wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2026 – 08:42 am BST

PDB ID	:	6HIF / pdb_00006hif
Title	:	Kuenenia stuttgartiensis hydrazine dehydrogenase complex
Authors	:	Akram, M.; Dietl, A.; Mersdorf, U.; Prinz, S.; Maalcke, W.; Keltjens, J.; Ferousi, C.; de Almeida, N.M.; Reimann, J.; Kartal, B.; Jetten, M.S.M.; Parey, K.; Barends, T.R.M.
Deposited on	:	2018-08-29
Resolution	:	2.80 Å(reported)

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

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

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

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

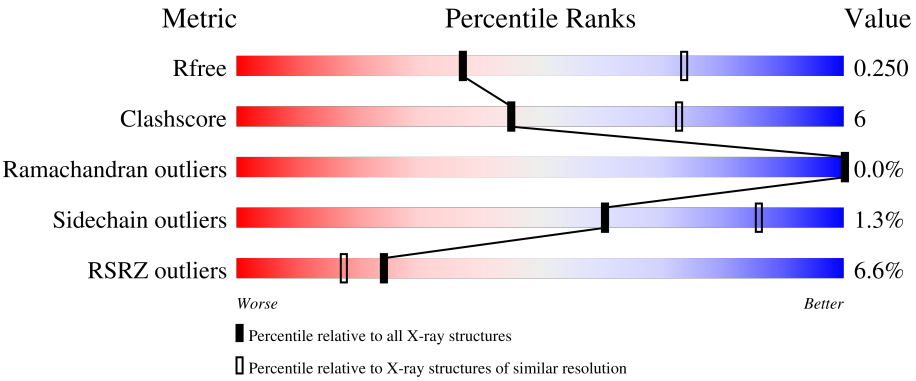
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	582	3% 79% 12% 9%
1	B	582	2% 80% 11% 9%
1	C	582	% 81% 11% 9%
1	D	582	4% 73% 18% • 9%

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Mol	Chain	Length	Quality of chain
1	E	582	5% 81% 10% 9%
1	F	582	14% 80% 11% 9%
1	G	582	% 78% 13% 9%
1	H	582	% 78% 13% 9%
1	I	582	70% 19% 9%
1	J	582	% 79% 12% 9%
1	K	582	% 79% 13% 9%
1	L	582	% 80% 11% 9%
1	M	582	2% 82% 9% 9%
1	N	582	2% 80% 11% 9%
1	O	582	% 80% 11% 9%
1	P	582	2% 80% 11% 9%
1	Q	582	2% 79% 13% 9%
1	R	582	2% 78% 13% 9%
1	S	582	12% 80% 11% 9%
1	T	582	8% 80% 11% 9%
1	U	582	12% 82% 9% 9%
1	V	582	14% 81% 10% 9%
1	W	582	17% 79% 12% 9%
1	X	582	19% 80% 12% 9%
2	Y	114	5% 68% 8% 25%
2	Z	114	16% 69% 5% 25%
2	a	114	9% 68% 5% 25%
2	b	114	10% 67% 7% 25%
2	c	114	7% 68% 5% 25%

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Mol	Chain	Length	Quality of chain
2	d	114	8% 68% 7% 25%
2	e	114	6% 68% 7% 25%
2	f	114	14% 69% 5% 25%
2	g	114	7% 68% 6% 25%
2	h	114	18% 68% 6% 25%
2	i	114	31% 68% 5% 25%
2	j	114	13% 67% 9% 25%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	A	600	X	-	-	-
3	HEC	A	601	X	-	-	-
3	HEC	A	602	X	-	-	-
3	HEC	A	604	X	-	-	-
3	HEC	A	605	X	-	-	-
3	HEC	A	606	X	-	-	-
3	HEC	A	607	X	-	-	-
3	HEC	B	600	X	-	-	-
3	HEC	B	601	X	-	-	-
3	HEC	B	602	X	-	-	-
3	HEC	B	604	X	-	-	-
3	HEC	B	605	X	-	-	-
3	HEC	B	606	X	-	-	-
3	HEC	B	607	X	-	-	-
3	HEC	C	600	X	-	-	-
3	HEC	C	601	X	-	-	-
3	HEC	C	602	X	-	-	-
3	HEC	C	604	X	-	-	-
3	HEC	C	605	X	-	-	-
3	HEC	C	606	X	-	-	-
3	HEC	C	607	X	-	-	-
3	HEC	D	600	X	-	-	-
3	HEC	D	601	X	-	-	-
3	HEC	D	602	X	-	-	-
3	HEC	D	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	D	605	X	-	-	-
3	HEC	D	606	X	-	-	-
3	HEC	E	600	X	-	-	-
3	HEC	E	601	X	-	-	-
3	HEC	E	602	X	-	-	-
3	HEC	E	604	X	-	-	-
3	HEC	E	605	X	-	-	-
3	HEC	E	606	X	-	-	-
3	HEC	E	607	X	-	-	-
3	HEC	F	600	X	-	-	-
3	HEC	F	601	X	-	-	-
3	HEC	F	602	X	-	-	-
3	HEC	F	604	X	-	-	-
3	HEC	F	605	X	-	-	-
3	HEC	F	606	X	-	-	-
3	HEC	F	607	X	-	-	-
3	HEC	G	600	X	-	-	-
3	HEC	G	601	X	-	-	-
3	HEC	G	602	X	-	-	-
3	HEC	G	604	X	-	-	-
3	HEC	G	605	X	-	-	-
3	HEC	G	606	X	-	-	-
3	HEC	G	607	X	-	-	-
3	HEC	H	600	X	-	-	-
3	HEC	H	601	X	-	-	-
3	HEC	H	602	X	-	-	-
3	HEC	H	604	X	-	-	-
3	HEC	H	605	X	-	-	-
3	HEC	H	606	X	-	-	-
3	HEC	H	607	X	-	-	-
3	HEC	I	600	X	-	-	-
3	HEC	I	601	X	-	-	-
3	HEC	I	602	X	-	-	-
3	HEC	I	604	X	-	-	-
3	HEC	I	605	X	-	-	-
3	HEC	I	606	X	-	-	-
3	HEC	I	607	X	-	-	-
3	HEC	J	600	X	-	-	-
3	HEC	J	601	X	-	-	-
3	HEC	J	602	X	-	-	-
3	HEC	J	604	X	-	-	-
3	HEC	J	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	J	606	X	-	-	-
3	HEC	J	607	X	-	-	-
3	HEC	K	600	X	-	-	-
3	HEC	K	601	X	-	-	-
3	HEC	K	602	X	-	-	-
3	HEC	K	604	X	-	-	-
3	HEC	K	605	X	-	-	-
3	HEC	K	606	X	-	-	-
3	HEC	K	607	X	-	-	-
3	HEC	L	600	X	-	-	-
3	HEC	L	601	X	-	-	-
3	HEC	L	602	X	-	-	-
3	HEC	L	604	X	-	-	-
3	HEC	L	605	X	-	-	-
3	HEC	L	606	X	-	-	-
3	HEC	L	607	X	-	-	-
3	HEC	M	600	X	-	-	-
3	HEC	M	601	X	-	-	-
3	HEC	M	602	X	-	-	-
3	HEC	M	604	X	-	-	-
3	HEC	M	605	X	-	-	-
3	HEC	M	606	X	-	-	-
3	HEC	M	607	X	-	-	-
3	HEC	N	600	X	-	-	-
3	HEC	N	601	X	-	-	-
3	HEC	N	602	X	-	-	-
3	HEC	N	604	X	-	-	-
3	HEC	N	605	X	-	-	-
3	HEC	N	606	X	-	-	-
3	HEC	N	607	X	-	-	-
3	HEC	O	600	X	-	-	-
3	HEC	O	601	X	-	-	-
3	HEC	O	602	X	-	-	-
3	HEC	O	604	X	-	-	-
3	HEC	O	605	X	-	-	-
3	HEC	O	606	X	-	-	-
3	HEC	O	607	X	-	-	-
3	HEC	P	600	X	-	-	-
3	HEC	P	601	X	-	-	-
3	HEC	P	602	X	-	-	-
3	HEC	P	604	X	-	-	-
3	HEC	P	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	P	606	X	-	-	-
3	HEC	P	607	X	-	-	-
3	HEC	Q	600	X	-	-	-
3	HEC	Q	601	X	-	-	-
3	HEC	Q	602	X	-	-	-
3	HEC	Q	604	X	-	-	-
3	HEC	Q	605	X	-	-	-
3	HEC	Q	606	X	-	-	-
3	HEC	Q	607	X	-	-	-
3	HEC	R	600	X	-	-	-
3	HEC	R	601	X	-	-	-
3	HEC	R	602	X	-	-	-
3	HEC	R	604	X	-	-	-
3	HEC	R	605	X	-	-	-
3	HEC	R	606	X	-	-	-
3	HEC	R	607	X	-	-	-
3	HEC	S	600	X	-	-	-
3	HEC	S	601	X	-	-	-
3	HEC	S	602	X	-	-	-
3	HEC	S	604	X	-	-	-
3	HEC	S	605	X	-	-	-
3	HEC	S	606	X	-	-	-
3	HEC	S	607	X	-	-	-
3	HEC	T	600	X	-	-	-
3	HEC	T	601	X	-	-	-
3	HEC	T	602	X	-	-	-
3	HEC	T	604	X	-	-	-
3	HEC	T	605	X	-	-	-
3	HEC	T	606	X	-	-	-
3	HEC	T	607	X	-	-	-
3	HEC	U	600	X	-	-	-
3	HEC	U	601	X	-	-	-
3	HEC	U	602	X	-	-	-
3	HEC	U	604	X	-	-	-
3	HEC	U	605	X	-	-	-
3	HEC	U	606	X	-	-	-
3	HEC	U	607	X	-	-	-
3	HEC	V	600	X	-	-	-
3	HEC	V	601	X	-	-	-
3	HEC	V	602	X	-	-	-
3	HEC	V	604	X	-	-	-
3	HEC	V	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEC	V	606	X	-	-	-
3	HEC	V	607	X	-	-	-
3	HEC	W	600	X	-	-	-
3	HEC	W	601	X	-	-	-
3	HEC	W	602	X	-	-	-
3	HEC	W	604	X	-	-	-
3	HEC	W	605	X	-	-	-
3	HEC	W	606	X	-	-	-
3	HEC	W	607	X	-	-	-
3	HEC	X	600	X	-	-	-
3	HEC	X	601	X	-	-	-
3	HEC	X	602	X	-	-	-
3	HEC	X	604	X	-	-	-
3	HEC	X	605	X	-	-	-
3	HEC	X	606	X	-	-	-
3	HEC	X	607	X	-	-	-
4	SO4	G	610	-	-	X	-
4	SO4	J	611	-	-	X	-
5	GOL	H	614	-	-	X	-
5	GOL	H	615	-	-	X	-
5	GOL	I	614	-	-	X	-
5	GOL	K	614	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 118753 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 Hydrazine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	A	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	B	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	C	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	D	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	E	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	F	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	H	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	I	527	Total	C	N	O	S	0	0	0
			4201	2633	739	793	36			
1	J	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	K	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	L	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	M	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	N	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	O	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	P	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	R	531	Total	C	N	O	S	0	1	0
			4237	2653	749	799	36			
1	S	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	T	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	U	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	V	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	W	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			
1	X	531	Total	C	N	O	S	0	0	0
			4226	2647	745	798	36			

- Molecule 2 is a protein called hdh assembly factor Kustc1130.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	Z	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	a	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	b	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	c	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	d	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	e	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	f	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	g	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	h	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			
2	i	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			

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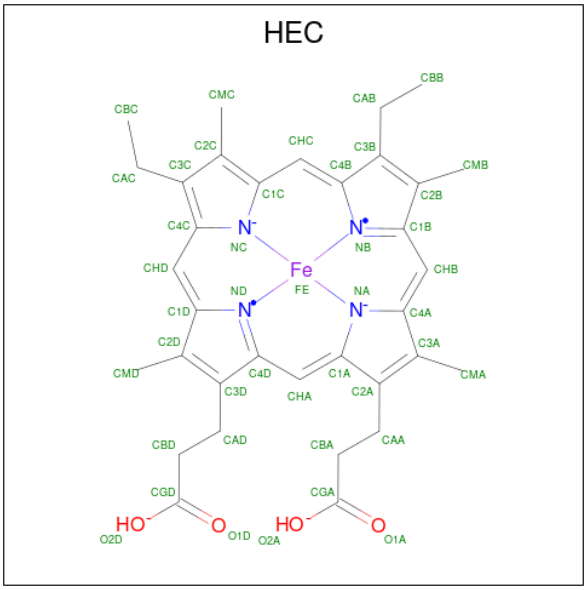
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	j	86	Total	C	N	O	S	0	0	0
			640	403	110	125	2			

- Molecule 3 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	J	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	R	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	S	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	T	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	U	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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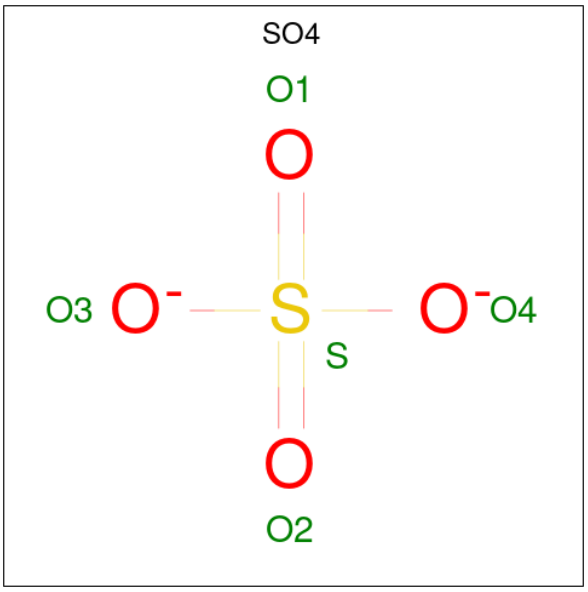
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	W	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	X	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	G	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	F	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	I	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	J	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	K	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	M	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	N	1	Total O S 5 4 1	0	0
4	O	1	Total O S 5 4 1	0	0
4	O	1	Total O S 5 4 1	0	0
4	O	1	Total O S 5 4 1	0	0
4	P	1	Total O S 5 4 1	0	0
4	Q	1	Total O S 5 4 1	0	0
4	Q	1	Total O S 5 4 1	0	0
4	Q	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	S	1	Total O S 5 4 1	0	0

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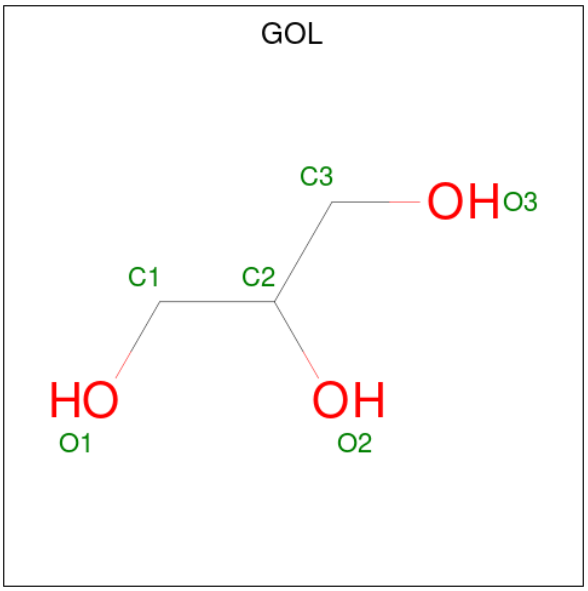
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	S	1	Total O S 5 4 1	0	0
4	T	1	Total O S 5 4 1	0	0
4	U	1	Total O S 5 4 1	0	0
4	U	1	Total O S 5 4 1	0	0
4	U	1	Total O S 5 4 1	0	0
4	V	1	Total O S 5 4 1	0	0
4	V	1	Total O S 5 4 1	0	0
4	V	1	Total O S 5 4 1	0	0
4	W	1	Total O S 5 4 1	0	0
4	X	1	Total O S 5 4 1	0	0
4	X	1	Total O S 5 4 1	0	0
4	X	1	Total O S 5 4 1	0	0
4	Y	1	Total O S 5 4 1	0	0
4	Y	1	Total O S 5 4 1	0	0
4	a	1	Total O S 5 4 1	0	0
4	c	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	I	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	K	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0
5	K	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total K 1 1	0	0
6	K	1	Total K 1 1	0	0
6	Q	1	Total K 1 1	0	0
6	X	1	Total K 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	78	Total O 78 78	0	0
7	A	33	Total O 33 33	0	0
7	B	40	Total O 40 40	0	0
7	C	36	Total O 36 36	0	0
7	D	21	Total O 21 21	0	0
7	E	21	Total O 21 21	0	0
7	F	24	Total O 24 24	0	0
7	H	70	Total O 70 70	0	0
7	I	62	Total O 62 62	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	J	78	Total O 78 78	0	0
7	K	57	Total O 57 57	0	0
7	L	69	Total O 69 69	0	0
7	M	27	Total O 27 27	0	0
7	N	37	Total O 37 37	0	0
7	O	40	Total O 40 40	0	0
7	P	50	Total O 50 50	0	0
7	Q	48	Total O 48 48	0	0
7	R	49	Total O 49 49	0	0
7	S	4	Total O 4 4	0	0
7	T	15	Total O 15 15	0	0
7	U	15	Total O 15 15	0	0
7	V	17	Total O 17 17	0	0
7	W	12	Total O 12 12	0	0
7	X	13	Total O 13 13	0	0
7	Y	2	Total O 2 2	0	0
7	Z	1	Total O 1 1	0	0
7	a	2	Total O 2 2	0	0
7	b	2	Total O 2 2	0	0
7	c	2	Total O 2 2	0	0
7	d	2	Total O 2 2	0	0

Continued on next page...

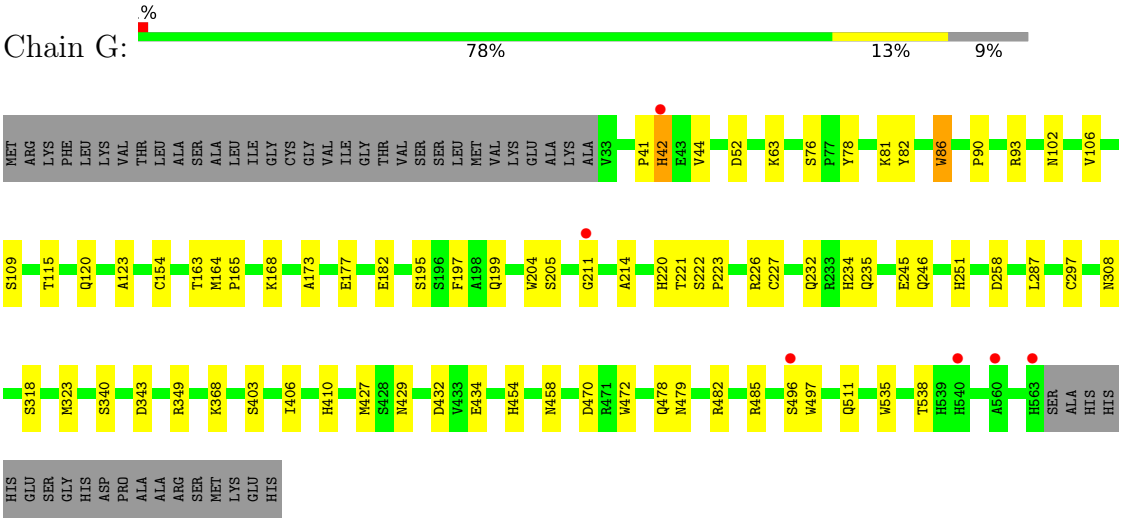
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	e	2	Total O 2 2	0	0
7	f	2	Total O 2 2	0	0
7	g	1	Total O 1 1	0	0
7	i	2	Total O 2 2	0	0
7	j	1	Total O 1 1	0	0

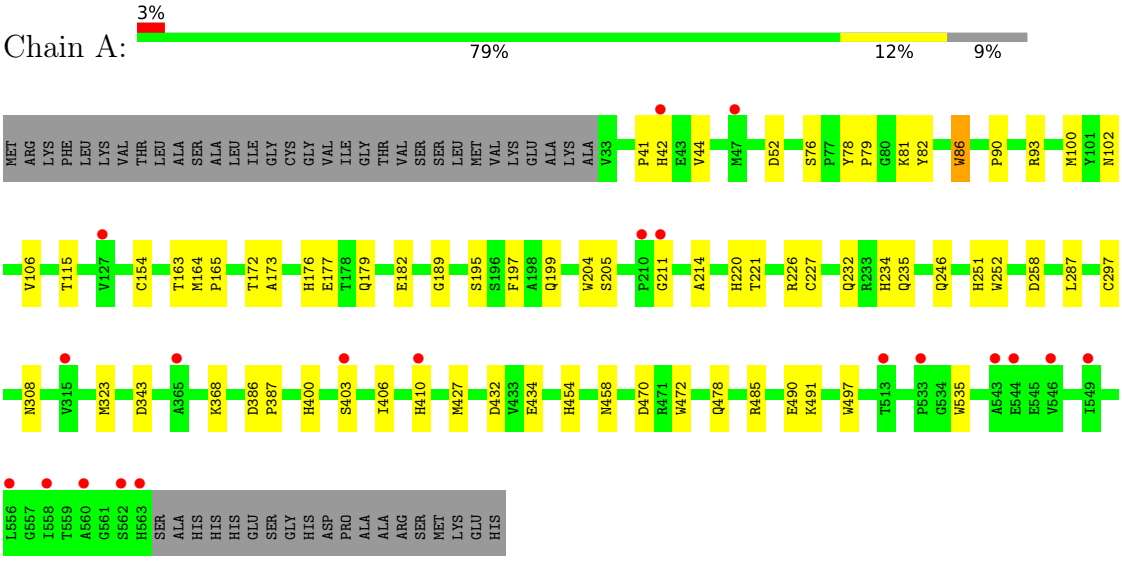
3 Residue-property plots (i)

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

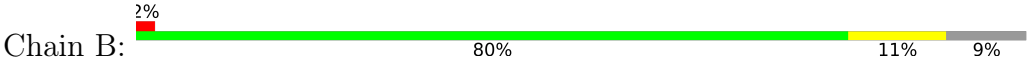
• Molecule 1: Hydrazine dehydrogenase

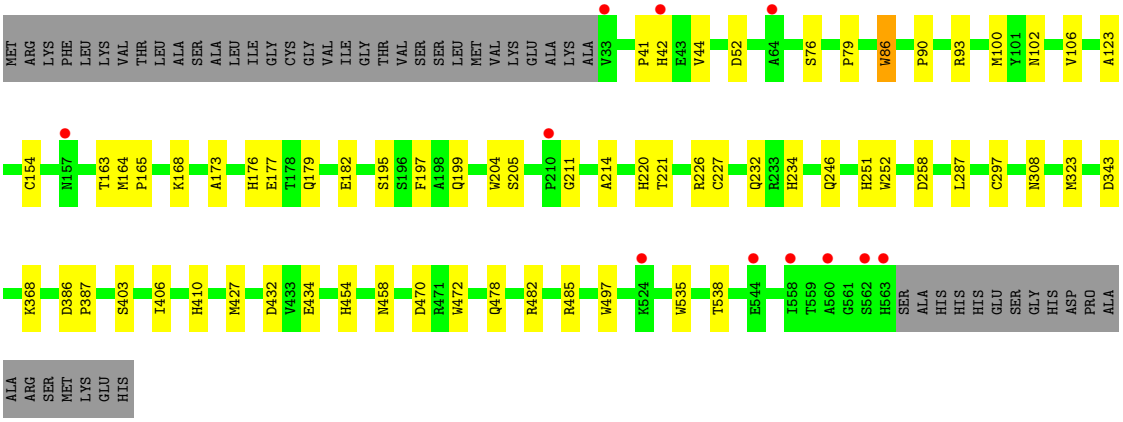


• Molecule 1: Hydrazine dehydrogenase



• Molecule 1: Hydrazine dehydrogenase

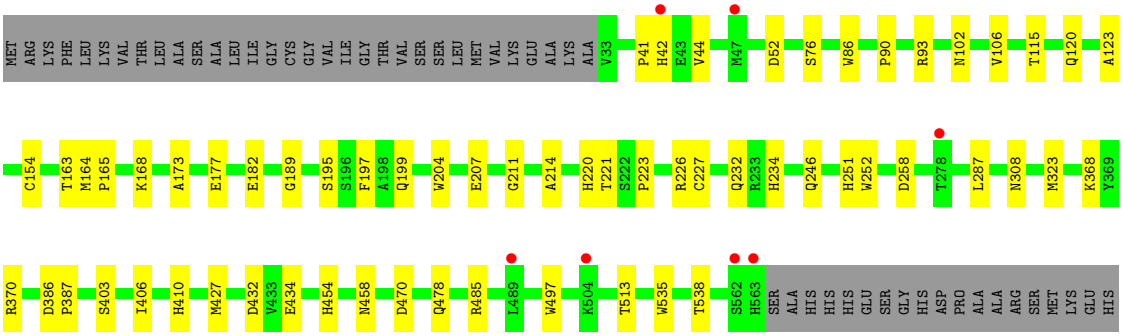




• Molecule 1: Hydrazine dehydrogenase

Chain C:

