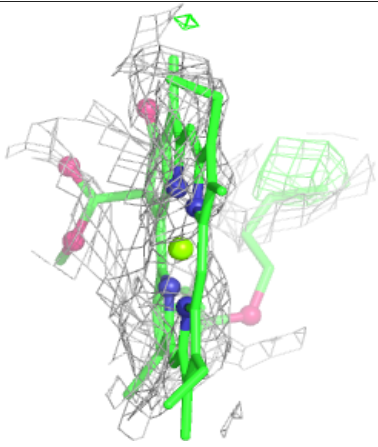
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CLA L 1502:

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

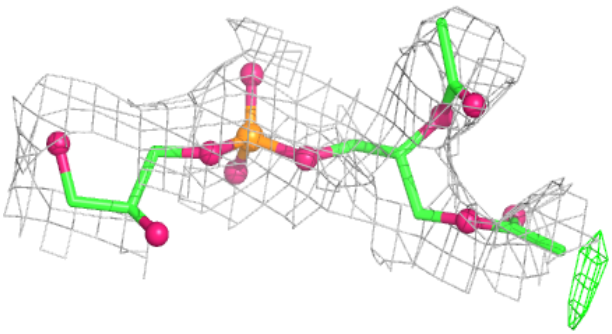


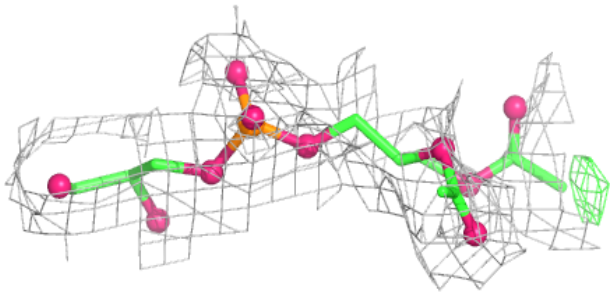


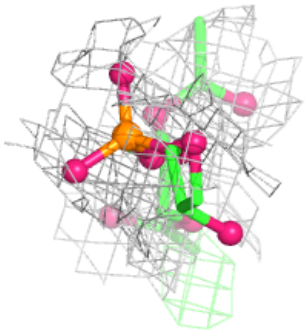


Electron density around LHG B 5006:

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



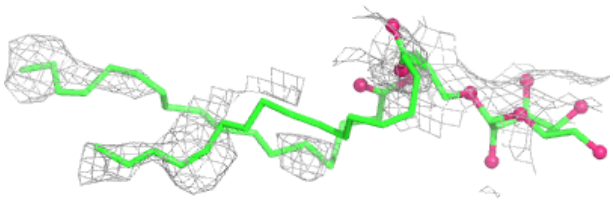




Electron density around LMG B 5005:

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

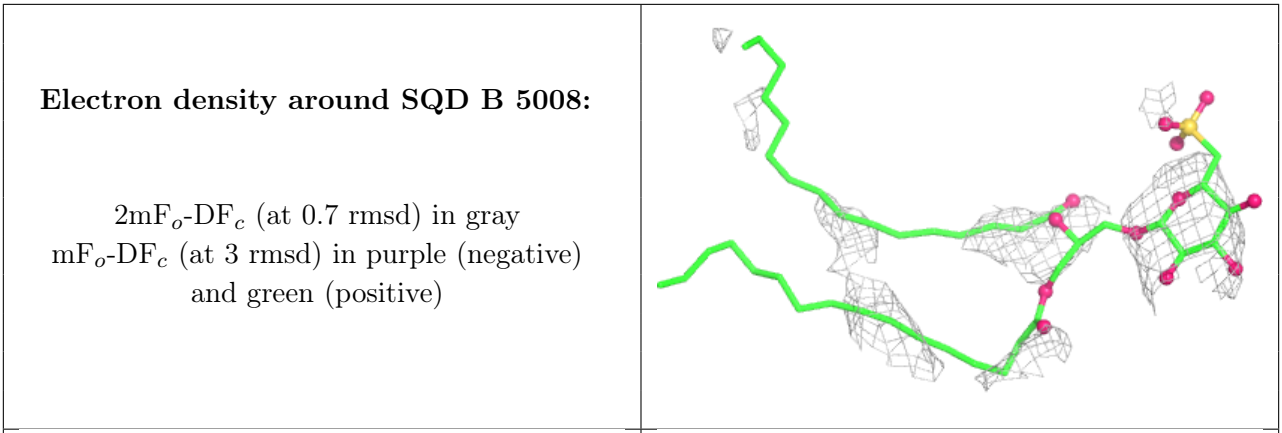






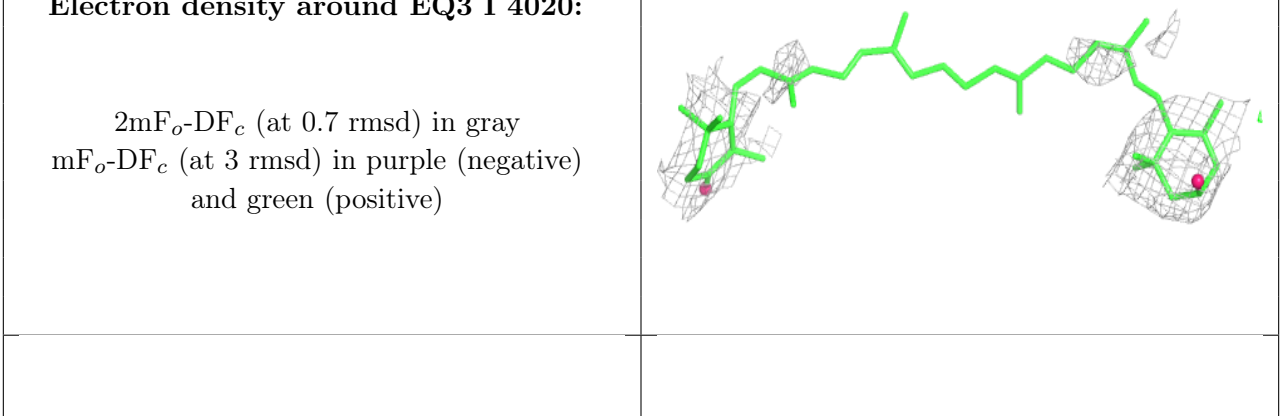
Electron density around SQD B 5008:

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



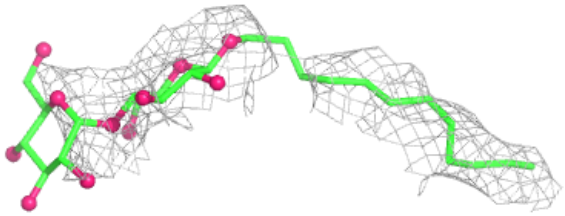
Electron density around EQ3 I 4020:

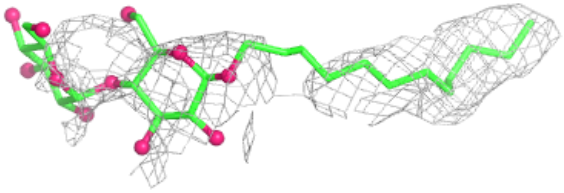
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT F 6001:

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

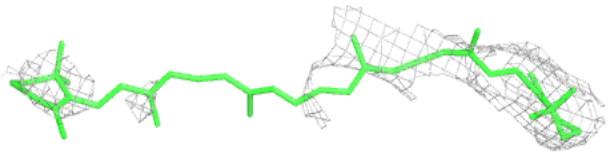


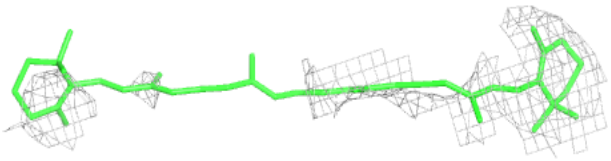


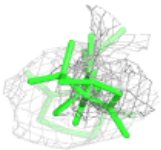


Electron density around BCR K 4001:

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

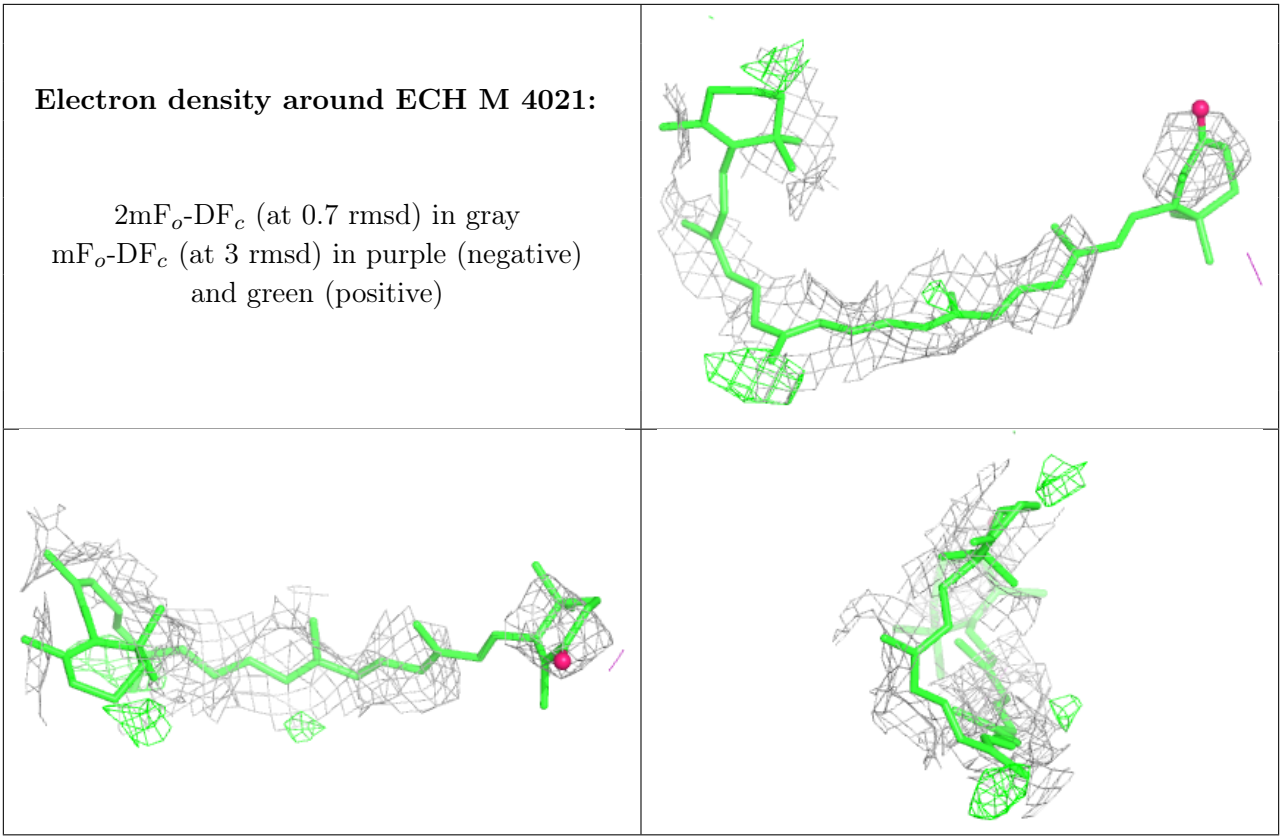






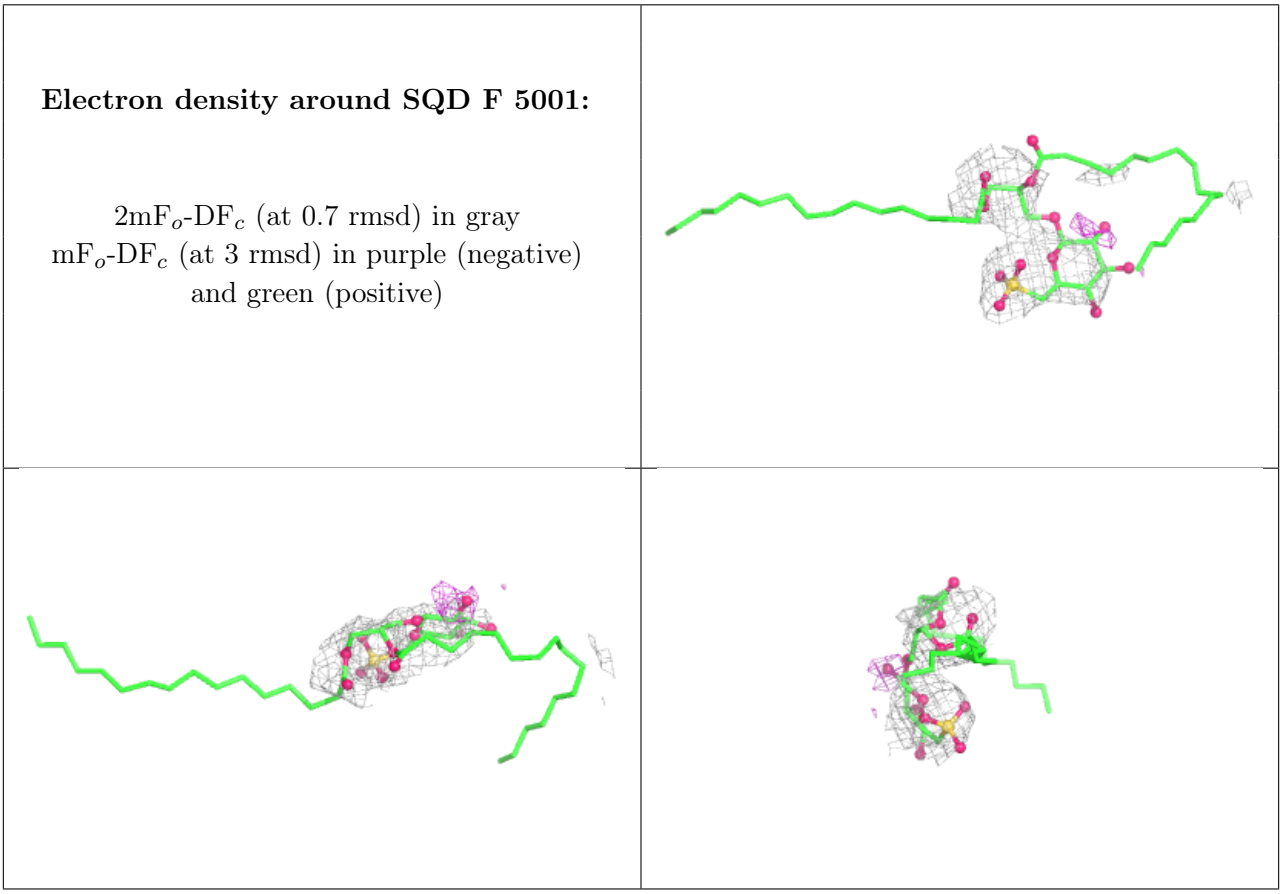
Electron density around ECH M 4021:

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



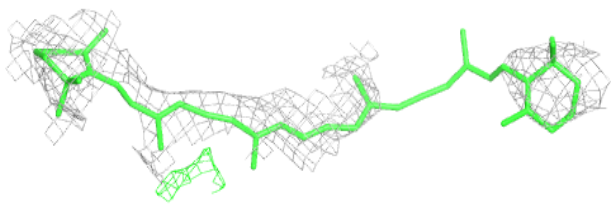
Electron density around SQD F 5001:

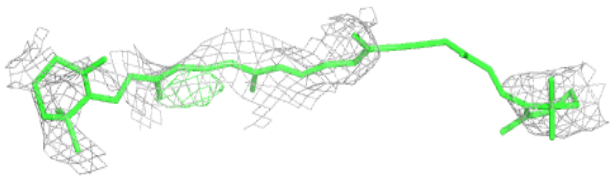
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

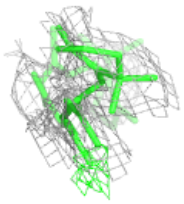


Electron density around BCR A 4001:

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

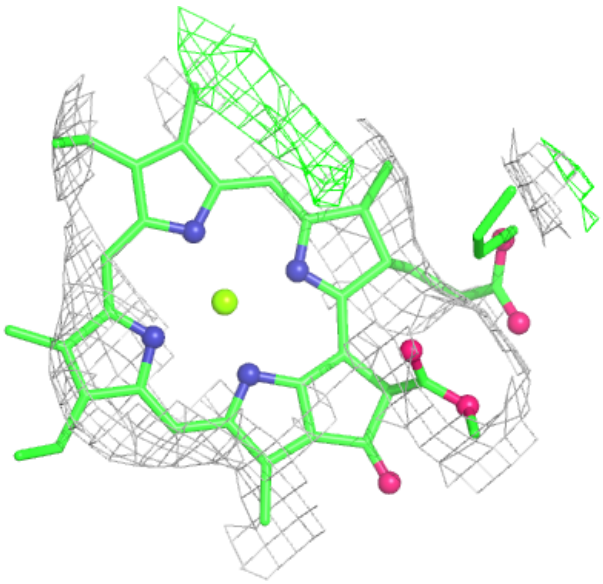


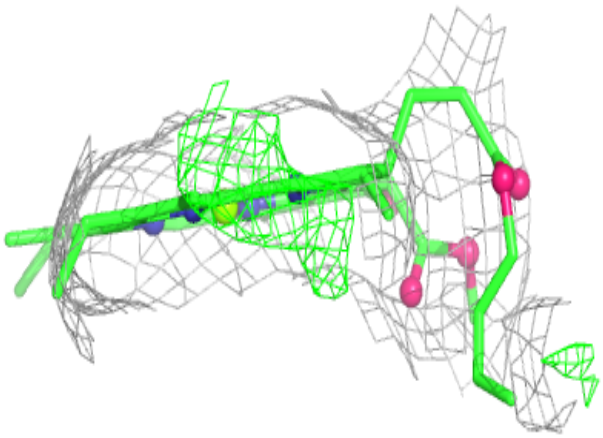


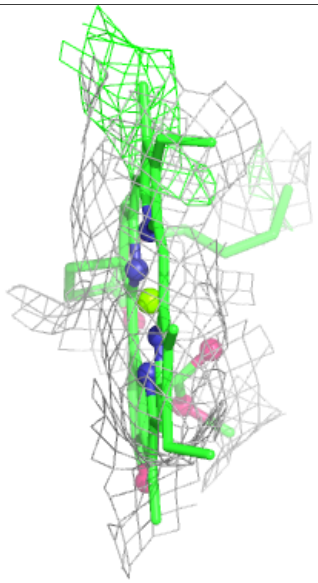


Electron density around CLA B 1207:

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

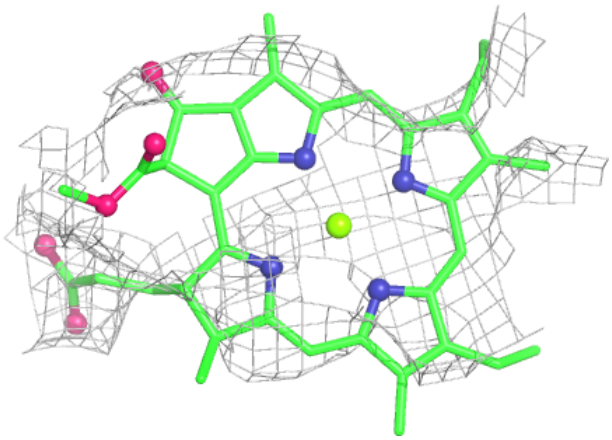


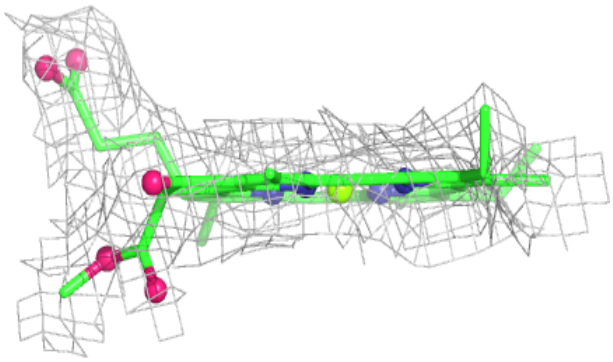


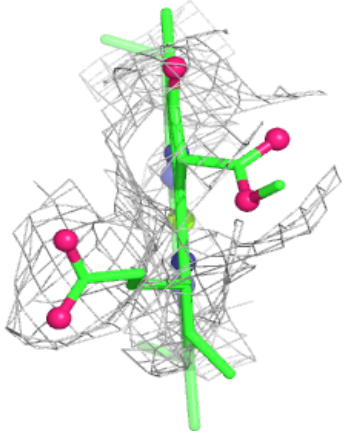


Electron density around CLA K 1401:

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

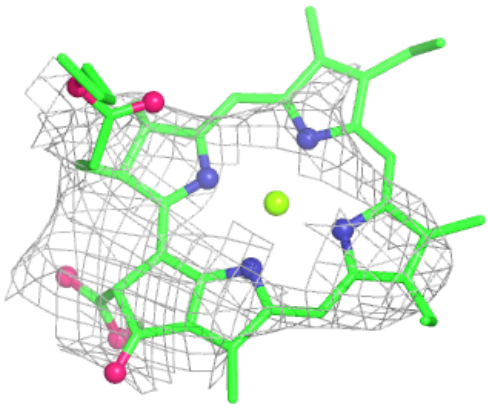


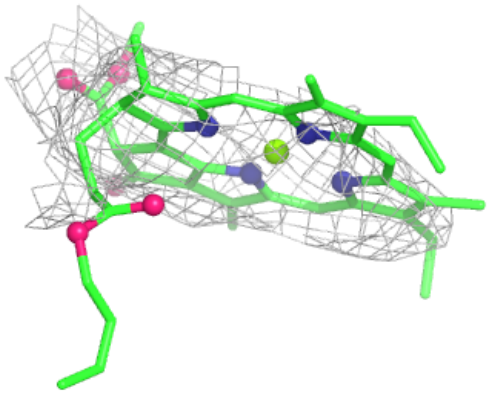


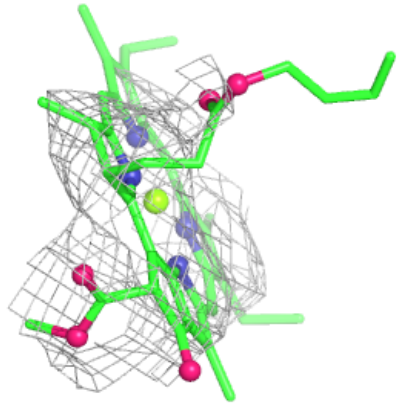


Electron density around CLA A 1113:

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

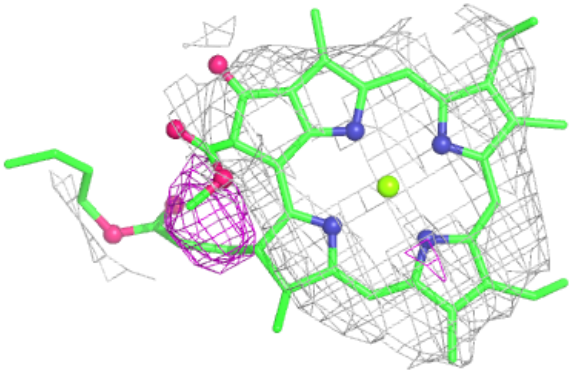


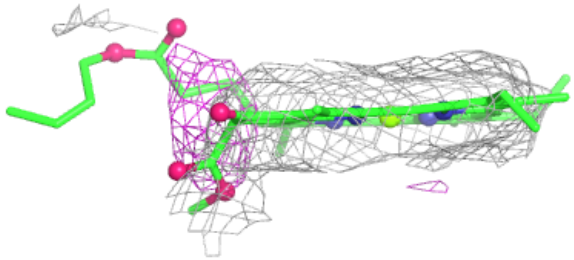


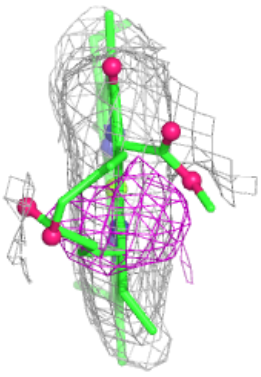


Electron density around CLA B 1240:

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

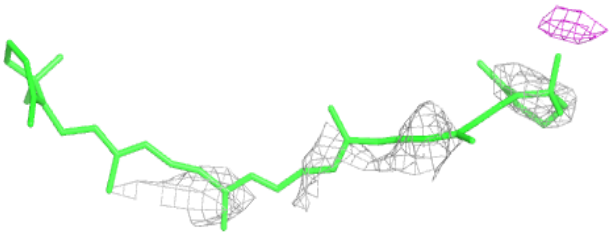


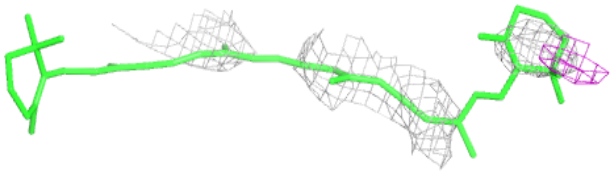


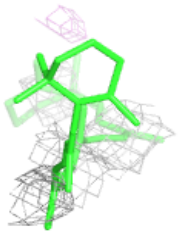


Electron density around BCR I 4018:

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

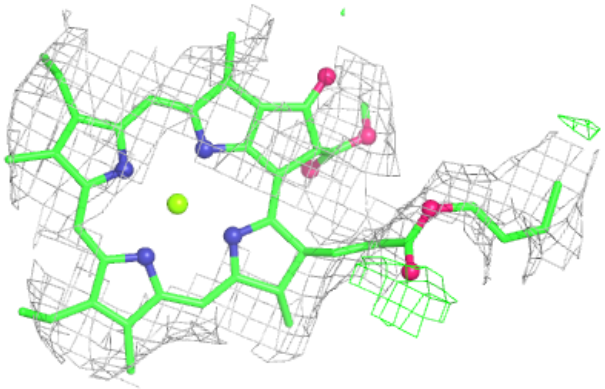


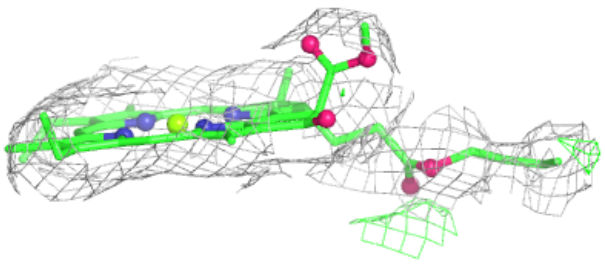


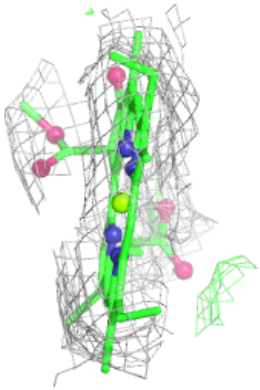


Electron density around CLA B 1219:

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

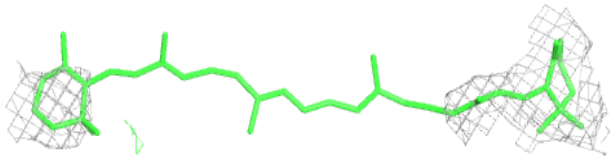


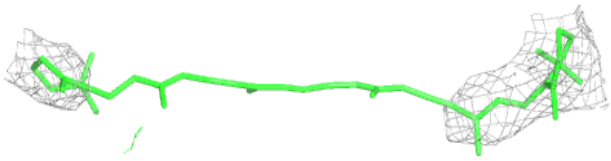


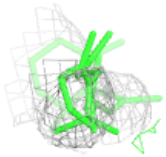


Electron density around BCR A 4003:

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

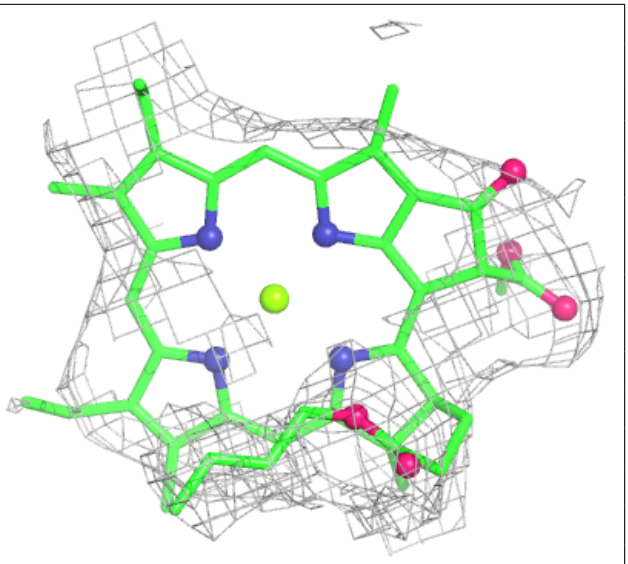


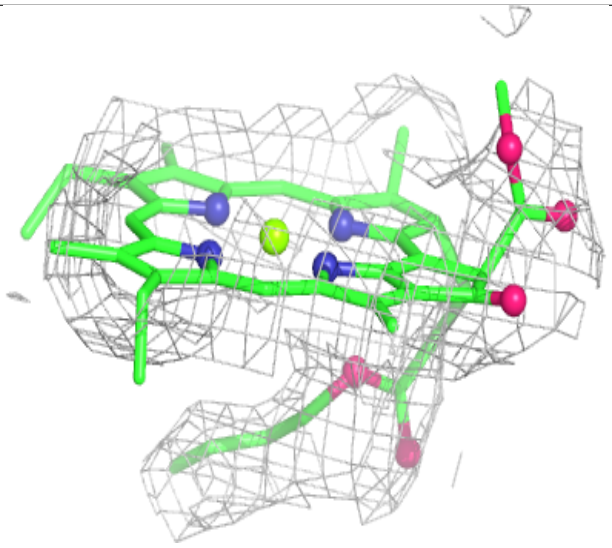




Electron density around CLA B 1217:

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

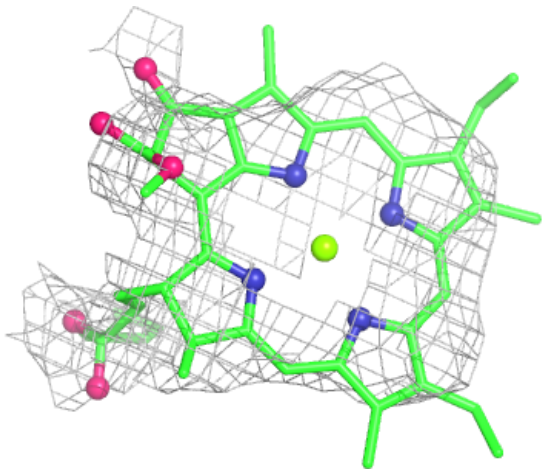


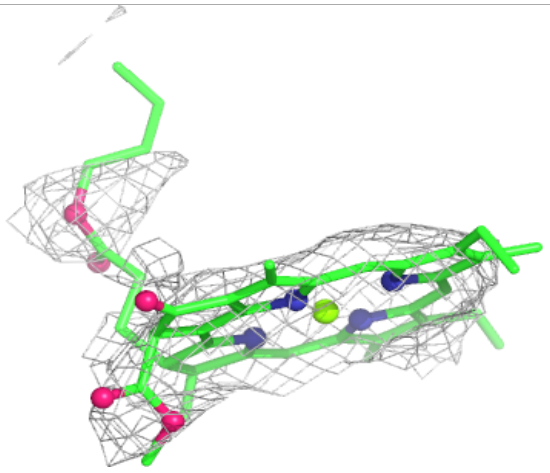


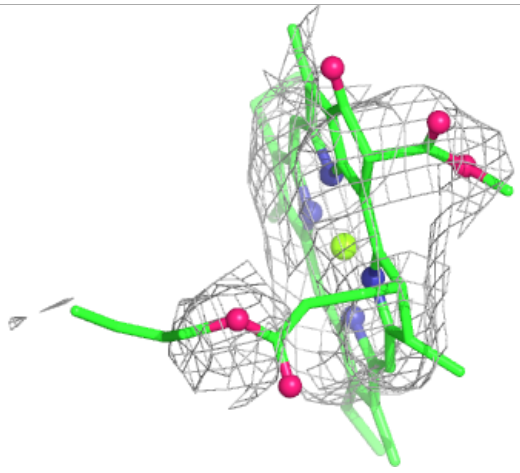


Electron density around CLA J 1303:

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

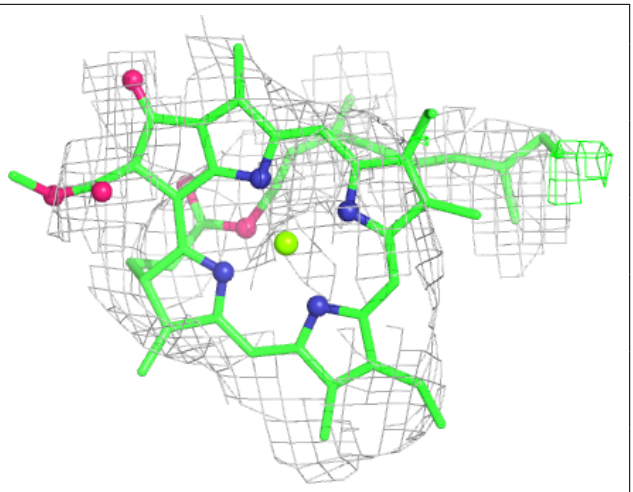


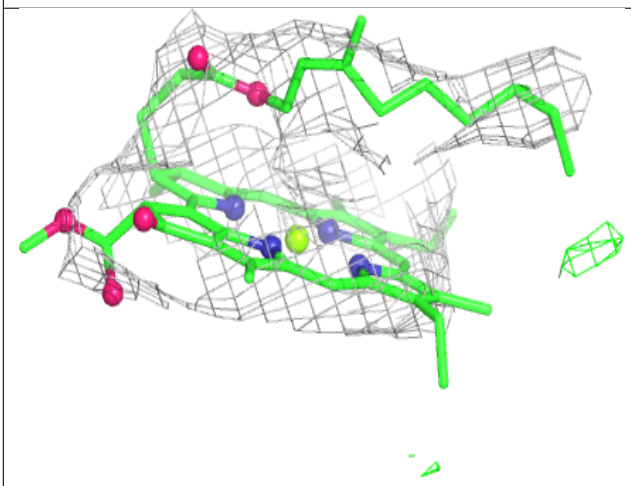


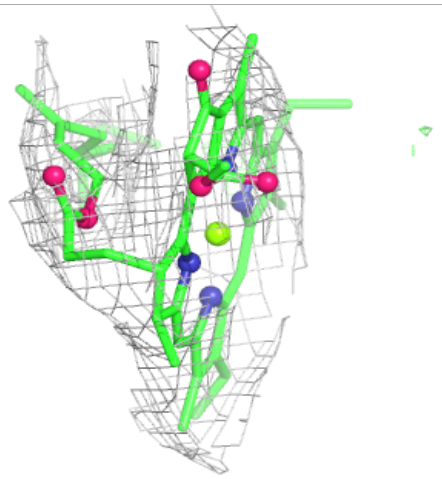


Electron density around CLA A 1115:

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

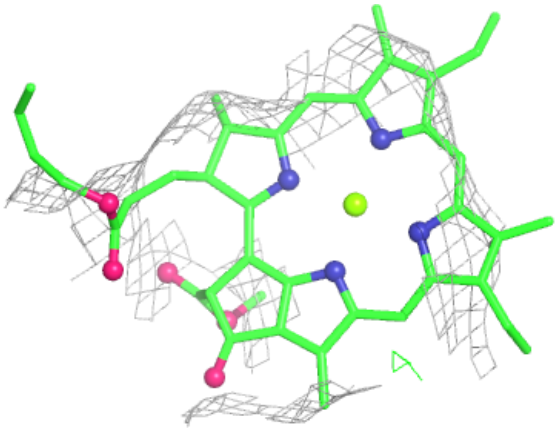


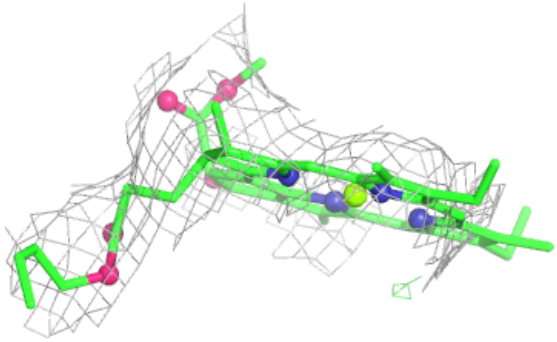


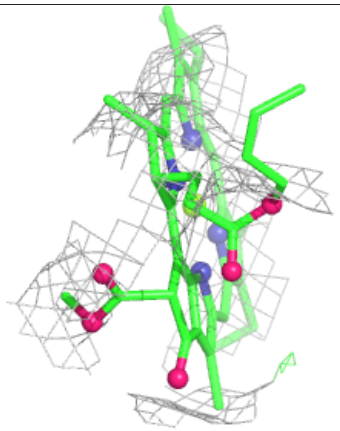


Electron density around CLA K 1402:

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

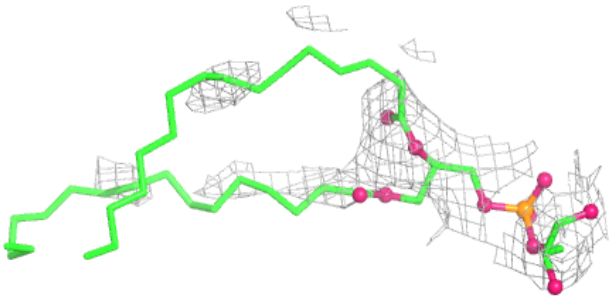


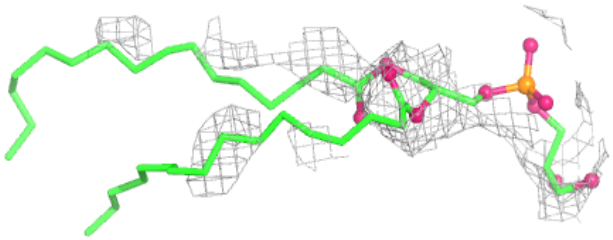




Electron density around LHG A 5003:

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

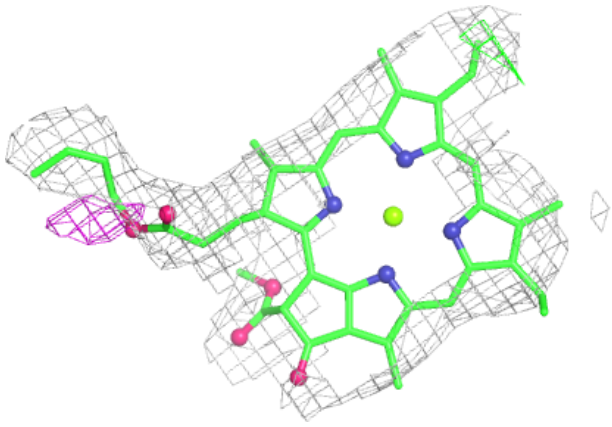


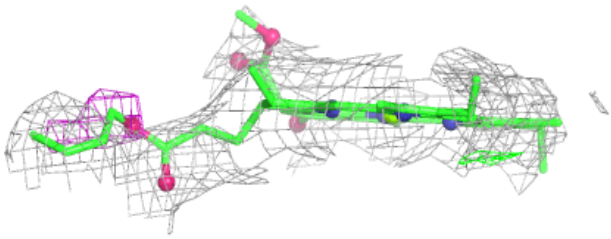


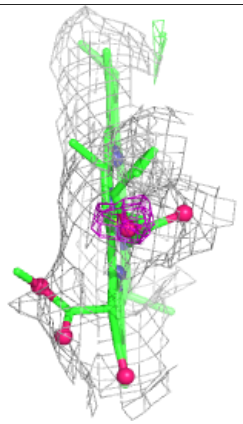


Electron density around CLA F 1302:

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

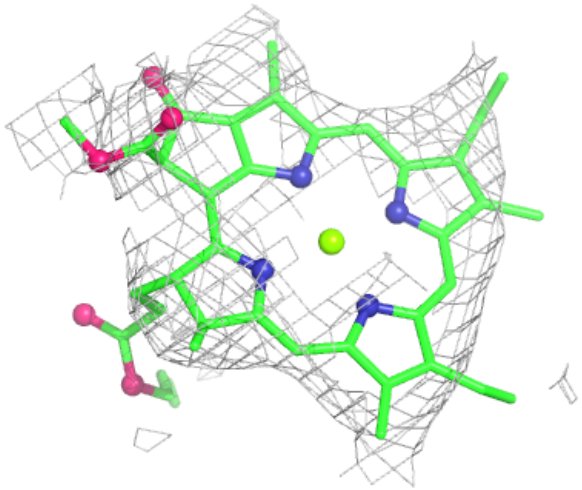


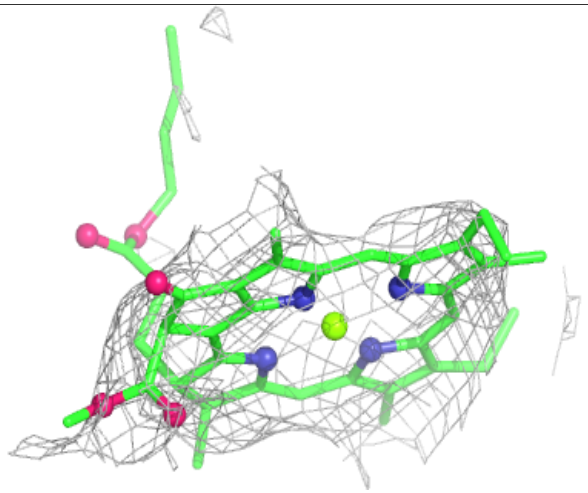


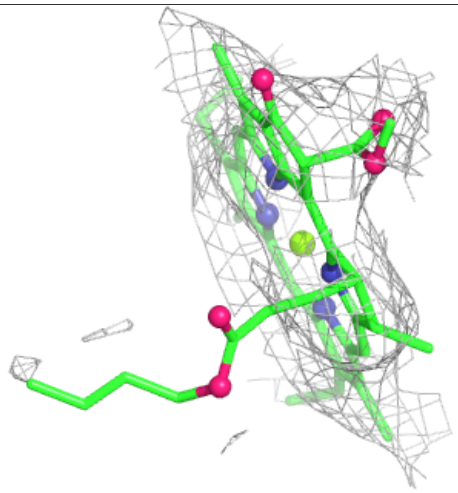


Electron density around CLA B 1212:

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

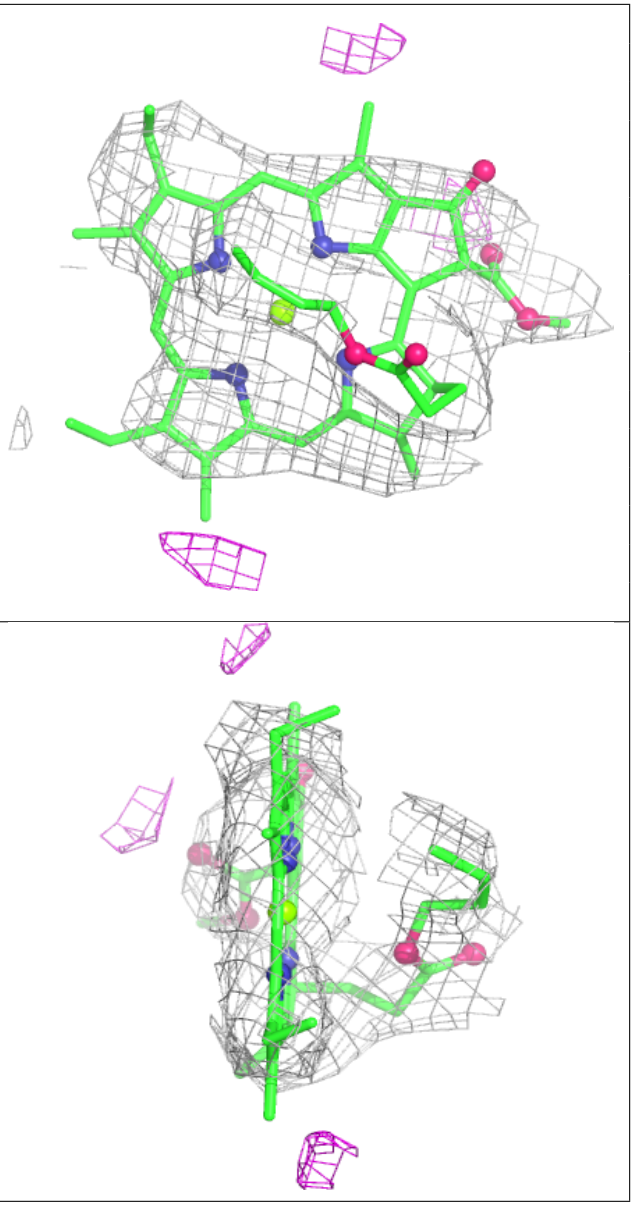






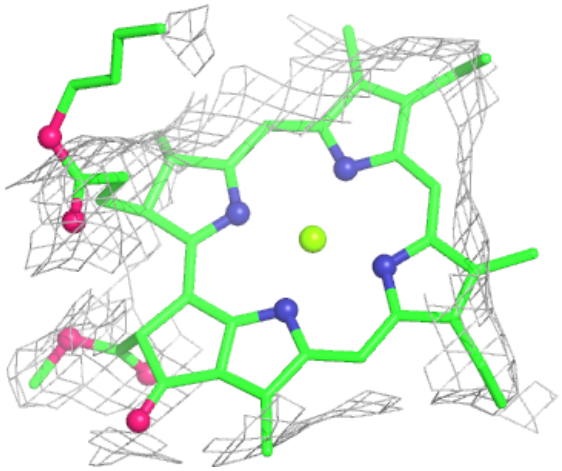
Electron density around CLA B 1204:

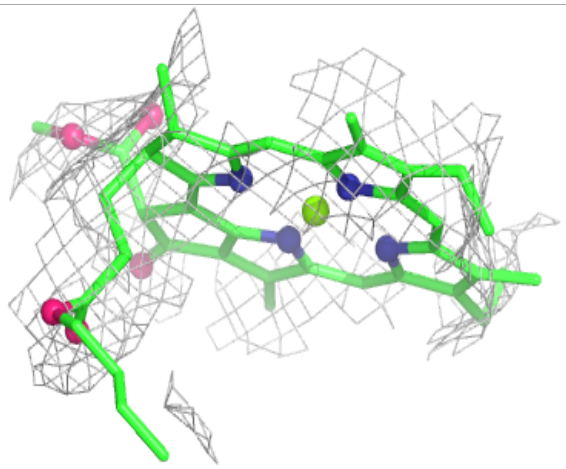
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

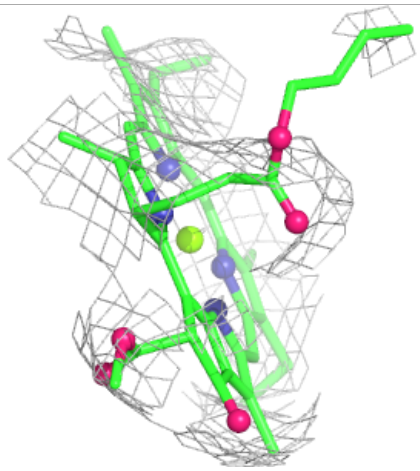


Electron density around CLA A 1114:

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

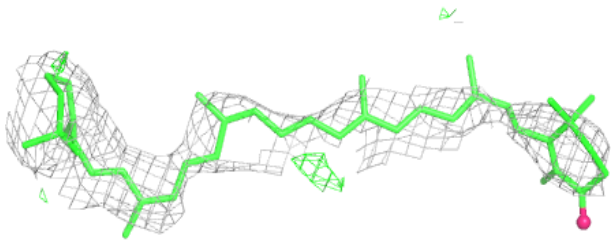


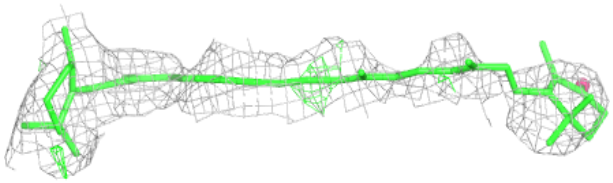


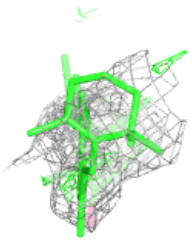


Electron density around ECH B 4006:

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

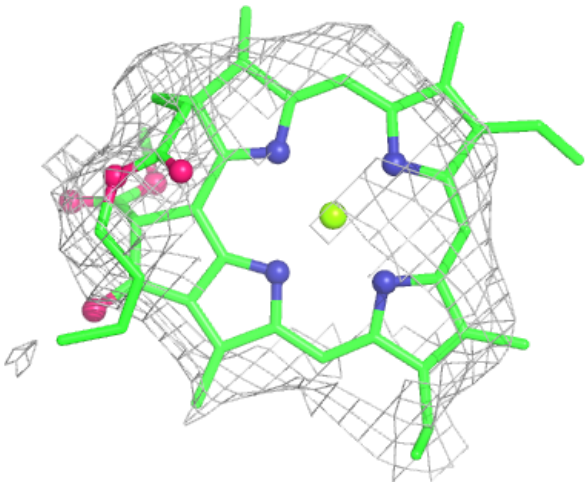


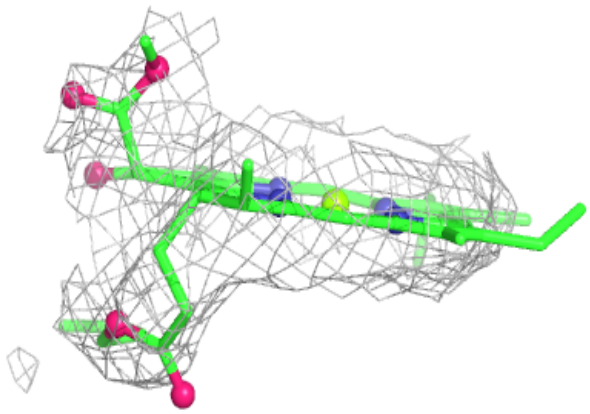


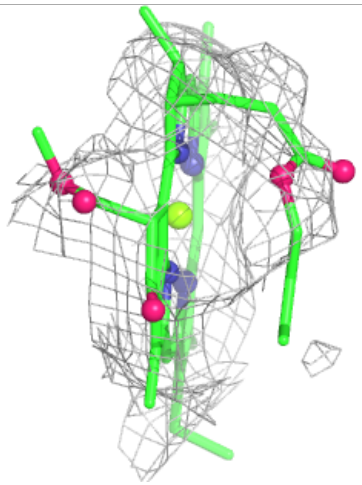


Electron density around CLA J 1302:

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

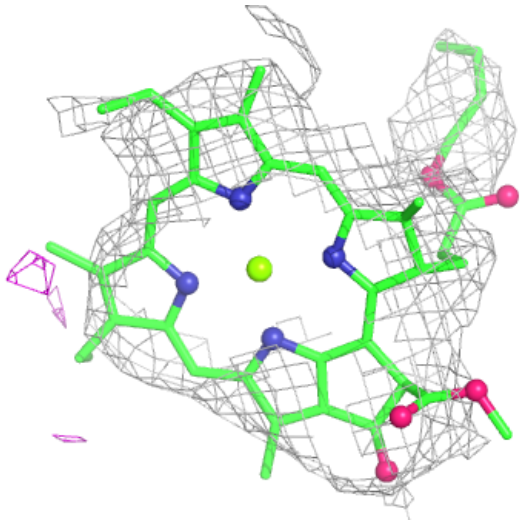


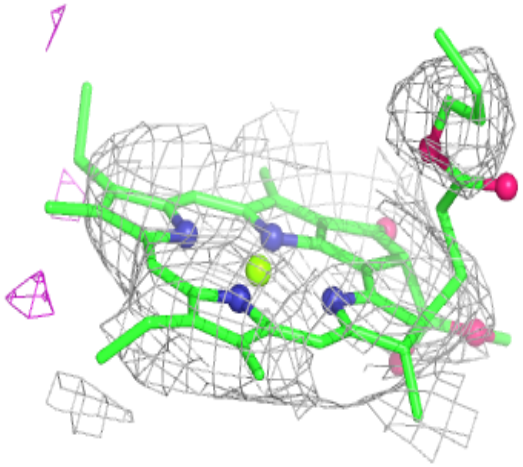




Electron density around CLA A 1133:

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

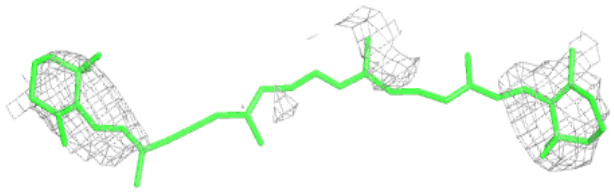




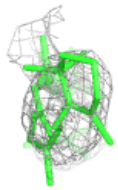


Electron density around BCR B 4004:

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

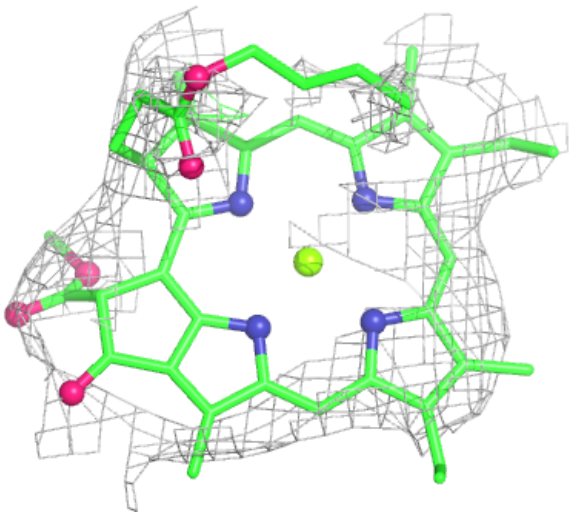


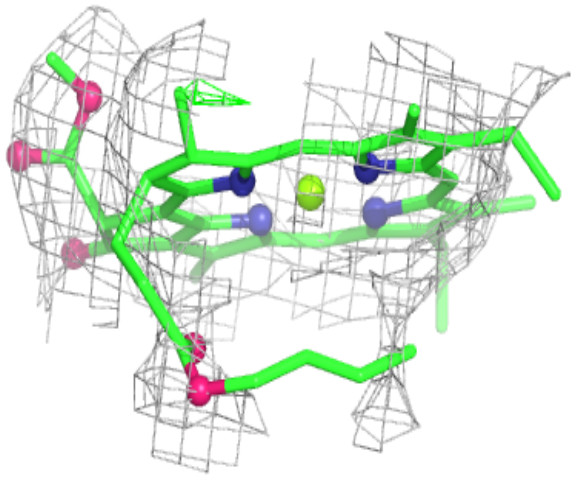


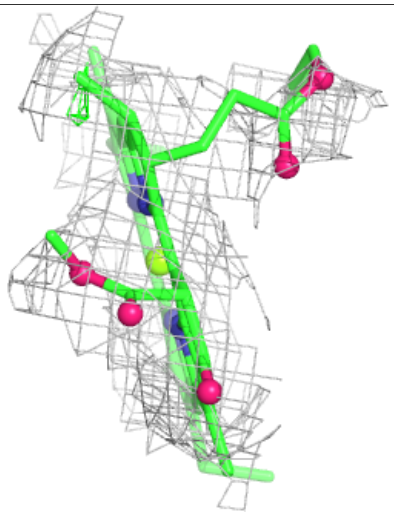


Electron density around CLA B 1209:

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

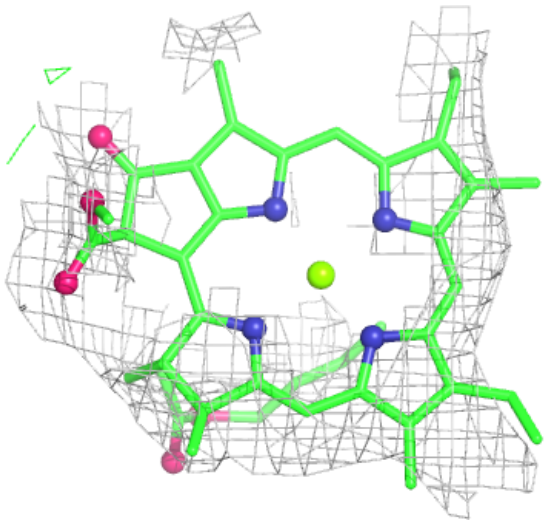


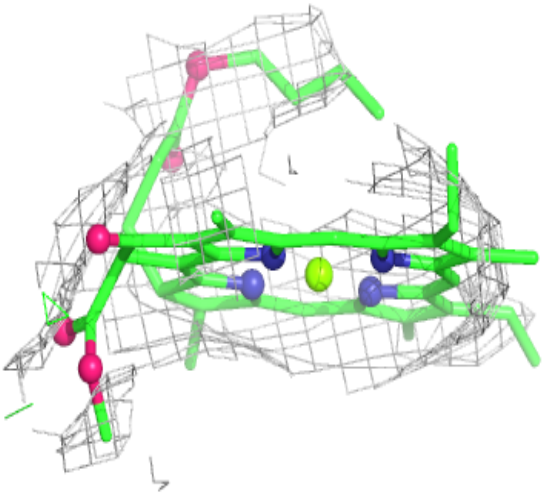


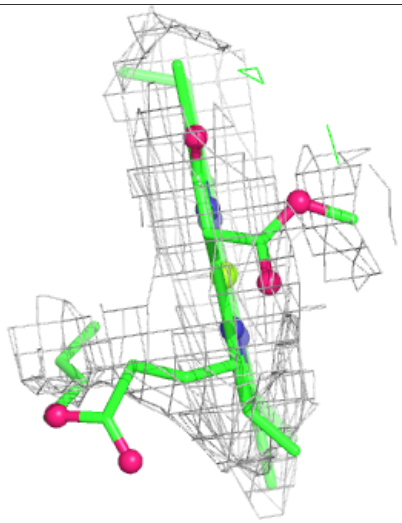


Electron density around CLA A 1120:

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

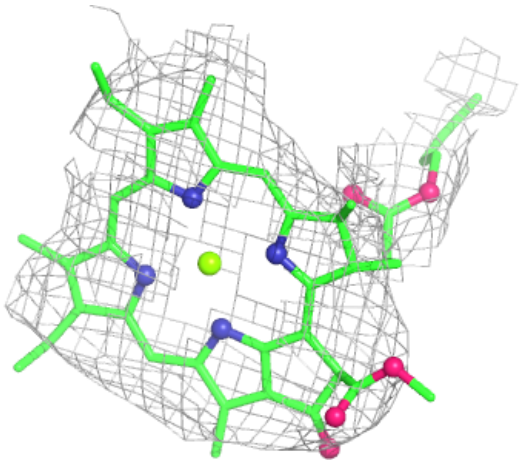


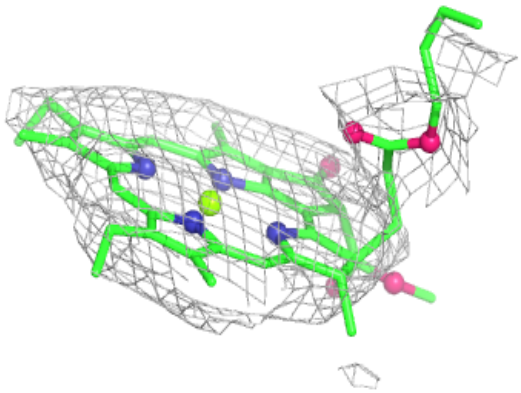




Electron density around CLA A 1108:

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

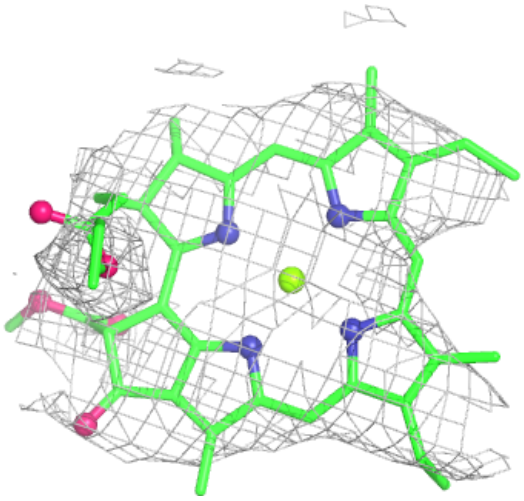


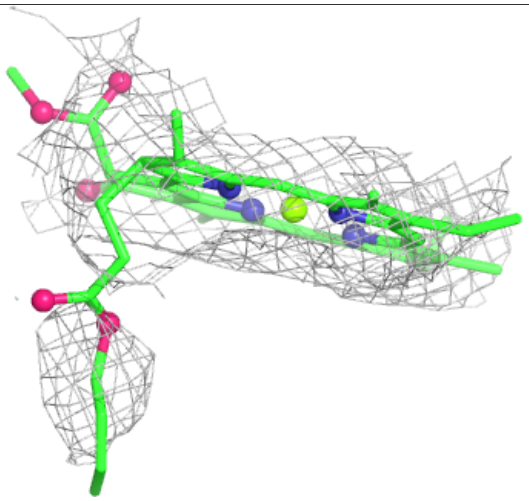




Electron density around CLA B 1208:

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

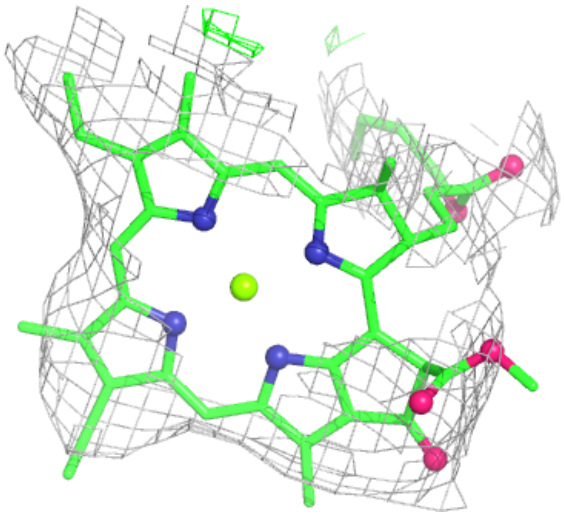


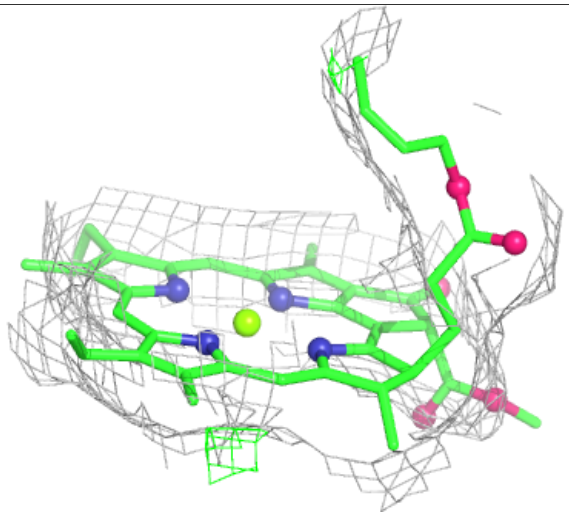


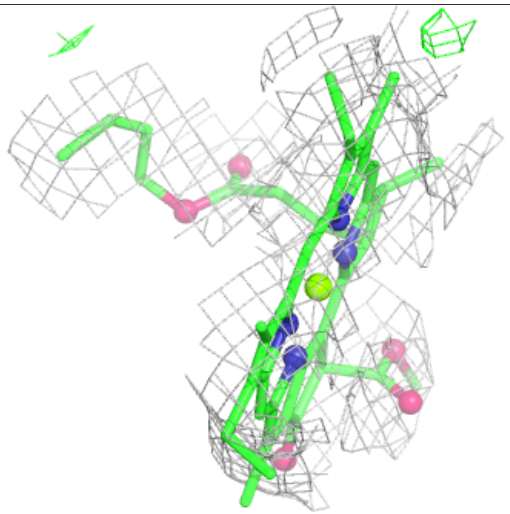


Electron density around CLA A 1130:

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

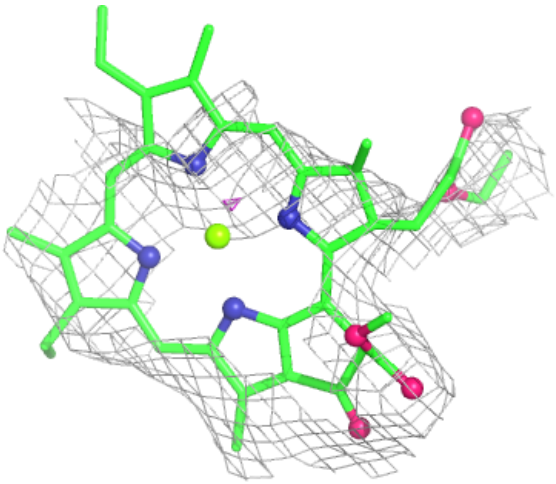


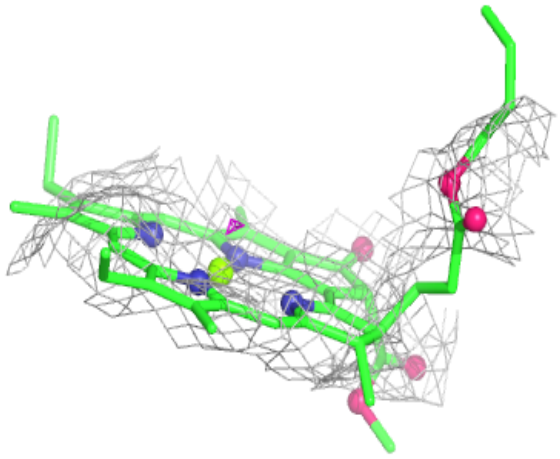


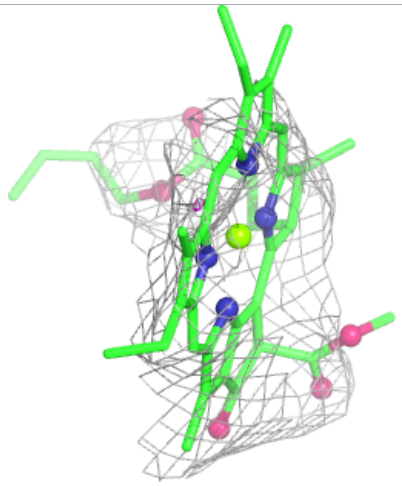


Electron density around CLA A 1112:

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

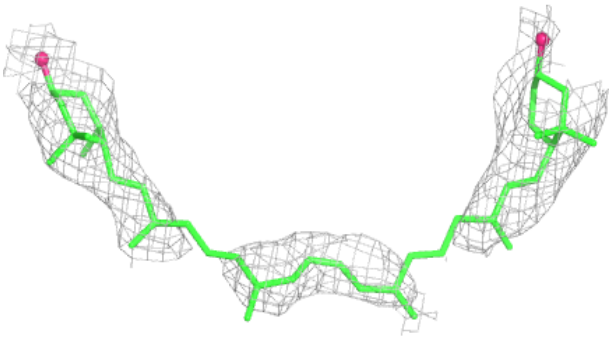


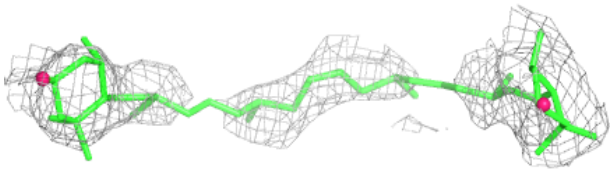


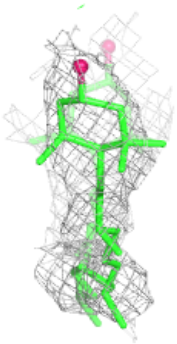


Electron density around C7Z F 4016:

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

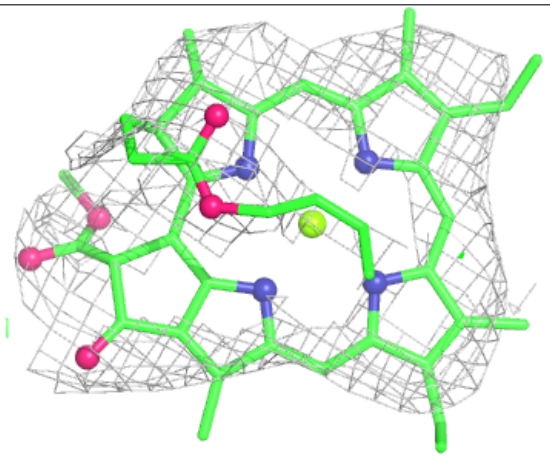


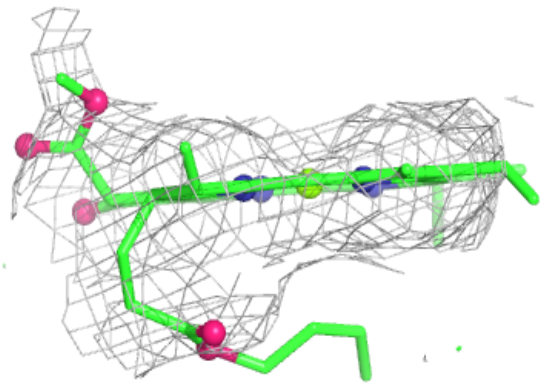


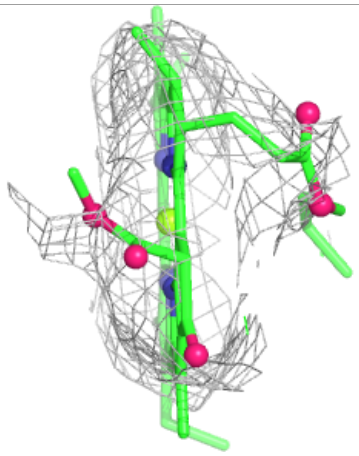


Electron density around CLA B 1213:

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

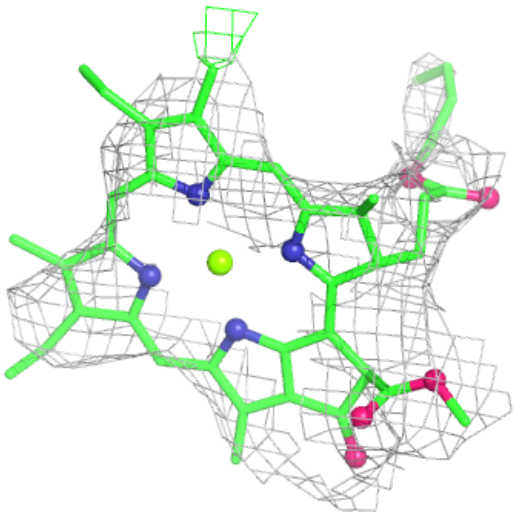


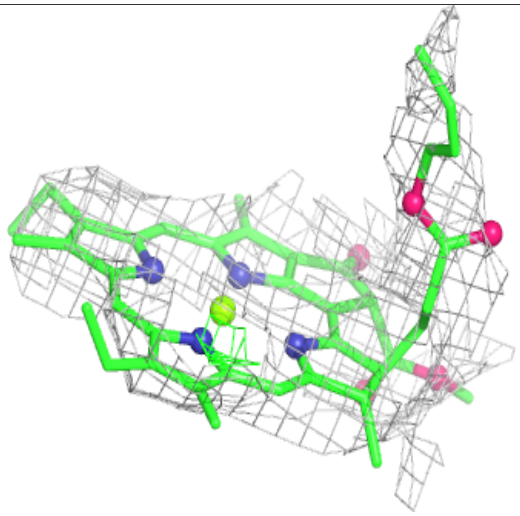


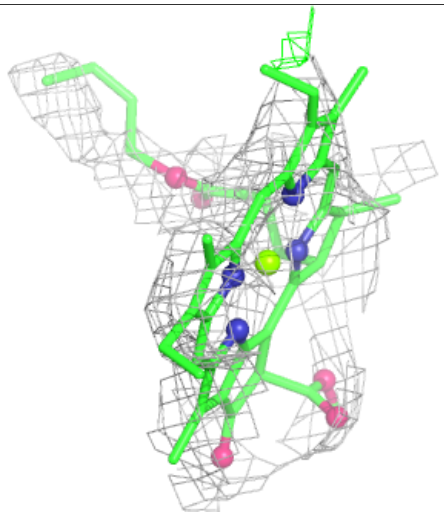


Electron density around CLA B 1216:

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

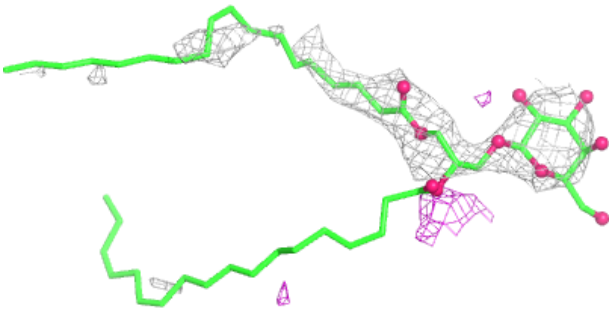


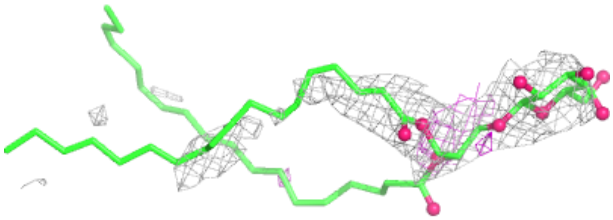


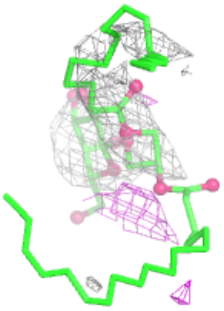


Electron density around LMG B 5002:

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

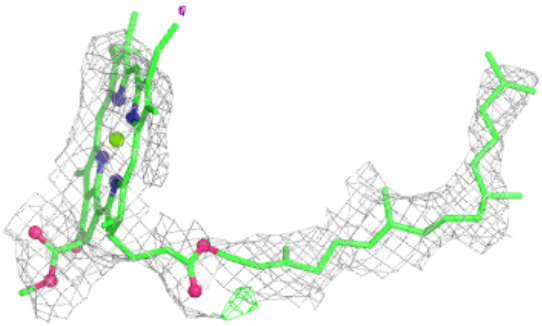


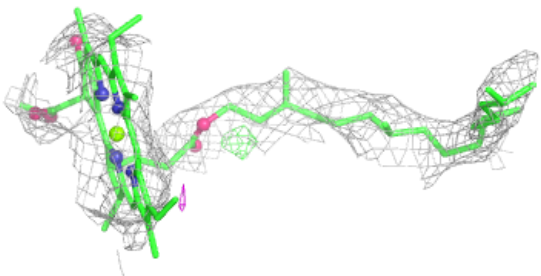


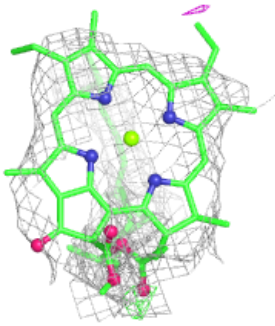


Electron density around CLA A 1105:

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

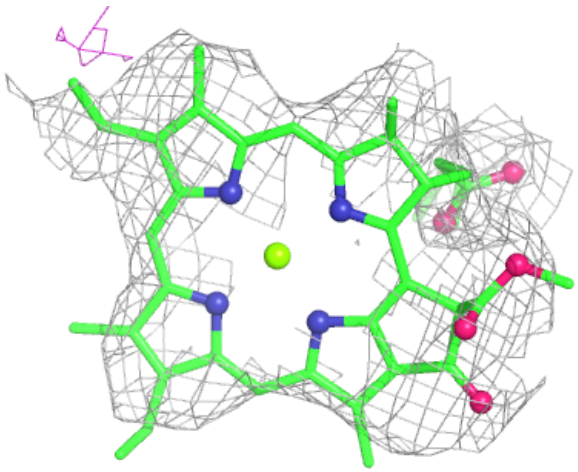


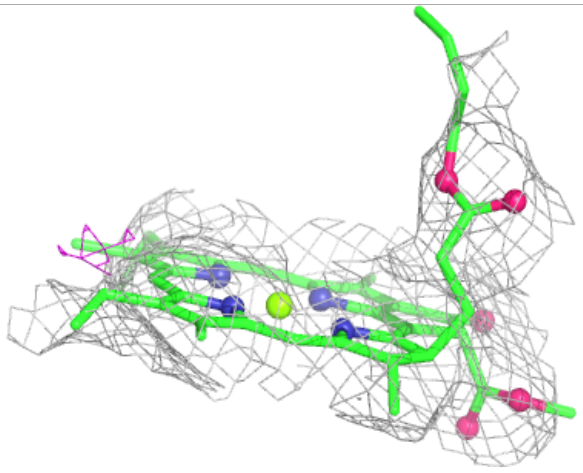


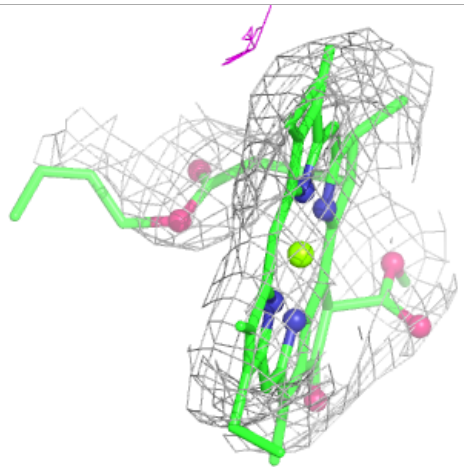


Electron density around CLA B 1201:

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

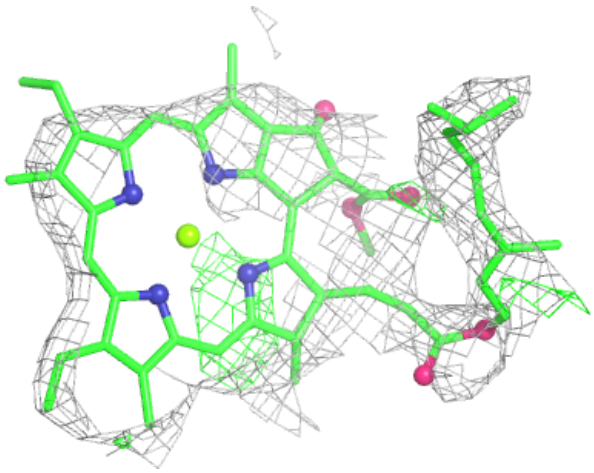


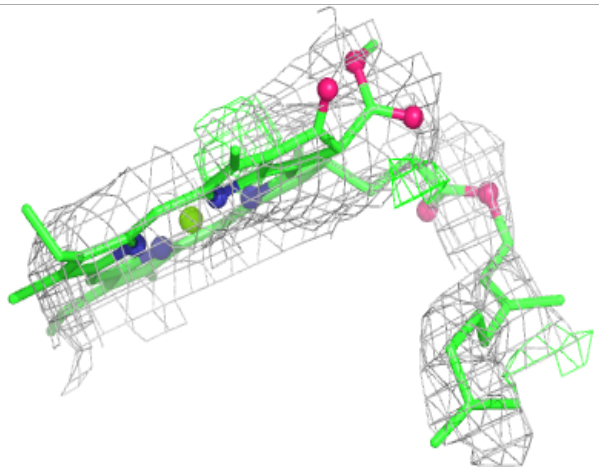


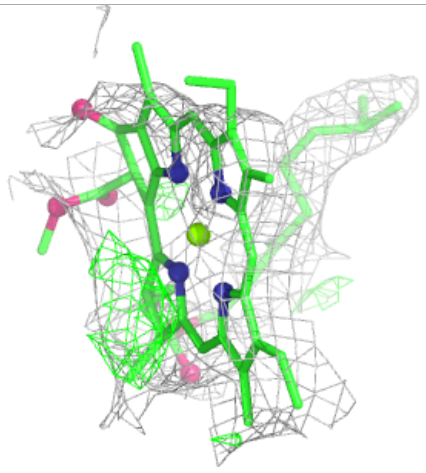


Electron density around CLA A 1011:

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

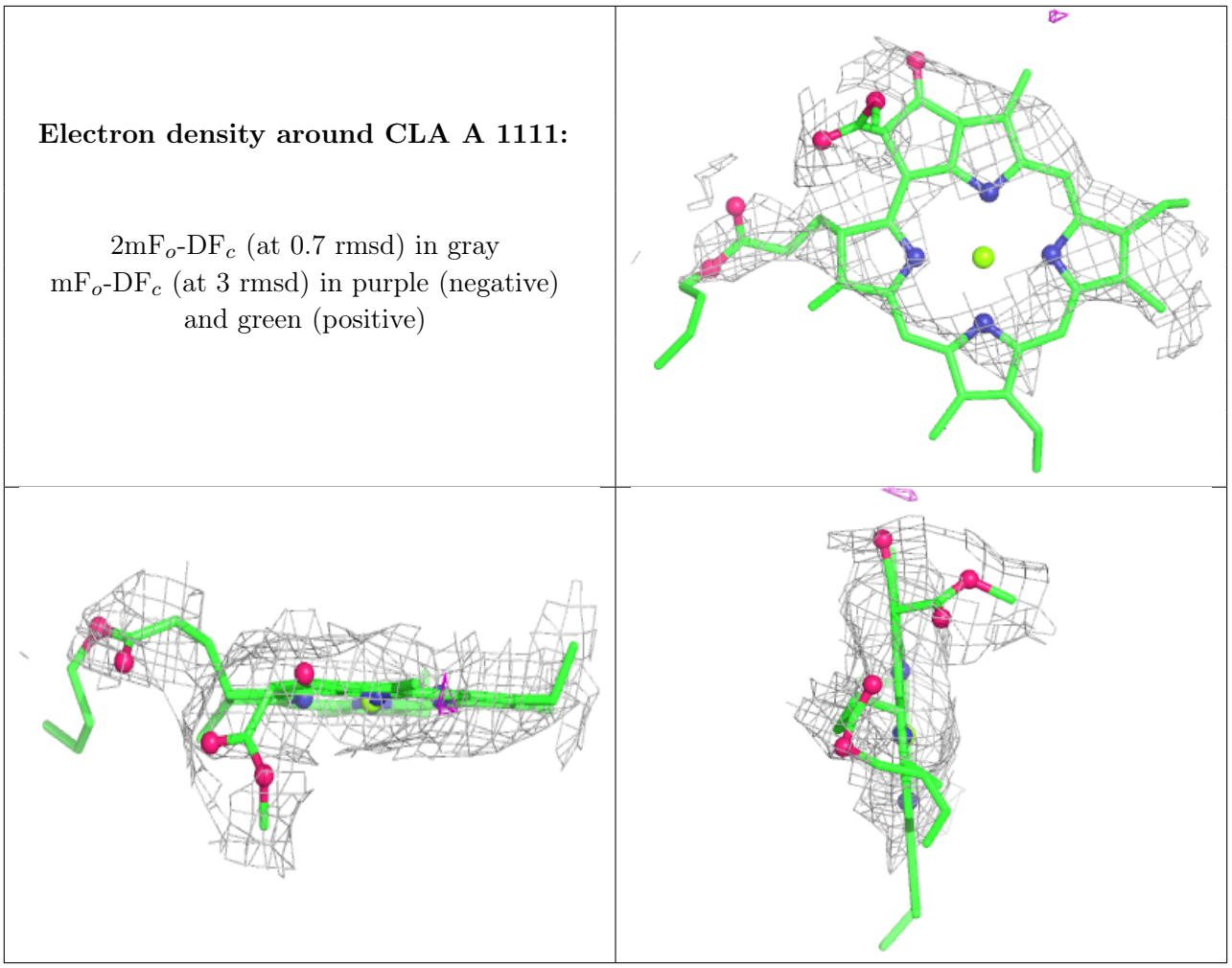






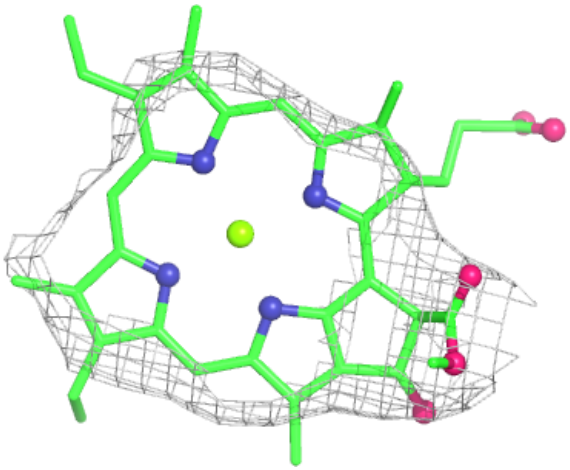
Electron density around CLA A 1111:

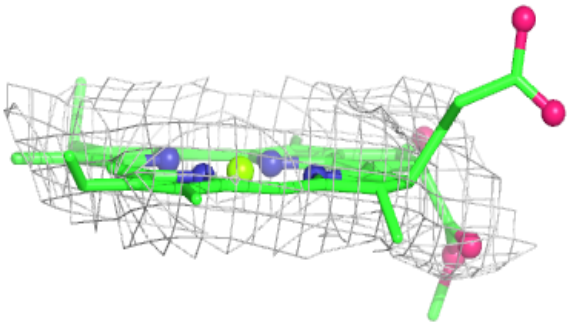
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

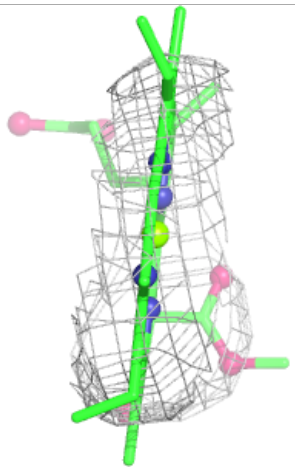


Electron density around CLA A 1141:

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

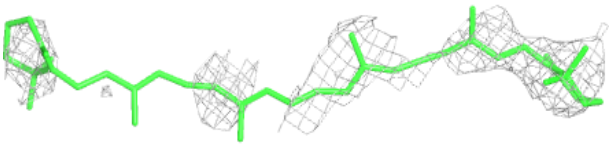


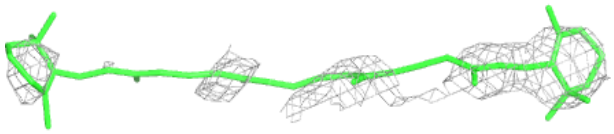


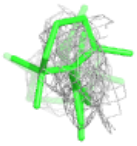


Electron density around BCR A 4007:

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

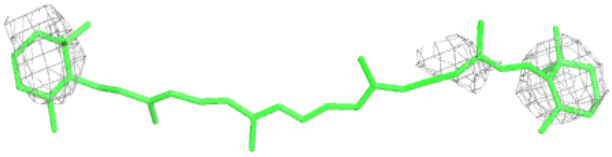


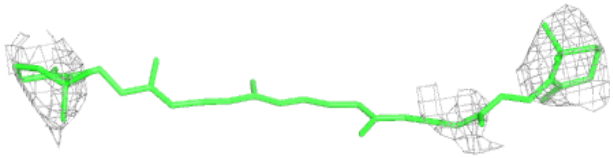


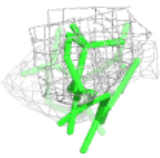


Electron density around BCR A 4008:

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

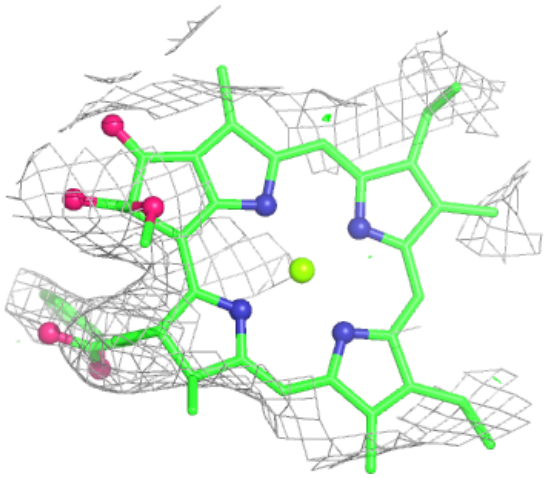


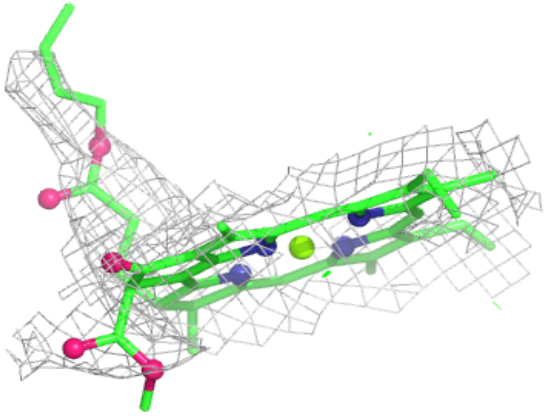


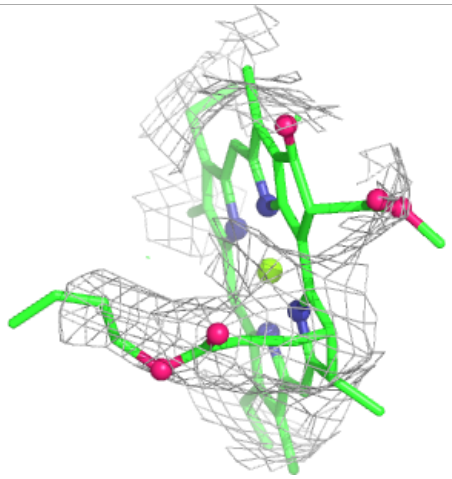


Electron density around CLA B 1211:

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

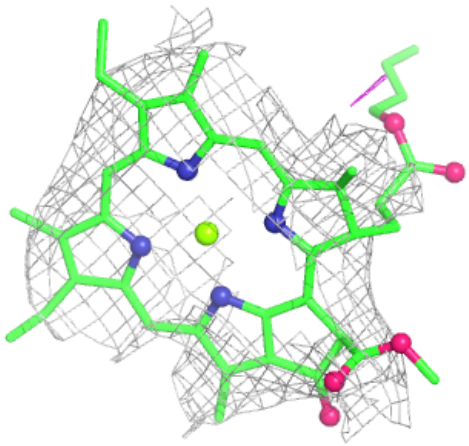


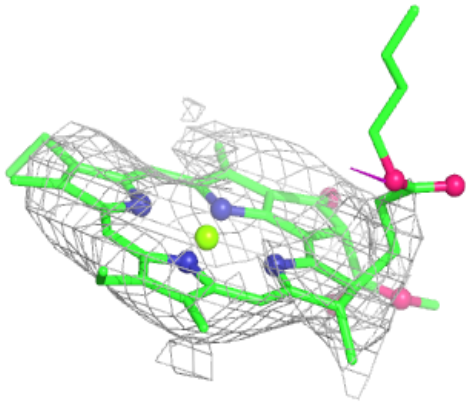


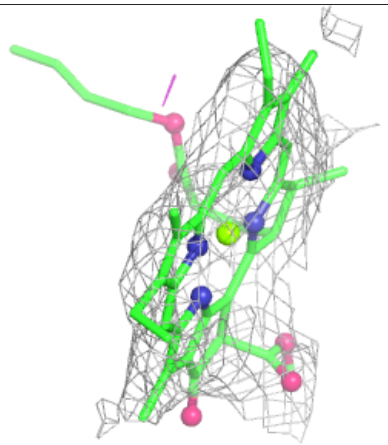


Electron density around CLA A 1129:

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

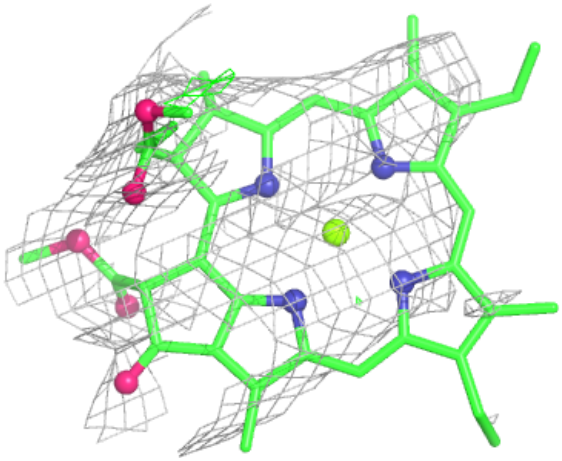


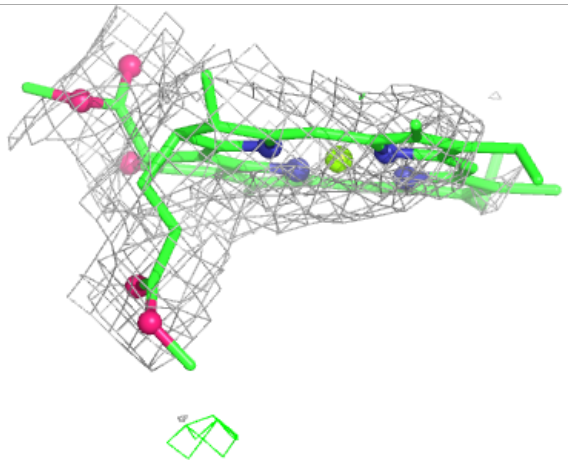


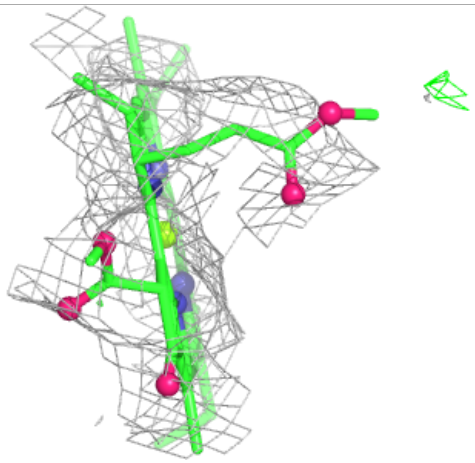


Electron density around CLA A 1119:

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

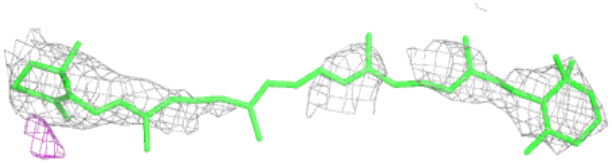


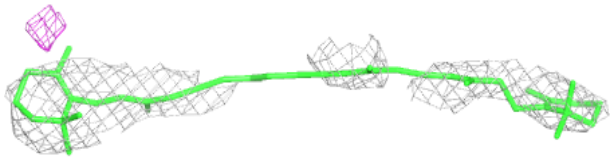


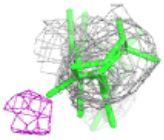


Electron density around BCR A 4012:

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

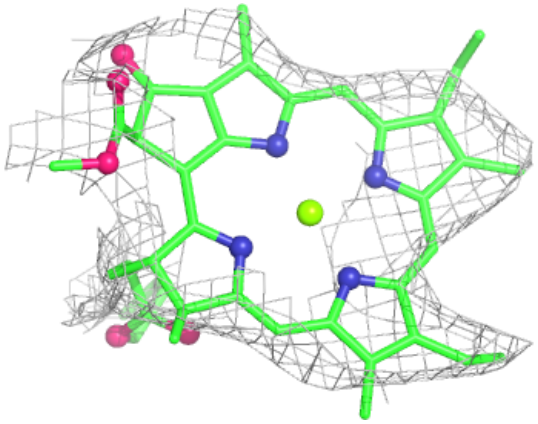


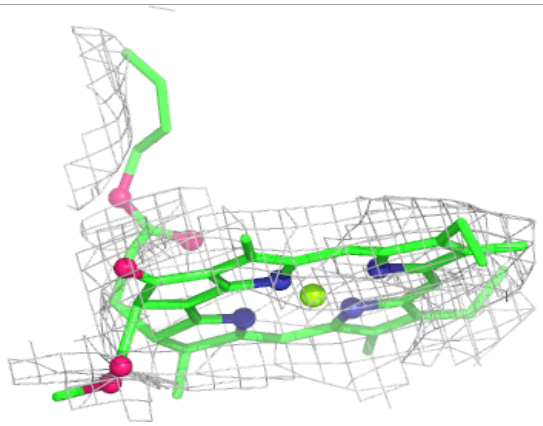


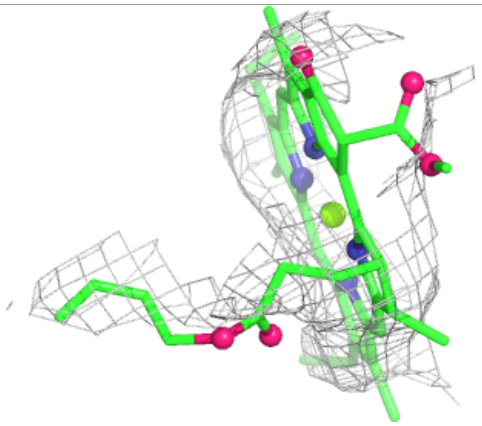


Electron density around CLA A 1134:

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

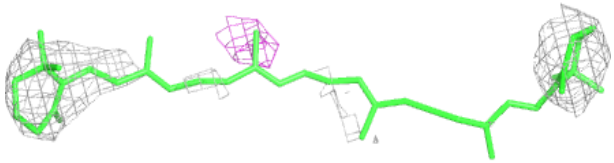


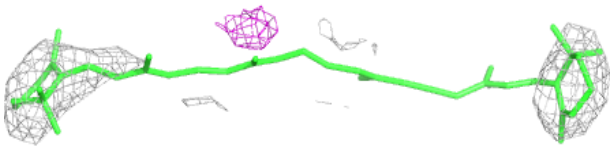


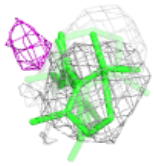


Electron density around BCR B 4017:

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

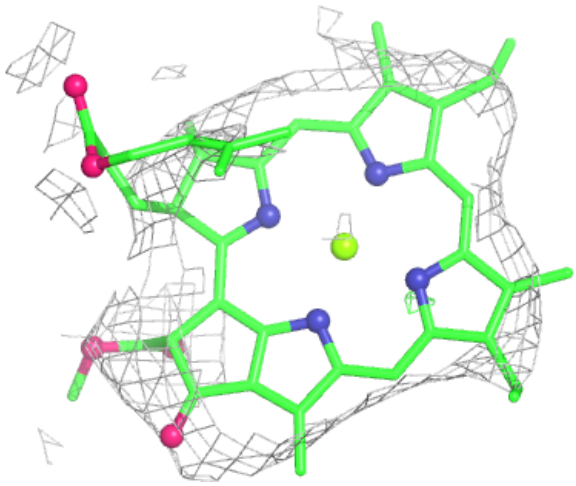


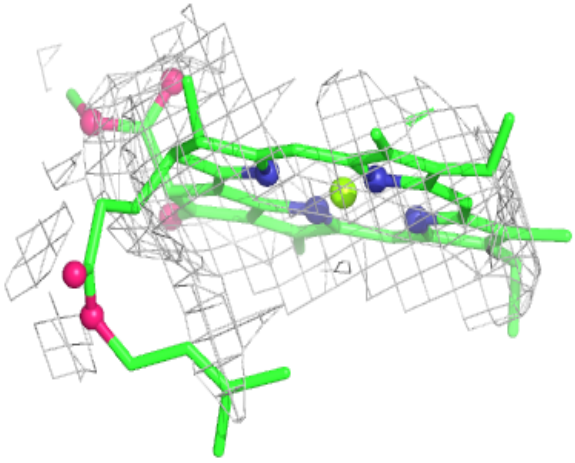


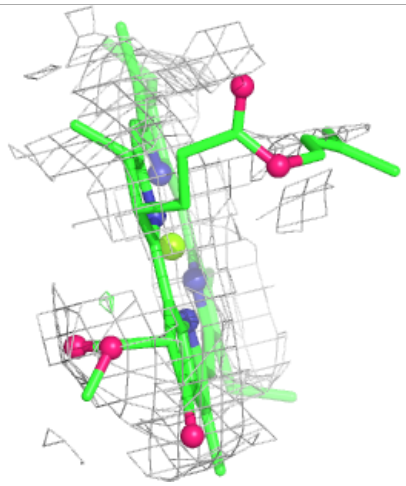


Electron density around CLA A 1118:

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

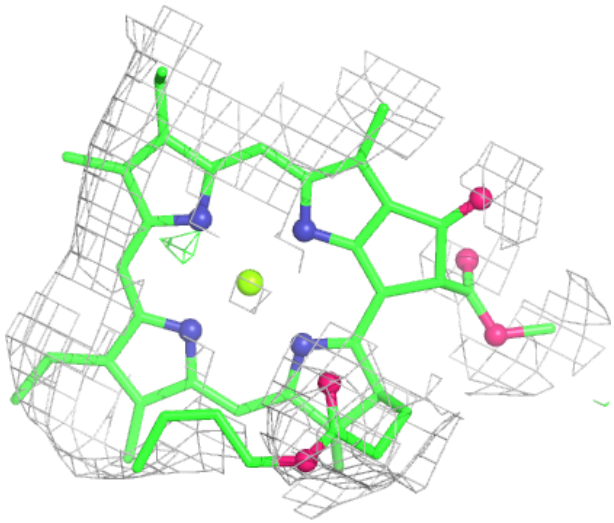


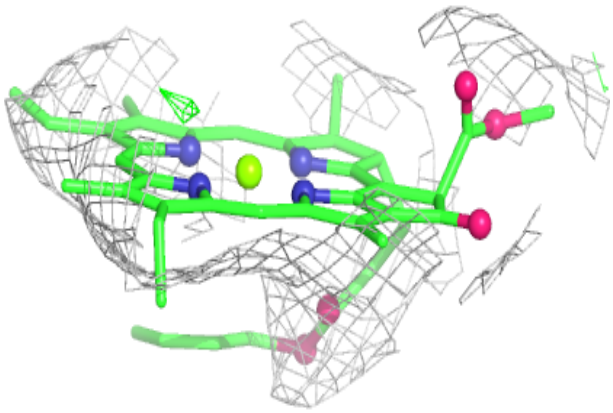




Electron density around CLA B 1218:

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

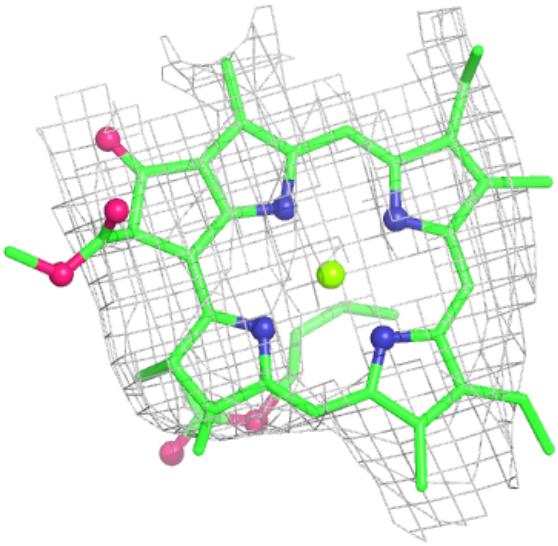


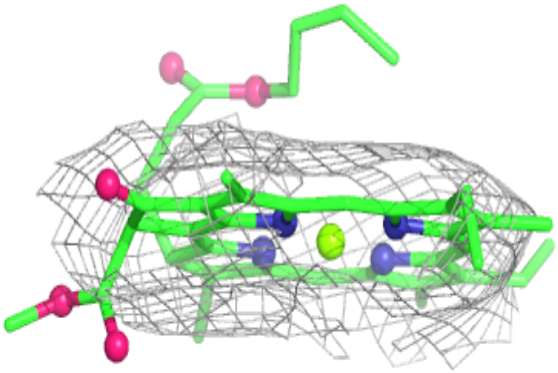


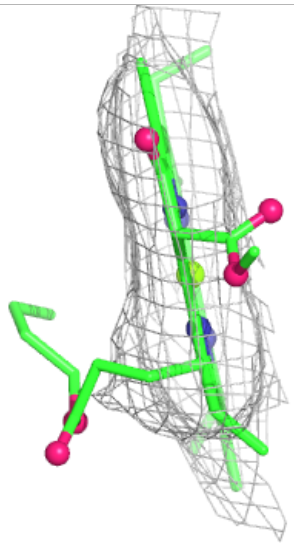


Electron density around CLA A 1121:

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

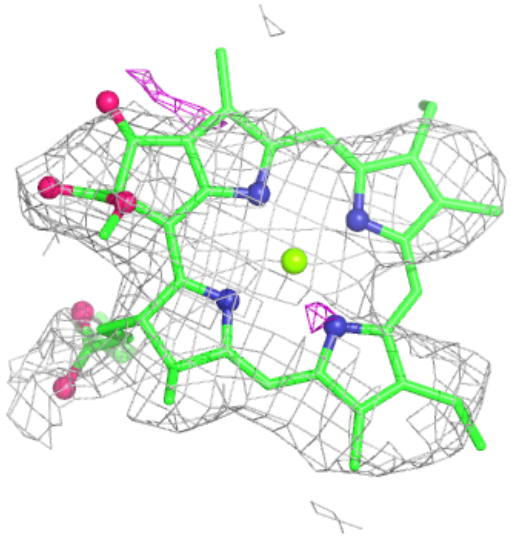


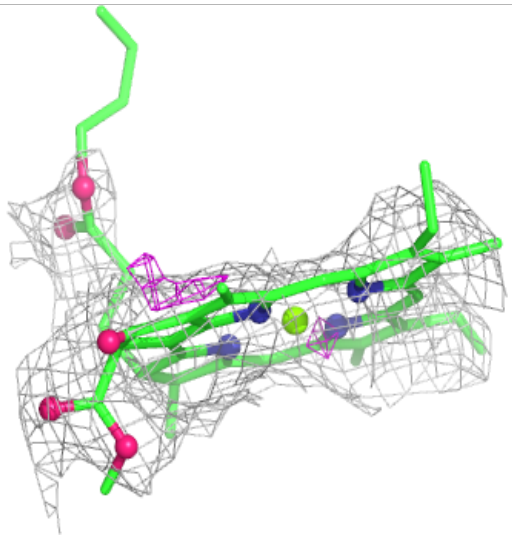


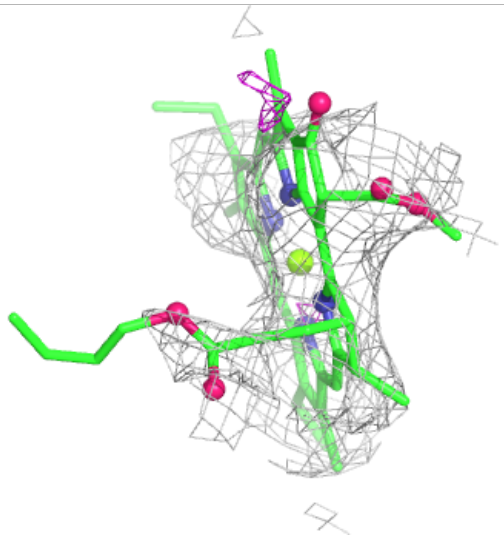


Electron density around CLA B 1226:

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

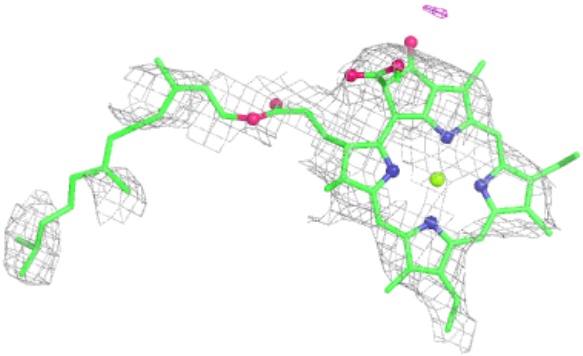


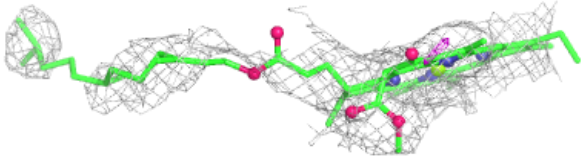


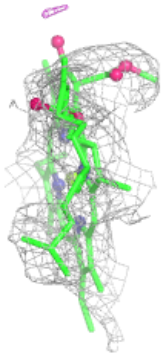


Electron density around CLA B 1234:

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

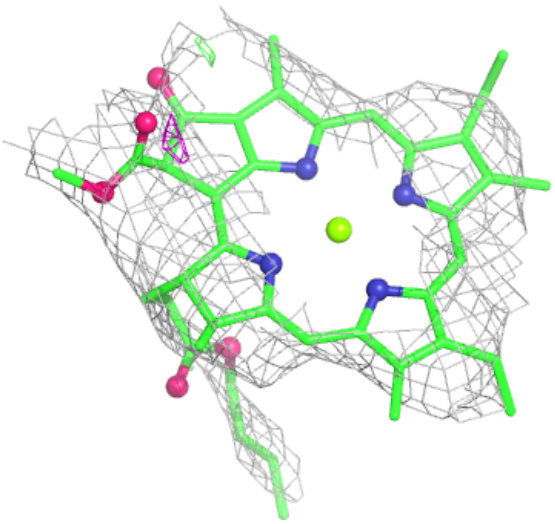


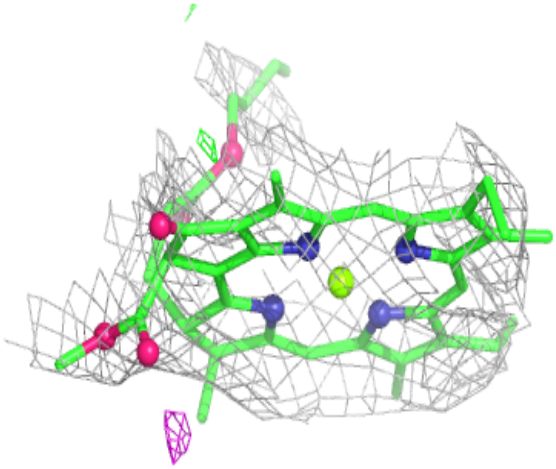


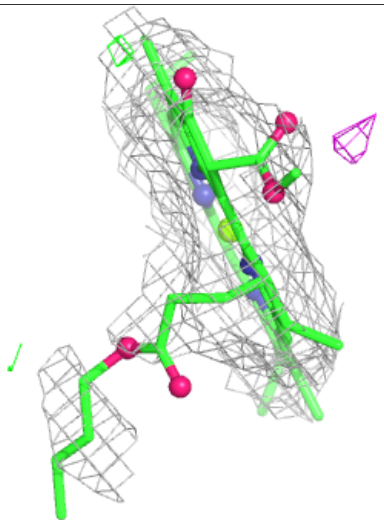


Electron density around CLA A 1122:

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

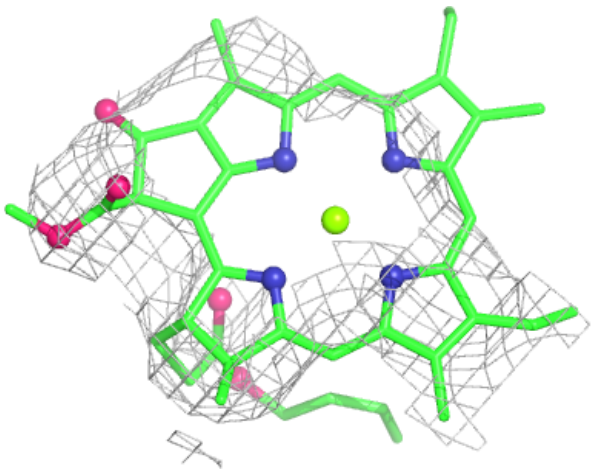


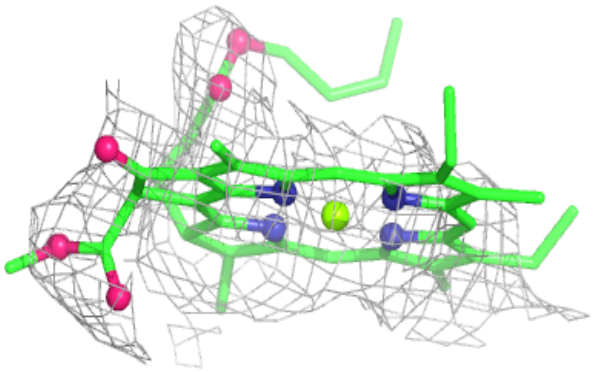


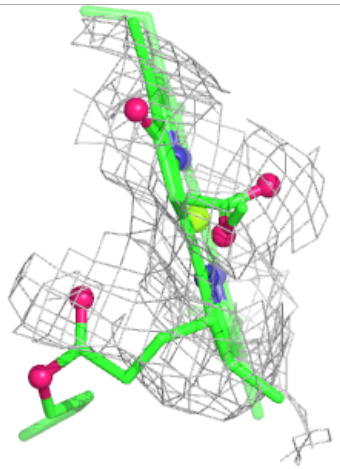


Electron density around CLA A 1110:

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

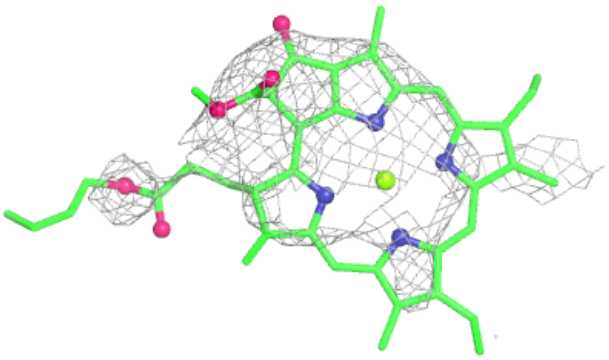


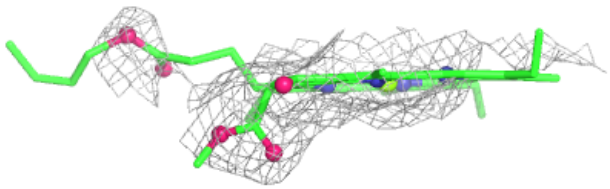


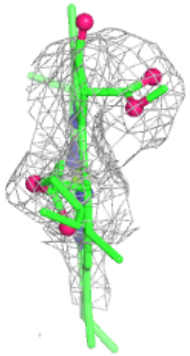


Electron density around CLA A 1135:

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

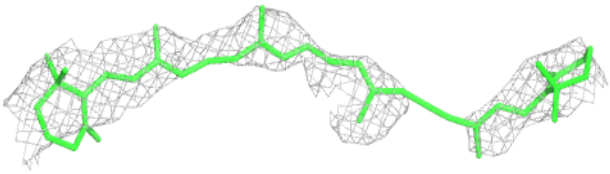


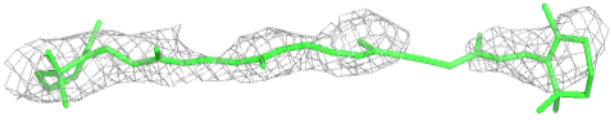


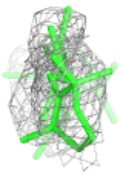


Electron density around BCR B 4005:

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

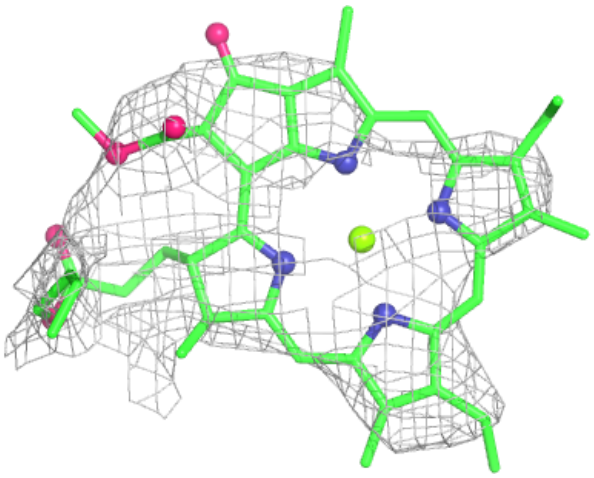


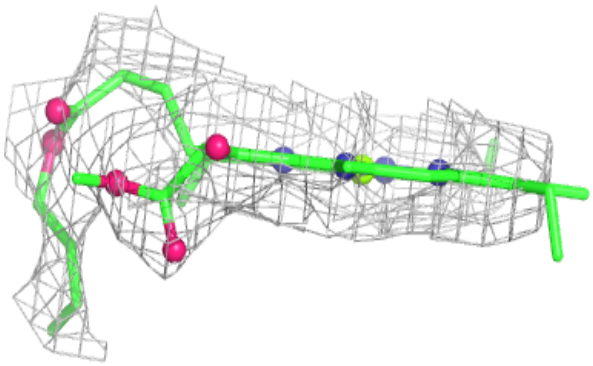


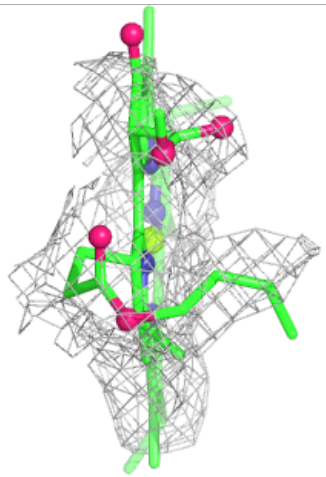


Electron density around CLA B 1203:

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

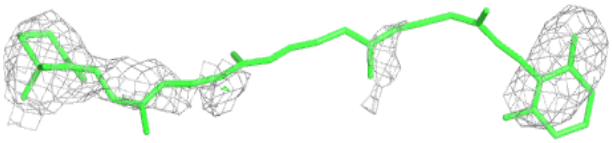


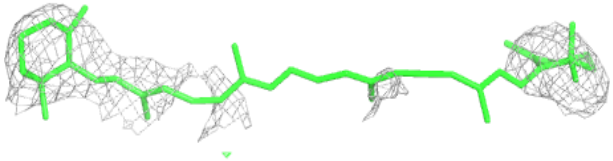


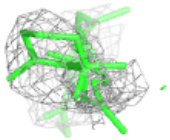


Electron density around BCR B 4018:

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

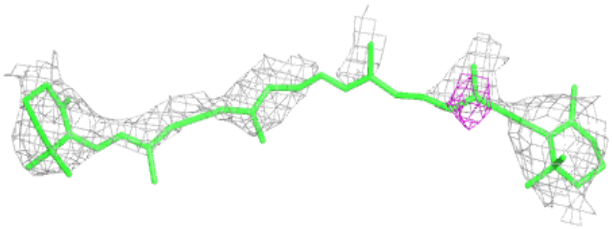


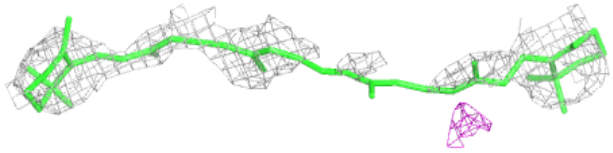


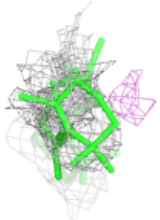


Electron density around BCR B 4010:

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

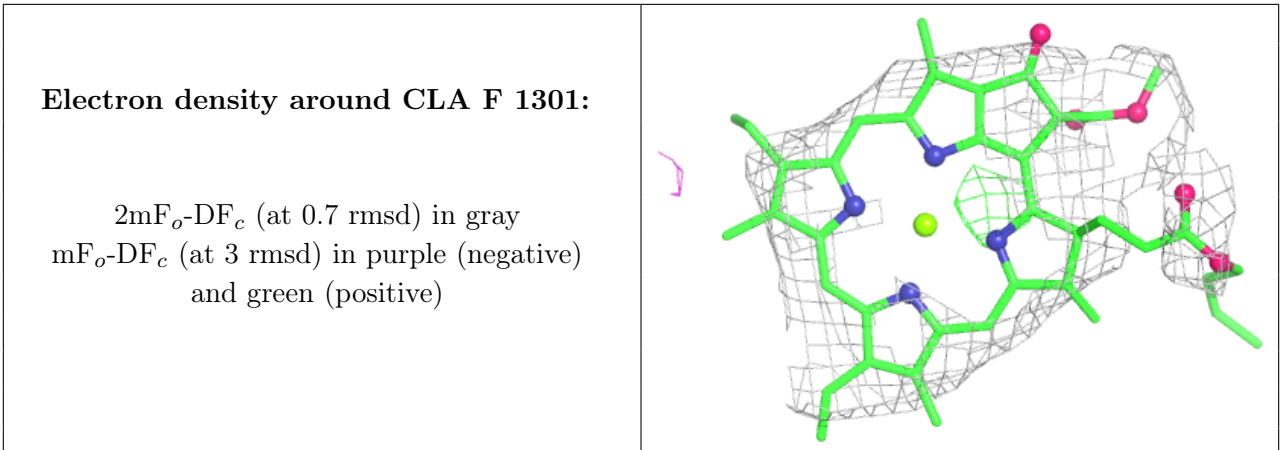


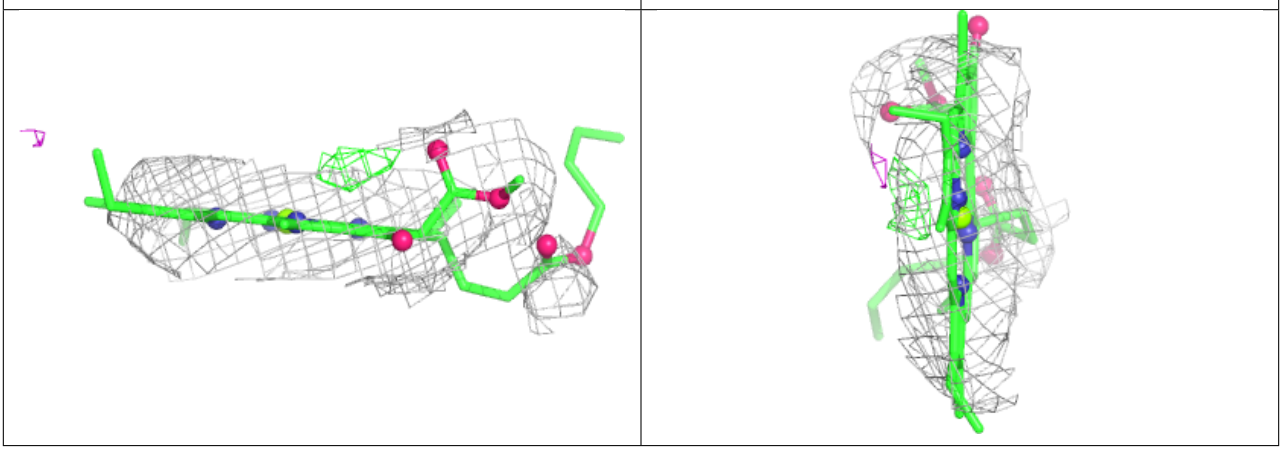




Electron density around CLA F 1301:

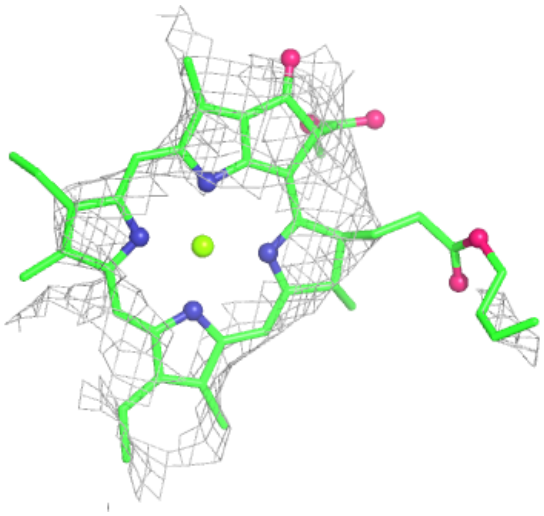
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

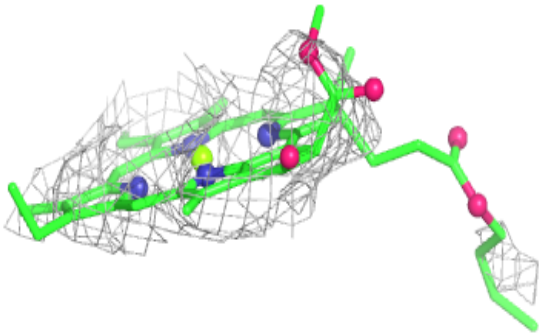




Electron density around CLA A 1125:

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

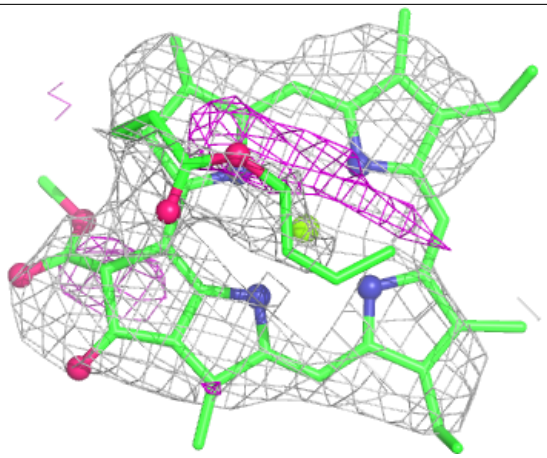


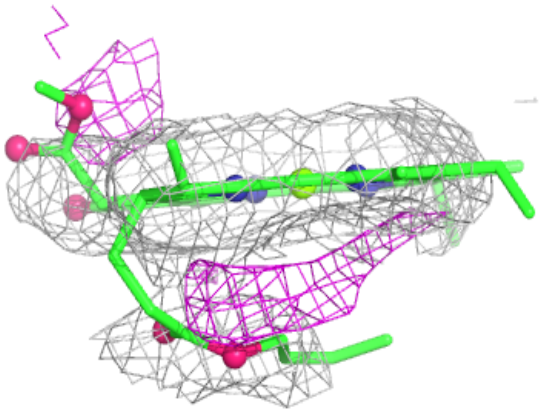


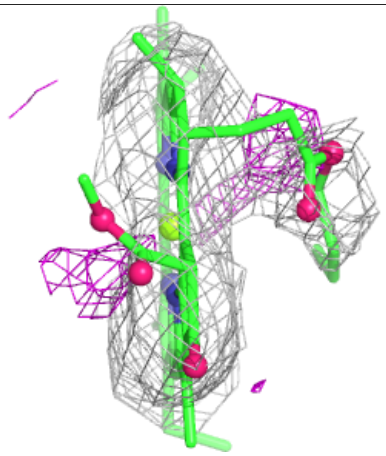


Electron density around CLA B 1205:

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

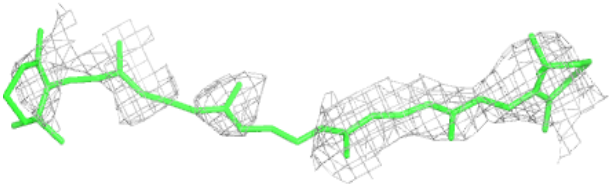


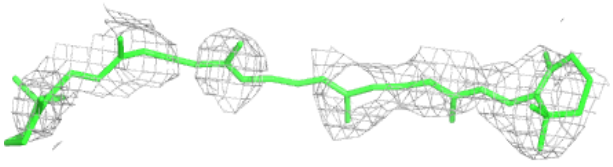




Electron density around BCR J 4013:

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

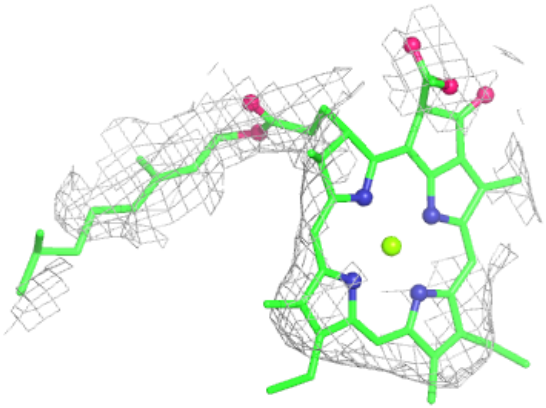


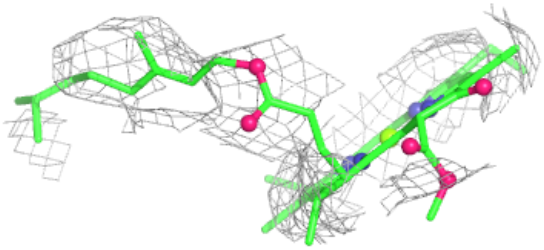


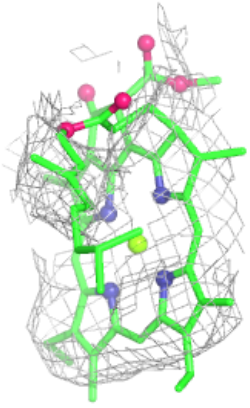


Electron density around CLA A 1132:

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

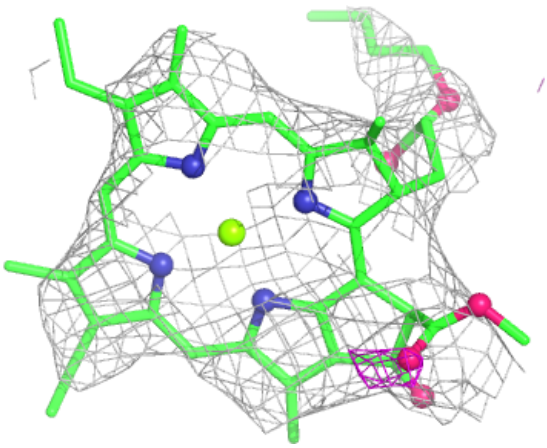


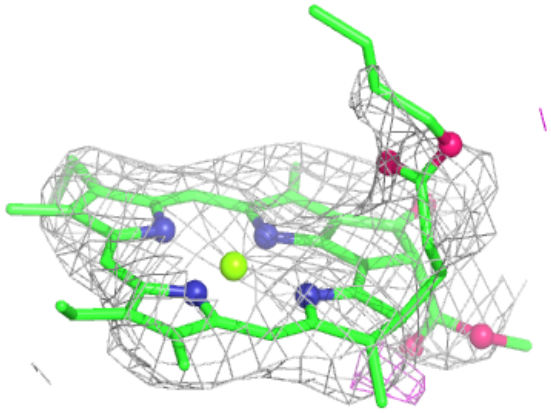


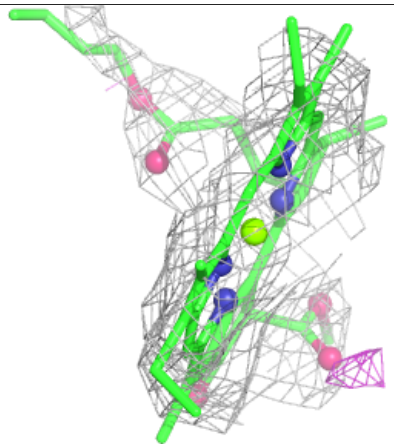


Electron density around CLA B 1228:

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

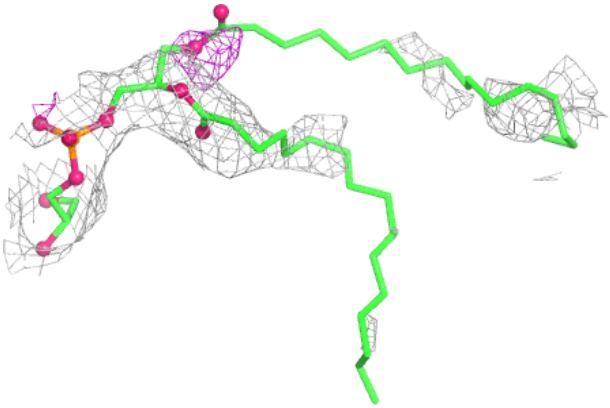


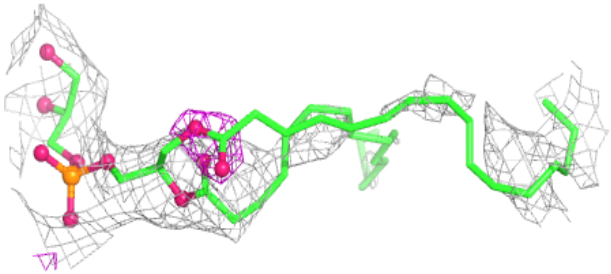




Electron density around LHG B 5004:

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

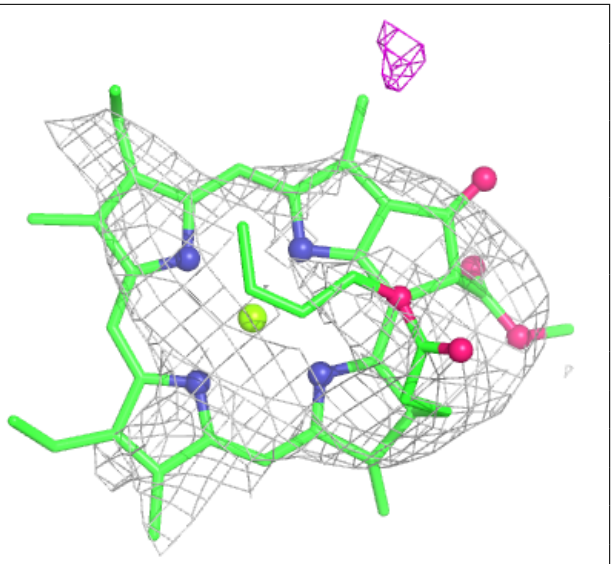


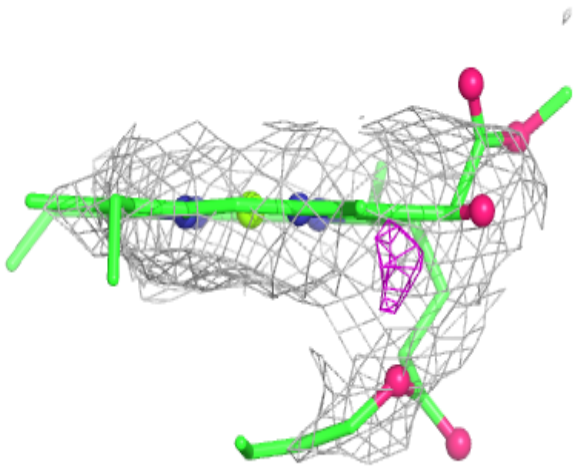


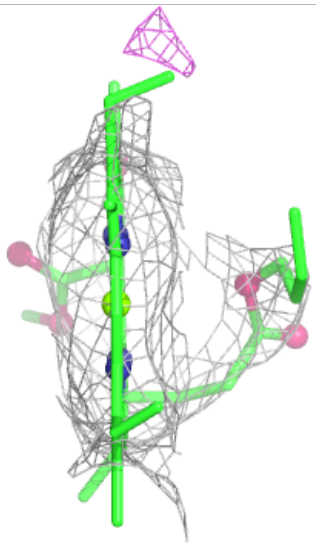


Electron density around CLA A 1136:

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

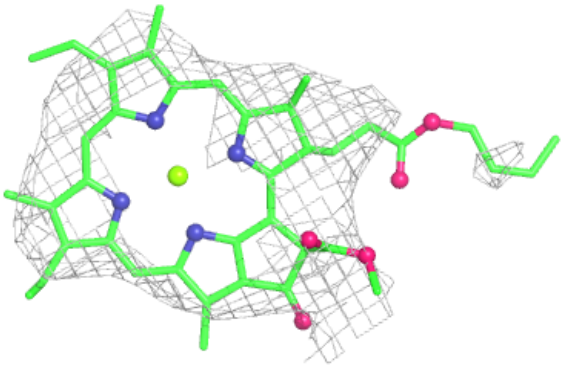


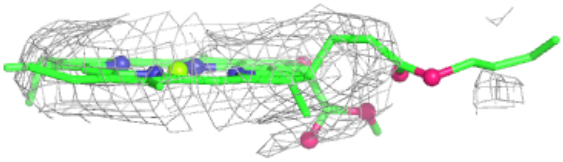


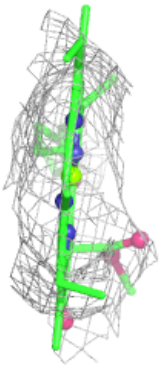


Electron density around CLA A 1131:

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

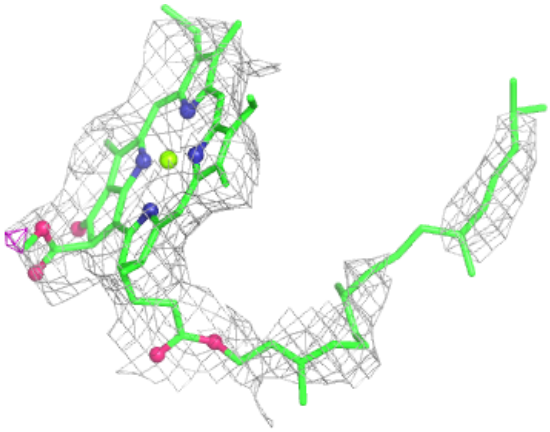


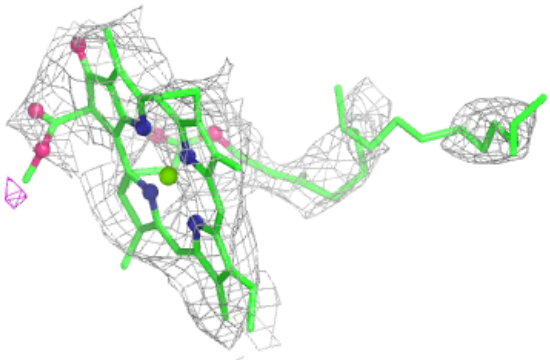


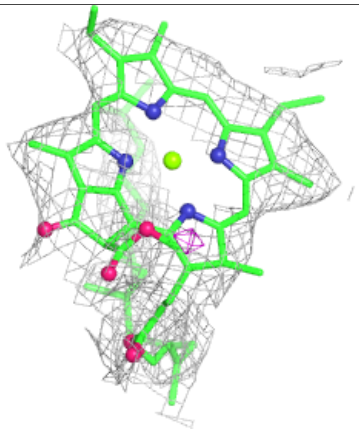


Electron density around CLA A 1102:

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

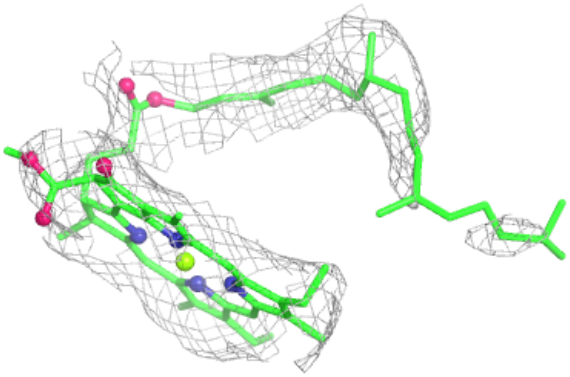


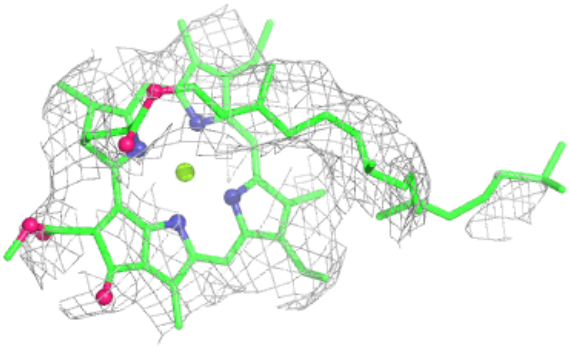


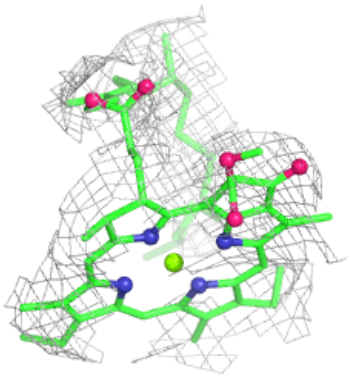


Electron density around CLA A 1109:

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

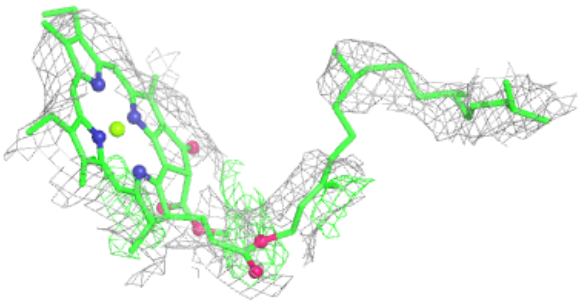


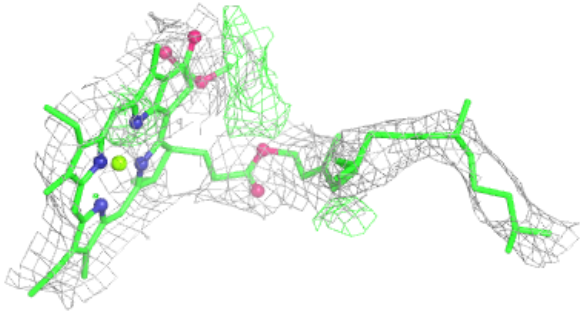


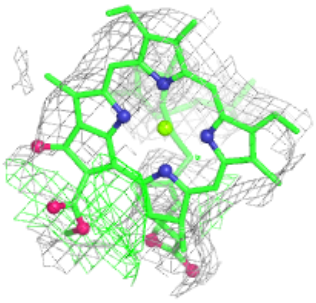


Electron density around CLA B 1021:

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

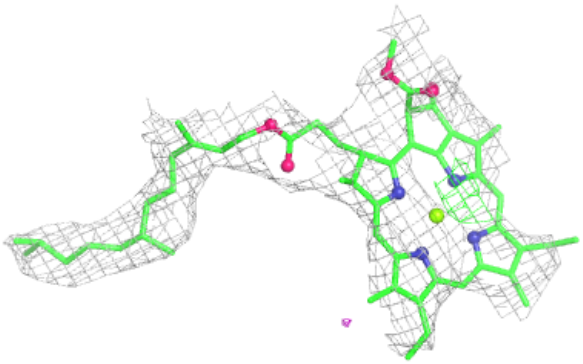


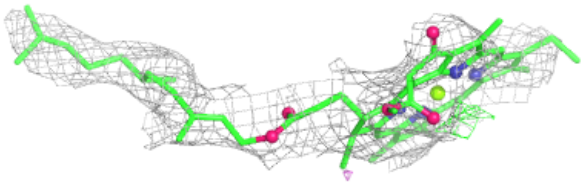


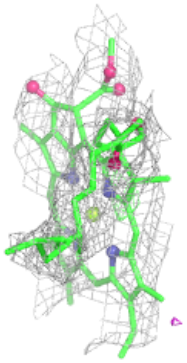


Electron density around CLA B 1022:

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

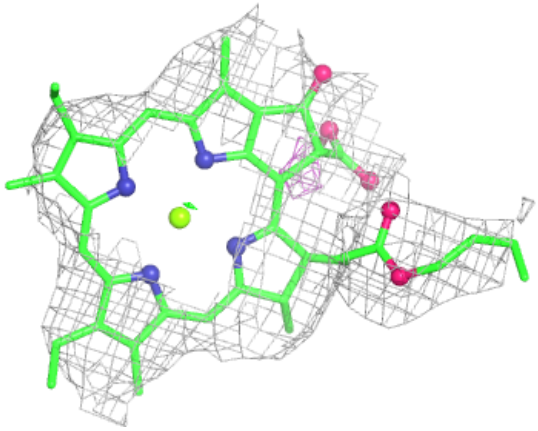


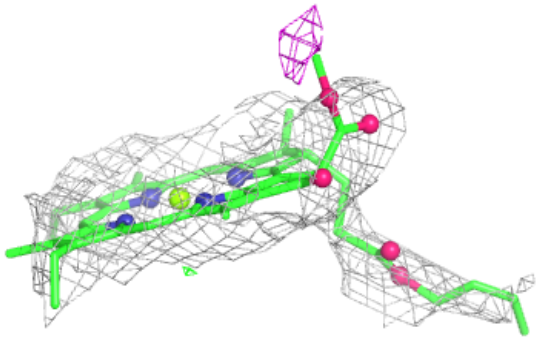


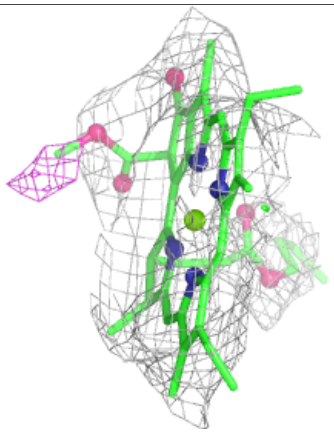


Electron density around CLA B 1220:

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

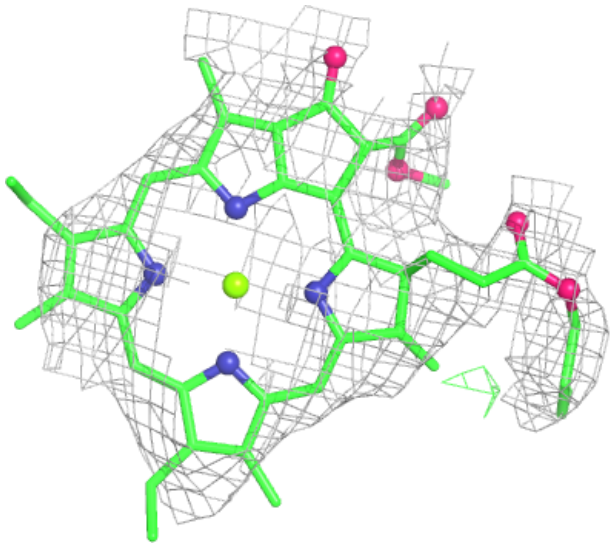


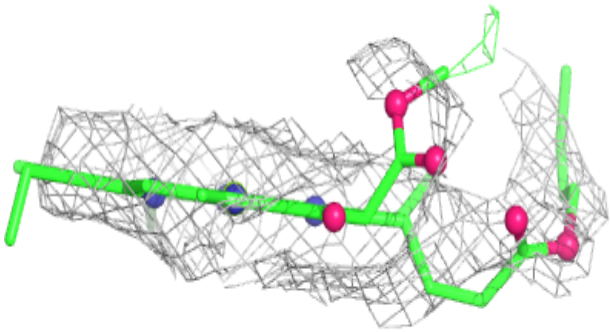


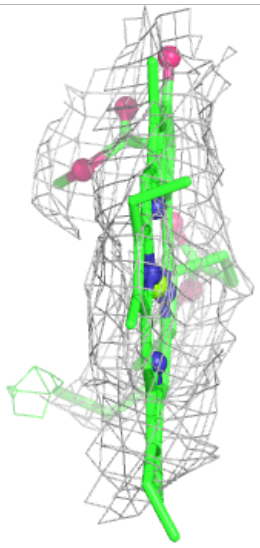


Electron density around CLA B 1221:

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

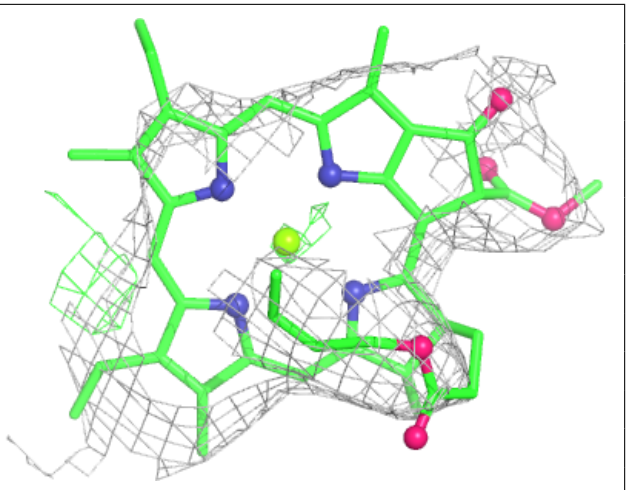


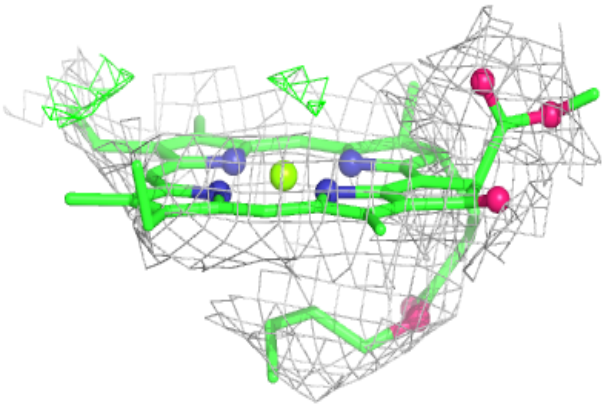




Electron density around CLA A 1116:

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

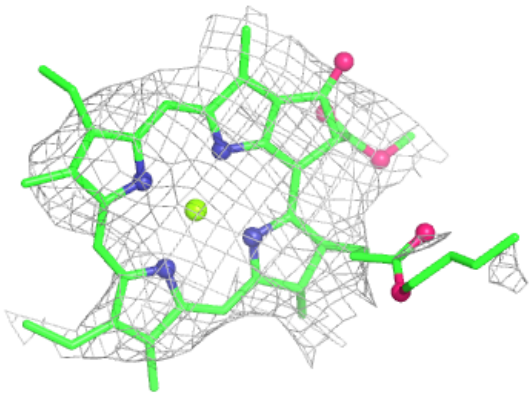


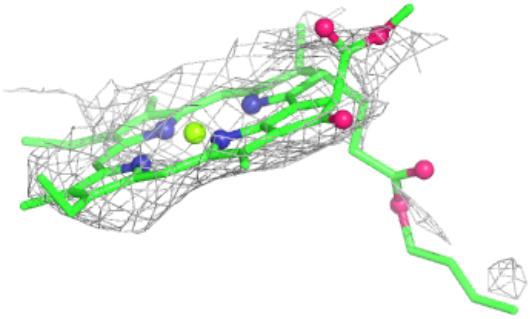


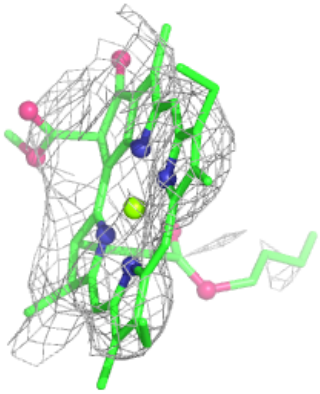


Electron density around CLA A 1137:

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

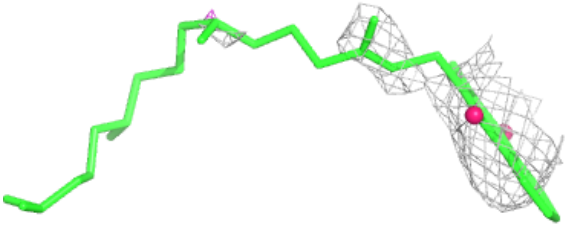


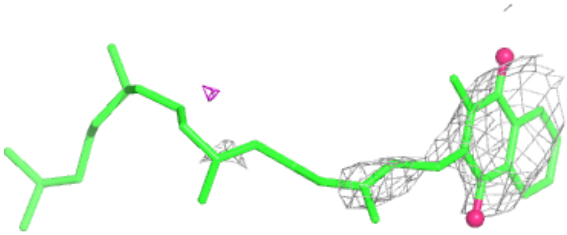


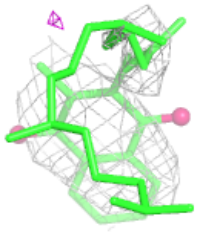


Electron density around PQN B 2002:

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

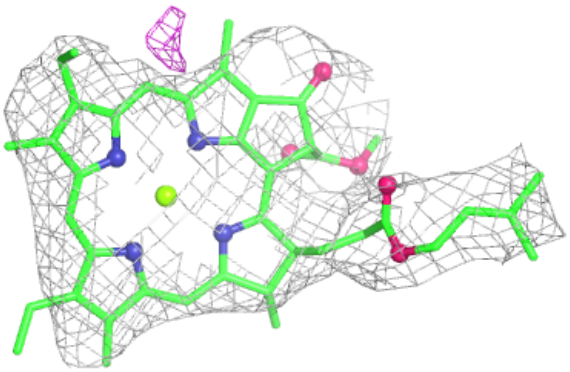


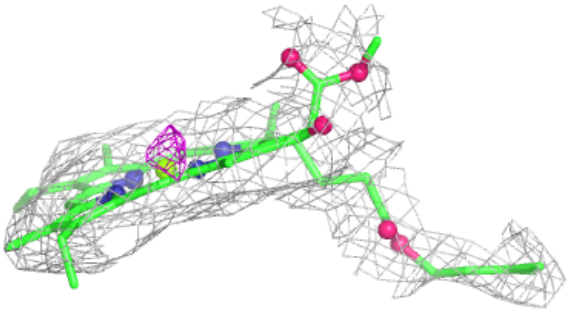


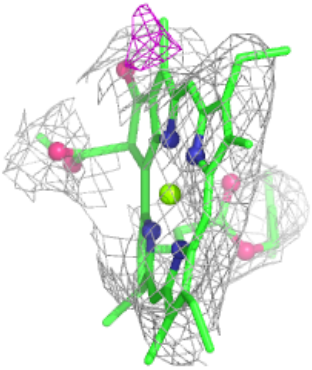


Electron density around CLA A 1107:

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

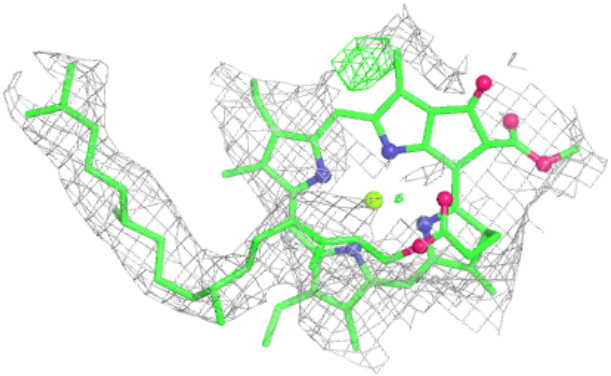


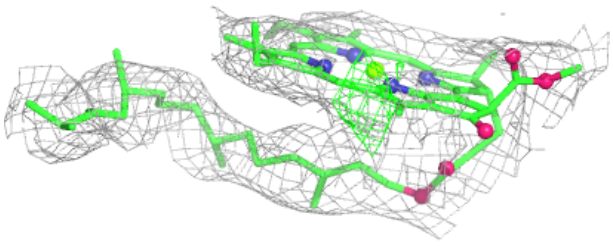


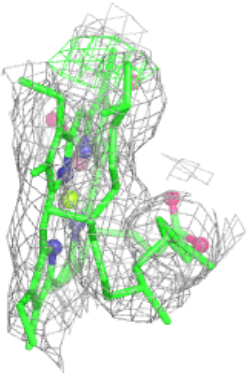


Electron density around CLA B 1235:

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

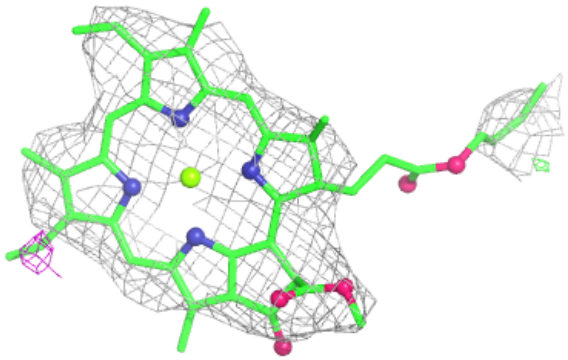


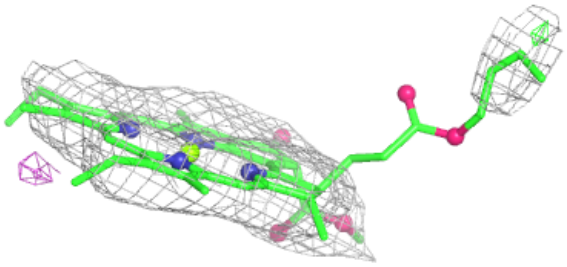


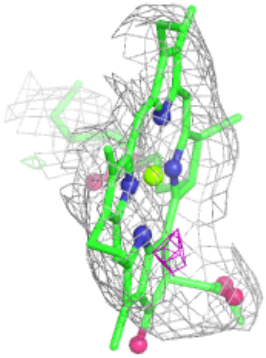


Electron density around CLA B 1239:

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

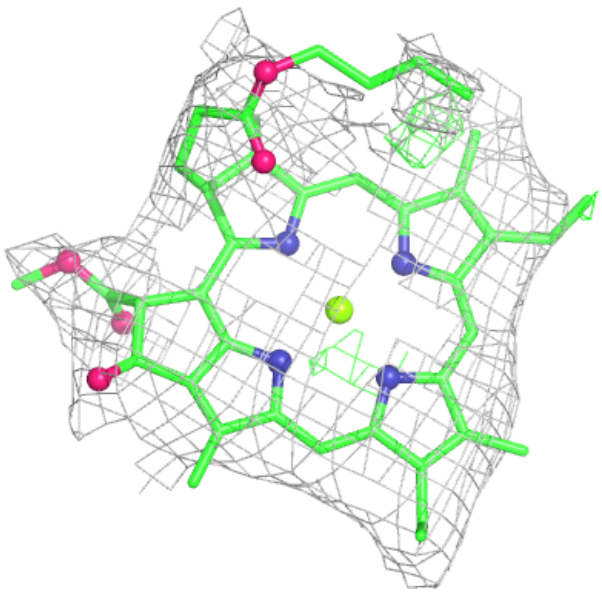


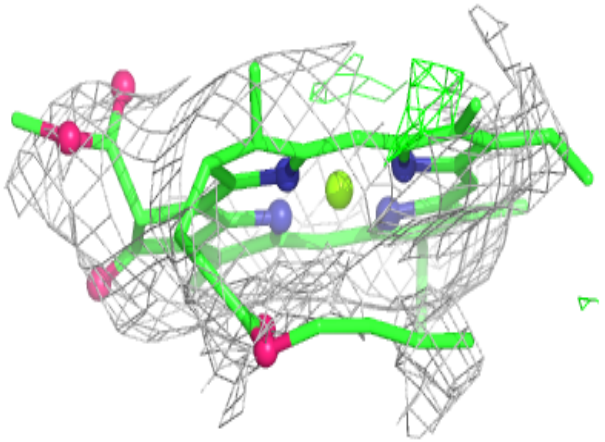


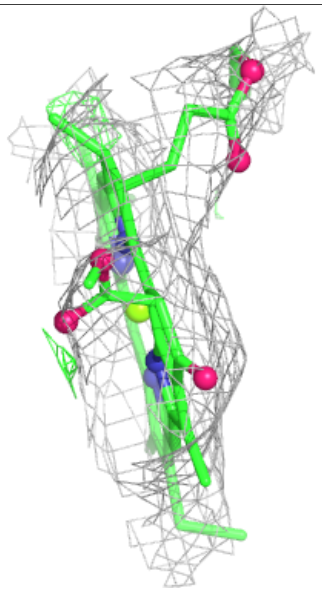


Electron density around CLA B 1215:

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

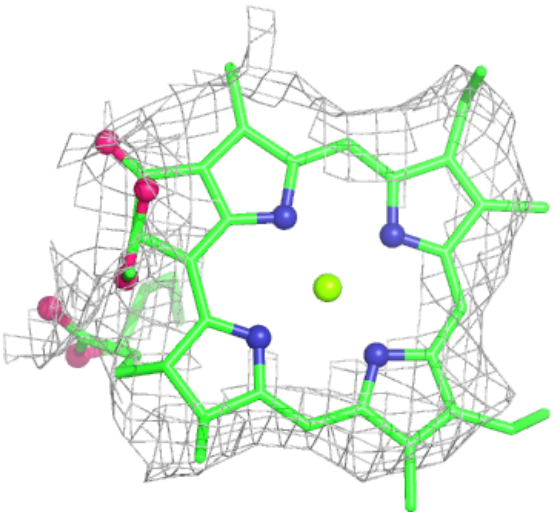




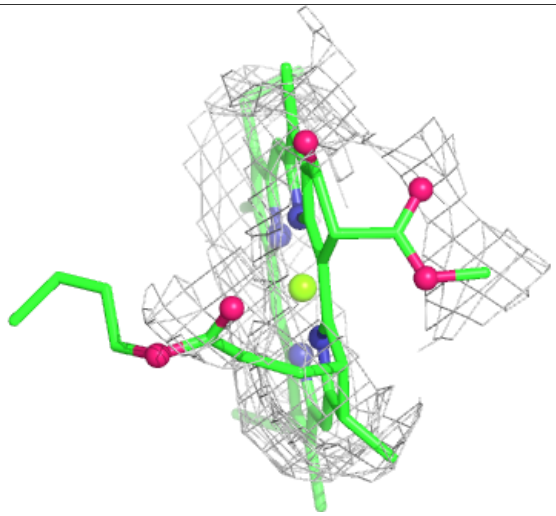


Electron density around CLA B 1238:

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

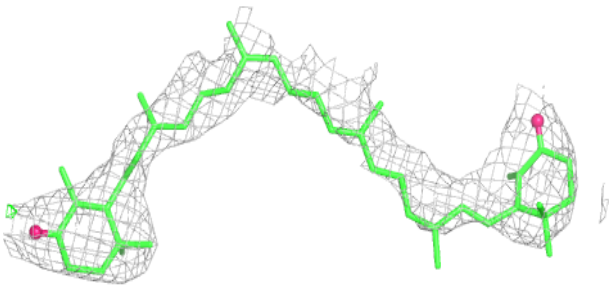


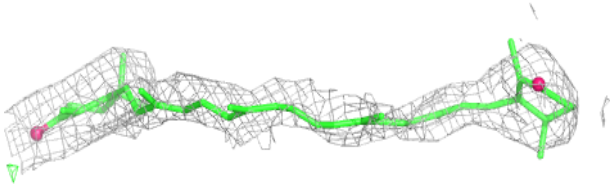


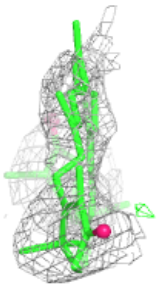


Electron density around 45D B 4011:

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

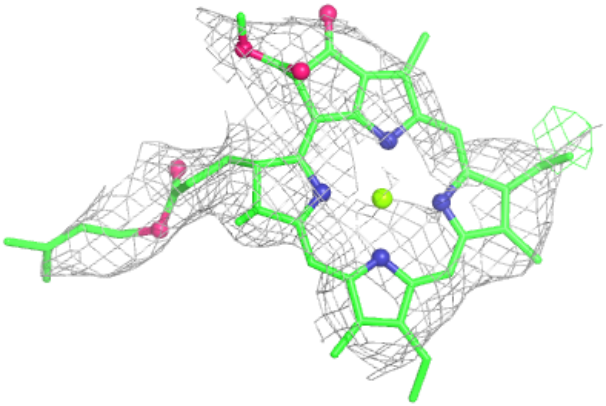


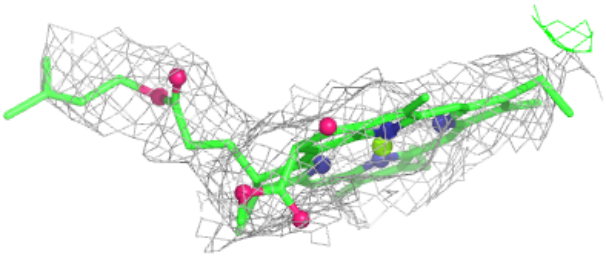


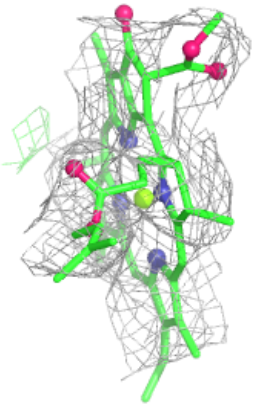


Electron density around CLA B 1222:

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

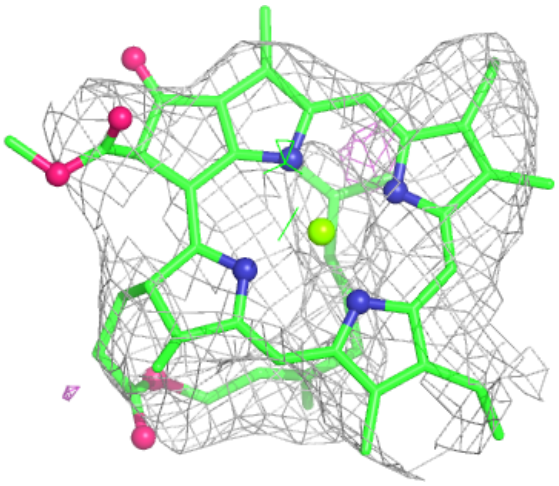


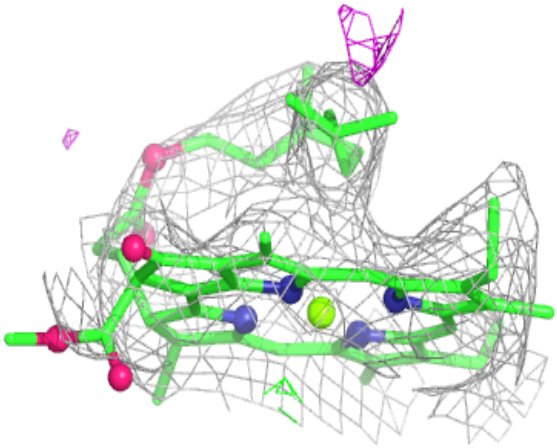




Electron density around CLA B 1224:

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

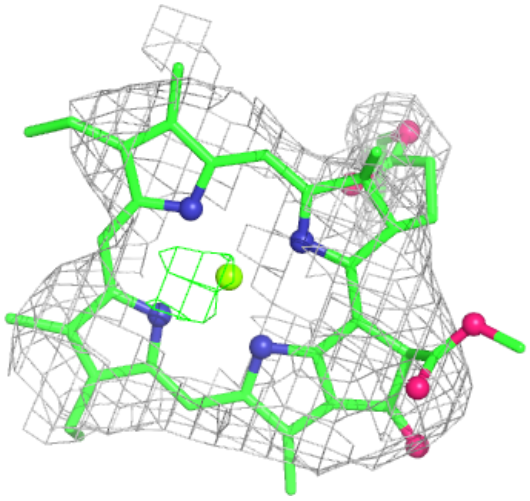


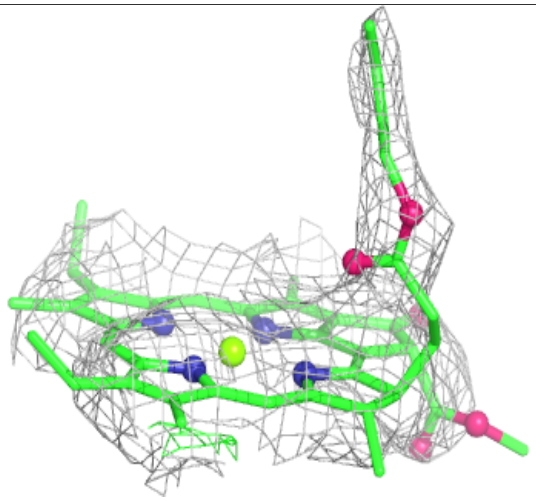


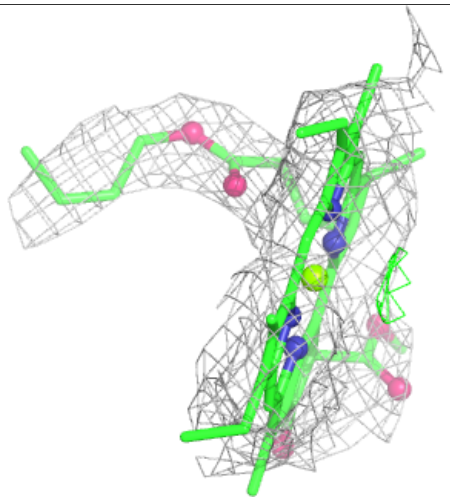


Electron density around CLA B 1225:

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

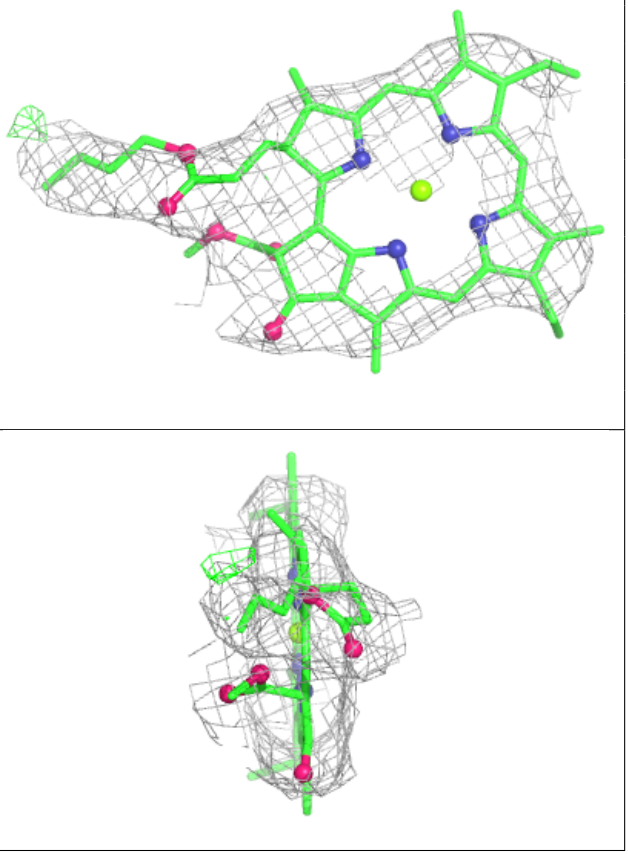






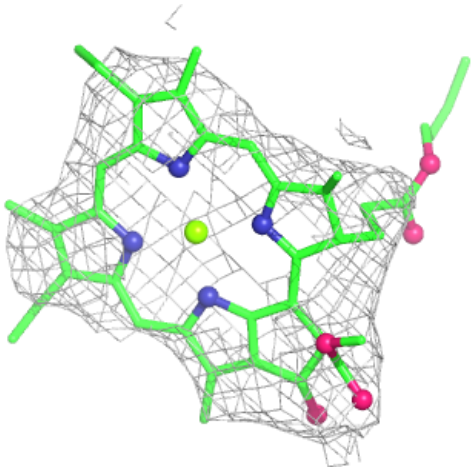
Electron density around CLA A 1101:

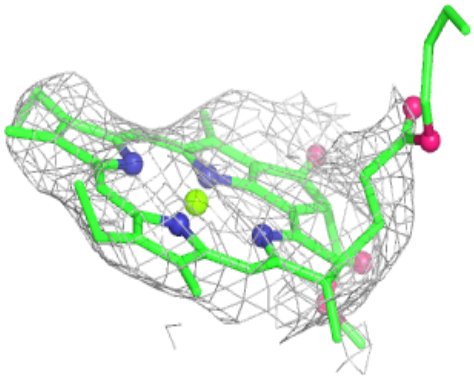
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

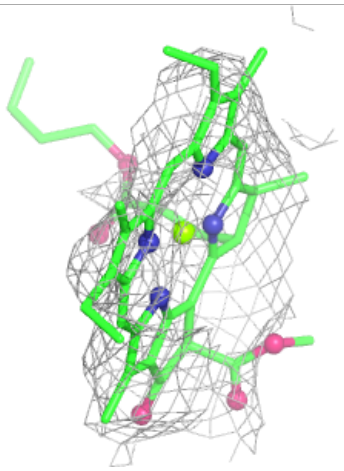


Electron density around CLA B 1227:

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

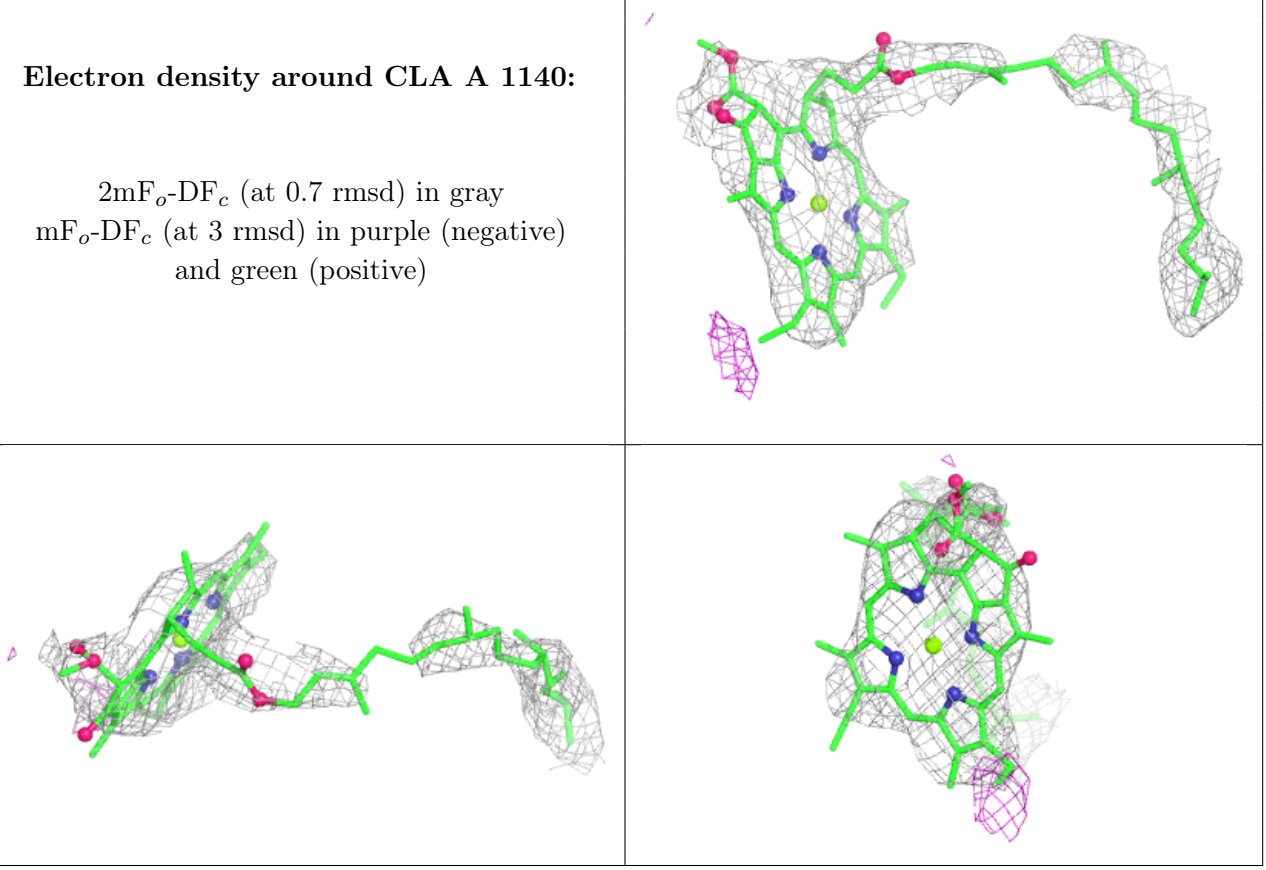






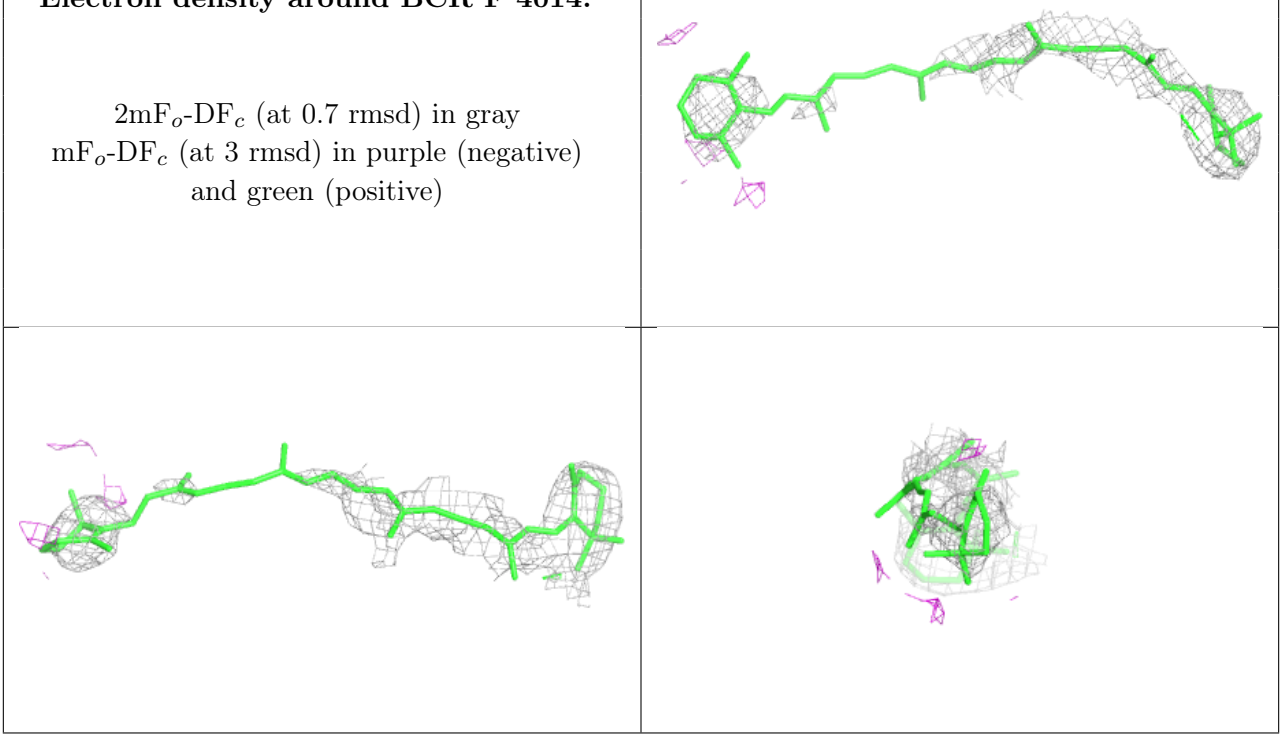
Electron density around CLA A 1140:

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



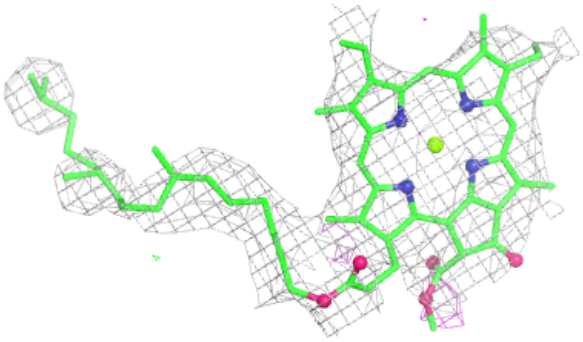
Electron density around BCR F 4014:

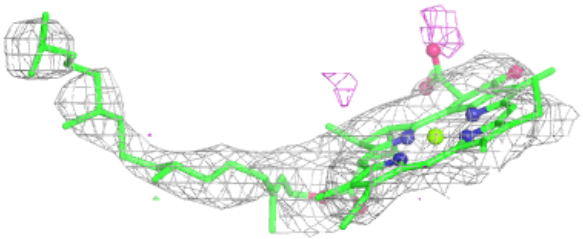
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA A 1013:

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

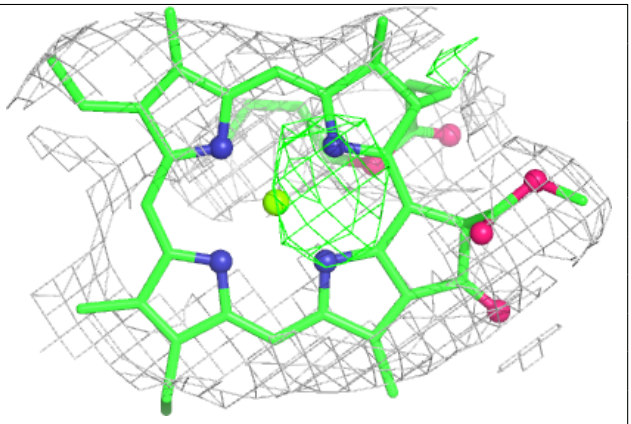


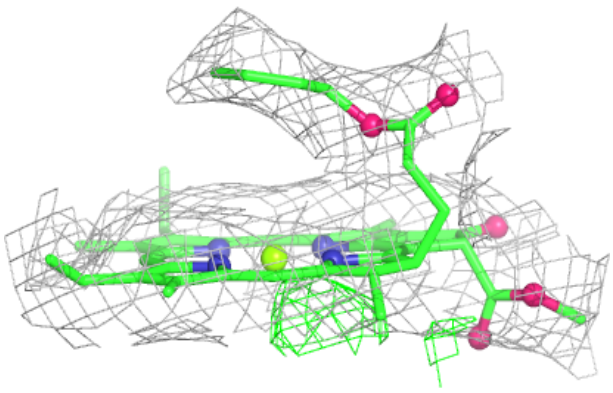


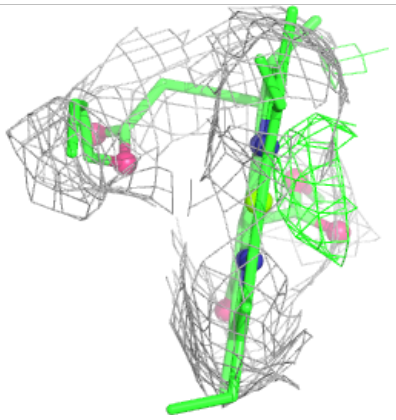


Electron density around CLA B 1237:

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

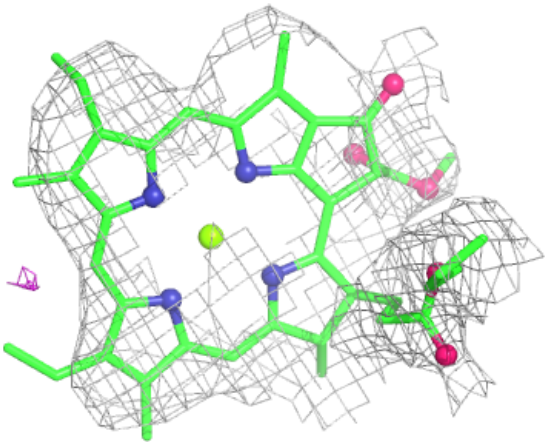


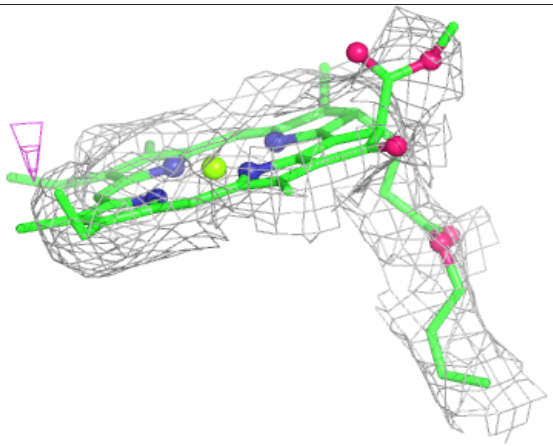


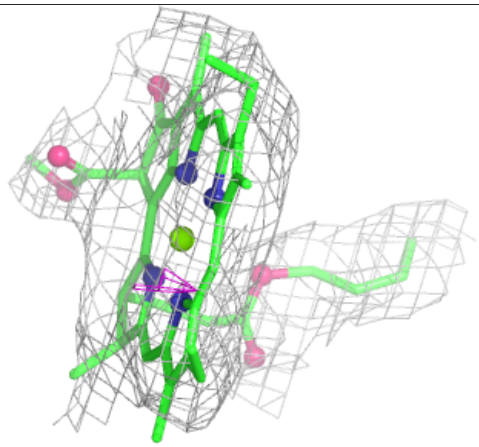


Electron density around CLA B 1236:

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

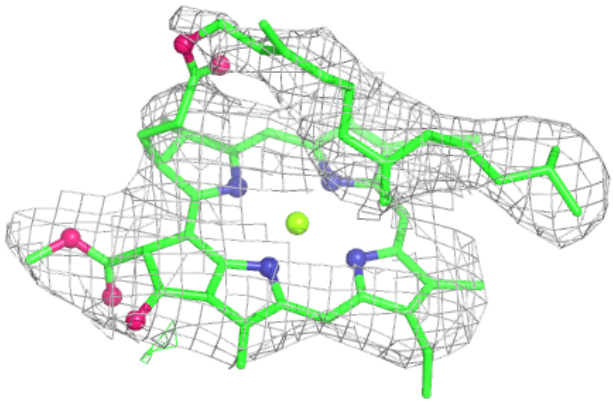


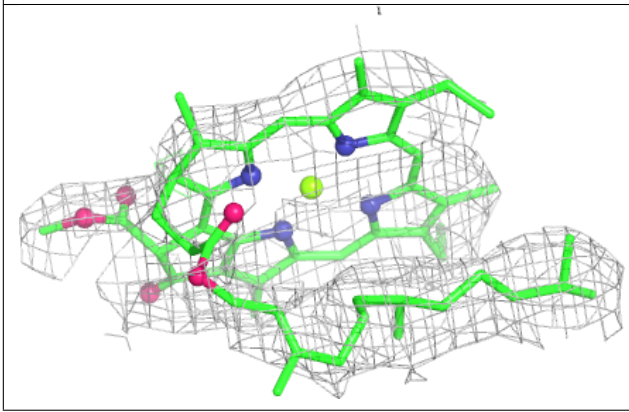


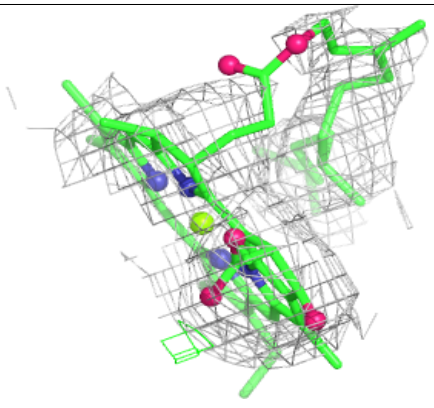


Electron density around CLA B 1214:

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

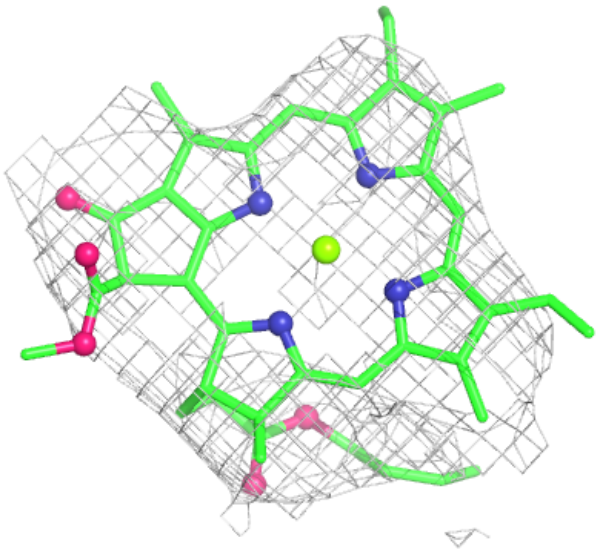


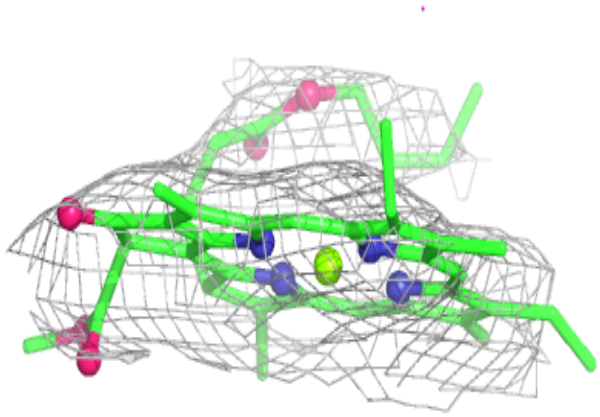


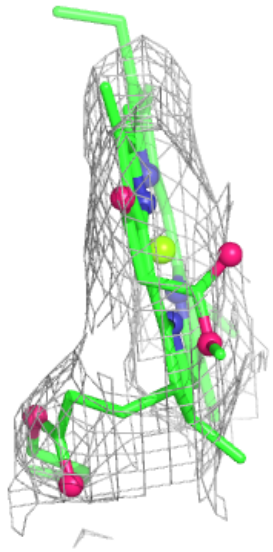


Electron density around CLA A 1117:

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

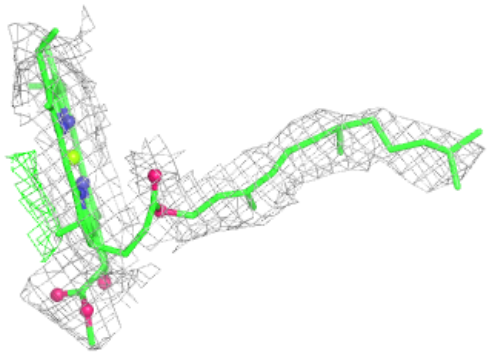


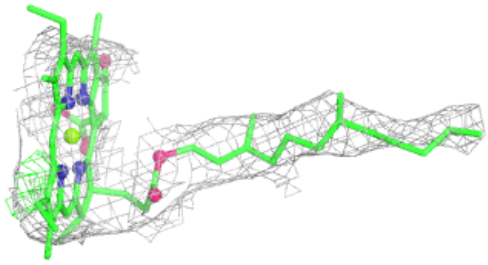


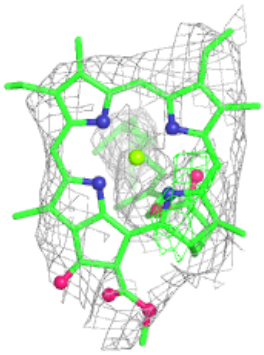


Electron density around CLA A 1126:

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

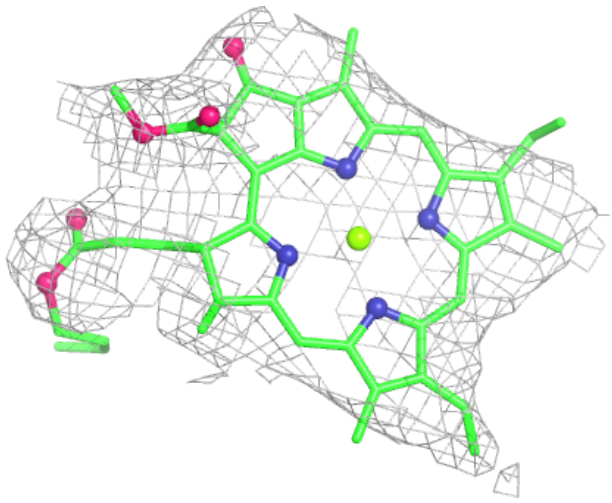


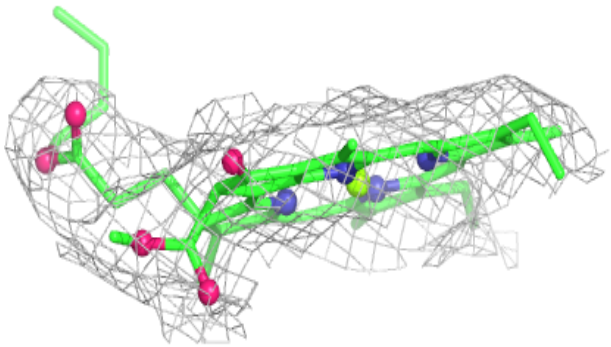


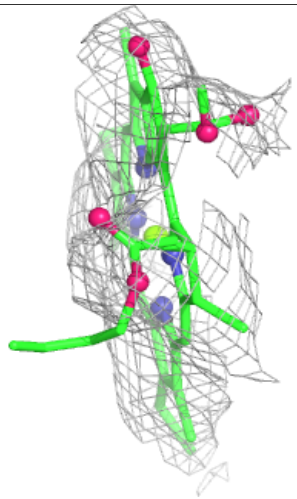


Electron density around CLA B 1206:

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

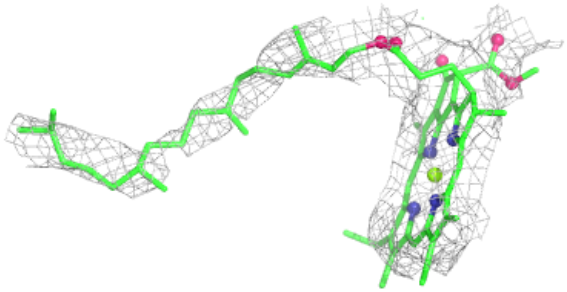


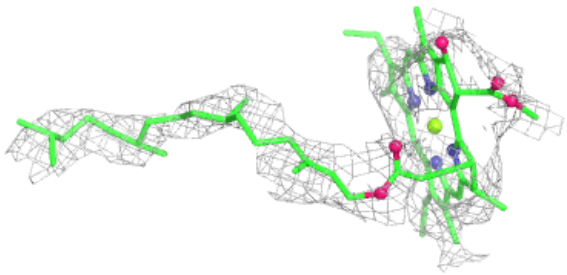


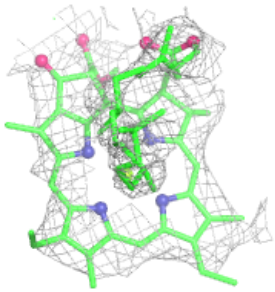


Electron density around CLA A 1128:

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

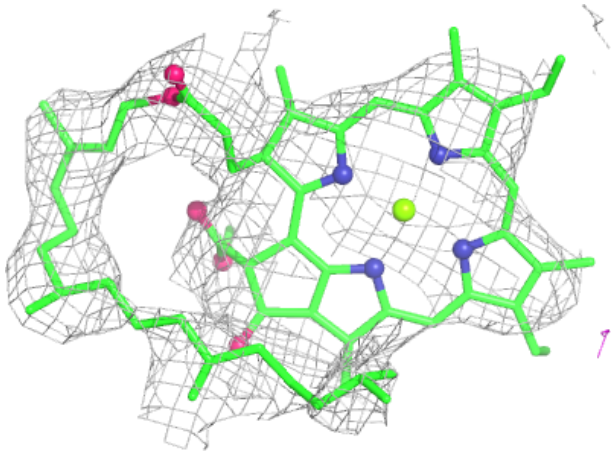


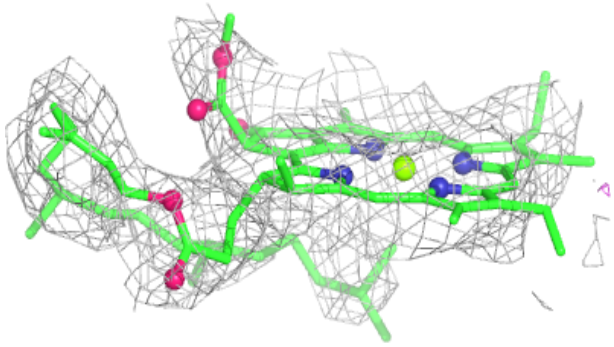


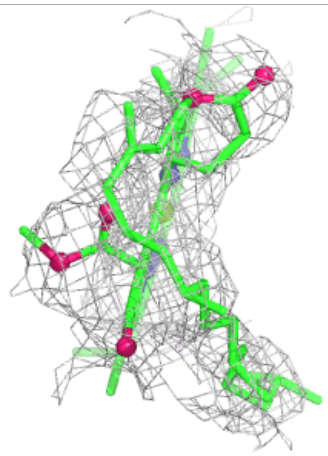


Electron density around CLA B 1202:

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

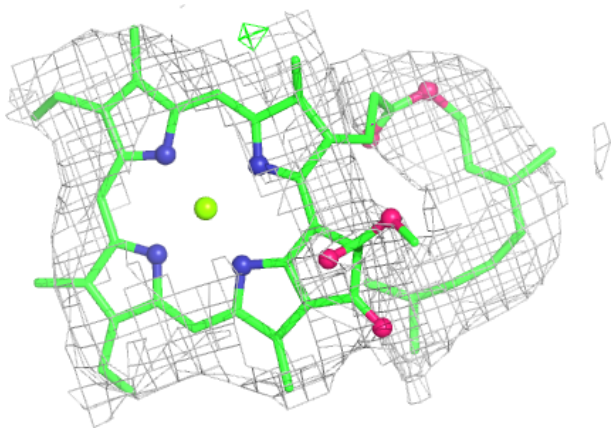


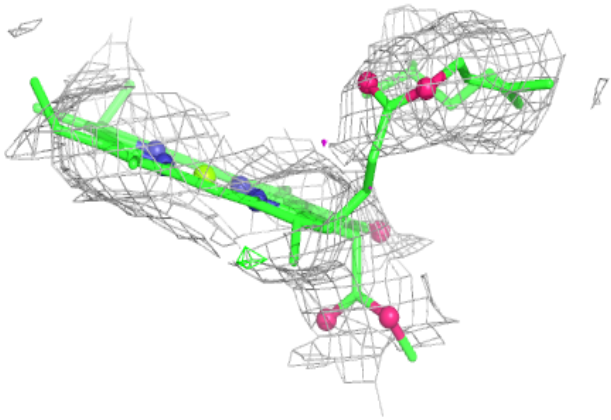


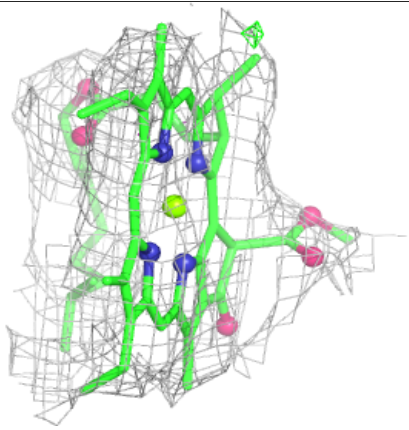


Electron density around CLA B 1229:

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

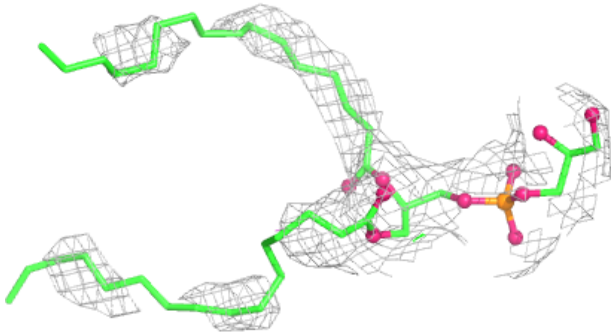


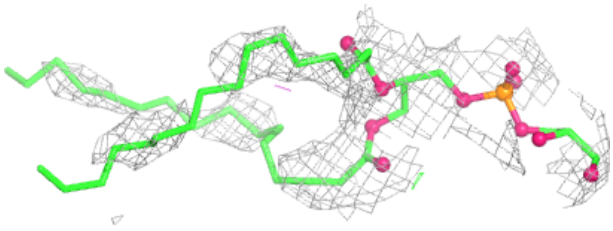




Electron density around LHG A 5001:

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

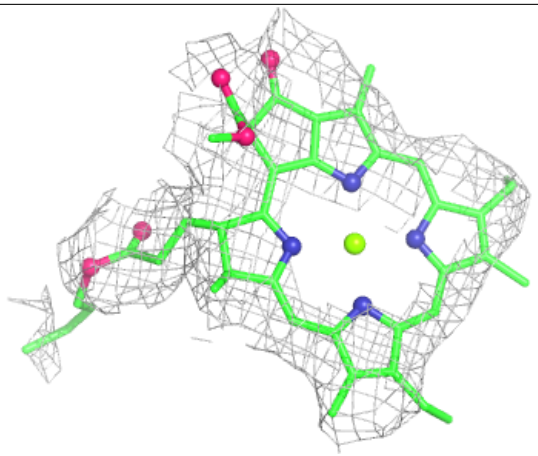


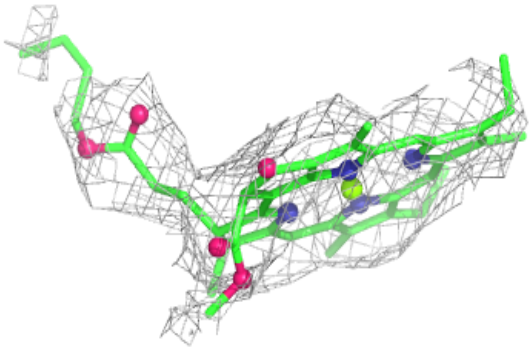


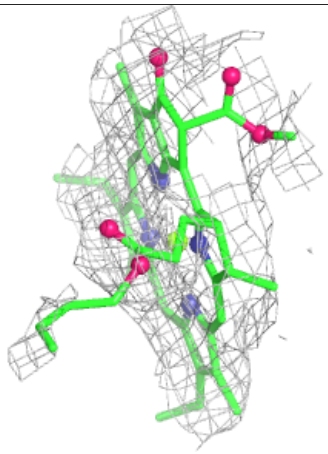


Electron density around CLA B 1230:

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

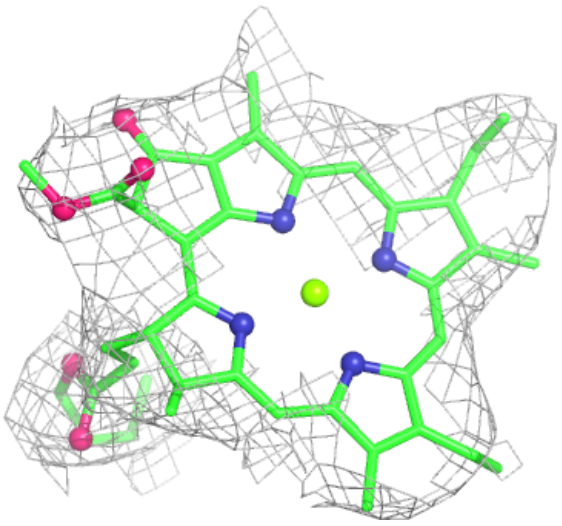


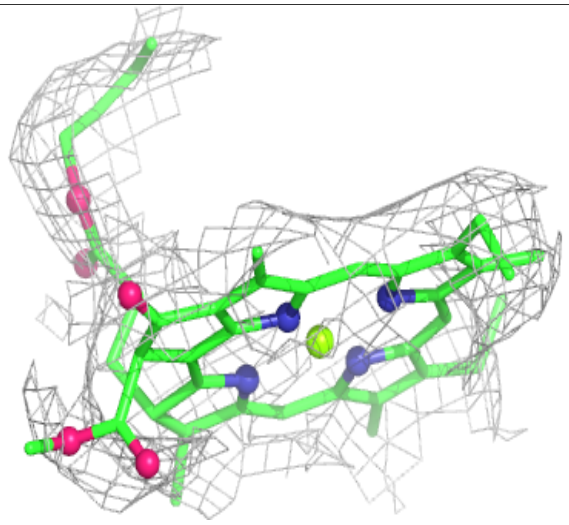


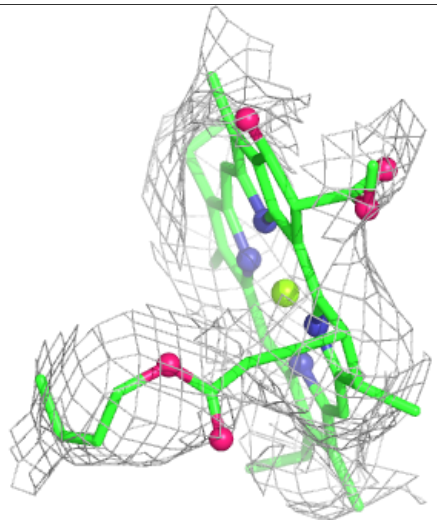


Electron density around CLA B 1232:

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

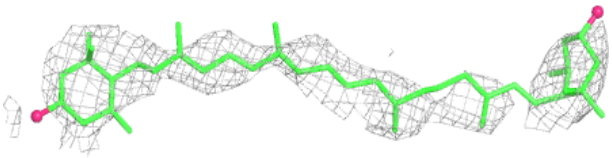


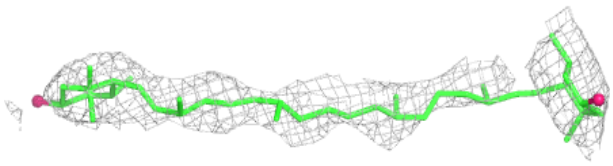


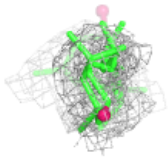


Electron density around C7Z J 4015:

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

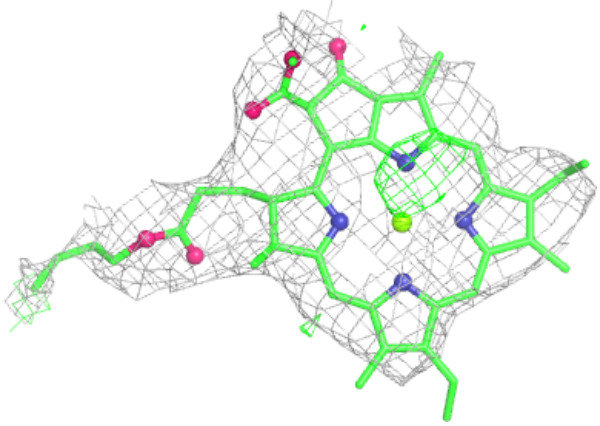


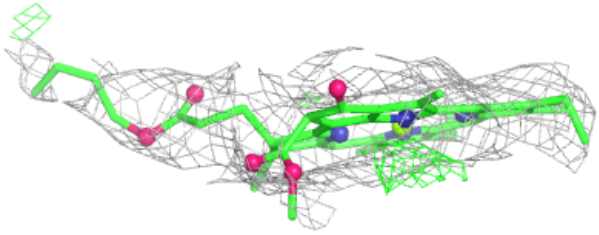


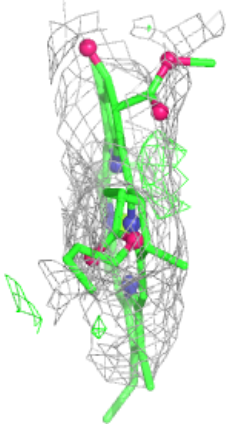


Electron density around CLA A 1012:

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

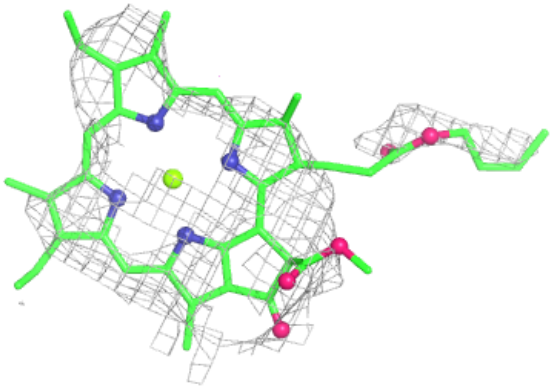


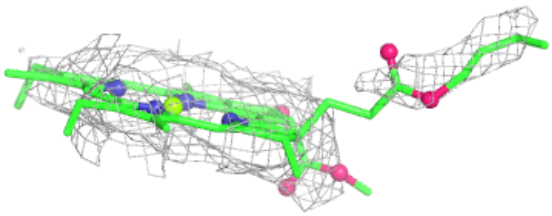


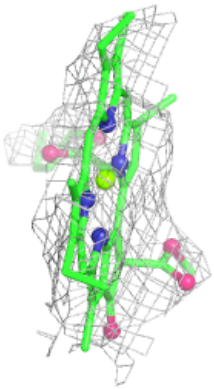


Electron density around CLA B 1223:

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

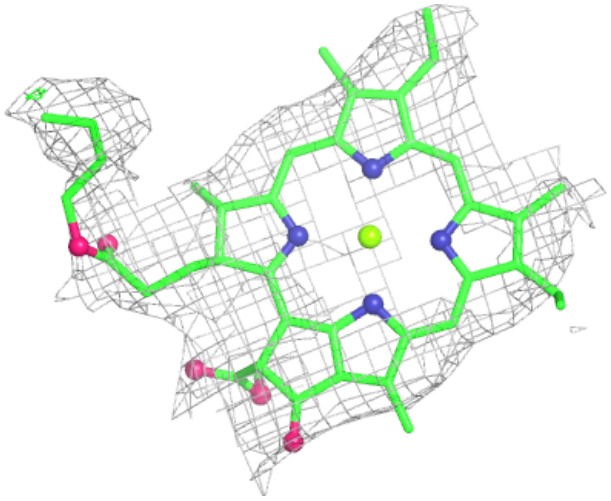


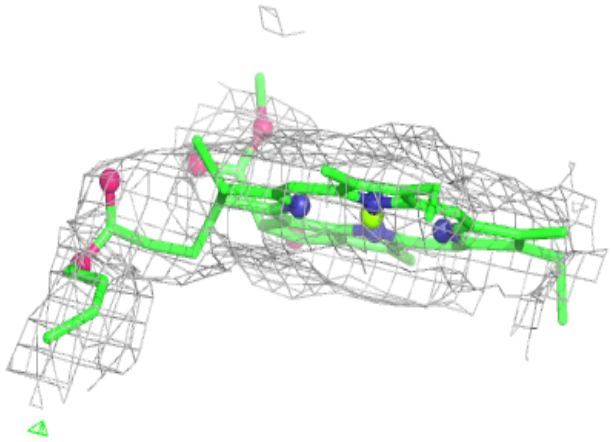




Electron density around CLA B 1210:

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

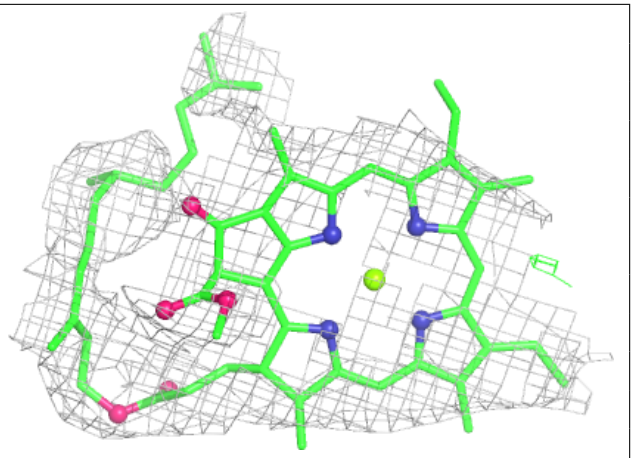


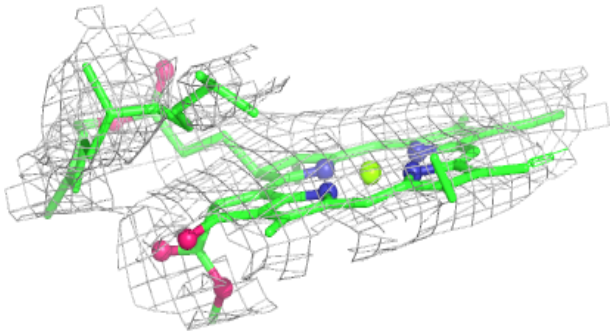


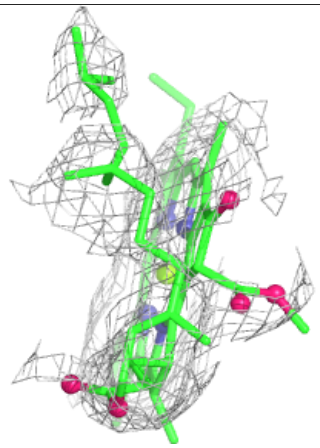


Electron density around CLA A 1123:

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

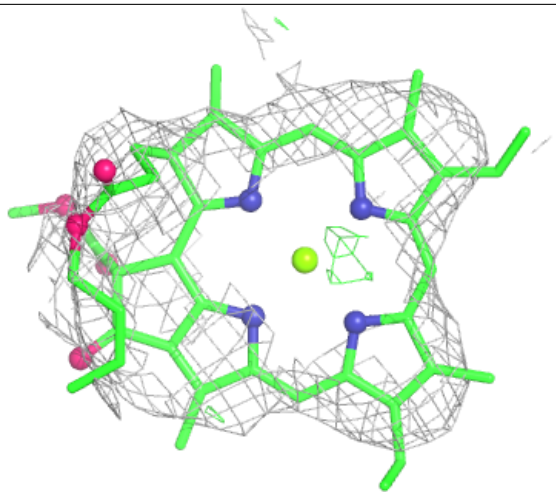


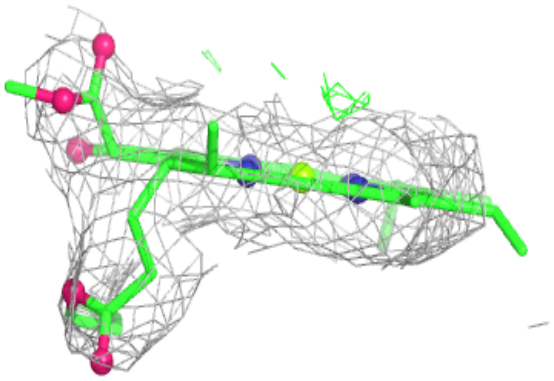


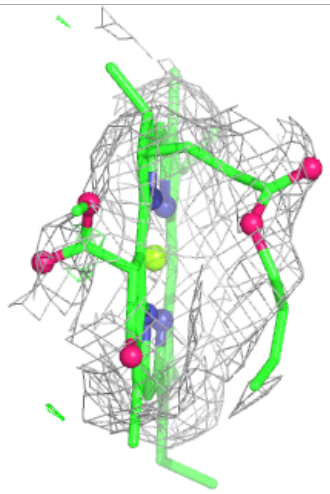


Electron density around CLA A 1127:

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

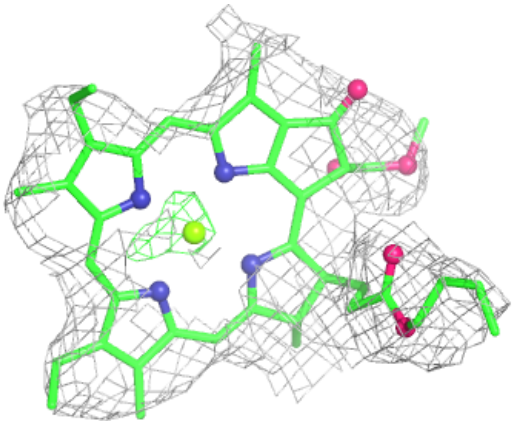


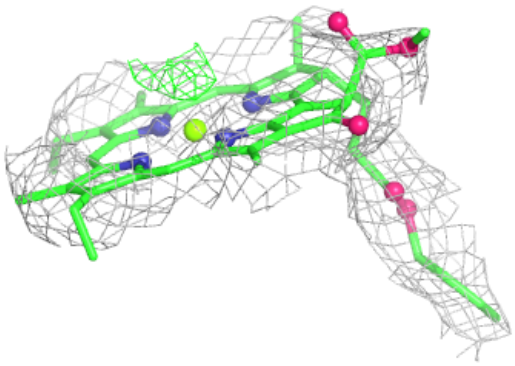


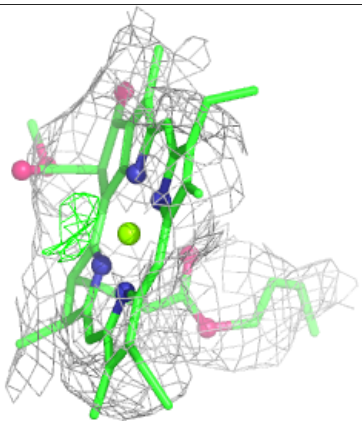


Electron density around CLA B 1231:

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

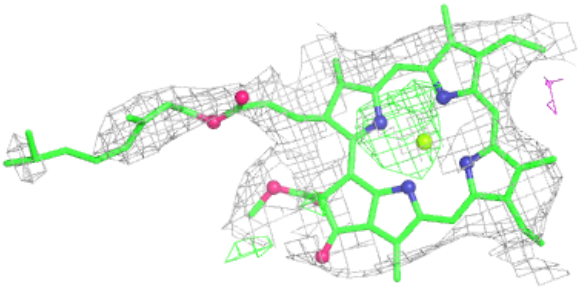


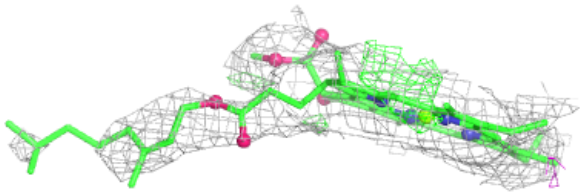


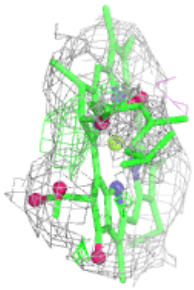


Electron density around CLA A 1139:

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

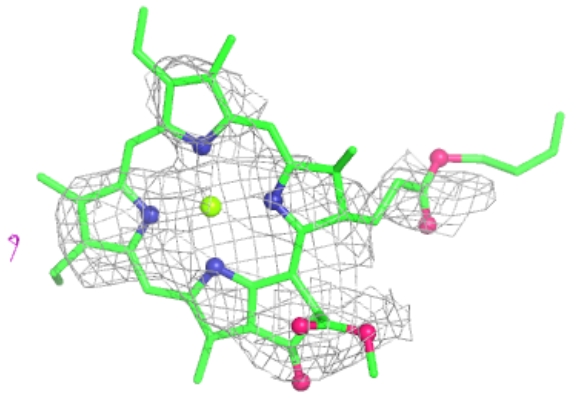


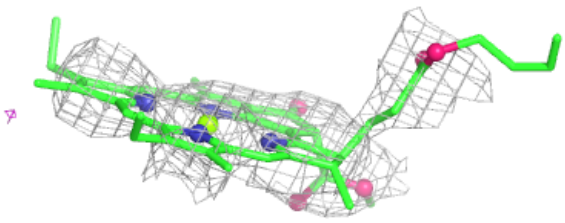


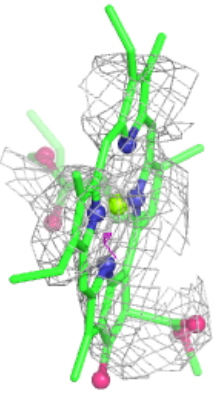


Electron density around CLA A 1124:

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

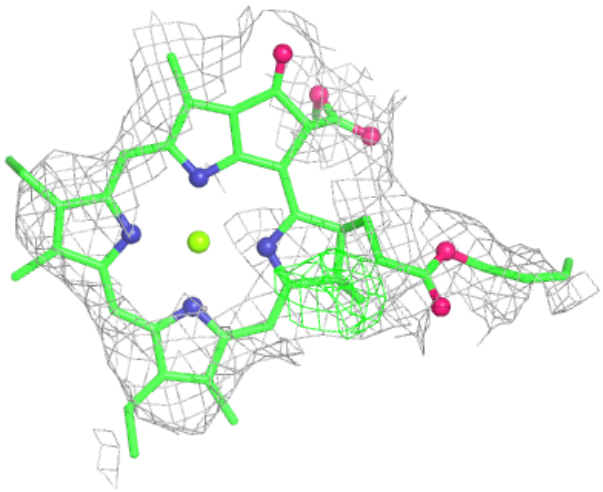


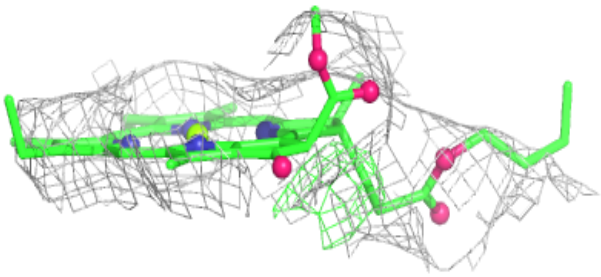


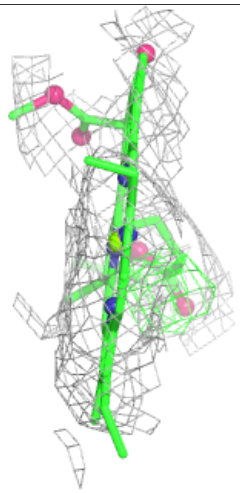


Electron density around CLA A 1103:

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

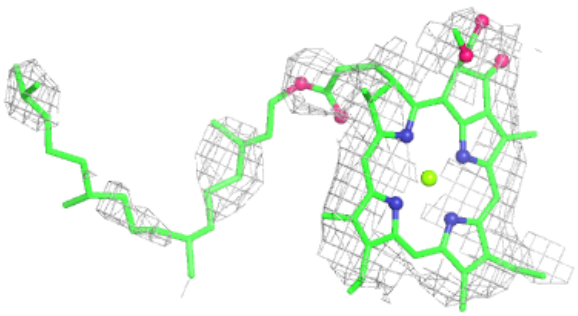


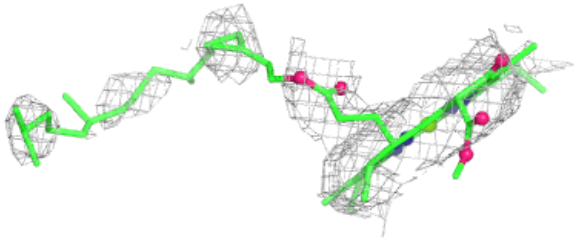




Electron density around CLA A 1106:

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

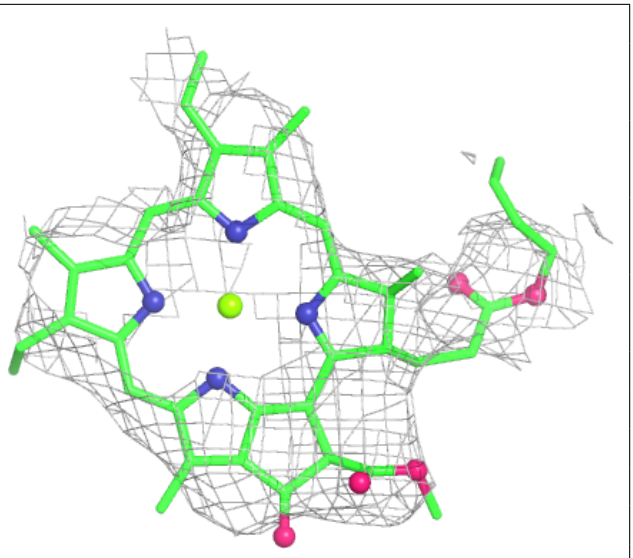


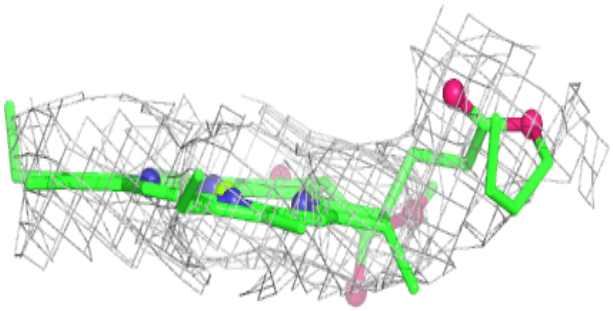


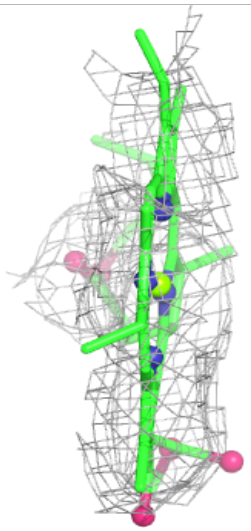


Electron density around CLA B 1023:

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

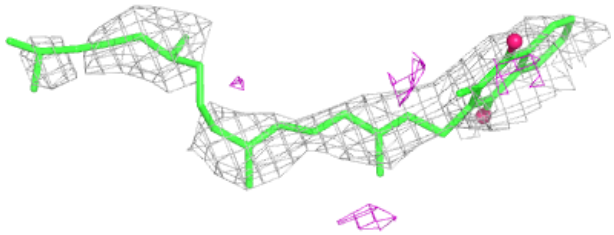


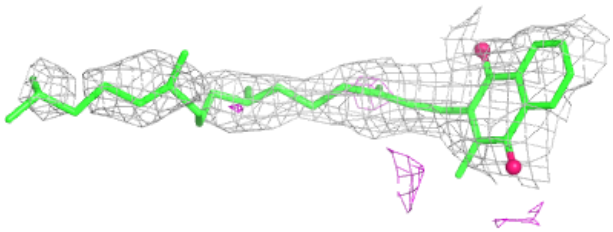


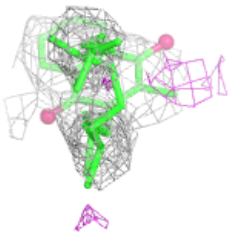


Electron density around PQN A 2001:

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

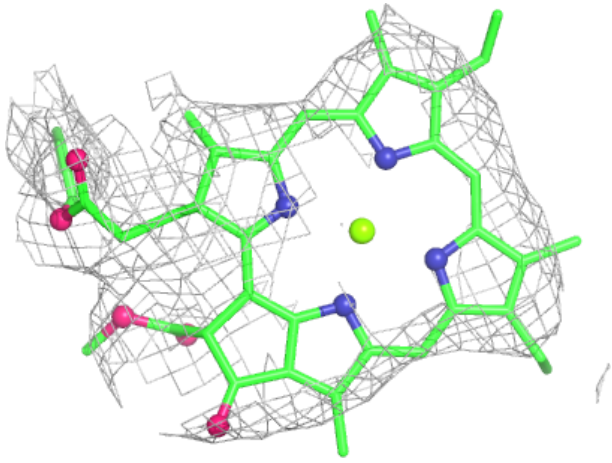


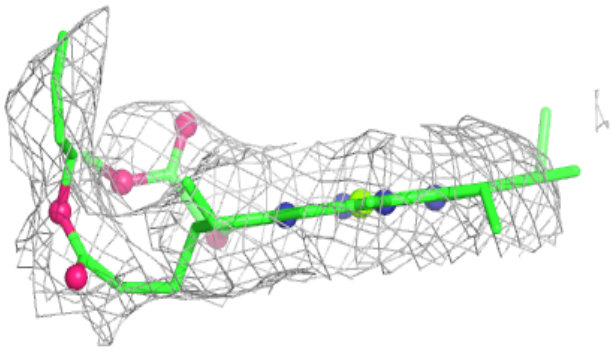




Electron density around CLA A 1104:

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

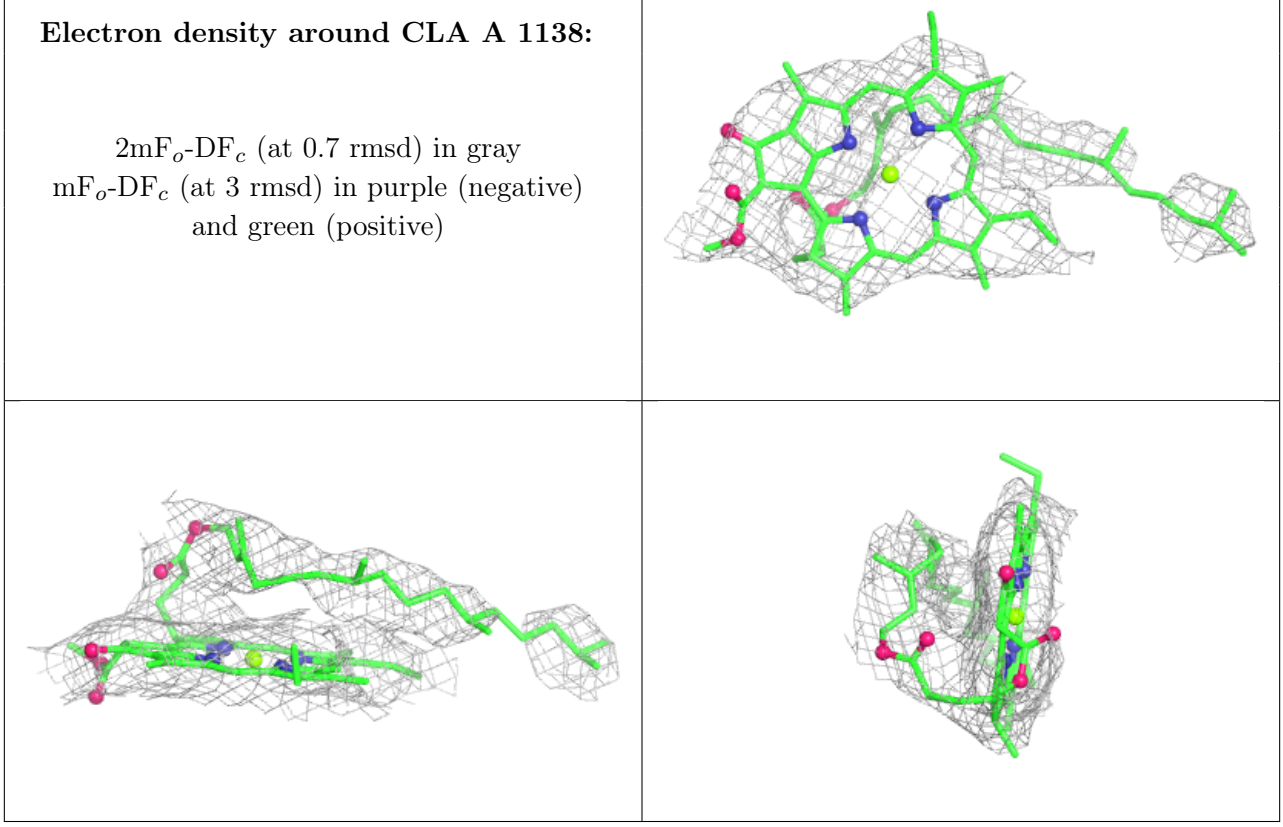






Electron density around CLA A 1138:

$2mF_o$-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.