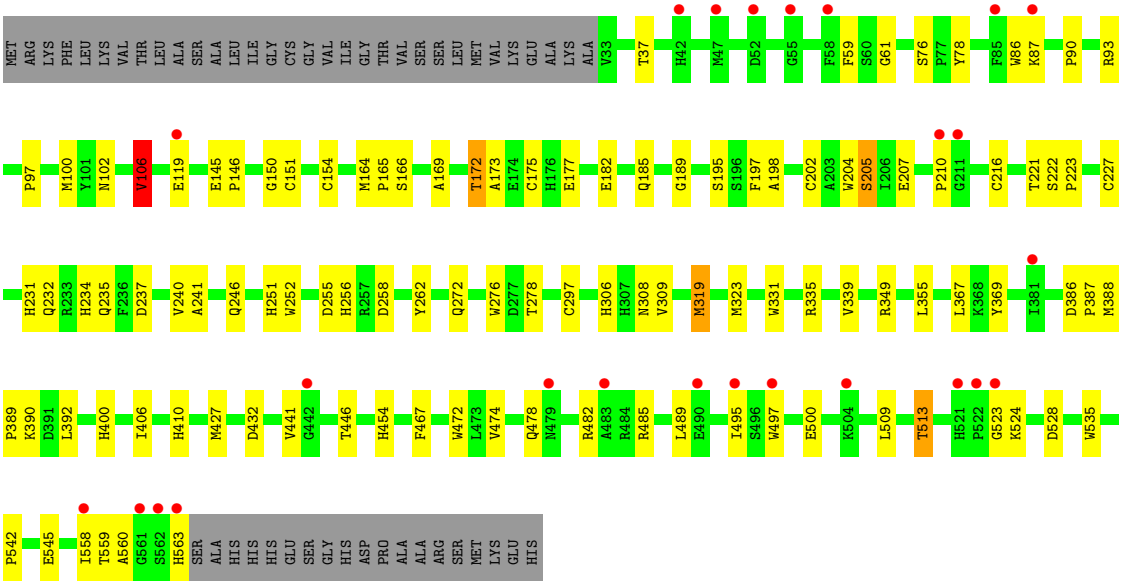




• Molecule 1: Hydrazine dehydrogenase

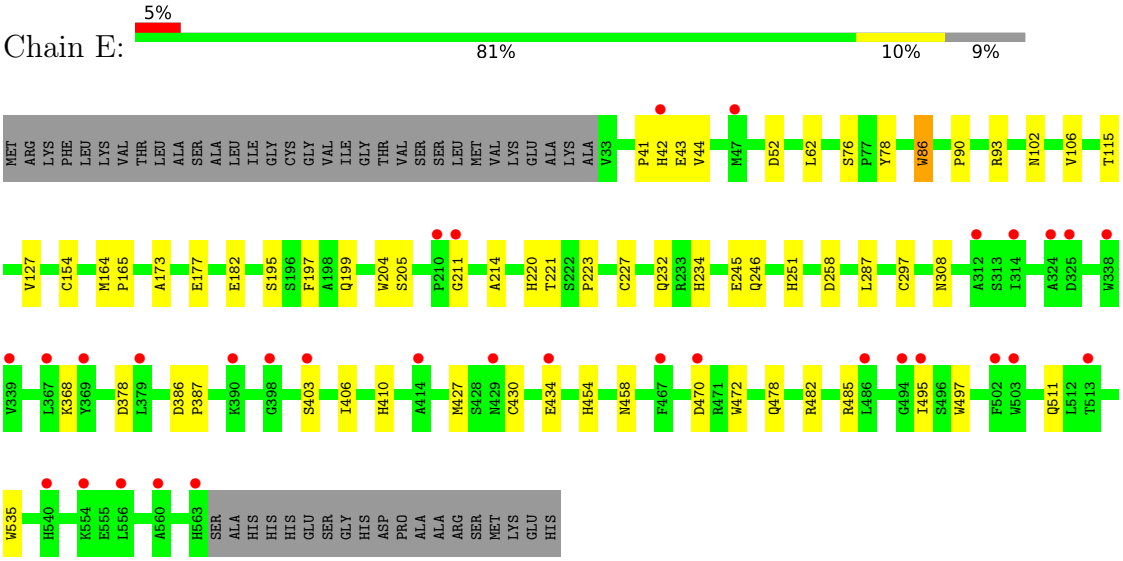
Chain D:





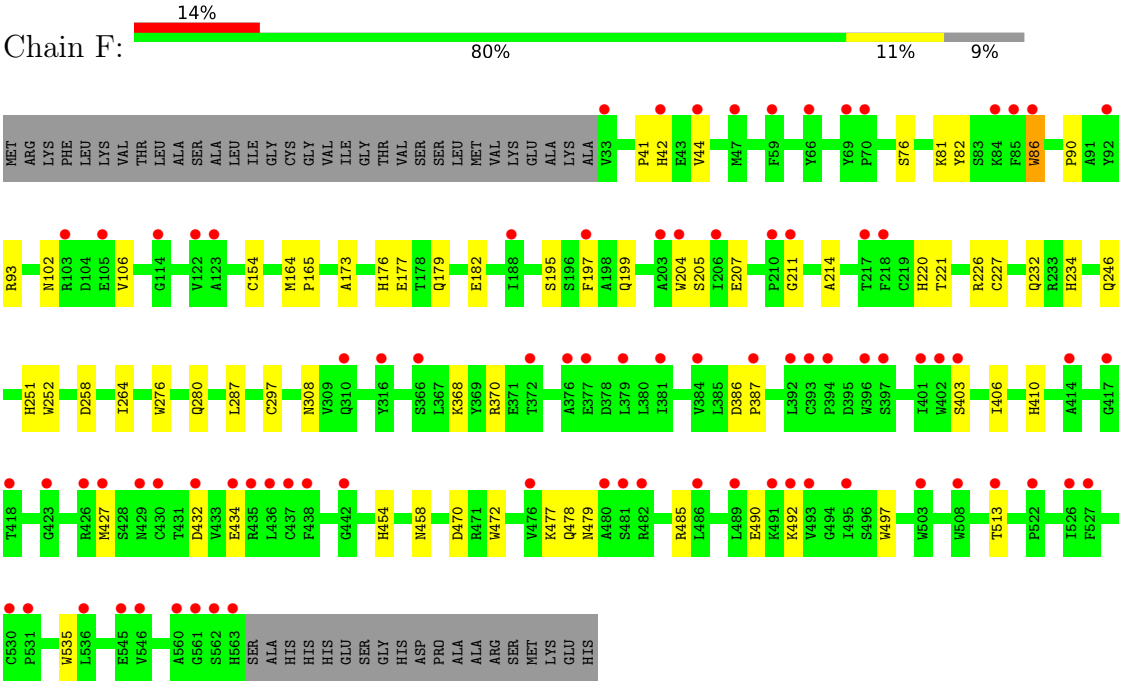
• Molecule 1: Hydrazine dehydrogenase

Chain E:



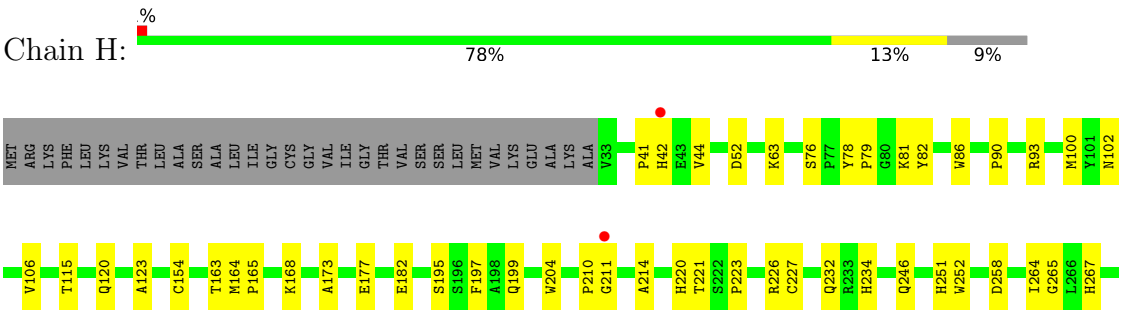
• Molecule 1: Hydrazine dehydrogenase

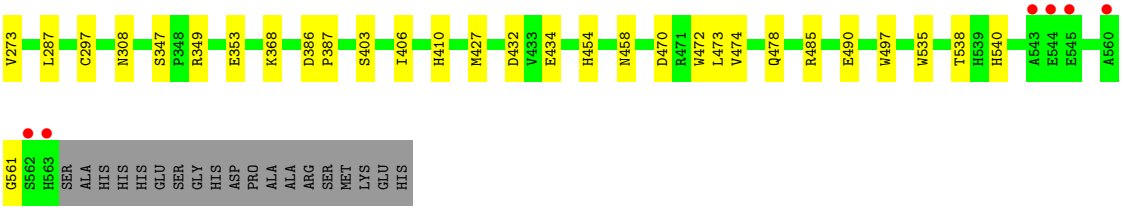
Chain F:



• Molecule 1: Hydrazine dehydrogenase

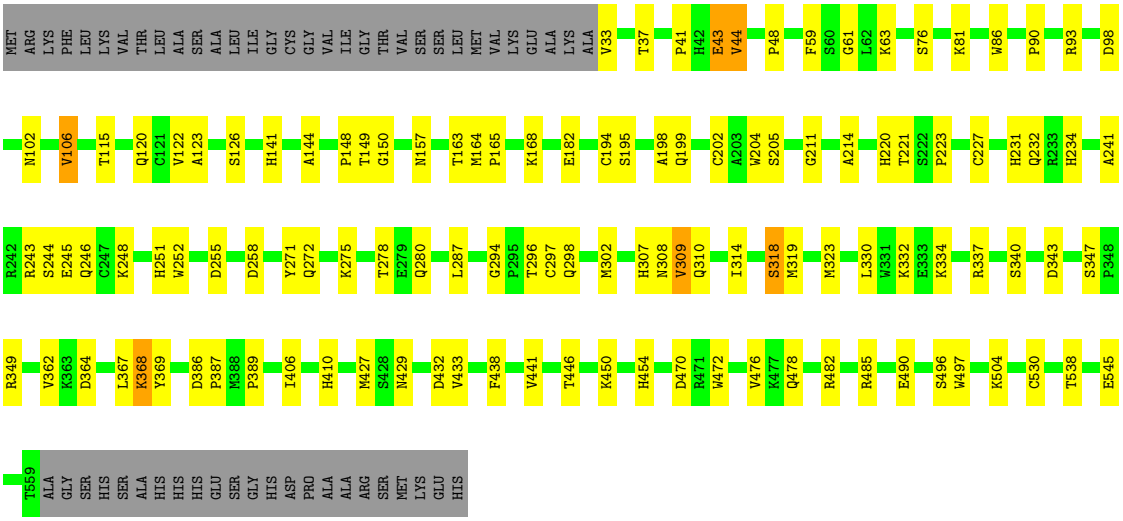
Chain H:





• Molecule 1: Hydrazine dehydrogenase

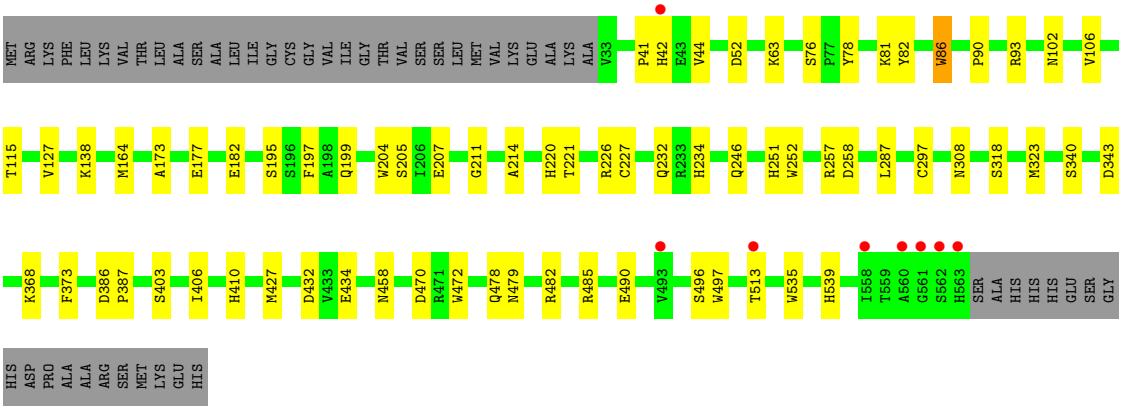
Chain I:



• Molecule 1: Hydrazine dehydrogenase

Chain J:

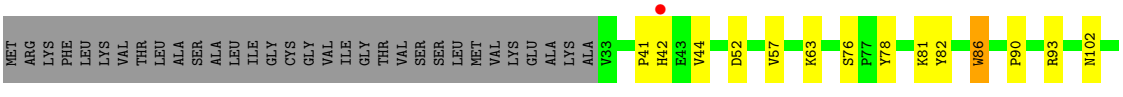


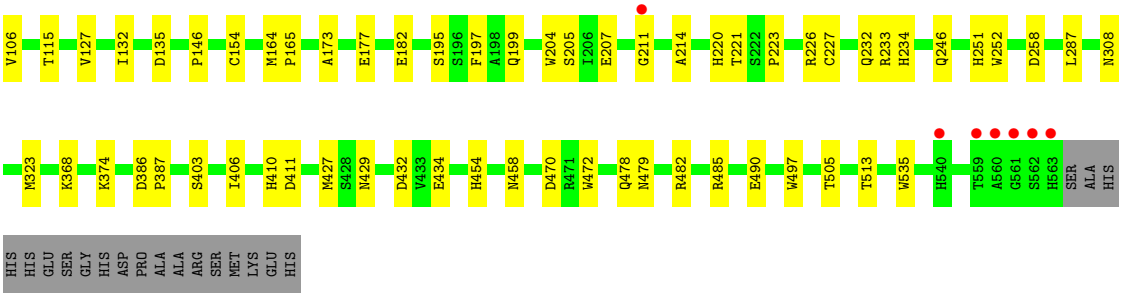


• Molecule 1: Hydrazine dehydrogenase

Chain K:



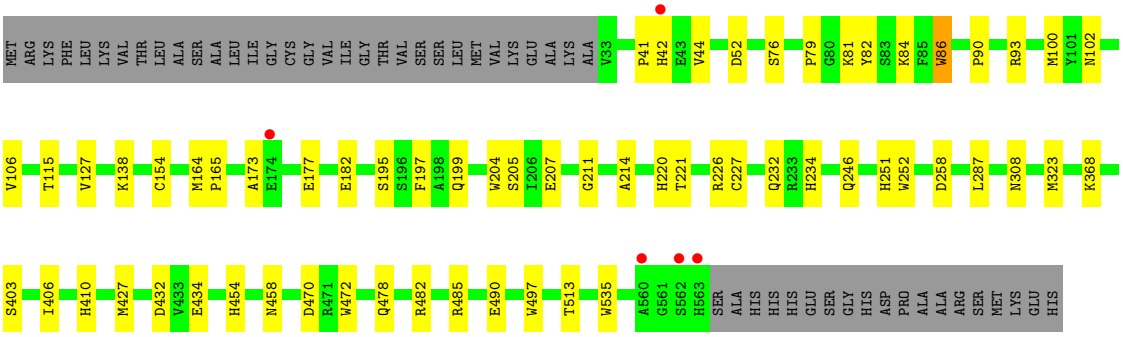




• Molecule 1: Hydrazine dehydrogenase

Chain L:

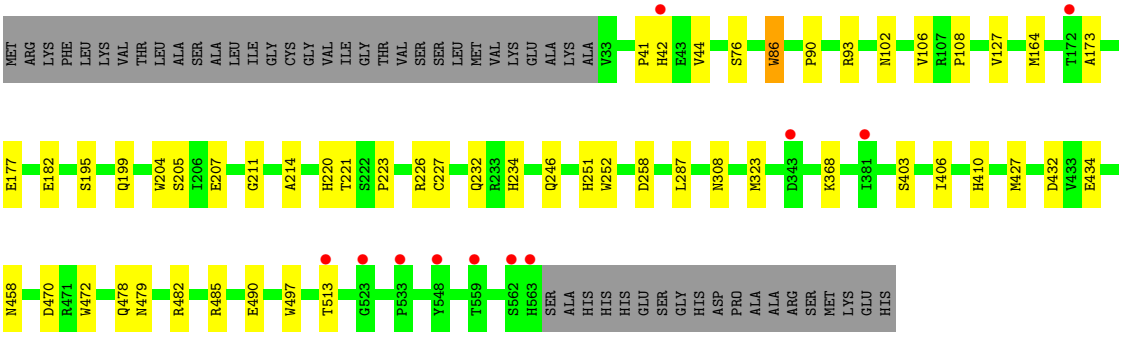




• Molecule 1: Hydrazine dehydrogenase

Chain M:

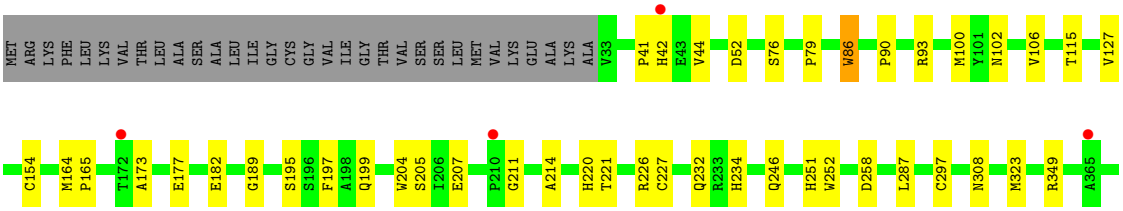




• Molecule 1: Hydrazine dehydrogenase

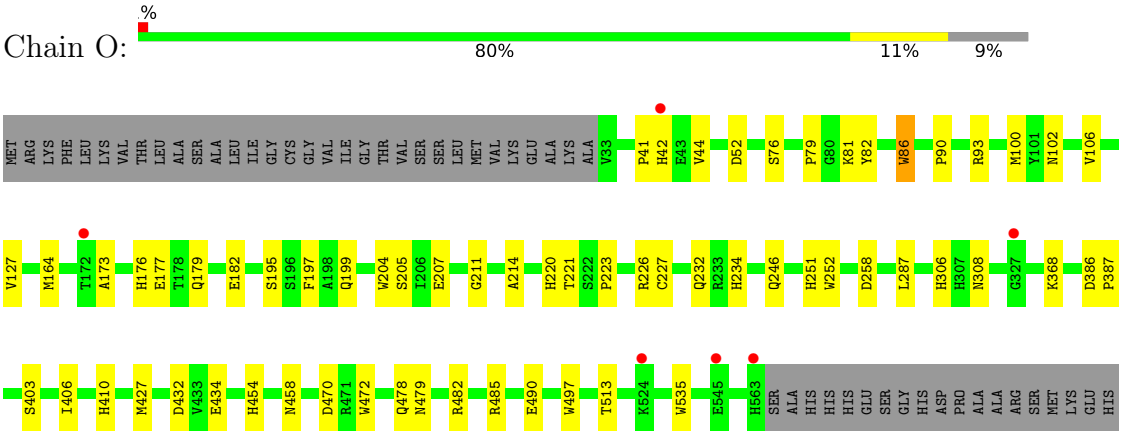
Chain N:



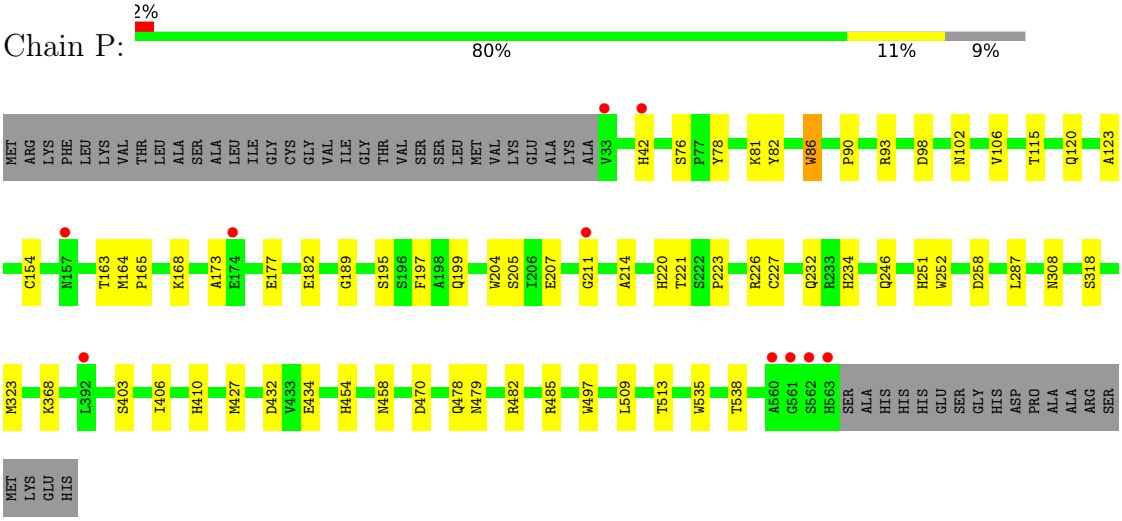




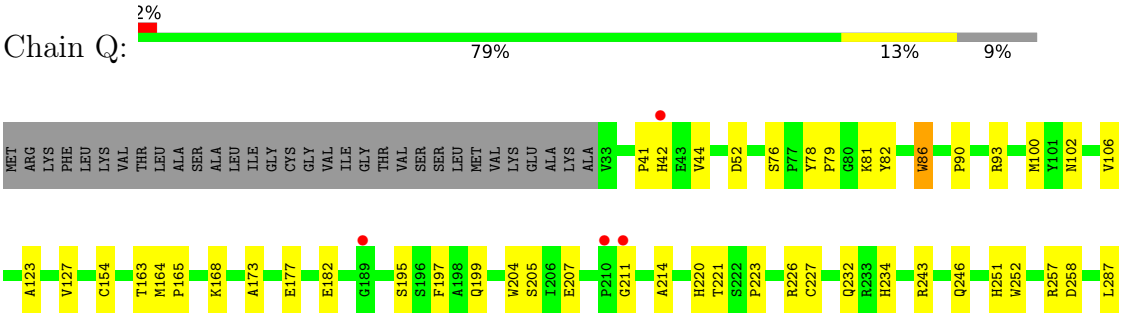
• Molecule 1: Hydrazine dehydrogenase

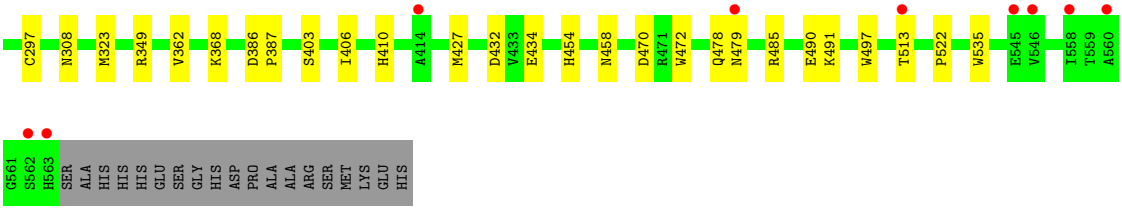


• Molecule 1: Hydrazine dehydrogenase



• Molecule 1: Hydrazine dehydrogenase

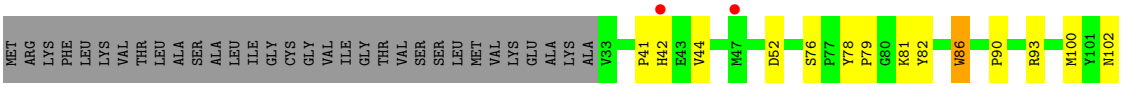


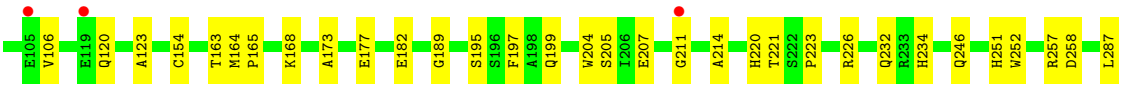


• Molecule 1: Hydrazine dehydrogenase

Chain R:







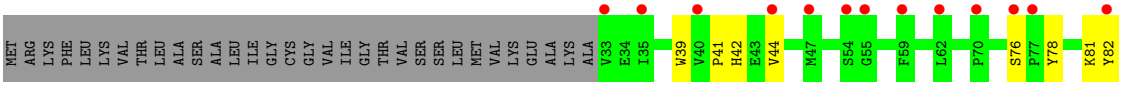


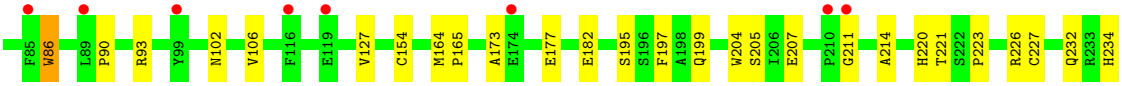


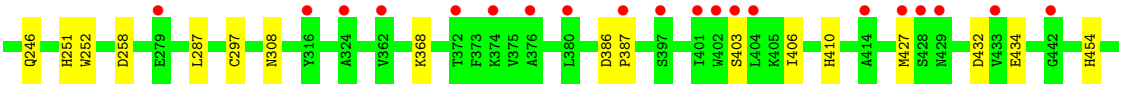
• Molecule 1: Hydrazine dehydrogenase

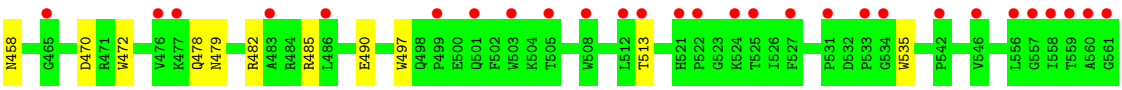
Chain S:

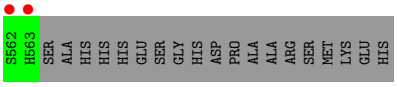








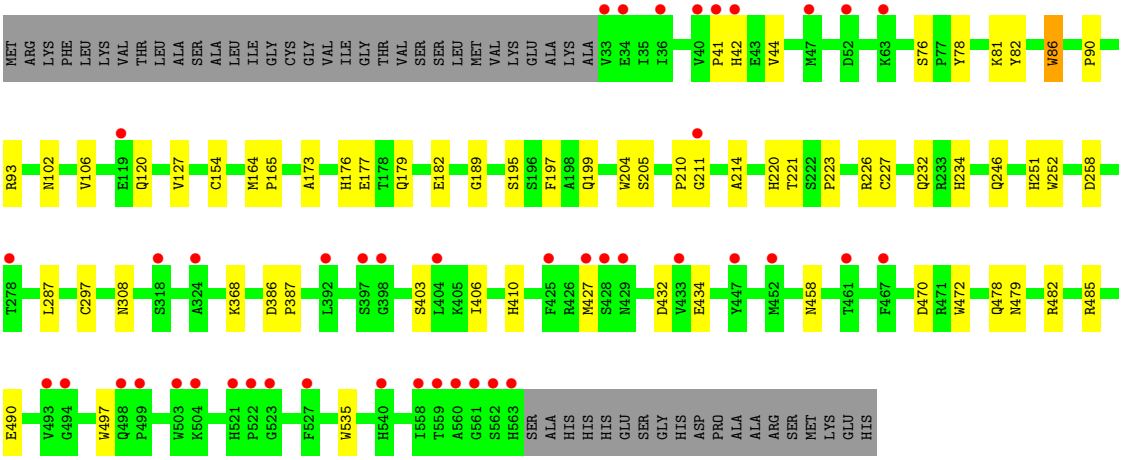




• Molecule 1: Hydrazine dehydrogenase

Chain T:

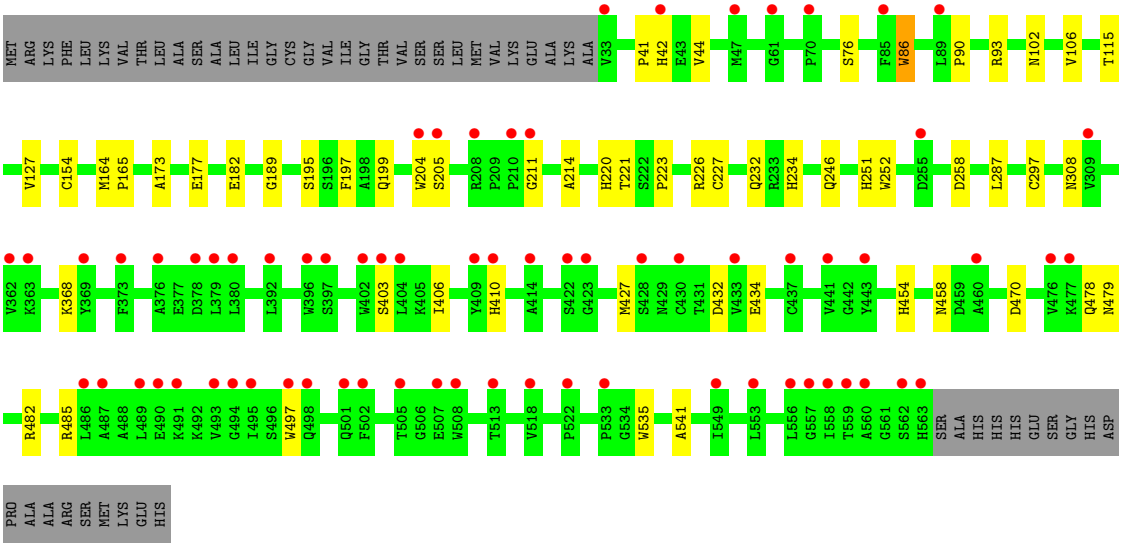




• Molecule 1: Hydrazine dehydrogenase

Chain U:

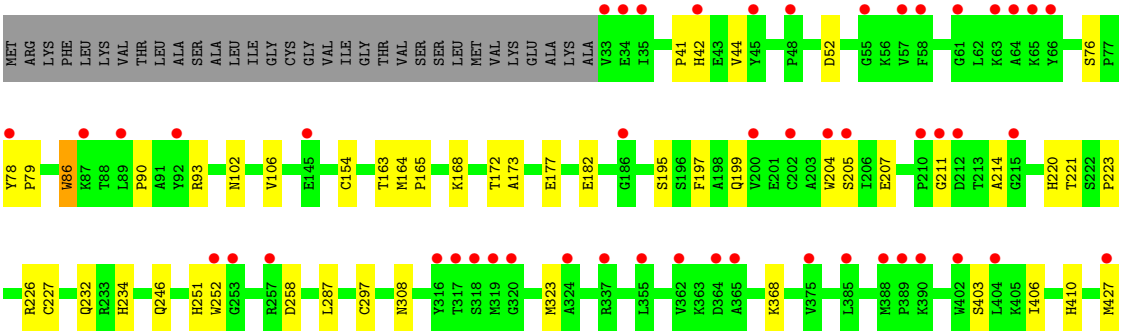


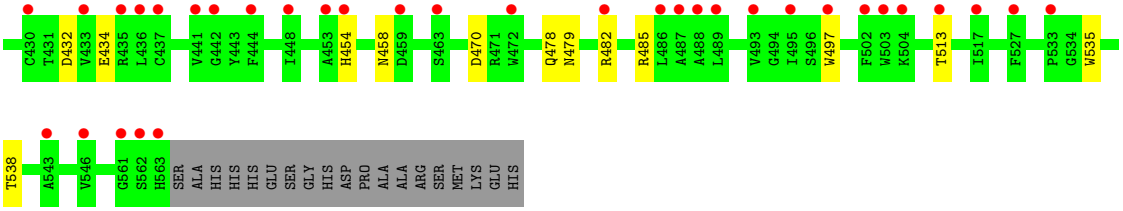


• Molecule 1: Hydrazine dehydrogenase

Chain V:

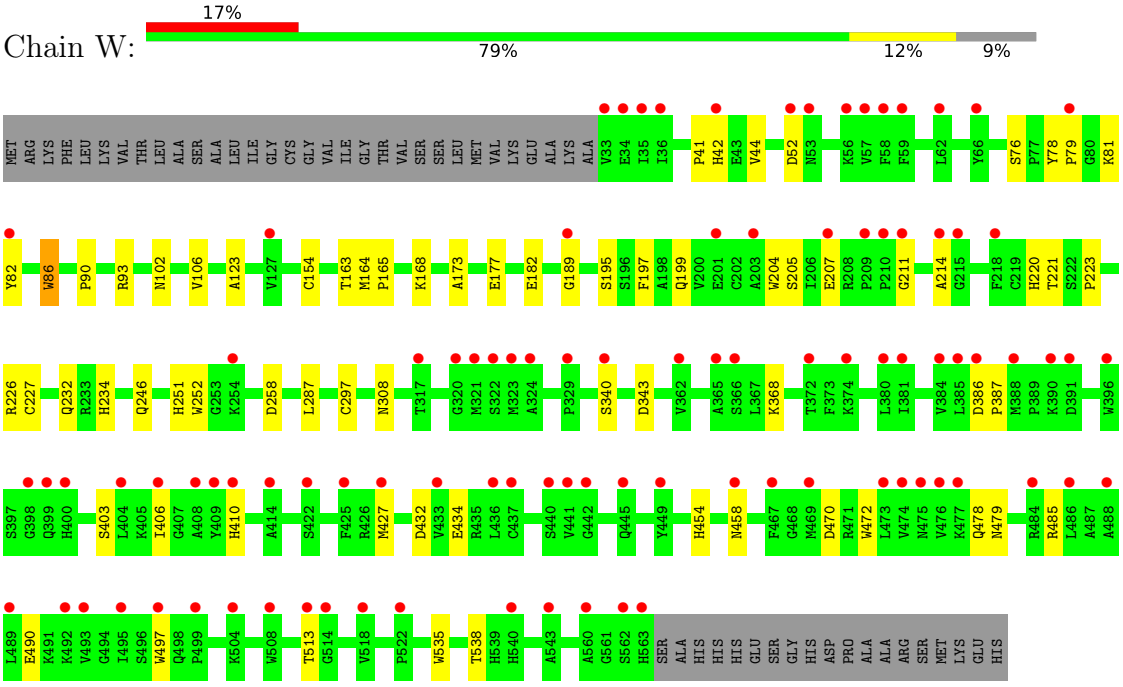






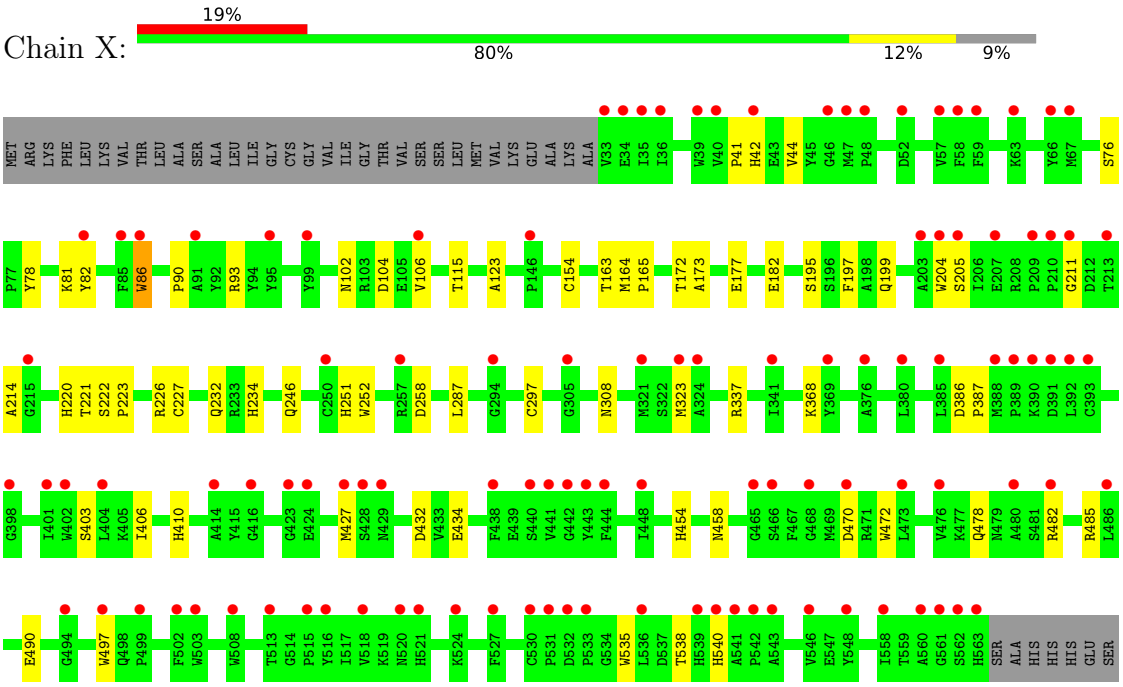
• Molecule 1: Hydrazine dehydrogenase

Chain W:



• Molecule 1: Hydrazine dehydrogenase

Chain X:

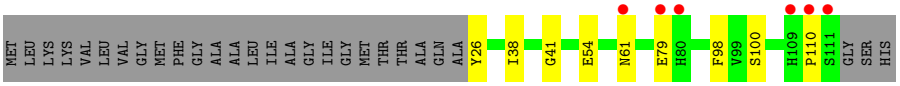




• Molecule 2: hdh assembly factor Kustc1130

Chain Y:

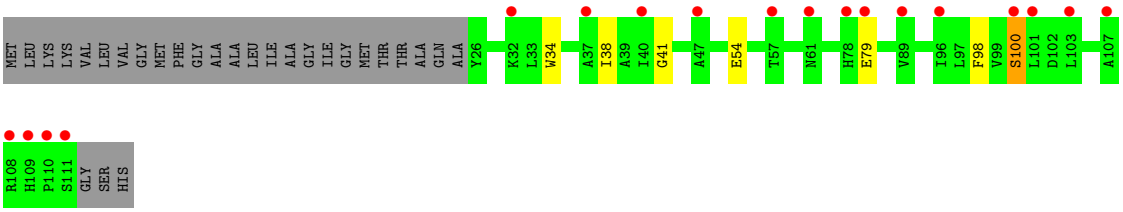




• Molecule 2: hdh assembly factor Kustc1130

Chain Z:

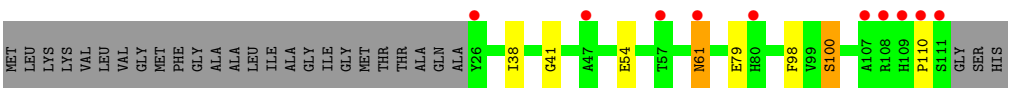




• Molecule 2: hdh assembly factor Kustc1130

Chain a:

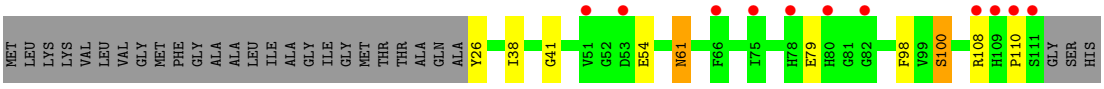




• Molecule 2: hdh assembly factor Kustc1130

Chain b:

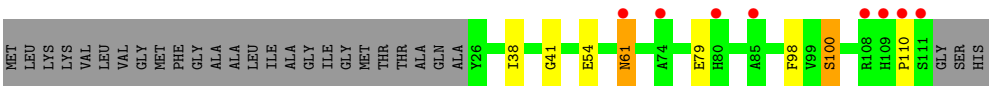




• Molecule 2: hdh assembly factor Kustc1130

Chain c:

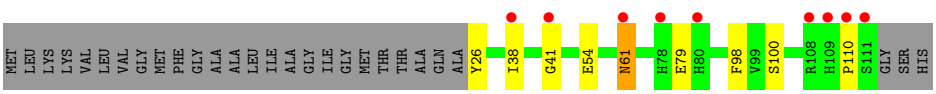




• Molecule 2: hdh assembly factor Kustc1130

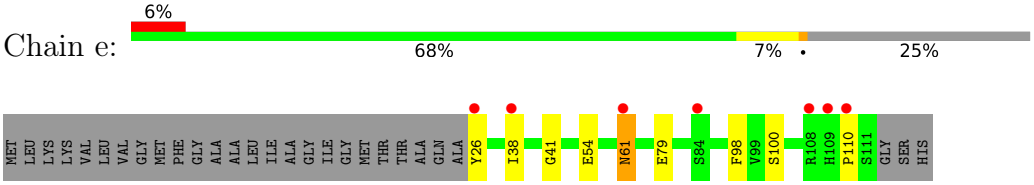
Chain d:





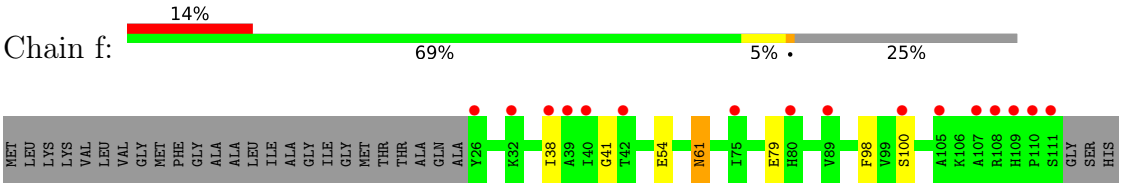
• Molecule 2: hdh assembly factor Kustc1130

Chain e:



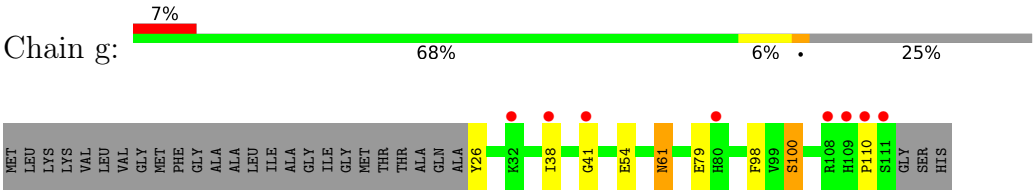
• Molecule 2: hdh assembly factor Kustc1130

Chain f:



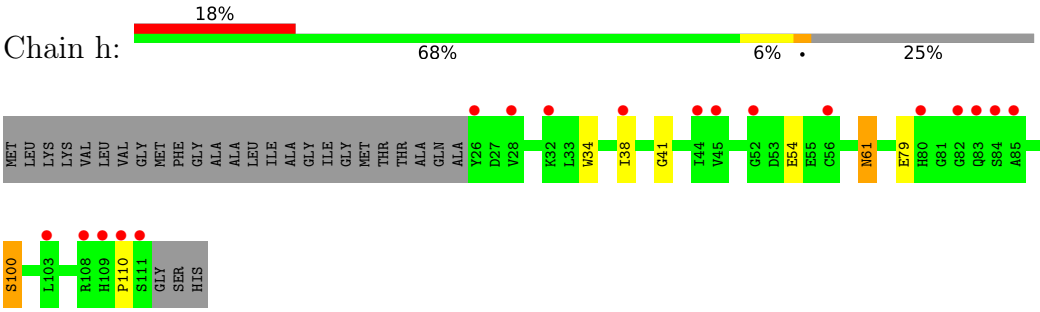
• Molecule 2: hdh assembly factor Kustc1130

Chain g:



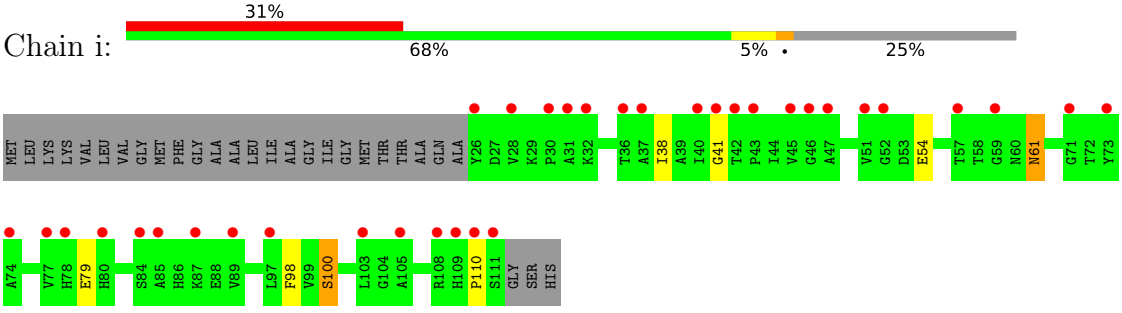
• Molecule 2: hdh assembly factor Kustc1130

Chain h:



• Molecule 2: hdh assembly factor Kustc1130

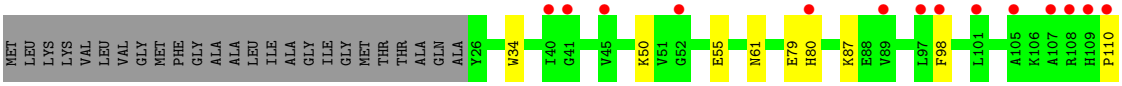
Chain i:



• Molecule 2: hdh assembly factor Kustc1130

Chain j:




MET LEU LYS LYS VAL LEU VAL GLY MET PHE GLY ALA ALA LEU ILE ALA GLY ILE GLY MET THR THR ALA GLN ALA Y26 W34 I40 G41 V45 K50 V51 G52 E55 N61 E79 H80 K87 E88 V89 L97 F98 L101 A105 K106 A107 R108 H109 P110


S111 GLY SER HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	211.86Å 211.86Å 398.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.71 – 2.80 93.71 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (93.71-2.80) 96.6 (93.71-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.221 , 0.238 0.220 , 0.250	Depositor DCC
R_{free} test set	30022 reflections (6.09%)	wwPDB-VP
Wilson B-factor (Å^2)	58.7	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 54.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	118753	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: GOL, HEC, SO4, K

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	0.44	0/4355	0.91	0/5901
1	B	0.45	0/4355	0.90	0/5901
1	C	0.45	0/4355	0.92	0/5901
1	D	0.44	0/4355	0.95	0/5901
1	E	0.44	0/4355	0.91	0/5901
1	F	0.44	0/4355	0.91	0/5901
1	G	0.45	0/4355	0.91	0/5901
1	H	0.45	0/4355	0.91	0/5901
1	I	0.46	0/4329	0.95	0/5866
1	J	0.45	0/4355	0.90	0/5901
1	K	0.45	0/4355	0.90	0/5901
1	L	0.45	0/4355	0.91	0/5901
1	M	0.44	0/4355	0.91	0/5901
1	N	0.44	0/4355	0.91	0/5901
1	O	0.45	0/4355	0.90	0/5901
1	P	0.45	0/4355	0.91	0/5901
1	Q	0.45	0/4355	0.91	0/5901
1	R	0.45	0/4366	0.90	0/5915
1	S	0.44	0/4355	0.91	0/5901
1	T	0.44	0/4355	0.91	0/5901
1	U	0.44	0/4355	0.91	0/5901
1	V	0.44	0/4355	0.91	0/5901
1	W	0.44	0/4355	0.91	0/5901
1	X	0.44	0/4355	0.91	0/5901
2	Y	0.47	0/653	0.77	1/887 (0.1%)
2	Z	0.47	0/653	0.78	0/887
2	a	0.47	0/653	0.78	1/887 (0.1%)
2	b	0.47	0/653	0.77	1/887 (0.1%)
2	c	0.47	0/653	0.78	1/887 (0.1%)
2	d	0.48	0/653	0.78	1/887 (0.1%)
2	e	0.48	0/653	0.78	1/887 (0.1%)
2	f	0.47	0/653	0.78	1/887 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	g	0.47	0/653	0.78	1/887 (0.1%)
2	h	0.47	0/653	0.77	1/887 (0.1%)
2	i	0.48	0/653	0.77	1/887 (0.1%)
2	j	0.47	0/653	0.77	0/887
All	All	0.45	0/112341	0.90	10/152247 (0.0%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	c	61	ASN	CB-CA-C	-5.58	101.53	110.79
2	e	61	ASN	CB-CA-C	-5.47	101.70	110.79
2	Y	61	ASN	CB-CA-C	-5.40	101.82	110.79
2	h	61	ASN	CB-CA-C	-5.36	101.89	110.79
2	d	61	ASN	CB-CA-C	-5.34	101.93	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4226	0	3941	52	1
1	B	4226	0	3941	51	0
1	C	4226	0	3941	52	0
1	D	4226	0	3941	75	0
1	E	4226	0	3941	49	0
1	F	4226	0	3941	46	0
1	G	4226	0	3941	71	2
1	H	4226	0	3941	80	0
1	I	4201	0	3921	101	0
1	J	4226	0	3941	62	1
1	K	4226	0	3941	70	0
1	L	4226	0	3941	53	0
1	M	4226	0	3941	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	4226	0	3941	51	0
1	O	4226	0	3941	51	0
1	P	4226	0	3941	55	0
1	Q	4226	0	3941	58	1
1	R	4237	0	3953	59	1
1	S	4226	0	3941	44	0
1	T	4226	0	3941	45	0
1	U	4226	0	3941	41	0
1	V	4226	0	3941	47	0
1	W	4226	0	3941	52	0
1	X	4226	0	3941	52	0
2	Y	640	0	627	5	0
2	Z	640	0	627	4	0
2	a	640	0	627	5	0
2	b	640	0	627	7	0
2	c	640	0	627	6	0
2	d	640	0	627	6	0
2	e	640	0	627	6	0
2	f	640	0	627	4	0
2	g	640	0	627	6	0
2	h	640	0	627	7	0
2	i	640	0	627	6	0
2	j	640	0	627	10	0
3	A	344	0	236	11	0
3	B	344	0	236	12	0
3	C	344	0	236	12	0
3	D	344	0	237	14	0
3	E	344	0	236	13	0
3	F	344	0	236	12	0
3	G	344	0	236	15	0
3	H	344	0	236	11	0
3	I	344	0	237	24	0
3	J	344	0	236	12	0
3	K	344	0	236	15	0
3	L	344	0	236	14	0
3	M	344	0	236	11	0
3	N	344	0	236	14	0
3	O	344	0	236	11	0
3	P	344	0	236	13	0
3	Q	344	0	236	17	0
3	R	344	0	236	14	0
3	S	344	0	236	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	T	344	0	236	11	0
3	U	344	0	236	14	0
3	V	344	0	236	14	0
3	W	344	0	236	17	0
3	X	344	0	236	14	0
4	A	15	0	0	0	0
4	B	10	0	0	1	0
4	C	15	0	0	0	0
4	D	5	0	0	0	0
4	E	10	0	0	0	0
4	F	10	0	0	0	0
4	G	30	0	0	3	0
4	H	25	0	0	1	0
4	I	20	0	0	0	0
4	J	15	0	0	2	0
4	K	15	0	0	0	0
4	L	20	0	0	1	0
4	M	20	0	0	0	0
4	N	15	0	0	1	0
4	O	15	0	0	0	0
4	P	5	0	0	0	0
4	Q	15	0	0	1	0
4	R	15	0	0	0	0
4	S	10	0	0	0	0
4	T	5	0	0	0	0
4	U	15	0	0	0	0
4	V	15	0	0	0	0
4	W	5	0	0	0	0
4	X	15	0	0	1	0
4	Y	10	0	0	0	0
4	a	5	0	0	0	0
4	c	5	0	0	0	0
5	A	18	0	24	2	0
5	D	6	0	8	0	0
5	G	12	0	16	2	0
5	H	12	0	16	20	0
5	I	18	0	24	5	0
5	J	12	0	16	3	0
5	K	24	0	32	14	0
5	L	6	0	8	1	0
6	H	1	0	0	0	0
6	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	1	0	0	0	0
6	X	1	0	0	0	0
7	A	33	0	0	3	0
7	B	40	0	0	2	0
7	C	36	0	0	0	0
7	D	21	0	0	0	0
7	E	21	0	0	2	0
7	F	24	0	0	0	0
7	G	78	0	0	8	0
7	H	70	0	0	4	0
7	I	62	0	0	1	0
7	J	78	0	0	4	0
7	K	57	0	0	5	0
7	L	69	0	0	1	0
7	M	27	0	0	1	0
7	N	37	0	0	0	0
7	O	40	0	0	0	0
7	P	50	0	0	3	0
7	Q	48	0	0	4	0
7	R	49	0	0	5	0
7	S	4	0	0	0	0
7	T	15	0	0	1	0
7	U	15	0	0	0	0
7	V	17	0	0	0	0
7	W	12	0	0	0	0
7	X	13	0	0	0	0
7	Y	2	0	0	0	0
7	Z	1	0	0	0	0
7	a	2	0	0	0	0
7	b	2	0	0	0	0
7	c	2	0	0	1	0
7	d	2	0	0	0	0
7	e	2	0	0	0	0
7	f	2	0	0	0	0
7	g	1	0	0	0	0
7	i	2	0	0	0	0
7	j	1	0	0	0	0
All	All	118753	0	107910	1326	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1326 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:H:267:HIS:HD1	5:H:614:GOL:H11	1.06	1.14
1:H:267:HIS:ND1	5:H:614:GOL:H11	1.65	1.12
1:H:267:HIS:HD1	5:H:614:GOL:C1	1.74	1.01
1:H:267:HIS:CE1	5:H:614:GOL:H31	2.01	0.96
1:I:406:ILE:H	1:I:410:HIS:HD2	1.14	0.95

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LYS:O	1:R:496:SER:OG[1_545]	1.83	0.37
1:G:42:HIS:NE2	1:J:496:SER:CB[2_555]	2.03	0.17
1:G:496:SER:OG	1:Q:491:LYS:O[1_655]	2.18	0.02

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	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	B	529/582 (91%)	514 (97%)	15 (3%)	0	100	100
1	C	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	D	529/582 (91%)	491 (93%)	36 (7%)	2 (0%)	30	60
1	E	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	F	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
1	G	529/582 (91%)	516 (98%)	13 (2%)	0	100	100
1	H	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	I	525/582 (90%)	502 (96%)	23 (4%)	0	100	100
1	J	529/582 (91%)	516 (98%)	13 (2%)	0	100	100
1	K	529/582 (91%)	513 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	M	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
1	N	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	O	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	P	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	Q	529/582 (91%)	514 (97%)	15 (3%)	0	100	100
1	R	530/582 (91%)	515 (97%)	15 (3%)	0	100	100
1	S	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	T	529/582 (91%)	511 (97%)	18 (3%)	0	100	100
1	U	529/582 (91%)	513 (97%)	16 (3%)	0	100	100
1	V	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	W	529/582 (91%)	512 (97%)	17 (3%)	0	100	100
1	X	529/582 (91%)	515 (97%)	14 (3%)	0	100	100
2	Y	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	Z	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
2	a	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	b	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	c	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	d	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	e	84/114 (74%)	82 (98%)	2 (2%)	0	100	100
2	f	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	g	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	h	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	i	84/114 (74%)	83 (99%)	1 (1%)	0	100	100
2	j	84/114 (74%)	79 (94%)	5 (6%)	0	100	100
All	All	13701/15336 (89%)	13279 (97%)	420 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	256	HIS
1	D	106	VAL

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	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	B	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	C	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	D	451/491 (92%)	435 (96%)	16 (4%)	32	67
1	E	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	F	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	G	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	H	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	I	449/491 (91%)	429 (96%)	20 (4%)	24	58
1	J	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	K	451/491 (92%)	446 (99%)	5 (1%)	65	87
1	L	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	M	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	N	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	O	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	P	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	Q	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	R	452/491 (92%)	448 (99%)	4 (1%)	70	89
1	S	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	T	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	U	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	V	451/491 (92%)	448 (99%)	3 (1%)	76	91
1	W	451/491 (92%)	447 (99%)	4 (1%)	70	89
1	X	451/491 (92%)	446 (99%)	5 (1%)	65	87
2	Y	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	Z	68/86 (79%)	65 (96%)	3 (4%)	25	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	a	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	b	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	c	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	d	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	e	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	f	68/86 (79%)	66 (97%)	2 (3%)	37	73
2	g	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	h	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	i	68/86 (79%)	65 (96%)	3 (4%)	25	59
2	j	68/86 (79%)	67 (98%)	1 (2%)	57	84
All	All	11639/12816 (91%)	11485 (99%)	154 (1%)	61	86

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	42	HIS
2	f	79	GLU
1	X	42	HIS
2	a	79	GLU
2	i	54	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 233 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	478	GLN
1	X	246	GLN
1	P	102	ASN
1	X	179	GLN
1	U	520	ASN

5.3.3 RNA

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 286 ligands modelled in this entry, 4 are monoatomic - leaving 282 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	$\#\|Z\| > 2$
3	HEC	A	604	1	50,50,50	1.76	12 (24%)	68,82,82	1.61	14 (20%)
5	GOL	I	615	-	5,5,5	0.33	0	5,5,5	0.36	0
4	SO4	A	610	-	4,4,4	0.32	0	6,6,6	0.14	0
3	HEC	O	603	1,7	50,50,50	2.63	15 (30%)	68,82,82	2.79	21 (30%)
4	SO4	V	609	-	4,4,4	0.40	0	6,6,6	0.28	0
4	SO4	G	610	-	4,4,4	0.29	0	6,6,6	0.09	0
3	HEC	T	600	1	50,50,50	1.71	8 (16%)	68,82,82	1.72	19 (27%)
3	HEC	Q	607	1	50,50,50	1.69	8 (16%)	68,82,82	1.62	14 (20%)
4	SO4	Q	611	-	4,4,4	0.35	0	6,6,6	0.14	0
3	HEC	U	601	1	50,50,50	1.71	8 (16%)	68,82,82	1.65	15 (22%)
3	HEC	C	601	1	50,50,50	1.71	8 (16%)	68,82,82	1.66	14 (20%)
3	HEC	I	603	1,7	50,50,50	2.57	14 (28%)	68,82,82	3.26	24 (35%)
3	HEC	R	605	1	50,50,50	1.70	9 (18%)	68,82,82	1.68	19 (27%)
3	HEC	J	606	1	50,50,50	1.72	8 (16%)	68,82,82	1.62	14 (20%)
4	SO4	V	611	-	4,4,4	0.34	0	6,6,6	0.05	0
3	HEC	R	600	1	50,50,50	1.72	8 (16%)	68,82,82	1.66	16 (23%)
4	SO4	L	611	-	4,4,4	0.33	0	6,6,6	0.09	0
3	HEC	F	605	1	50,50,50	1.73	10 (20%)	68,82,82	1.65	18 (26%)
3	HEC	P	600	1	50,50,50	1.73	8 (16%)	68,82,82	1.71	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	HEC	L	605	1	50,50,50	1.71	8 (16%)	68,82,82	1.70	17 (25%)
3	HEC	J	600	1	50,50,50	1.68	9 (18%)	68,82,82	1.71	18 (26%)
3	HEC	K	602	1	50,50,50	1.72	9 (18%)	68,82,82	1.63	13 (19%)
3	HEC	F	606	1	50,50,50	1.73	9 (18%)	68,82,82	1.64	15 (22%)
3	HEC	K	606	1	50,50,50	1.73	9 (18%)	68,82,82	1.64	17 (25%)
3	HEC	R	604	1	50,50,50	1.72	10 (20%)	68,82,82	1.67	14 (20%)
4	SO4	G	609	-	4,4,4	0.35	0	6,6,6	0.08	0
3	HEC	G	601	1	50,50,50	1.69	7 (14%)	68,82,82	1.68	15 (22%)
4	SO4	J	611	-	4,4,4	0.29	0	6,6,6	0.09	0
5	GOL	J	613	-	5,5,5	0.27	0	5,5,5	0.49	0
3	HEC	X	601	1	50,50,50	1.72	8 (16%)	68,82,82	1.68	15 (22%)
3	HEC	J	605	1	50,50,50	1.73	10 (20%)	68,82,82	1.66	18 (26%)
3	HEC	Q	604	1	50,50,50	1.72	9 (18%)	68,82,82	1.64	14 (20%)
4	SO4	U	611	-	4,4,4	0.32	0	6,6,6	0.08	0
3	HEC	V	602	1	50,50,50	1.73	9 (18%)	68,82,82	1.62	13 (19%)
3	HEC	K	605	1	50,50,50	1.75	9 (18%)	68,82,82	1.63	16 (23%)
3	HEC	X	606	1	50,50,50	1.73	9 (18%)	68,82,82	1.62	15 (22%)
4	SO4	I	611	-	4,4,4	0.34	0	6,6,6	0.07	0
3	HEC	X	604	1	50,50,50	1.75	11 (22%)	68,82,82	1.64	15 (22%)
4	SO4	Y	202	-	4,4,4	0.33	0	6,6,6	0.11	0
3	HEC	S	606	1	50,50,50	1.75	9 (18%)	68,82,82	1.61	15 (22%)
4	SO4	K	609	-	4,4,4	0.21	0	6,6,6	0.34	0
3	HEC	N	600	1	50,50,50	1.72	9 (18%)	68,82,82	1.71	18 (26%)
3	HEC	P	604	1	50,50,50	1.70	8 (16%)	68,82,82	1.67	16 (23%)
4	SO4	G	611	-	4,4,4	0.34	0	6,6,6	0.10	0
3	HEC	F	607	1	50,50,50	1.73	9 (18%)	68,82,82	1.57	11 (16%)
3	HEC	J	602	1	50,50,50	1.77	10 (20%)	68,82,82	1.60	14 (20%)
3	HEC	C	603	1	50,50,50	2.56	15 (30%)	68,82,82	2.77	16 (23%)
4	SO4	K	611	-	4,4,4	0.36	0	6,6,6	0.06	0
3	HEC	L	607	1	50,50,50	1.71	9 (18%)	68,82,82	1.58	12 (17%)
5	GOL	I	613	-	5,5,5	0.26	0	5,5,5	0.24	0
3	HEC	L	602	1	50,50,50	1.73	10 (20%)	68,82,82	1.60	14 (20%)
3	HEC	T	601	1	50,50,50	1.73	9 (18%)	68,82,82	1.65	14 (20%)
4	SO4	H	611	-	4,4,4	0.32	0	6,6,6	0.21	0
5	GOL	K	614	-	5,5,5	0.18	0	5,5,5	0.37	0
3	HEC	F	604	1	50,50,50	1.73	9 (18%)	68,82,82	1.64	13 (19%)
3	HEC	W	606	1	50,50,50	1.75	9 (18%)	68,82,82	1.63	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	W	602	1	50,50,50	1.73	9 (18%)	68,82,82	1.67	14 (20%)
4	SO4	R	611	-	4,4,4	0.31	0	6,6,6	0.06	0
3	HEC	A	602	1	50,50,50	1.75	10 (20%)	68,82,82	1.67	16 (23%)
4	SO4	O	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	A	607	1	50,50,50	1.78	9 (18%)	68,82,82	1.52	12 (17%)
3	HEC	P	605	1	50,50,50	1.74	10 (20%)	68,82,82	1.67	16 (23%)
3	HEC	C	602	1	50,50,50	1.72	9 (18%)	68,82,82	1.64	15 (22%)
4	SO4	M	610	-	4,4,4	0.32	0	6,6,6	0.09	0
3	HEC	D	603	1,7	50,50,50	2.62	14 (28%)	68,82,82	2.98	22 (32%)
5	GOL	H	614	-	5,5,5	0.41	0	5,5,5	0.77	0
3	HEC	S	603	1,7	50,50,50	2.66	14 (28%)	68,82,82	2.79	21 (30%)
3	HEC	B	601	1	50,50,50	1.75	9 (18%)	68,82,82	1.68	14 (20%)
3	HEC	U	605	1	50,50,50	1.73	9 (18%)	68,82,82	1.68	16 (23%)
3	HEC	R	601	1	50,50,50	1.70	7 (14%)	68,82,82	1.66	14 (20%)
3	HEC	K	600	1	50,50,50	1.68	8 (16%)	68,82,82	1.71	18 (26%)
3	HEC	D	606	1	50,50,50	1.73	9 (18%)	68,82,82	1.59	15 (22%)
3	HEC	N	606	1	50,50,50	1.72	11 (22%)	68,82,82	1.63	15 (22%)
3	HEC	V	604	1	50,50,50	1.74	9 (18%)	68,82,82	1.67	14 (20%)
3	HEC	R	602	1	50,50,50	1.70	9 (18%)	68,82,82	1.63	14 (20%)
3	HEC	R	607	1	50,50,50	1.75	9 (18%)	68,82,82	1.61	15 (22%)
3	HEC	D	604	1	50,50,50	1.74	10 (20%)	68,82,82	1.67	11 (16%)
3	HEC	G	607	1	50,50,50	1.72	10 (20%)	68,82,82	1.58	12 (17%)
4	SO4	a	201	-	4,4,4	0.34	0	6,6,6	0.08	0
3	HEC	M	605	1	50,50,50	1.71	10 (20%)	68,82,82	1.71	16 (23%)
4	SO4	Q	610	-	4,4,4	0.33	0	6,6,6	0.11	0
3	HEC	E	605	1	50,50,50	1.74	9 (18%)	68,82,82	1.63	15 (22%)
3	HEC	E	602	1	50,50,50	1.72	9 (18%)	68,82,82	1.68	15 (22%)
3	HEC	K	601	1	50,50,50	1.76	10 (20%)	68,82,82	1.71	14 (20%)
3	HEC	F	600	1	50,50,50	1.74	9 (18%)	68,82,82	1.69	18 (26%)
3	HEC	E	606	1	50,50,50	1.73	9 (18%)	68,82,82	1.63	15 (22%)
3	HEC	F	601	1	50,50,50	1.73	9 (18%)	68,82,82	1.67	14 (20%)
4	SO4	B	610	-	4,4,4	0.37	0	6,6,6	0.09	0
3	HEC	B	605	1	50,50,50	1.72	10 (20%)	68,82,82	1.65	16 (23%)
4	SO4	N	611	-	4,4,4	0.33	0	6,6,6	0.09	0
3	HEC	N	604	1	50,50,50	1.72	9 (18%)	68,82,82	1.66	14 (20%)
4	SO4	H	612	-	4,4,4	0.35	0	6,6,6	0.07	0
5	GOL	G	615	-	5,5,5	0.45	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	K	607	1	50,50,50	1.77	10 (20%)	68,82,82	1.56	11 (16%)
4	SO4	N	609	-	4,4,4	0.37	0	6,6,6	0.13	0
3	HEC	L	606	1	50,50,50	1.69	9 (18%)	68,82,82	1.69	19 (27%)
4	SO4	I	609	-	4,4,4	0.35	0	6,6,6	0.34	0
4	SO4	B	609	-	4,4,4	0.30	0	6,6,6	0.13	0
4	SO4	C	609	-	4,4,4	0.32	0	6,6,6	0.14	0
3	HEC	H	601	1	50,50,50	1.72	10 (20%)	68,82,82	1.71	15 (22%)
3	HEC	A	606	1	50,50,50	1.73	8 (16%)	68,82,82	1.65	16 (23%)
4	SO4	U	610	-	4,4,4	0.33	0	6,6,6	0.07	0
3	HEC	T	605	1	50,50,50	1.73	9 (18%)	68,82,82	1.68	18 (26%)
4	SO4	K	610	-	4,4,4	0.34	0	6,6,6	0.10	0
3	HEC	T	607	1	50,50,50	1.72	10 (20%)	68,82,82	1.57	12 (17%)
3	HEC	V	601	1	50,50,50	1.71	8 (16%)	68,82,82	1.68	15 (22%)
4	SO4	F	610	-	4,4,4	0.33	0	6,6,6	0.08	0
4	SO4	M	609	-	4,4,4	0.35	0	6,6,6	0.09	0
3	HEC	H	603	1,7	50,50,50	2.57	14 (28%)	68,82,82	2.77	19 (27%)
3	HEC	A	600	1	50,50,50	1.70	8 (16%)	68,82,82	1.72	18 (26%)
3	HEC	V	605	1	50,50,50	1.75	10 (20%)	68,82,82	1.66	18 (26%)
4	SO4	X	609	-	4,4,4	0.33	0	6,6,6	0.14	0
3	HEC	E	607	1	50,50,50	1.73	12 (24%)	68,82,82	1.61	12 (17%)
3	HEC	G	600	1	50,50,50	1.71	8 (16%)	68,82,82	1.70	18 (26%)
3	HEC	J	603	1,7	50,50,50	2.58	14 (28%)	68,82,82	2.81	20 (29%)
3	HEC	V	606	1	50,50,50	1.74	10 (20%)	68,82,82	1.68	18 (26%)
4	SO4	D	609	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	H	609	-	4,4,4	0.36	0	6,6,6	0.10	0
5	GOL	A	613	-	5,5,5	0.41	0	5,5,5	0.35	0
4	SO4	G	612	-	4,4,4	0.34	0	6,6,6	0.12	0
3	HEC	J	607	1	50,50,50	1.76	10 (20%)	68,82,82	1.55	11 (16%)
3	HEC	M	600	1	50,50,50	1.72	8 (16%)	68,82,82	1.69	18 (26%)
3	HEC	E	600	1	50,50,50	1.73	8 (16%)	68,82,82	1.70	16 (23%)
3	HEC	K	603	1,7	50,50,50	2.59	15 (30%)	68,82,82	2.77	20 (29%)
3	HEC	W	605	1	50,50,50	1.76	12 (24%)	68,82,82	1.64	17 (25%)
3	HEC	P	606	1	50,50,50	1.71	8 (16%)	68,82,82	1.63	14 (20%)
4	SO4	S	610	-	4,4,4	0.35	0	6,6,6	0.08	0
4	SO4	H	610	-	4,4,4	0.36	0	6,6,6	0.05	0
3	HEC	C	607	1	50,50,50	1.72	9 (18%)	68,82,82	1.54	11 (16%)
4	SO4	V	610	-	4,4,4	0.35	0	6,6,6	0.12	0
4	SO4	J	609	-	4,4,4	0.36	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	F	602	1	50,50,50	1.73	9 (18%)	68,82,82	1.62	16 (23%)
3	HEC	B	600	1	50,50,50	1.72	10 (20%)	68,82,82	1.71	19 (27%)
3	HEC	C	605	1	50,50,50	1.69	9 (18%)	68,82,82	1.71	18 (26%)
3	HEC	O	607	1	50,50,50	1.70	7 (14%)	68,82,82	1.60	13 (19%)
3	HEC	U	603	1,7	50,50,50	2.59	14 (28%)	68,82,82	2.77	20 (29%)
3	HEC	U	606	1	50,50,50	1.73	9 (18%)	68,82,82	1.64	14 (20%)
3	HEC	H	604	1	50,50,50	1.75	10 (20%)	68,82,82	1.61	14 (20%)
3	HEC	K	604	1	50,50,50	1.72	10 (20%)	68,82,82	1.66	14 (20%)
4	SO4	C	610	-	4,4,4	0.34	0	6,6,6	0.12	0
3	HEC	N	601	1	50,50,50	1.75	9 (18%)	68,82,82	1.64	13 (19%)
3	HEC	D	601	1	50,50,50	1.72	9 (18%)	68,82,82	1.61	12 (17%)
3	HEC	G	602	1	50,50,50	1.69	10 (20%)	68,82,82	1.64	14 (20%)
3	HEC	V	607	1	50,50,50	1.73	10 (20%)	68,82,82	1.56	11 (16%)
3	HEC	X	607	1	50,50,50	1.73	8 (16%)	68,82,82	1.56	12 (17%)
4	SO4	M	612	-	4,4,4	0.34	0	6,6,6	0.14	0
3	HEC	Q	606	1	50,50,50	1.72	10 (20%)	68,82,82	1.62	15 (22%)
3	HEC	I	601	1	50,50,50	1.77	12 (24%)	68,82,82	1.74	17 (25%)
4	SO4	C	611	-	4,4,4	0.34	0	6,6,6	0.16	0
3	HEC	L	601	1	50,50,50	1.67	8 (16%)	68,82,82	1.66	15 (22%)
3	HEC	P	603	1,7	50,50,50	2.58	14 (28%)	68,82,82	2.79	20 (29%)
3	HEC	O	601	1	50,50,50	1.73	10 (20%)	68,82,82	1.69	14 (20%)
4	SO4	Q	609	-	4,4,4	0.34	0	6,6,6	0.14	0
4	SO4	S	609	-	4,4,4	0.34	0	6,6,6	0.05	0
3	HEC	M	601	1	50,50,50	1.73	9 (18%)	68,82,82	1.65	14 (20%)
4	SO4	R	609	-	4,4,4	0.32	0	6,6,6	0.25	0
3	HEC	E	601	1	50,50,50	1.71	8 (16%)	68,82,82	1.67	14 (20%)
5	GOL	H	615	-	5,5,5	0.46	0	5,5,5	0.57	0
5	GOL	I	614	-	5,5,5	0.23	0	5,5,5	0.19	0
5	GOL	K	615	-	5,5,5	0.33	0	5,5,5	0.20	0
3	HEC	T	603	1	50,50,50	2.70	14 (28%)	68,82,82	2.82	21 (30%)
3	HEC	M	607	1	50,50,50	1.74	9 (18%)	68,82,82	1.61	14 (20%)
4	SO4	N	610	-	4,4,4	0.35	0	6,6,6	0.13	0
3	HEC	H	605	1	50,50,50	1.73	9 (18%)	68,82,82	1.65	18 (26%)
3	HEC	L	600	1	50,50,50	1.67	7 (14%)	68,82,82	1.70	17 (25%)
4	SO4	H	613	-	4,4,4	0.33	0	6,6,6	0.23	0
3	HEC	C	600	1	50,50,50	1.71	8 (16%)	68,82,82	1.70	17 (25%)
3	HEC	J	604	1	50,50,50	1.71	10 (20%)	68,82,82	1.68	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	M	604	1	50,50,50	1.73	10 (20%)	68,82,82	1.67	14 (20%)
4	SO4	I	612	-	4,4,4	0.36	0	6,6,6	0.06	0
3	HEC	O	600	1	50,50,50	1.71	9 (18%)	68,82,82	1.71	19 (27%)
4	SO4	O	609	-	4,4,4	0.36	0	6,6,6	0.08	0
4	SO4	W	609	-	4,4,4	0.35	0	6,6,6	0.10	0
4	SO4	O	611	-	4,4,4	0.32	0	6,6,6	0.08	0
3	HEC	T	606	1	50,50,50	1.73	9 (18%)	68,82,82	1.64	14 (20%)
3	HEC	I	600	1	50,50,50	1.70	8 (16%)	68,82,82	1.70	16 (23%)
3	HEC	Q	601	1	50,50,50	1.74	8 (16%)	68,82,82	1.68	14 (20%)
3	HEC	D	605	1	50,50,50	1.73	9 (18%)	68,82,82	1.62	15 (22%)
3	HEC	B	603	1	50,50,50	2.61	14 (28%)	68,82,82	2.79	18 (26%)
3	HEC	S	607	1	50,50,50	1.73	9 (18%)	68,82,82	1.57	12 (17%)
4	SO4	E	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	D	602	1	50,50,50	1.72	10 (20%)	68,82,82	1.66	17 (25%)
3	HEC	R	603	1	50,50,50	2.61	15 (30%)	68,82,82	2.76	18 (26%)
3	HEC	H	607	1	50,50,50	1.71	11 (22%)	68,82,82	1.61	13 (19%)
3	HEC	G	604	1	50,50,50	1.72	8 (16%)	68,82,82	1.70	15 (22%)
5	GOL	K	612	-	5,5,5	0.39	0	5,5,5	0.33	0
3	HEC	V	600	1	50,50,50	1.73	8 (16%)	68,82,82	1.70	18 (26%)
3	HEC	F	603	1,7	50,50,50	2.61	14 (28%)	68,82,82	2.85	19 (27%)
3	HEC	S	604	1	50,50,50	1.75	11 (22%)	68,82,82	1.64	14 (20%)
4	SO4	X	611	-	4,4,4	0.34	0	6,6,6	0.07	0
3	HEC	W	607	1	50,50,50	1.76	11 (22%)	68,82,82	1.59	13 (19%)
3	HEC	B	602	1	50,50,50	1.71	9 (18%)	68,82,82	1.66	14 (20%)
3	HEC	B	606	1	50,50,50	1.72	10 (20%)	68,82,82	1.69	18 (26%)
4	SO4	F	609	-	4,4,4	0.34	0	6,6,6	0.13	0
3	HEC	B	604	1	50,50,50	1.70	10 (20%)	68,82,82	1.70	15 (22%)
4	SO4	J	610	-	4,4,4	0.32	0	6,6,6	0.13	0
4	SO4	T	609	-	4,4,4	0.35	0	6,6,6	0.08	0
3	HEC	G	603	1,7	50,50,50	2.62	15 (30%)	68,82,82	2.79	18 (26%)
3	HEC	M	603	1,7	50,50,50	2.64	16 (32%)	68,82,82	2.80	18 (26%)
3	HEC	X	603	1,7	50,50,50	2.63	14 (28%)	68,82,82	2.84	22 (32%)
3	HEC	M	602	1	50,50,50	1.76	11 (22%)	68,82,82	1.63	15 (22%)
3	HEC	S	601	1	50,50,50	1.75	9 (18%)	68,82,82	1.66	15 (22%)
3	HEC	N	605	1	50,50,50	1.74	11 (22%)	68,82,82	1.69	17 (25%)
3	HEC	U	600	1	50,50,50	1.72	8 (16%)	68,82,82	1.68	18 (26%)
3	HEC	N	602	1	50,50,50	1.77	9 (18%)	68,82,82	1.64	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	GOL	L	613	-	5,5,5	0.25	0	5,5,5	0.35	0
3	HEC	B	607	1	50,50,50	1.75	10 (20%)	68,82,82	1.61	14 (20%)
3	HEC	E	604	1	50,50,50	1.73	10 (20%)	68,82,82	1.66	16 (23%)
3	HEC	I	605	1	50,50,50	1.72	10 (20%)	68,82,82	1.72	16 (23%)
5	GOL	J	612	-	5,5,5	0.50	0	5,5,5	0.57	0
3	HEC	W	603	1,7	50,50,50	2.60	14 (28%)	68,82,82	2.80	21 (30%)
3	HEC	Q	605	1	50,50,50	1.73	10 (20%)	68,82,82	1.64	15 (22%)
3	HEC	W	601	1	50,50,50	1.74	10 (20%)	68,82,82	1.62	15 (22%)
5	GOL	G	616	-	5,5,5	0.19	0	5,5,5	0.42	0
3	HEC	D	600	1	50,50,50	1.75	9 (18%)	68,82,82	1.67	18 (26%)
3	HEC	H	600	1	50,50,50	1.72	9 (18%)	68,82,82	1.74	18 (26%)
3	HEC	G	605	1	50,50,50	1.66	8 (16%)	68,82,82	1.69	19 (27%)
3	HEC	S	600	1	50,50,50	1.76	10 (20%)	68,82,82	1.68	20 (29%)
4	SO4	X	610	-	4,4,4	0.33	0	6,6,6	0.05	0
4	SO4	A	609	-	4,4,4	0.30	0	6,6,6	0.12	0
3	HEC	X	605	1	50,50,50	1.74	9 (18%)	68,82,82	1.64	17 (25%)
5	GOL	A	612	-	5,5,5	0.28	0	5,5,5	0.28	0
4	SO4	G	613	-	4,4,4	0.29	0	6,6,6	0.37	0
3	HEC	L	603	1,7	50,50,50	2.53	14 (28%)	68,82,82	2.78	16 (23%)
3	HEC	I	602	1	50,50,50	1.74	9 (18%)	68,82,82	1.63	17 (25%)
4	SO4	c	201	-	4,4,4	0.35	0	6,6,6	0.09	0
5	GOL	K	613	-	5,5,5	0.23	0	5,5,5	0.34	0
3	HEC	W	604	1	50,50,50	1.75	10 (20%)	68,82,82	1.71	15 (22%)
3	HEC	C	606	1	50,50,50	1.73	8 (16%)	68,82,82	1.66	13 (19%)
3	HEC	H	602	1	50,50,50	1.72	9 (18%)	68,82,82	1.58	14 (20%)
3	HEC	H	606	1	50,50,50	1.75	9 (18%)	68,82,82	1.61	14 (20%)
3	HEC	O	602	1	50,50,50	1.71	9 (18%)	68,82,82	1.64	13 (19%)
3	HEC	A	603	1,7	50,50,50	2.63	14 (28%)	68,82,82	2.82	20 (29%)
3	HEC	L	604	1	50,50,50	1.73	9 (18%)	68,82,82	1.66	14 (20%)
3	HEC	W	600	1	50,50,50	1.72	9 (18%)	68,82,82	1.67	17 (25%)
3	HEC	C	604	1	50,50,50	1.74	9 (18%)	68,82,82	1.67	12 (17%)
3	HEC	N	607	1	50,50,50	1.74	8 (16%)	68,82,82	1.55	12 (17%)
3	HEC	O	604	1	50,50,50	1.73	9 (18%)	68,82,82	1.60	14 (20%)
5	GOL	A	614	-	5,5,5	0.35	0	5,5,5	0.18	0
4	SO4	P	609	-	4,4,4	0.33	0	6,6,6	0.14	0
3	HEC	I	607	1	50,50,50	1.72	10 (20%)	68,82,82	1.60	13 (19%)
3	HEC	Q	603	1,7	50,50,50	2.65	15 (30%)	68,82,82	2.85	19 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	I	604	1	50,50,50	1.75	9 (18%)	68,82,82	1.62	13 (19%)
3	HEC	U	607	1	50,50,50	1.72	9 (18%)	68,82,82	1.58	13 (19%)
3	HEC	U	602	1	50,50,50	1.74	10 (20%)	68,82,82	1.65	15 (22%)
4	SO4	M	611	-	4,4,4	0.35	0	6,6,6	0.11	0
4	SO4	A	611	-	4,4,4	0.32	0	6,6,6	0.16	0
4	SO4	U	609	-	4,4,4	0.32	0	6,6,6	0.26	0
3	HEC	U	604	1	50,50,50	1.72	10 (20%)	68,82,82	1.69	13 (19%)
3	HEC	A	605	1	50,50,50	1.73	9 (18%)	68,82,82	1.67	18 (26%)
3	HEC	Q	600	1	50,50,50	1.72	9 (18%)	68,82,82	1.69	17 (25%)
4	SO4	I	610	-	4,4,4	0.35	0	6,6,6	0.05	0
3	HEC	J	601	1	50,50,50	1.72	9 (18%)	68,82,82	1.67	15 (22%)
3	HEC	E	603	1,7	50,50,50	2.63	14 (28%)	68,82,82	2.81	22 (32%)
3	HEC	N	603	1,7	50,50,50	2.63	14 (28%)	68,82,82	2.79	20 (29%)
3	HEC	D	607	1	50,50,50	1.74	10 (20%)	68,82,82	1.62	15 (22%)
3	HEC	X	600	1	50,50,50	1.70	7 (14%)	68,82,82	1.73	20 (29%)
3	HEC	P	607	1	50,50,50	1.71	9 (18%)	68,82,82	1.58	12 (17%)
4	SO4	E	609	-	4,4,4	0.38	0	6,6,6	0.36	0
3	HEC	S	605	1	50,50,50	1.73	9 (18%)	68,82,82	1.63	18 (26%)
3	HEC	A	601	1	50,50,50	1.70	7 (14%)	68,82,82	1.68	14 (20%)
3	HEC	R	606	1	50,50,50	1.73	11 (22%)	68,82,82	1.70	17 (25%)
5	GOL	D	610	-	5,5,5	0.29	0	5,5,5	0.23	0
3	HEC	P	602	1	50,50,50	1.71	8 (16%)	68,82,82	1.62	13 (19%)
4	SO4	G	614	-	4,4,4	0.37	0	6,6,6	0.15	0
3	HEC	O	605	1	50,50,50	1.76	9 (18%)	68,82,82	1.69	16 (23%)
3	HEC	I	606	1	50,50,50	1.72	9 (18%)	68,82,82	1.74	16 (23%)
4	SO4	L	609	-	4,4,4	0.34	0	6,6,6	0.13	0
4	SO4	R	610	-	4,4,4	0.35	0	6,6,6	0.10	0
3	HEC	O	606	1	50,50,50	1.71	9 (18%)	68,82,82	1.67	20 (29%)
3	HEC	Q	602	1	50,50,50	1.72	8 (16%)	68,82,82	1.64	15 (22%)
4	SO4	L	610	-	4,4,4	0.30	0	6,6,6	0.16	0
4	SO4	L	612	-	4,4,4	0.36	0	6,6,6	0.10	0
3	HEC	S	602	1	50,50,50	1.71	9 (18%)	68,82,82	1.64	16 (23%)
4	SO4	Y	201	-	4,4,4	0.32	0	6,6,6	0.11	0
3	HEC	G	606	1	50,50,50	1.71	10 (20%)	68,82,82	1.69	19 (27%)
3	HEC	M	606	1	50,50,50	1.72	11 (22%)	68,82,82	1.69	15 (22%)
3	HEC	V	603	1,7	50,50,50	2.60	14 (28%)	68,82,82	2.77	18 (26%)
3	HEC	T	602	1	50,50,50	1.75	10 (20%)	68,82,82	1.61	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEC	P	601	1	50,50,50	1.73	9 (18%)	68,82,82	1.64	13 (19%)
3	HEC	X	602	1	50,50,50	1.72	9 (18%)	68,82,82	1.68	15 (22%)
3	HEC	T	604	1	50,50,50	1.73	11 (22%)	68,82,82	1.65	13 (19%)

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
3	HEC	A	604	1	1/1/3/7	6/14/54/54	-
5	GOL	I	615	-	-	2/4/4/4	-
3	HEC	O	603	1,7	-	2/14/54/54	-
3	HEC	T	600	1	1/1/3/7	7/14/54/54	-
3	HEC	Q	607	1	1/1/3/7	7/14/54/54	-
3	HEC	U	601	1	1/1/3/7	5/14/54/54	-
3	HEC	C	601	1	1/1/3/7	5/14/54/54	-
3	HEC	R	605	1	1/1/3/7	6/14/54/54	-
3	HEC	I	603	1,7	-	6/14/54/54	-
3	HEC	J	606	1	1/1/3/7	2/14/54/54	-
3	HEC	R	600	1	1/1/3/7	8/14/54/54	-
3	HEC	F	605	1	1/1/3/7	6/14/54/54	-
3	HEC	P	600	1	1/1/3/7	8/14/54/54	-
3	HEC	L	605	1	1/1/3/7	7/14/54/54	-
3	HEC	J	600	1	1/1/3/7	6/14/54/54	-
3	HEC	K	602	1	1/1/3/7	5/14/54/54	-
3	HEC	F	606	1	1/1/3/7	2/14/54/54	-
3	HEC	K	606	1	1/1/3/7	3/14/54/54	-
3	HEC	R	604	1	1/1/3/7	6/14/54/54	-
3	HEC	G	601	1	1/1/3/7	4/14/54/54	-
5	GOL	J	613	-	-	2/4/4/4	-
3	HEC	X	601	1	1/1/3/7	5/14/54/54	-
3	HEC	J	605	1	1/1/3/7	6/14/54/54	-
3	HEC	Q	604	1	1/1/3/7	6/14/54/54	-
3	HEC	V	602	1	1/1/3/7	5/14/54/54	-
3	HEC	K	605	1	1/1/3/7	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	X	606	1	1/1/3/7	2/14/54/54	-
3	HEC	X	604	1	1/1/3/7	6/14/54/54	-
3	HEC	S	606	1	1/1/3/7	2/14/54/54	-
3	HEC	N	600	1	1/1/3/7	6/14/54/54	-
3	HEC	P	604	1	1/1/3/7	6/14/54/54	-
3	HEC	F	607	1	1/1/3/7	4/14/54/54	-
3	HEC	J	602	1	1/1/3/7	5/14/54/54	-
3	HEC	C	603	1	-	1/14/54/54	-
5	GOL	K	614	-	-	4/4/4/4	-
3	HEC	L	607	1	1/1/3/7	5/14/54/54	-
5	GOL	I	613	-	-	4/4/4/4	-
3	HEC	L	602	1	1/1/3/7	5/14/54/54	-
3	HEC	T	601	1	1/1/3/7	5/14/54/54	-
3	HEC	F	604	1	1/1/3/7	6/14/54/54	-
3	HEC	W	606	1	1/1/3/7	2/14/54/54	-
3	HEC	W	602	1	1/1/3/7	5/14/54/54	-
3	HEC	A	602	1	1/1/3/7	5/14/54/54	-
3	HEC	A	607	1	1/1/3/7	6/14/54/54	-
3	HEC	P	605	1	1/1/3/7	6/14/54/54	-
3	HEC	C	602	1	1/1/3/7	5/14/54/54	-
3	HEC	D	603	1,7	-	5/14/54/54	-
5	GOL	H	614	-	-	4/4/4/4	-
3	HEC	S	603	1,7	-	3/14/54/54	-
3	HEC	B	601	1	1/1/3/7	5/14/54/54	-
3	HEC	U	605	1	1/1/3/7	6/14/54/54	-
3	HEC	R	601	1	1/1/3/7	4/14/54/54	-
3	HEC	K	600	1	1/1/3/7	8/14/54/54	-
3	HEC	D	606	1	1/1/3/7	2/14/54/54	-
3	HEC	N	606	1	1/1/3/7	3/14/54/54	-
3	HEC	V	604	1	1/1/3/7	6/14/54/54	-
3	HEC	R	602	1	1/1/3/7	5/14/54/54	-
3	HEC	R	607	1	1/1/3/7	7/14/54/54	-
3	HEC	D	604	1	1/1/3/7	5/14/54/54	-
3	HEC	G	607	1	1/1/3/7	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	M	605	1	1/1/3/7	8/14/54/54	-
3	HEC	E	605	1	1/1/3/7	7/14/54/54	-
3	HEC	E	602	1	1/1/3/7	5/14/54/54	-
3	HEC	K	601	1	1/1/3/7	5/14/54/54	-
3	HEC	F	600	1	1/1/3/7	7/14/54/54	-
3	HEC	E	606	1	1/1/3/7	2/14/54/54	-
3	HEC	F	601	1	1/1/3/7	4/14/54/54	-
3	HEC	B	605	1	1/1/3/7	6/14/54/54	-
3	HEC	N	604	1	1/1/3/7	6/14/54/54	-
5	GOL	G	615	-	-	2/4/4/4	-
3	HEC	K	607	1	1/1/3/7	7/14/54/54	-
3	HEC	L	606	1	1/1/3/7	2/14/54/54	-
3	HEC	H	601	1	1/1/3/7	6/14/54/54	-
3	HEC	A	606	1	1/1/3/7	2/14/54/54	-
3	HEC	T	605	1	1/1/3/7	6/14/54/54	-
3	HEC	T	607	1	1/1/3/7	5/14/54/54	-
3	HEC	V	601	1	1/1/3/7	5/14/54/54	-
3	HEC	H	603	1,7	-	3/14/54/54	-
3	HEC	A	600	1	1/1/3/7	6/14/54/54	-
3	HEC	V	605	1	1/1/3/7	6/14/54/54	-
3	HEC	E	607	1	1/1/3/7	7/14/54/54	-
3	HEC	G	600	1	1/1/3/7	6/14/54/54	-
3	HEC	V	606	1	1/1/3/7	2/14/54/54	-
3	HEC	J	603	1,7	-	2/14/54/54	-
5	GOL	A	613	-	-	2/4/4/4	-
3	HEC	J	607	1	1/1/3/7	6/14/54/54	-
3	HEC	M	600	1	1/1/3/7	8/14/54/54	-
3	HEC	E	600	1	1/1/3/7	7/14/54/54	-
3	HEC	W	605	1	1/1/3/7	6/14/54/54	-
3	HEC	K	603	1,7	-	3/14/54/54	-
3	HEC	P	606	1	1/1/3/7	2/14/54/54	-
3	HEC	C	607	1	1/1/3/7	6/14/54/54	-
3	HEC	F	602	1	1/1/3/7	5/14/54/54	-
3	HEC	B	600	1	1/1/3/7	8/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	C	605	1	1/1/3/7	6/14/54/54	-
3	HEC	O	607	1	1/1/3/7	7/14/54/54	-
3	HEC	U	603	1,7	-	1/14/54/54	-
3	HEC	U	606	1	1/1/3/7	2/14/54/54	-
3	HEC	H	604	1	1/1/3/7	6/14/54/54	-
3	HEC	K	604	1	1/1/3/7	6/14/54/54	-
3	HEC	N	601	1	1/1/3/7	4/14/54/54	-
3	HEC	D	601	1	1/1/3/7	4/14/54/54	-
3	HEC	G	602	1	1/1/3/7	5/14/54/54	-
3	HEC	V	607	1	1/1/3/7	7/14/54/54	-
3	HEC	X	607	1	1/1/3/7	6/14/54/54	-
3	HEC	Q	606	1	1/1/3/7	2/14/54/54	-
3	HEC	I	601	1	1/1/3/7	6/14/54/54	-
3	HEC	L	601	1	1/1/3/7	4/14/54/54	-
3	HEC	P	603	1,7	-	1/14/54/54	-
3	HEC	O	601	1	1/1/3/7	5/14/54/54	-
3	HEC	M	601	1	1/1/3/7	5/14/54/54	-
3	HEC	E	601	1	1/1/3/7	5/14/54/54	-
5	GOL	H	615	-	-	2/4/4/4	-
5	GOL	I	614	-	-	2/4/4/4	-
5	GOL	K	615	-	-	4/4/4/4	-
3	HEC	T	603	1	-	1/14/54/54	-
3	HEC	M	607	1	1/1/3/7	7/14/54/54	-
3	HEC	H	605	1	1/1/3/7	6/14/54/54	-
3	HEC	L	600	1	1/1/3/7	7/14/54/54	-
3	HEC	C	600	1	1/1/3/7	7/14/54/54	-
3	HEC	J	604	1	1/1/3/7	6/14/54/54	-
3	HEC	M	604	1	1/1/3/7	6/14/54/54	-
3	HEC	O	600	1	1/1/3/7	6/14/54/54	-
3	HEC	T	606	1	1/1/3/7	2/14/54/54	-
3	HEC	I	600	1	1/1/3/7	4/14/54/54	-
3	HEC	Q	601	1	1/1/3/7	5/14/54/54	-
3	HEC	D	605	1	1/1/3/7	8/14/54/54	-
3	HEC	S	607	1	1/1/3/7	7/14/54/54	-
3	HEC	B	603	1	-	1/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	D	602	1	1/1/3/7	4/14/54/54	-
3	HEC	R	603	1	-	1/14/54/54	-
3	HEC	H	607	1	1/1/3/7	6/14/54/54	-
3	HEC	G	604	1	1/1/3/7	6/14/54/54	-
5	GOL	K	612	-	-	2/4/4/4	-
3	HEC	V	600	1	1/1/3/7	7/14/54/54	-
3	HEC	F	603	1,7	-	1/14/54/54	-
3	HEC	S	604	1	1/1/3/7	6/14/54/54	-
3	HEC	W	607	1	1/1/3/7	6/14/54/54	-
3	HEC	B	602	1	1/1/3/7	5/14/54/54	-
3	HEC	B	606	1	1/1/3/7	3/14/54/54	-
3	HEC	B	604	1	1/1/3/7	6/14/54/54	-
3	HEC	G	603	1,7	-	3/14/54/54	-
3	HEC	M	603	1,7	-	3/14/54/54	-
3	HEC	X	603	1,7	-	3/14/54/54	-
3	HEC	M	602	1	1/1/3/7	5/14/54/54	-
3	HEC	S	601	1	1/1/3/7	4/14/54/54	-
3	HEC	N	605	1	1/1/3/7	7/14/54/54	-
3	HEC	U	600	1	1/1/3/7	6/14/54/54	-
3	HEC	N	602	1	1/1/3/7	5/14/54/54	-
5	GOL	L	613	-	-	2/4/4/4	-
3	HEC	B	607	1	1/1/3/7	7/14/54/54	-
3	HEC	E	604	1	1/1/3/7	6/14/54/54	-
3	HEC	I	605	1	1/1/3/7	9/14/54/54	-
5	GOL	J	612	-	-	4/4/4/4	-
3	HEC	W	603	1,7	-	3/14/54/54	-
3	HEC	Q	605	1	1/1/3/7	6/14/54/54	-
3	HEC	W	601	1	1/1/3/7	5/14/54/54	-
5	GOL	G	616	-	-	2/4/4/4	-
3	HEC	D	600	1	1/1/3/7	4/14/54/54	-
3	HEC	H	600	1	1/1/3/7	8/14/54/54	-
3	HEC	G	605	1	1/1/3/7	6/14/54/54	-
3	HEC	S	600	1	1/1/3/7	7/14/54/54	-
3	HEC	X	605	1	1/1/3/7	6/14/54/54	-
5	GOL	A	612	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	L	603	1,7	-	1/14/54/54	-
3	HEC	I	602	1	1/1/3/7	5/14/54/54	-
5	GOL	K	613	-	-	2/4/4/4	-
3	HEC	W	604	1	1/1/3/7	6/14/54/54	-
3	HEC	C	606	1	1/1/3/7	2/14/54/54	-
3	HEC	H	602	1	1/1/3/7	5/14/54/54	-
3	HEC	H	606	1	1/1/3/7	2/14/54/54	-
3	HEC	O	602	1	1/1/3/7	5/14/54/54	-
3	HEC	A	603	1,7	-	2/14/54/54	-
3	HEC	L	604	1	1/1/3/7	6/14/54/54	-
3	HEC	W	600	1	1/1/3/7	6/14/54/54	-
3	HEC	C	604	1	1/1/3/7	6/14/54/54	-
3	HEC	N	607	1	1/1/3/7	5/14/54/54	-
3	HEC	O	604	1	1/1/3/7	6/14/54/54	-
5	GOL	A	614	-	-	4/4/4/4	-
3	HEC	I	607	1	1/1/3/7	6/14/54/54	-
3	HEC	Q	603	1,7	-	2/14/54/54	-
3	HEC	I	604	1	1/1/3/7	7/14/54/54	-
3	HEC	U	607	1	1/1/3/7	7/14/54/54	-
3	HEC	U	602	1	1/1/3/7	5/14/54/54	-
3	HEC	U	604	1	1/1/3/7	6/14/54/54	-
3	HEC	A	605	1	1/1/3/7	6/14/54/54	-
3	HEC	Q	600	1	1/1/3/7	7/14/54/54	-
3	HEC	J	601	1	1/1/3/7	6/14/54/54	-
3	HEC	E	603	1,7	-	3/14/54/54	-
3	HEC	N	603	1,7	-	3/14/54/54	-
3	HEC	D	607	1	-	7/14/54/54	-
3	HEC	X	600	1	1/1/3/7	6/14/54/54	-
3	HEC	P	607	1	1/1/3/7	7/14/54/54	-
3	HEC	S	605	1	1/1/3/7	6/14/54/54	-
3	HEC	A	601	1	1/1/3/7	5/14/54/54	-
3	HEC	R	606	1	1/1/3/7	2/14/54/54	-
5	GOL	D	610	-	-	2/4/4/4	-
3	HEC	P	602	1	1/1/3/7	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEC	O	605	1	1/1/3/7	8/14/54/54	-
3	HEC	I	606	1	1/1/3/7	5/14/54/54	-
3	HEC	O	606	1	1/1/3/7	2/14/54/54	-
3	HEC	Q	602	1	1/1/3/7	5/14/54/54	-
3	HEC	S	602	1	1/1/3/7	5/14/54/54	-
3	HEC	G	606	1	1/1/3/7	2/14/54/54	-
3	HEC	M	606	1	1/1/3/7	2/14/54/54	-
3	HEC	V	603	1,7	-	1/14/54/54	-
3	HEC	T	602	1	1/1/3/7	5/14/54/54	-
3	HEC	P	601	1	1/1/3/7	6/14/54/54	-
3	HEC	X	602	1	1/1/3/7	5/14/54/54	-
3	HEC	T	604	1	1/1/3/7	6/14/54/54	-

The worst 5 of 1887 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	T	603	HEC	CHC-C4B	9.08	1.57	1.38
3	S	603	HEC	CHC-C4B	8.78	1.56	1.38
3	Q	603	HEC	CHC-C4B	8.76	1.56	1.38
3	O	603	HEC	CHC-C4B	8.73	1.56	1.38
3	M	603	HEC	CHC-C4B	8.71	1.56	1.38

The worst 5 of 3013 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	603	HEC	CBA-CAA-C2A	10.70	142.36	112.63
3	G	603	HEC	CHA-C1A-NA	-10.36	113.23	124.44
3	L	603	HEC	CHA-C1A-NA	-10.29	113.30	124.44
3	F	603	HEC	CHA-C1A-NA	-10.29	113.31	124.44
3	X	603	HEC	CHA-C1A-NA	-10.29	113.31	124.44

5 of 167 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	600	HEC	NA
3	G	601	HEC	NA
3	G	602	HEC	NA
3	G	604	HEC	NA
3	G	605	HEC	NA

5 of 1005 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	605	HEC	C4D-C3D-CAD-CBD
3	A	605	HEC	C4D-C3D-CAD-CBD
3	B	605	HEC	C4D-C3D-CAD-CBD
3	C	605	HEC	C4D-C3D-CAD-CBD
3	D	605	HEC	C4D-C3D-CAD-CBD

There are no ring outliers.

190 monomers are involved in 385 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	604	HEC	2	0
5	I	615	GOL	1	0
4	G	610	SO4	2	0
3	T	600	HEC	1	0
3	Q	607	HEC	3	0
3	U	601	HEC	3	0
3	C	601	HEC	1	0
3	I	603	HEC	3	0
3	R	605	HEC	7	0
3	J	606	HEC	1	0
3	R	600	HEC	1	0
3	F	605	HEC	5	0
3	P	600	HEC	1	0
3	L	605	HEC	4	0
3	J	600	HEC	1	0
3	K	602	HEC	2	0
3	F	606	HEC	2	0
3	K	606	HEC	2	0
3	R	604	HEC	3	0
4	G	609	SO4	1	0
3	G	601	HEC	3	0
4	J	611	SO4	2	0
5	J	613	GOL	3	0
3	X	601	HEC	2	0
3	J	605	HEC	5	0
3	Q	604	HEC	3	0
3	V	602	HEC	1	0
3	K	605	HEC	3	0
3	X	606	HEC	2	0
3	X	604	HEC	3	0
3	S	606	HEC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	N	600	HEC	1	0
3	P	604	HEC	3	0
3	F	607	HEC	1	0
3	J	602	HEC	1	0
3	L	607	HEC	3	0
3	L	602	HEC	1	0
3	T	601	HEC	1	0
5	K	614	GOL	10	0
3	F	604	HEC	3	0
3	W	606	HEC	2	0
3	W	602	HEC	1	0
3	A	602	HEC	1	0
3	A	607	HEC	3	0
3	P	605	HEC	4	0
3	C	602	HEC	1	0
3	D	603	HEC	2	0
5	H	614	GOL	11	0
3	B	601	HEC	1	0
3	U	605	HEC	5	0
3	R	601	HEC	1	0
3	K	600	HEC	2	0
3	D	606	HEC	2	0
3	N	606	HEC	2	0
3	V	604	HEC	3	0
3	R	607	HEC	3	0
3	D	604	HEC	2	0
3	G	607	HEC	3	0
3	M	605	HEC	4	0
3	E	605	HEC	6	0
3	E	602	HEC	1	0
3	K	601	HEC	5	0
3	F	600	HEC	2	0
3	E	606	HEC	1	0
3	F	601	HEC	1	0
3	B	605	HEC	5	0
3	N	604	HEC	3	0
5	G	615	GOL	1	0
3	K	607	HEC	3	0
3	L	606	HEC	2	0
4	B	609	SO4	1	0
3	H	601	HEC	1	0
3	A	606	HEC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	T	605	HEC	5	0
3	T	607	HEC	2	0
3	V	601	HEC	2	0
3	A	600	HEC	1	0
3	V	605	HEC	5	0
3	E	607	HEC	1	0
3	G	600	HEC	1	0
3	V	606	HEC	2	0
4	H	609	SO4	1	0
5	A	613	GOL	1	0
3	J	607	HEC	3	0
3	M	600	HEC	1	0
3	E	600	HEC	1	0
3	W	605	HEC	7	0
3	P	606	HEC	2	0
3	C	607	HEC	3	0
3	F	602	HEC	1	0
3	B	600	HEC	1	0
3	C	605	HEC	4	0
3	O	607	HEC	2	0
3	U	606	HEC	2	0
3	H	604	HEC	3	0
3	K	604	HEC	3	0
3	N	601	HEC	1	0
3	D	601	HEC	3	0
3	G	602	HEC	1	0
3	V	607	HEC	3	0
3	X	607	HEC	2	0
3	Q	606	HEC	2	0
3	I	601	HEC	5	0
3	L	601	HEC	3	0
3	O	601	HEC	2	0
4	Q	609	SO4	1	0
3	M	601	HEC	1	0
3	E	601	HEC	2	0
5	H	615	GOL	9	0
5	I	614	GOL	4	0
5	K	615	GOL	3	0
3	M	607	HEC	3	0
4	N	610	SO4	1	0
3	H	605	HEC	4	0
3	L	600	HEC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	600	HEC	1	0
3	J	604	HEC	3	0
3	M	604	HEC	2	0
3	O	600	HEC	2	0
3	T	606	HEC	1	0
3	I	600	HEC	2	0
3	Q	601	HEC	4	0
3	D	605	HEC	5	0
3	S	607	HEC	1	0
3	D	602	HEC	1	0
3	H	607	HEC	1	0
3	G	604	HEC	2	0
3	V	600	HEC	1	0
3	S	604	HEC	3	0
3	W	607	HEC	3	0
3	B	602	HEC	1	0
3	B	606	HEC	2	0
3	B	604	HEC	3	0
3	M	602	HEC	1	0
3	S	601	HEC	3	0
3	N	605	HEC	6	0
3	U	600	HEC	1	0
3	N	602	HEC	1	0
5	L	613	GOL	1	0
3	B	607	HEC	2	0
3	E	604	HEC	3	0
3	I	605	HEC	5	0
3	Q	605	HEC	6	0
3	W	601	HEC	3	0
5	G	616	GOL	1	0
3	D	600	HEC	2	0
3	H	600	HEC	1	0
3	G	605	HEC	5	0
3	S	600	HEC	1	0
4	X	610	SO4	1	0
3	X	605	HEC	6	0
5	A	612	GOL	1	0
3	I	602	HEC	2	0
5	K	613	GOL	1	0
3	W	604	HEC	3	0
3	C	606	HEC	2	0
3	H	602	HEC	1	0

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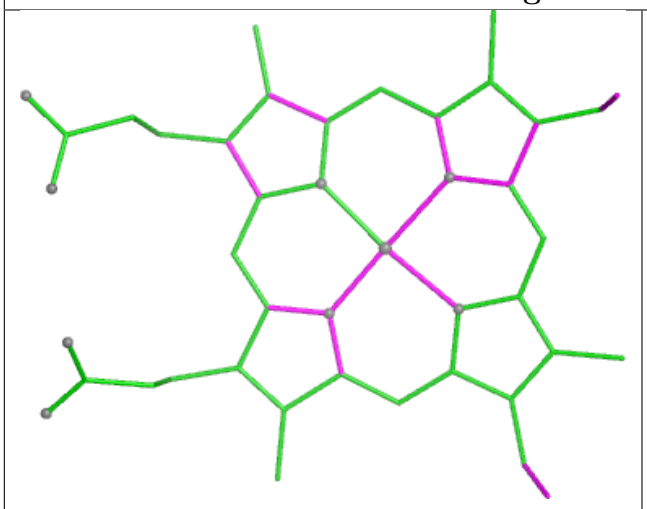
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	606	HEC	3	0
3	O	602	HEC	1	0
3	L	604	HEC	3	0
3	W	600	HEC	1	0
3	C	604	HEC	3	0
3	N	607	HEC	3	0
3	O	604	HEC	2	0
3	I	607	HEC	3	0
3	I	604	HEC	3	0
3	U	607	HEC	2	0
3	U	602	HEC	1	0
3	U	604	HEC	3	0
3	A	605	HEC	3	0
3	Q	600	HEC	2	0
3	J	601	HEC	1	0
3	X	600	HEC	1	0
3	P	607	HEC	2	0
3	S	605	HEC	6	0
3	A	601	HEC	1	0
3	R	606	HEC	2	0
3	P	602	HEC	1	0
3	O	605	HEC	2	0
3	I	606	HEC	3	0
3	O	606	HEC	2	0
3	Q	602	HEC	1	0
4	L	610	SO4	1	0
3	S	602	HEC	1	0
3	G	606	HEC	2	0
3	M	606	HEC	1	0
3	T	602	HEC	1	0
3	P	601	HEC	3	0
3	X	602	HEC	1	0
3	T	604	HEC	3	0

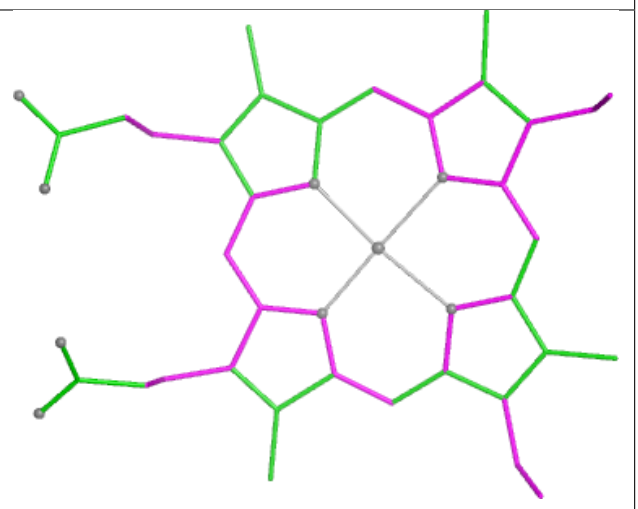
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

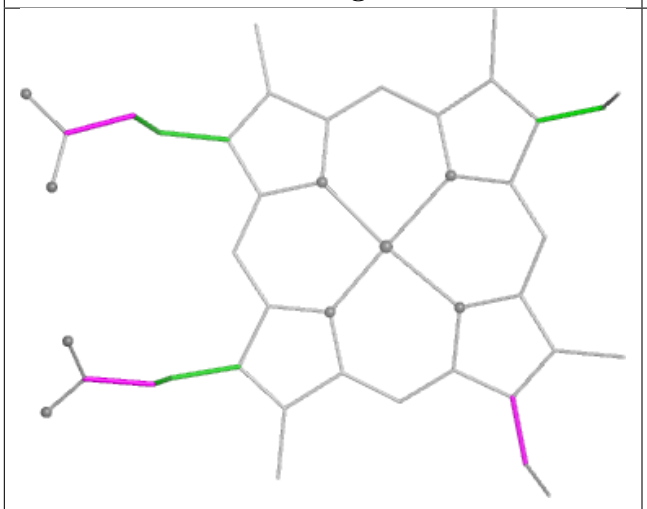
Ligand HEC A 604



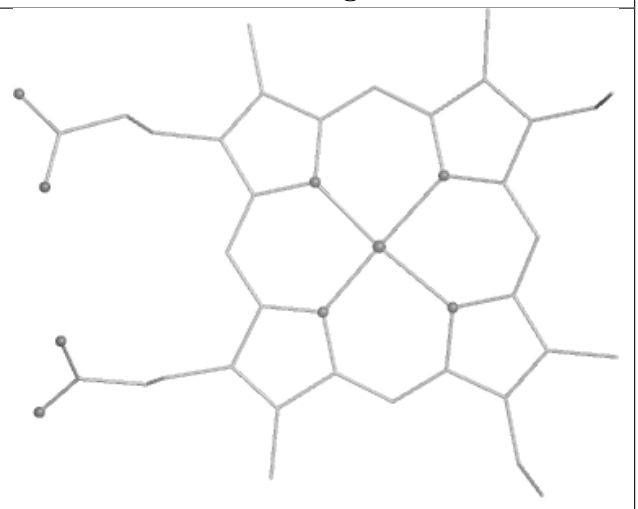
Bond lengths



Bond angles

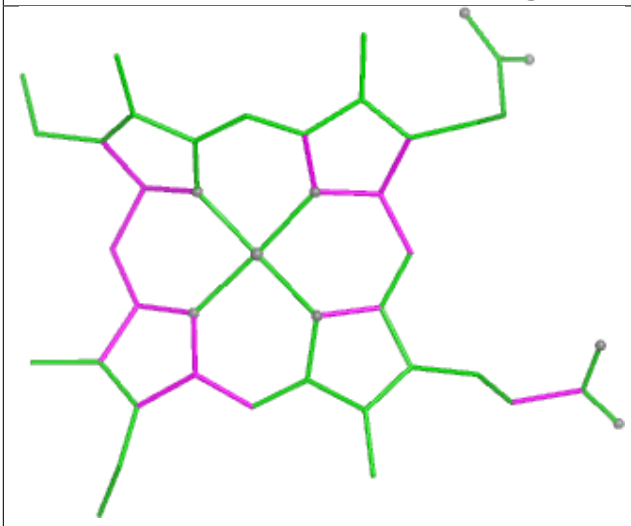


Torsions

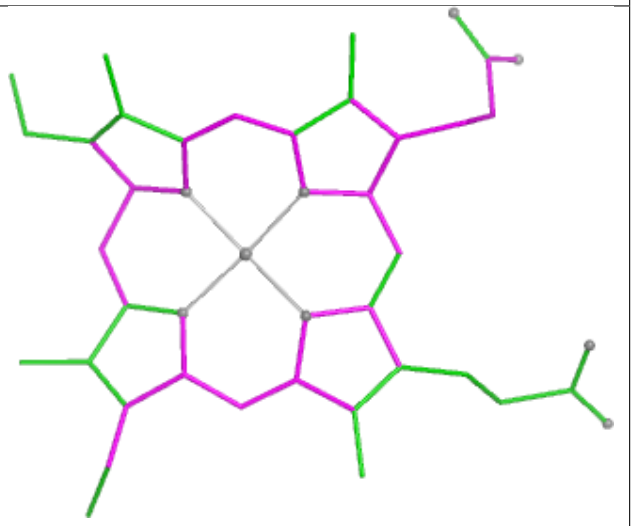


Rings

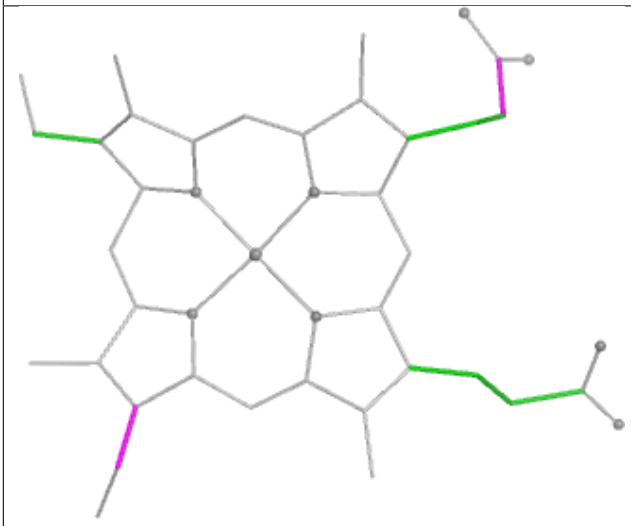
Ligand HEC O 603



Bond lengths



Bond angles



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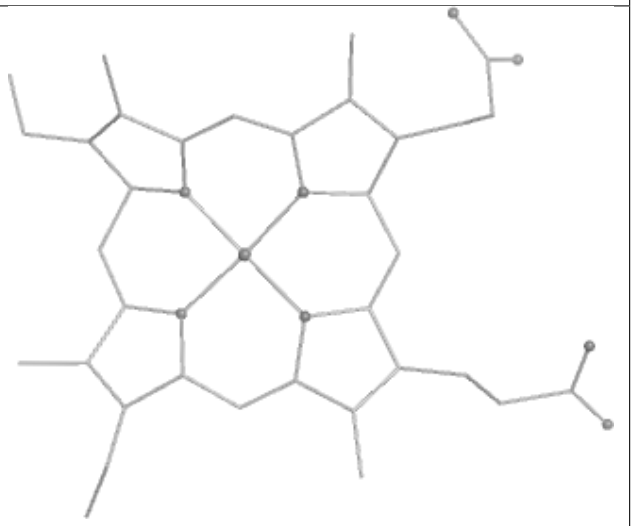
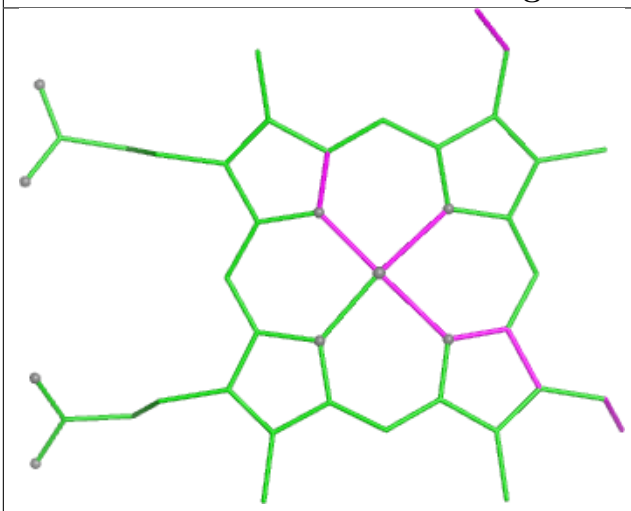


Rings

Ligand HEC T 600



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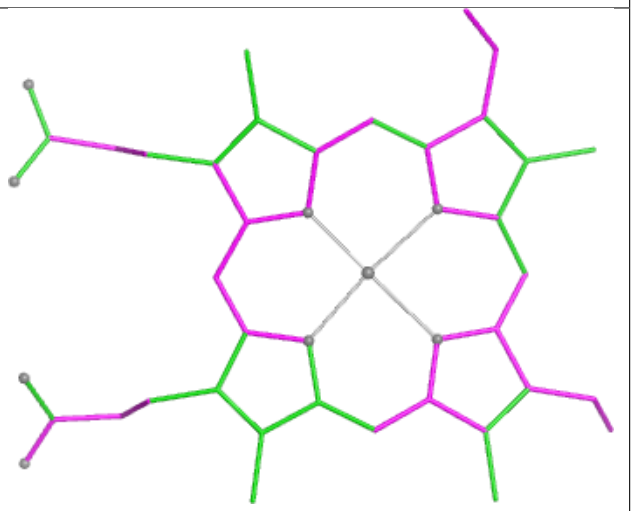

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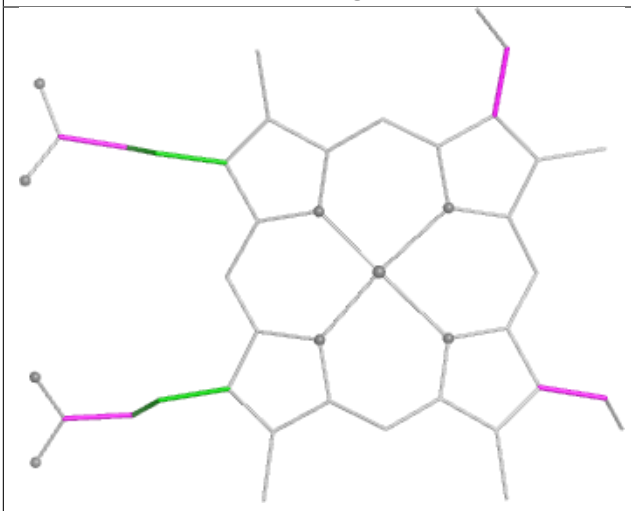

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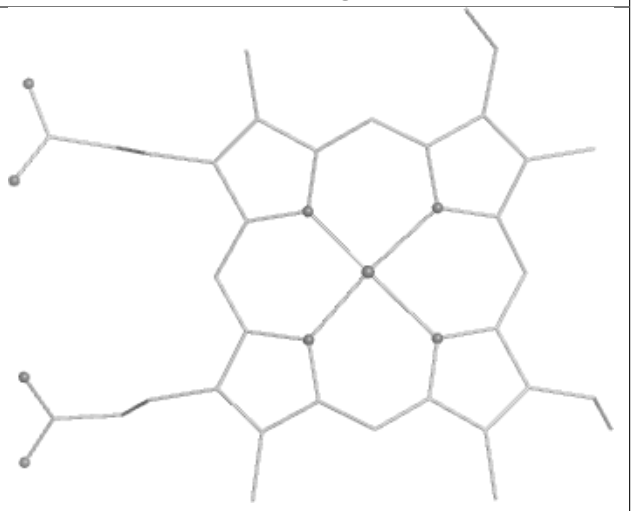
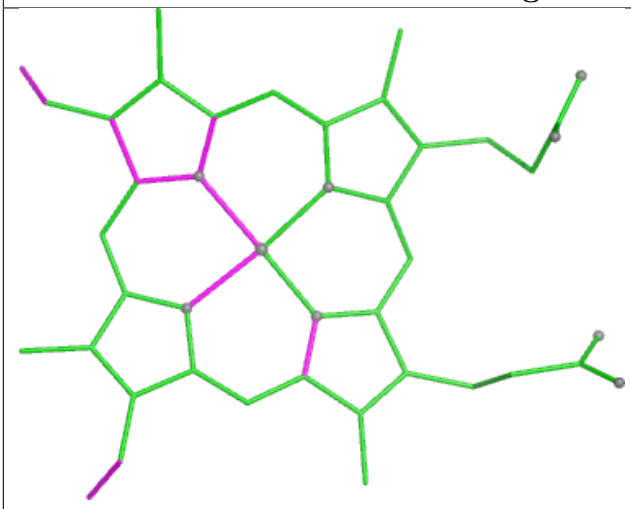


Rings

Ligand HEC Q 607



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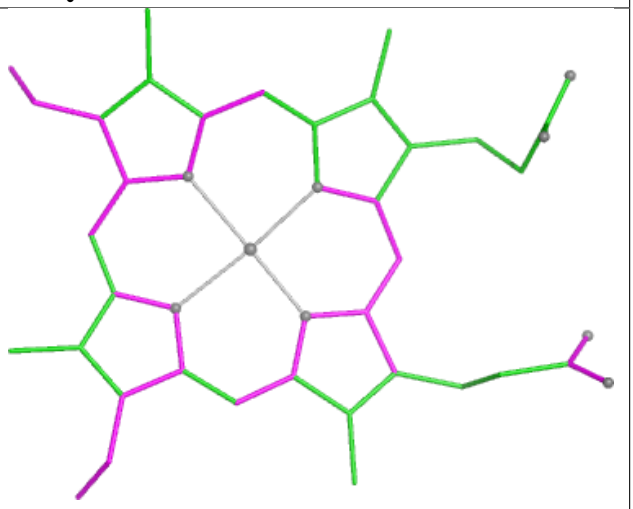

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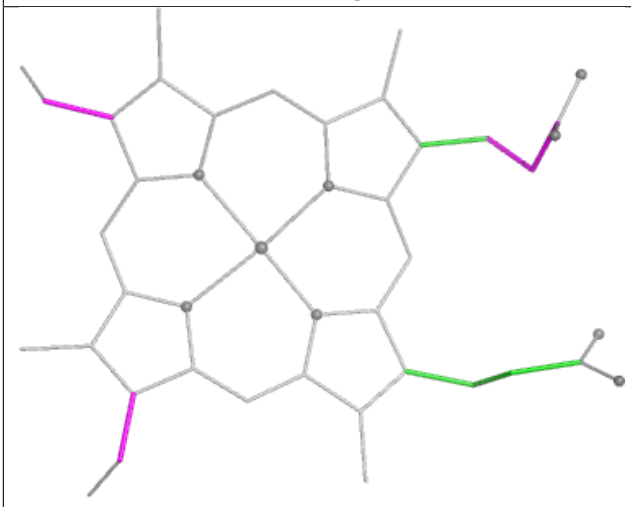

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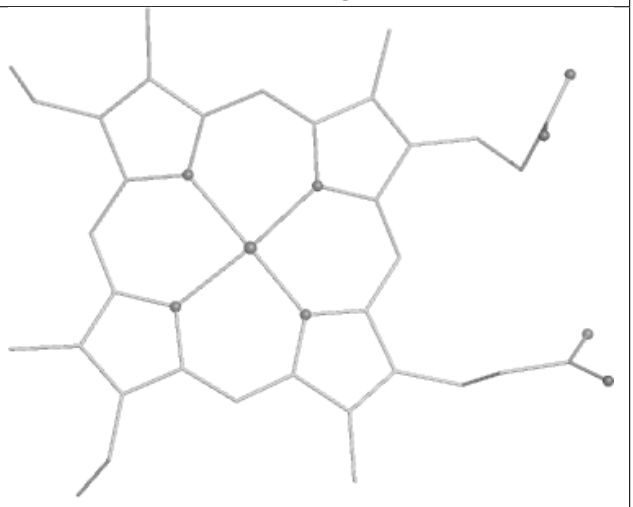
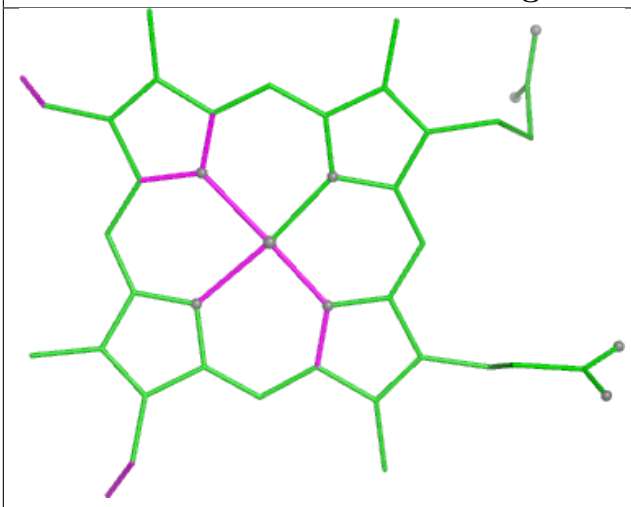
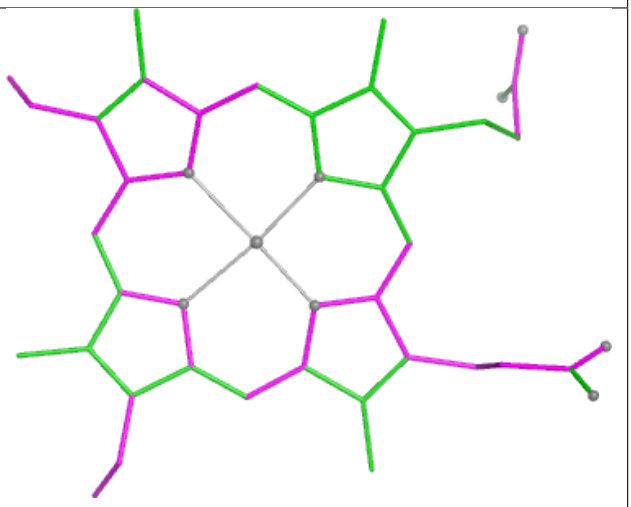


Rings

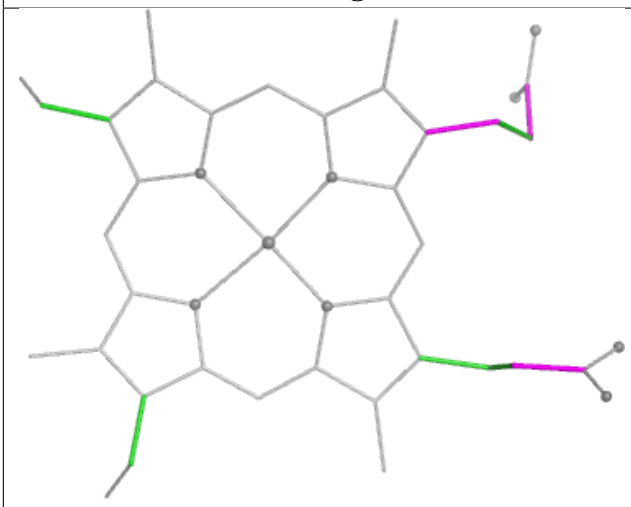
Ligand HEC U 601



Bond lengths



Bond angles



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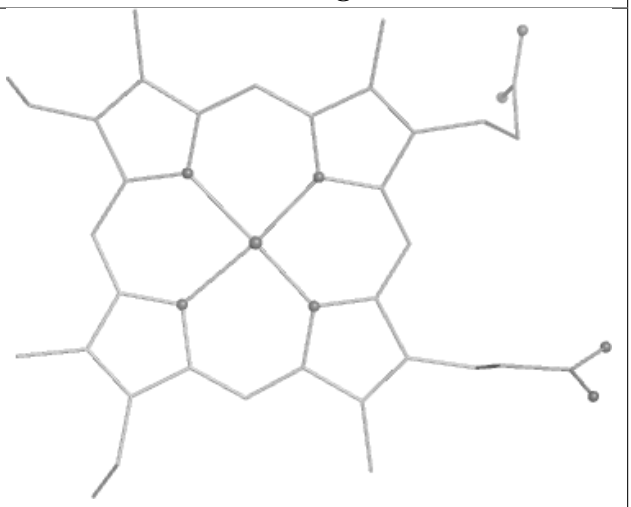
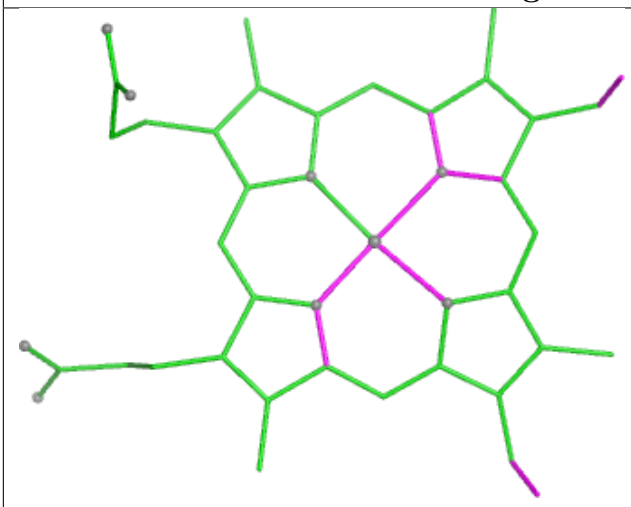


Rings

Ligand HEC C 601



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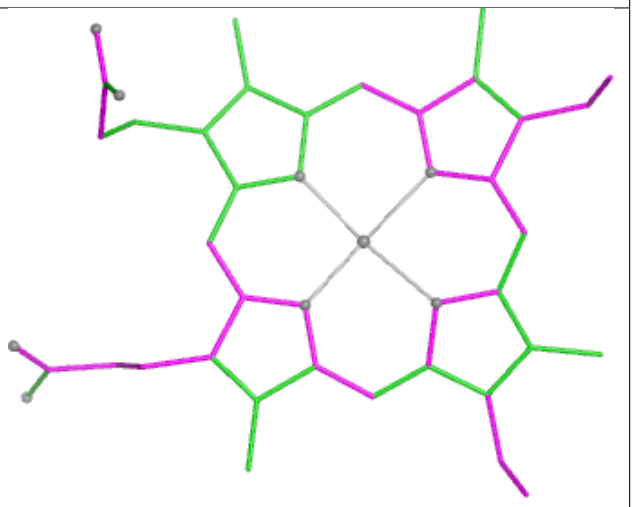
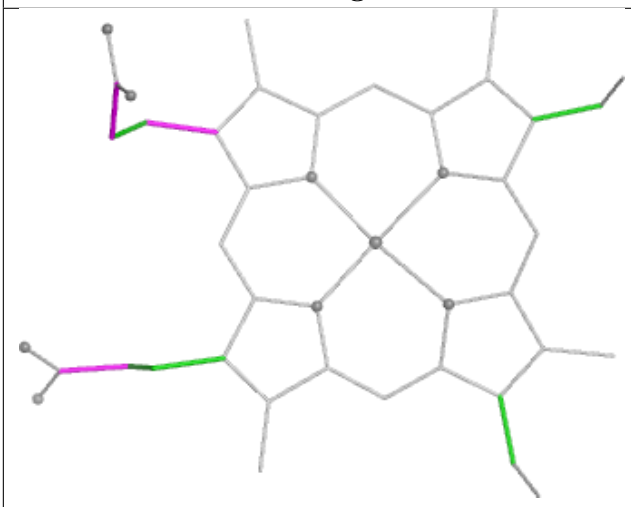


Bond angles



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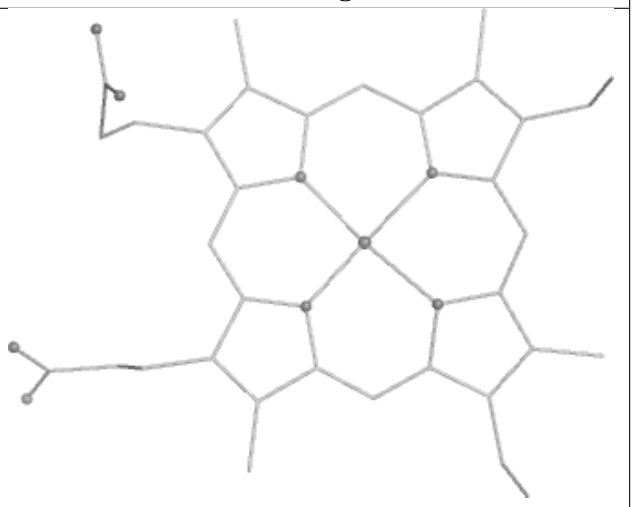
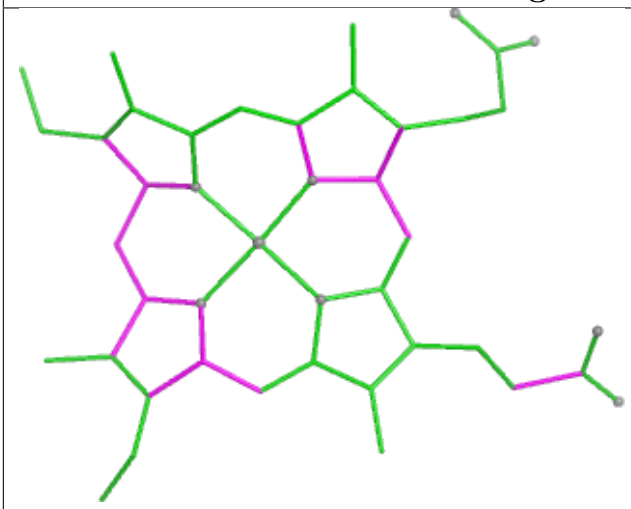
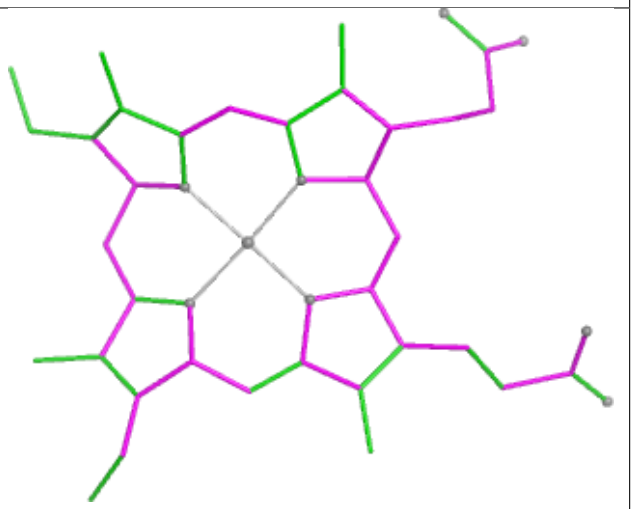


Rings

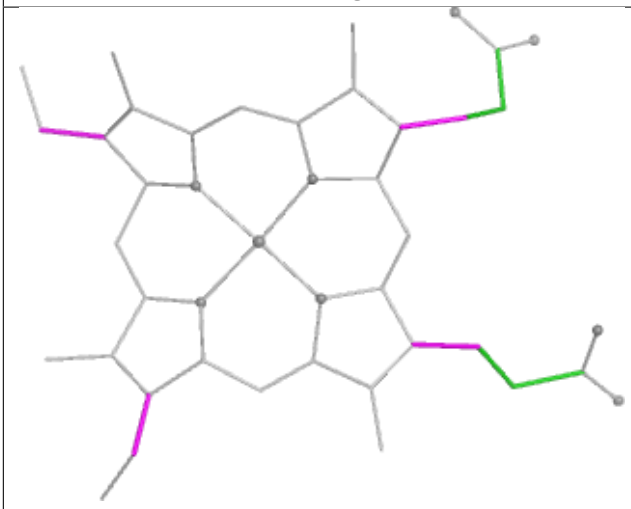
Ligand HEC I 603



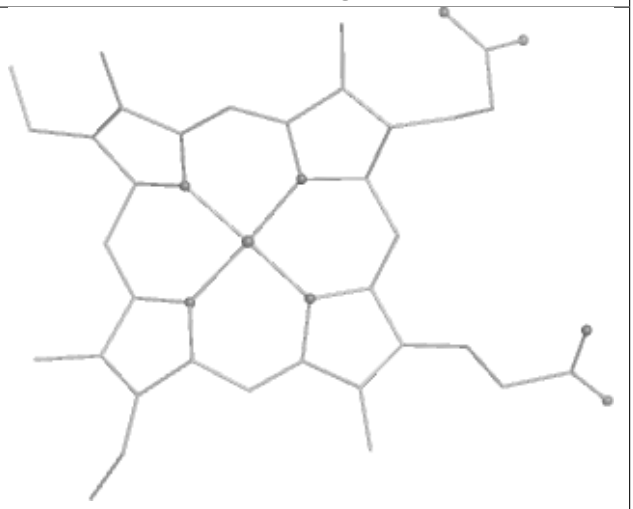
Bond lengths



Bond angles

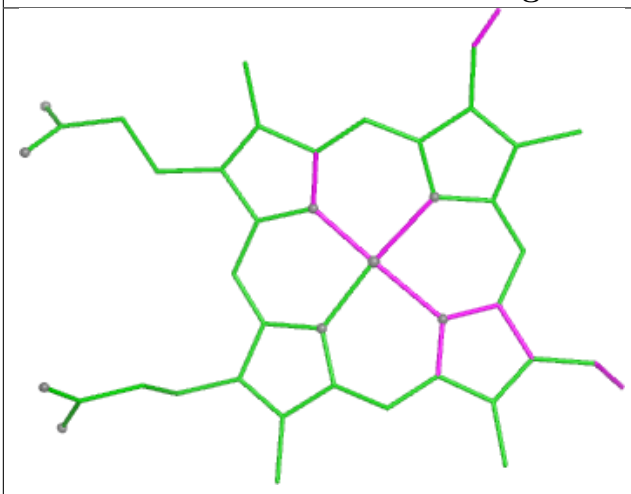


Torsions

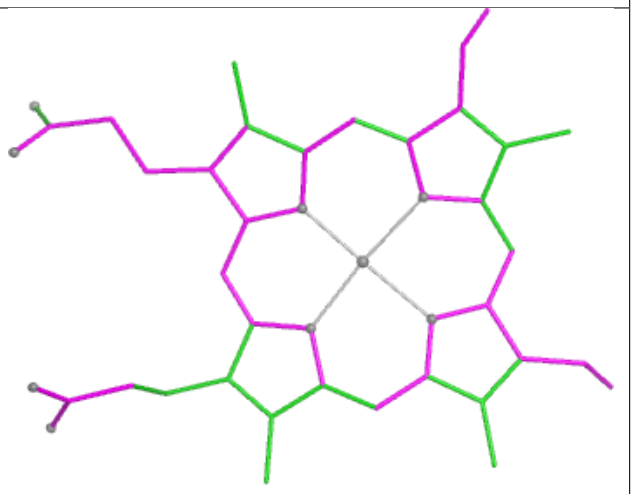


Rings

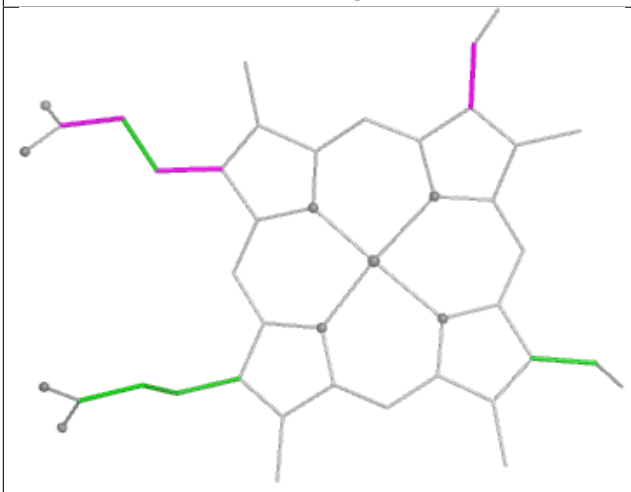
Ligand HEC R 605



Bond lengths



Bond angles



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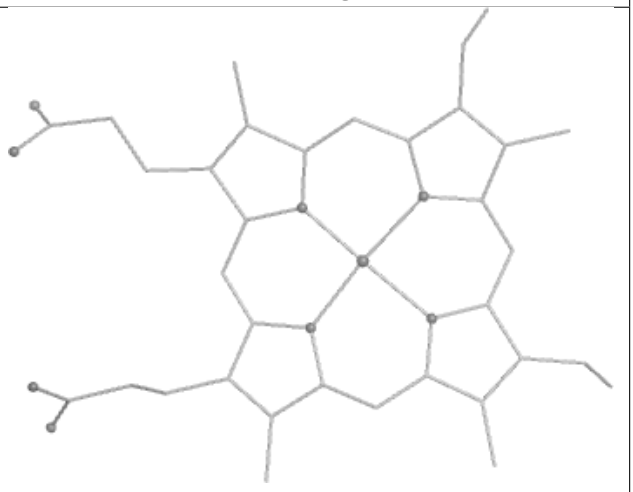
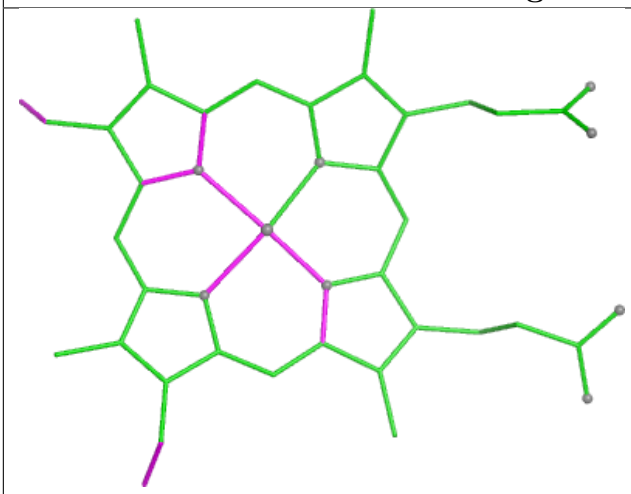


Rings

Ligand HEC J 606



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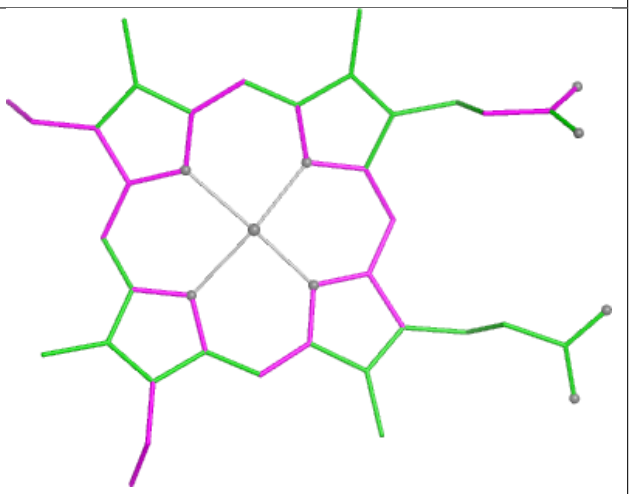

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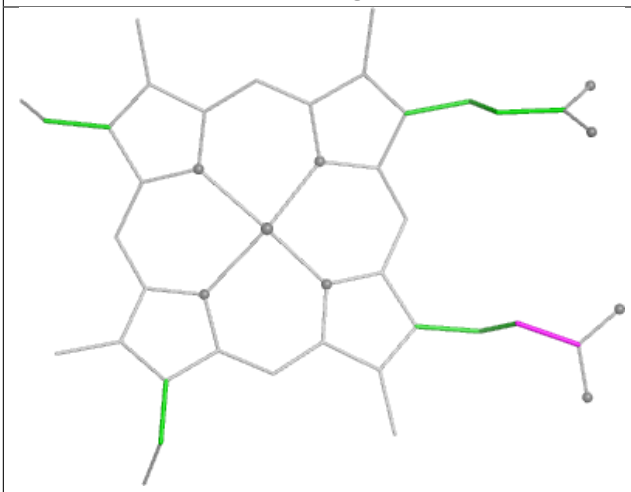

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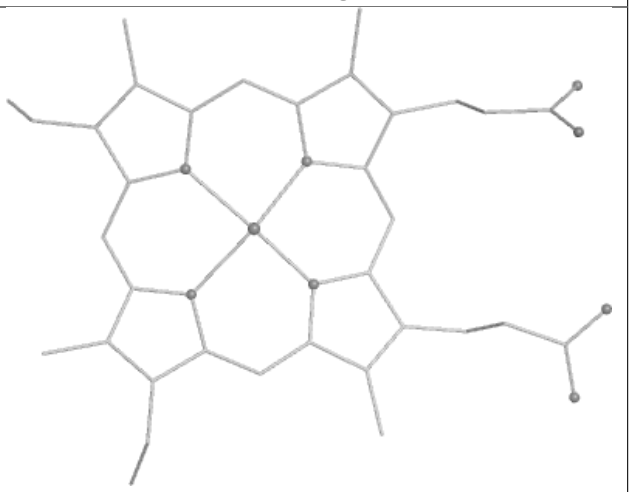

Rings

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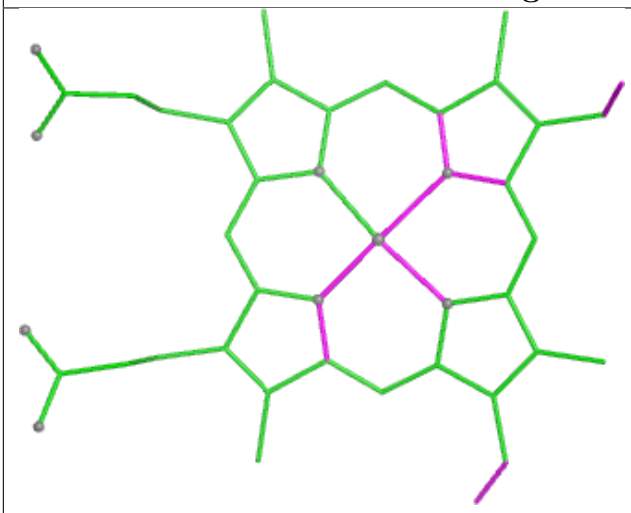

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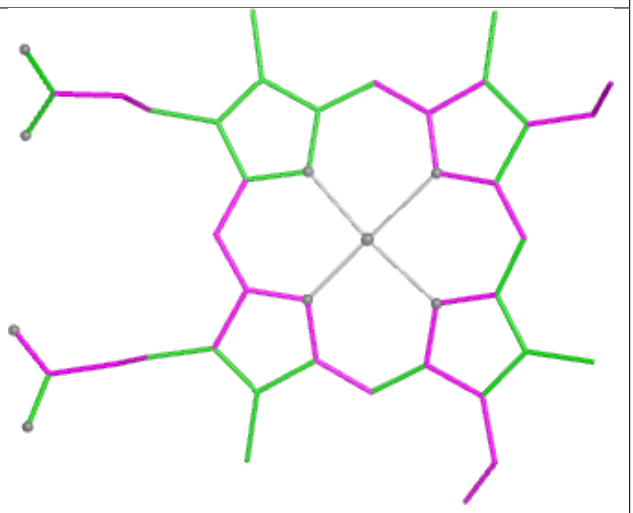

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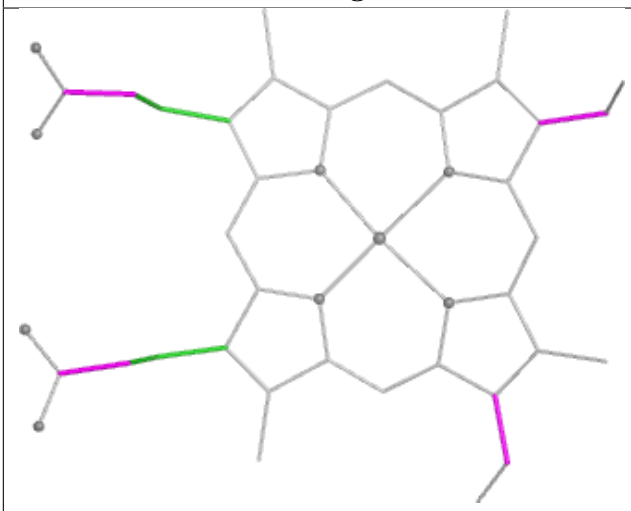

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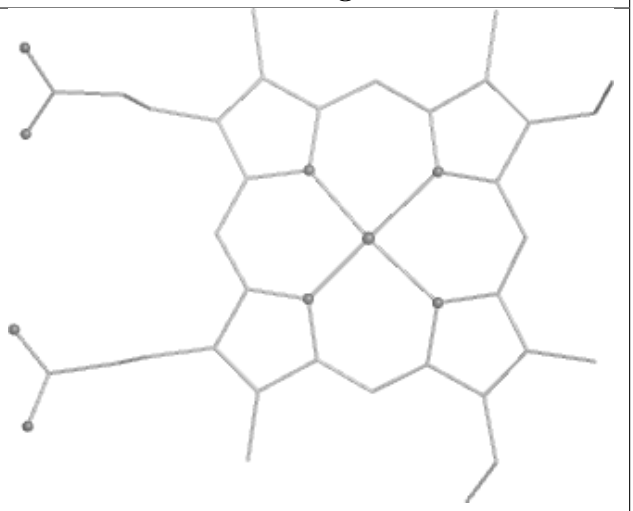

Rings

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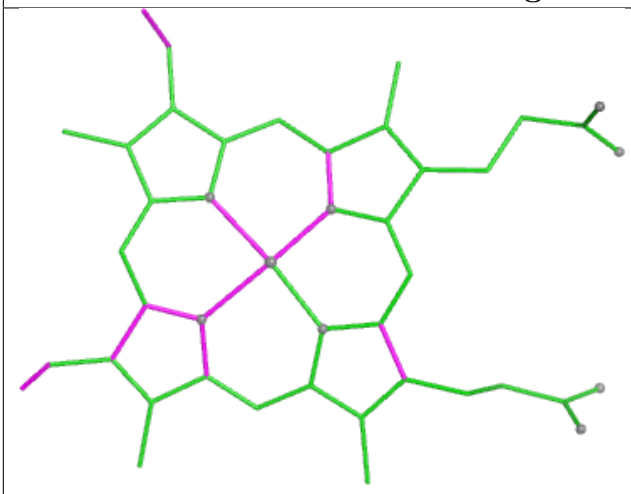

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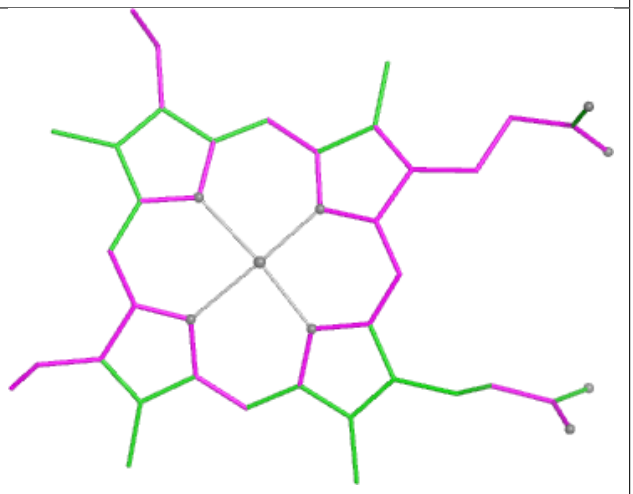

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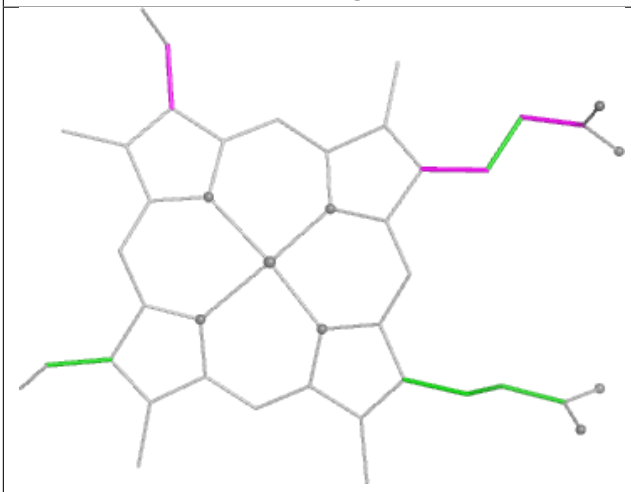

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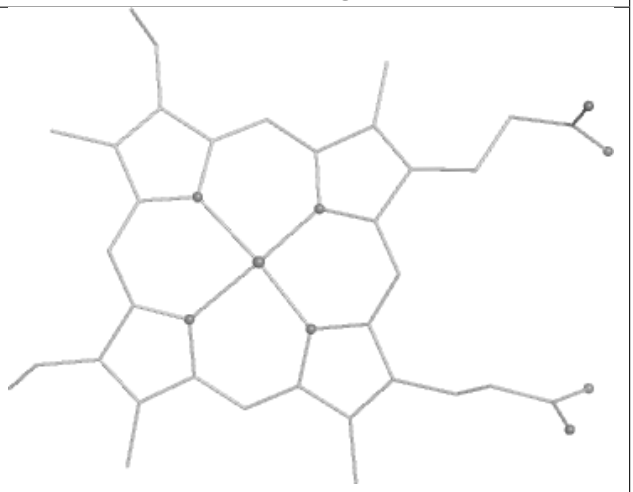

Rings

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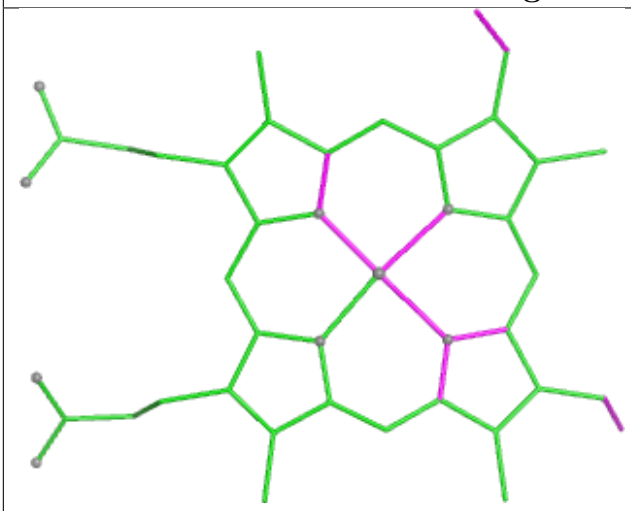

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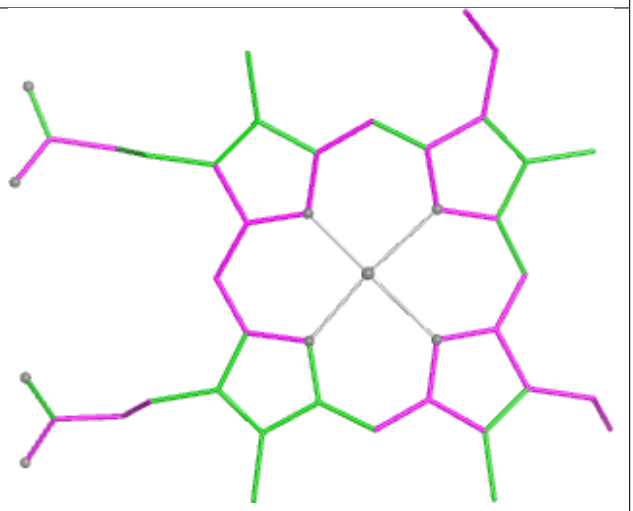

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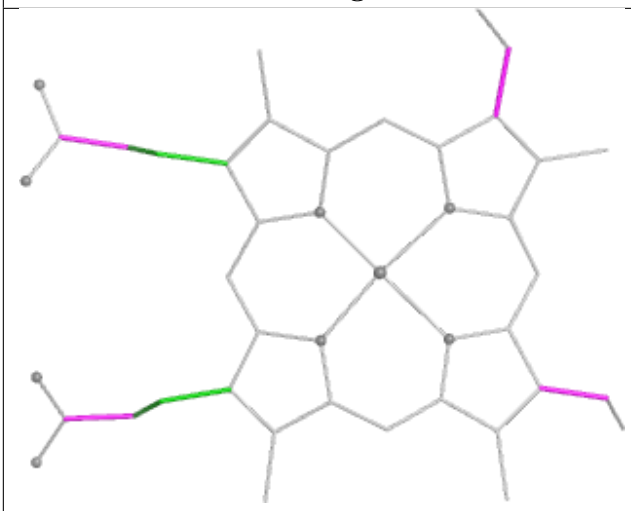

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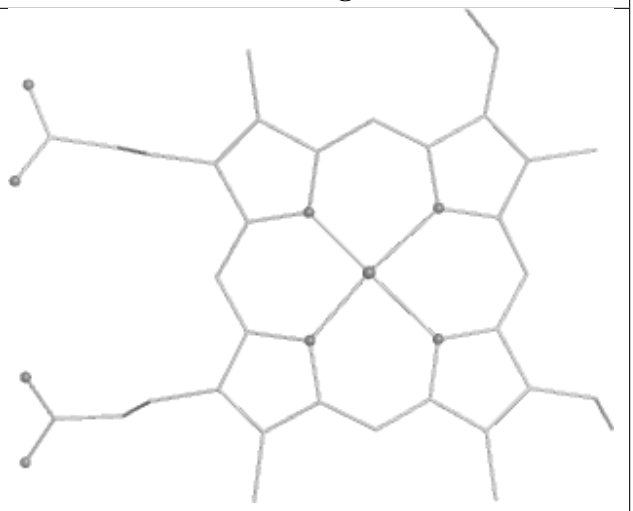

Rings

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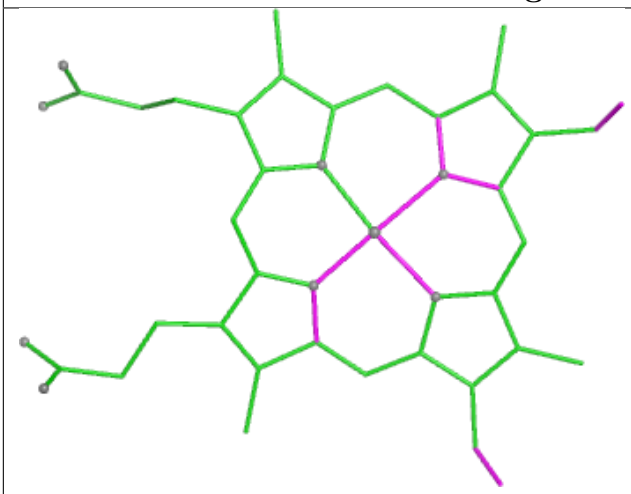

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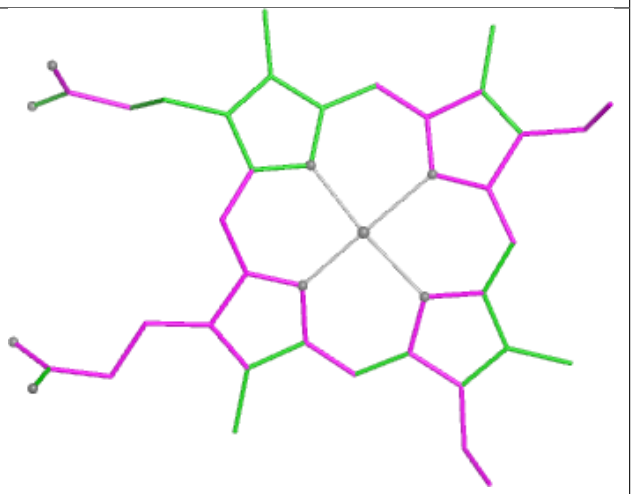

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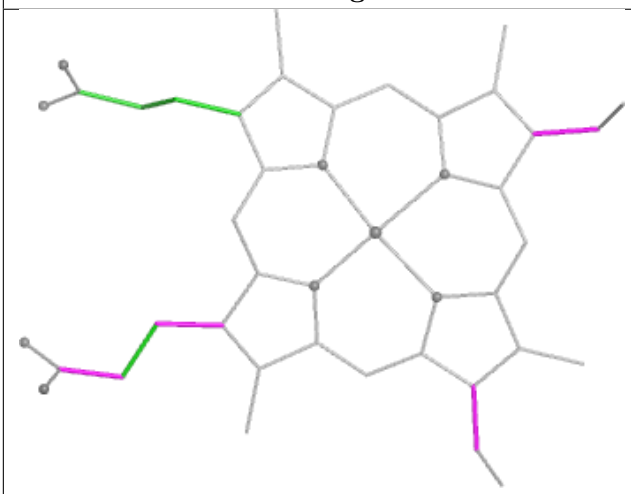

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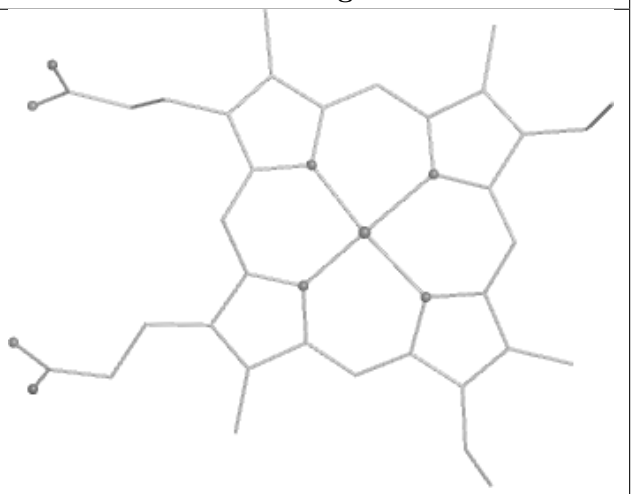
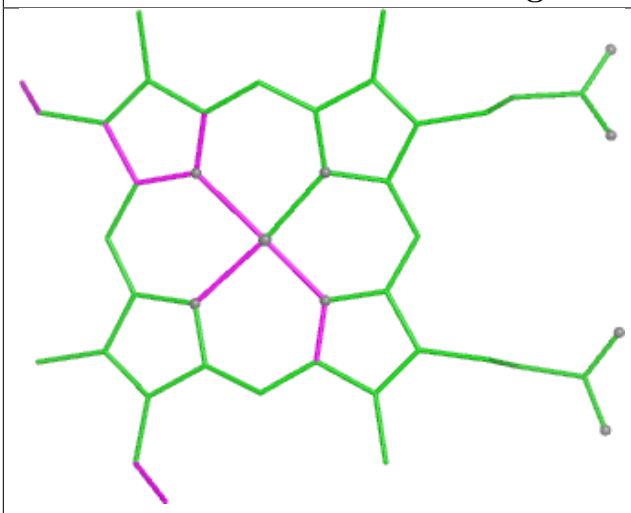


Rings

Ligand HEC J 600



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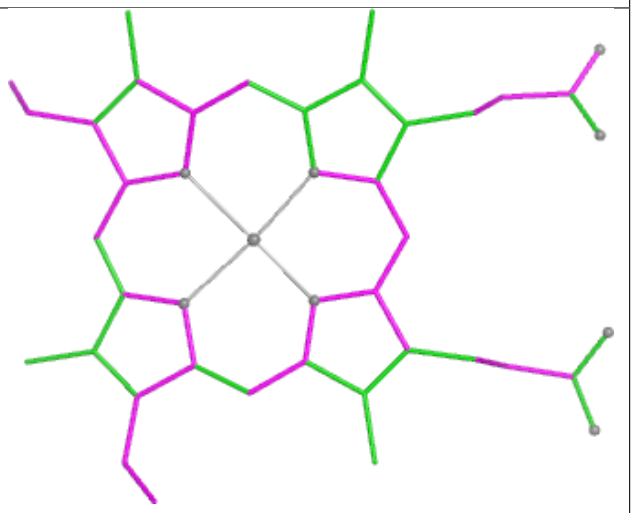

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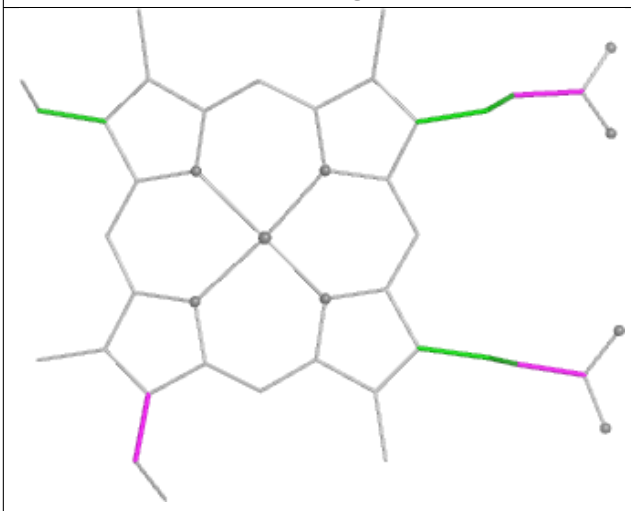

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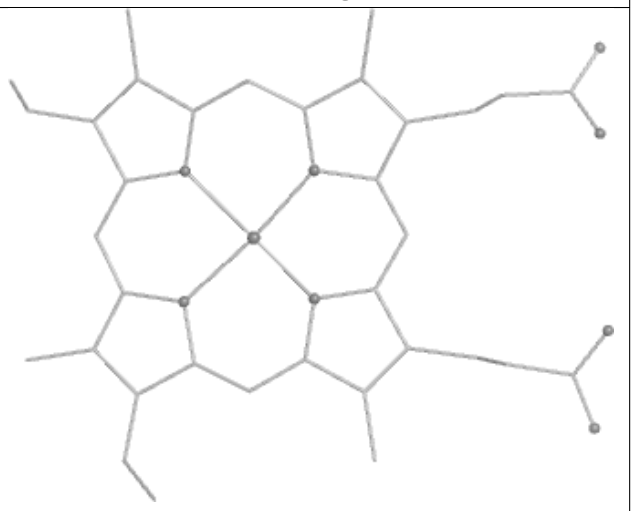
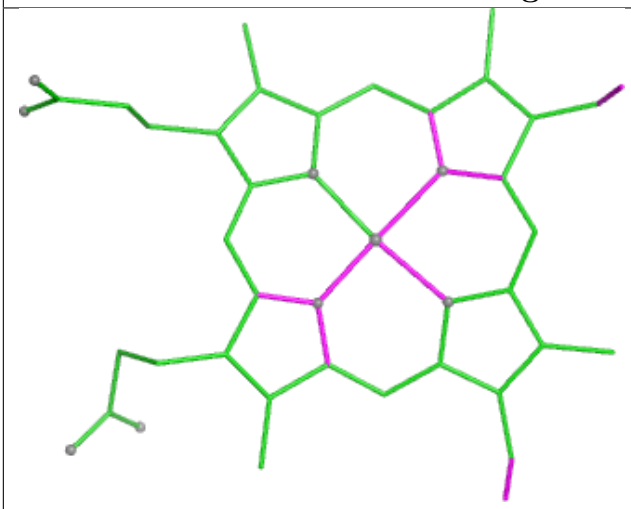


Rings

Ligand HEC K 602



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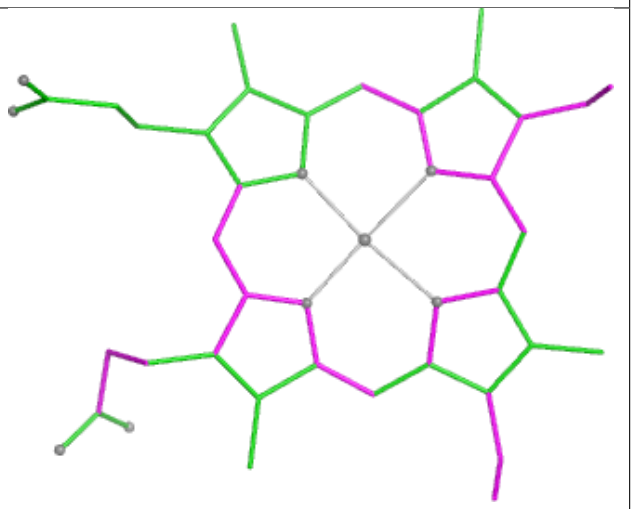

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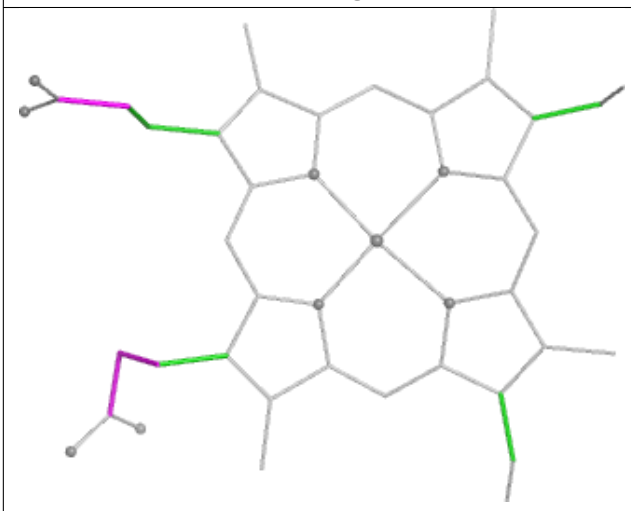

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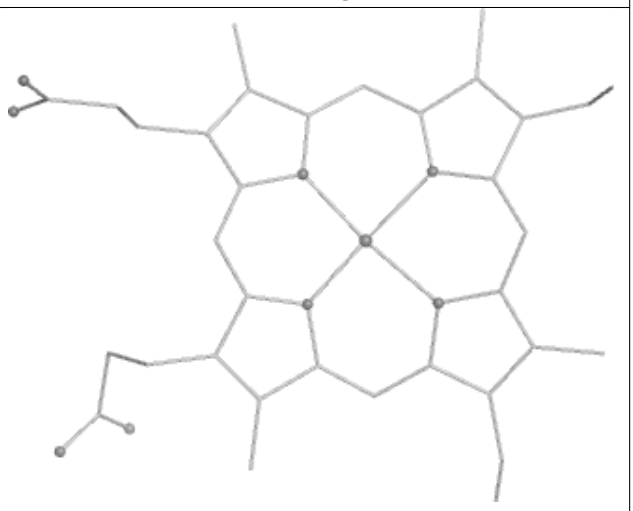

Rings

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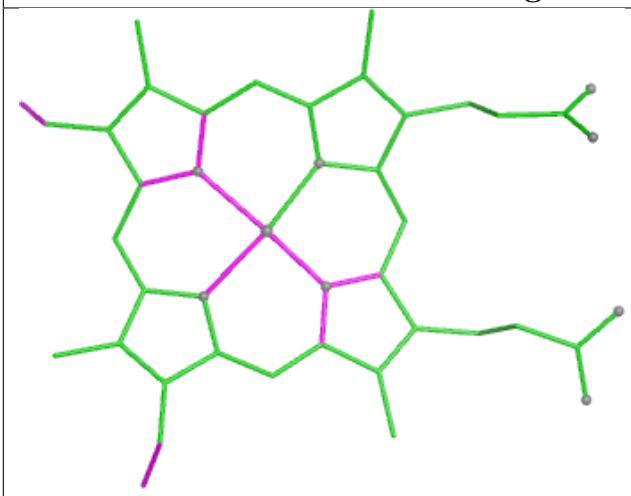

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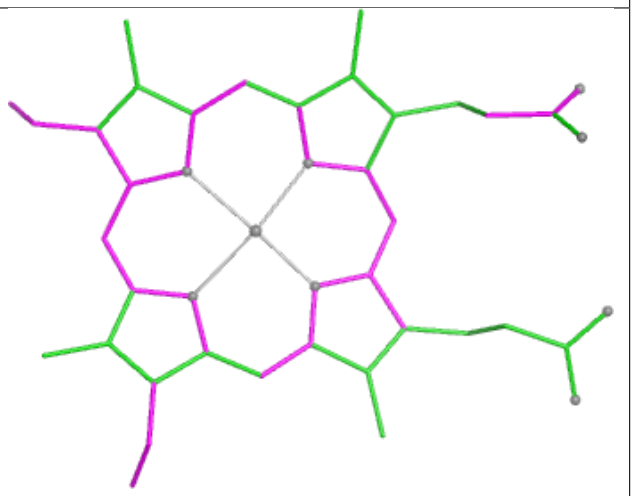

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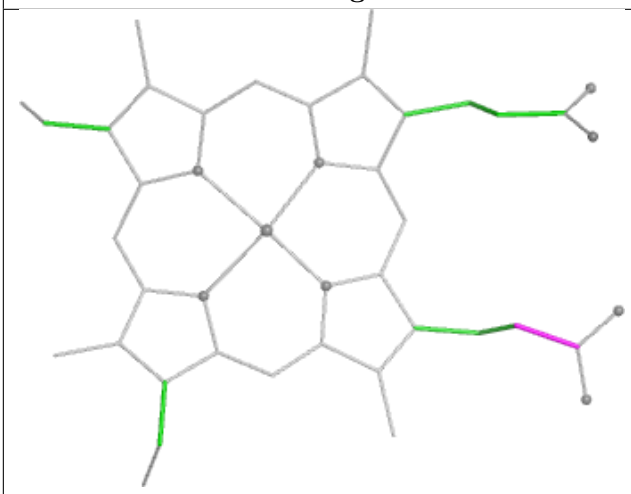

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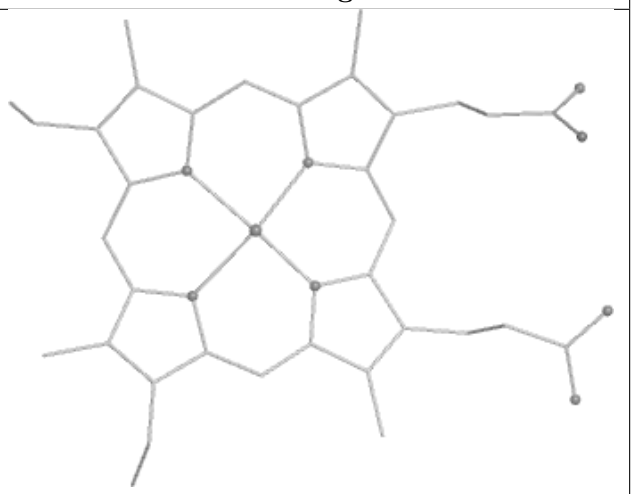

Rings

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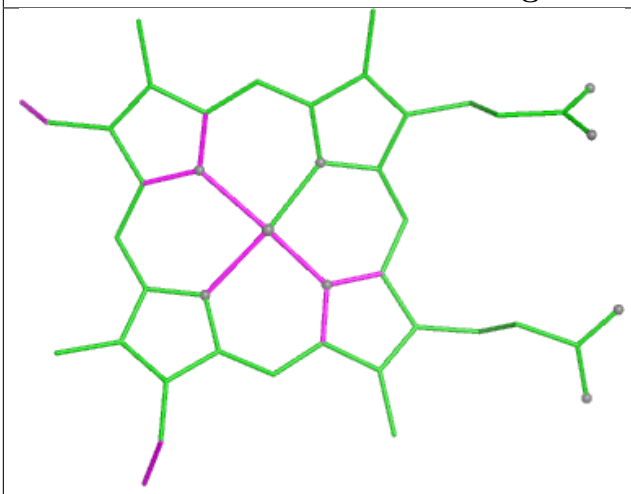

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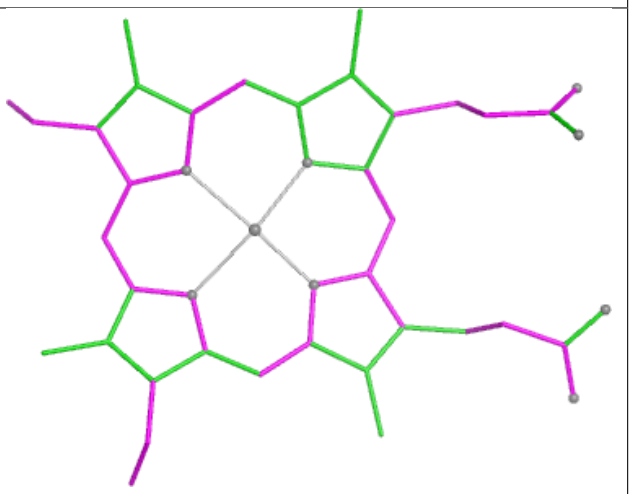

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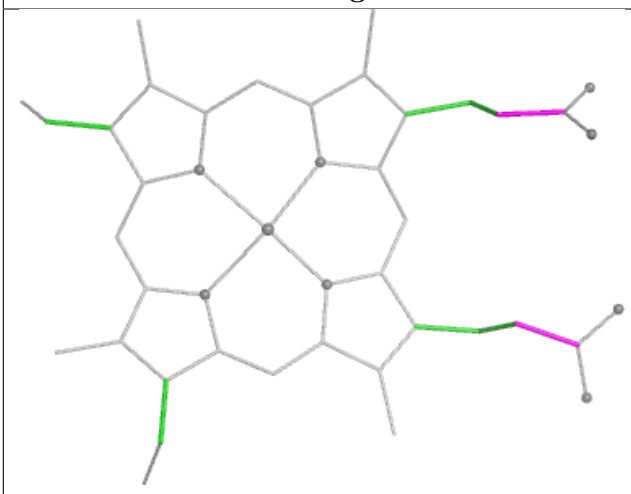

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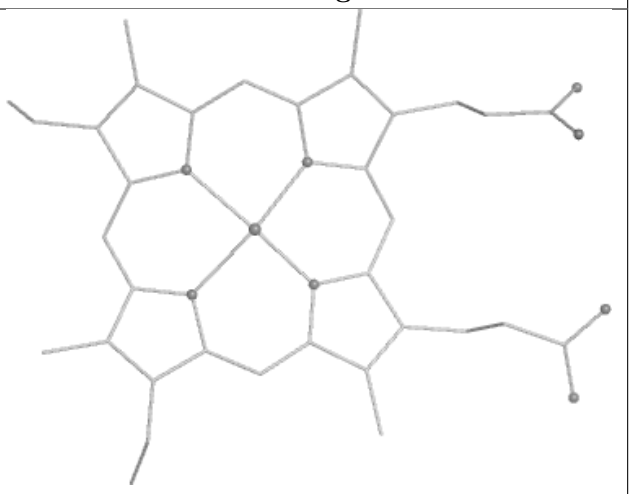

Rings

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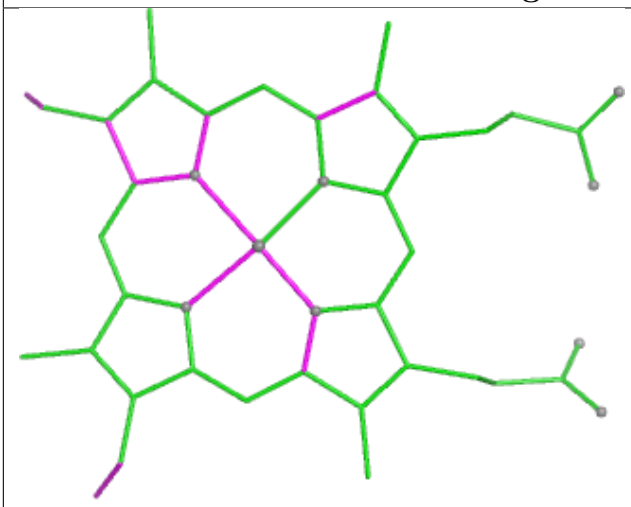

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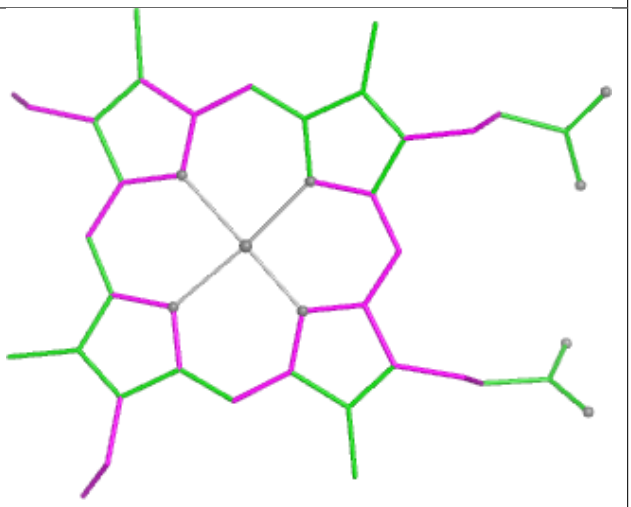

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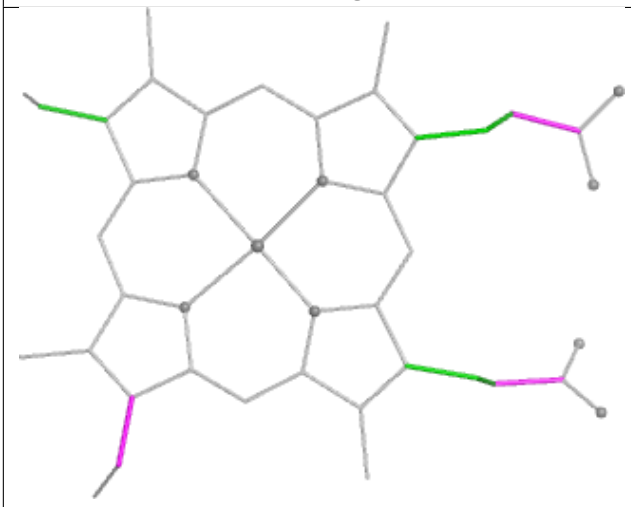

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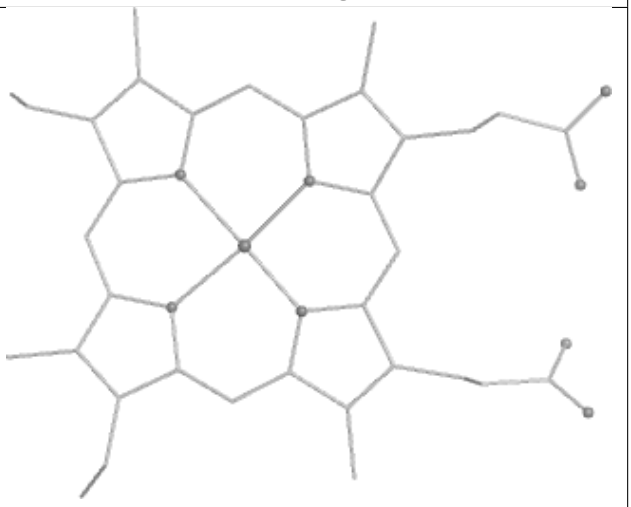

Rings

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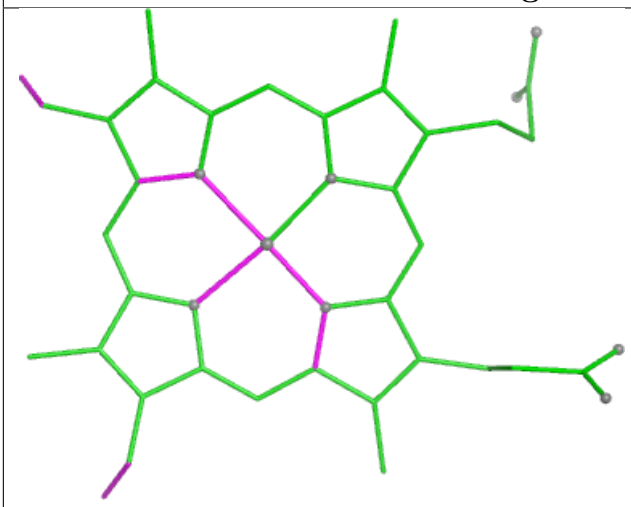

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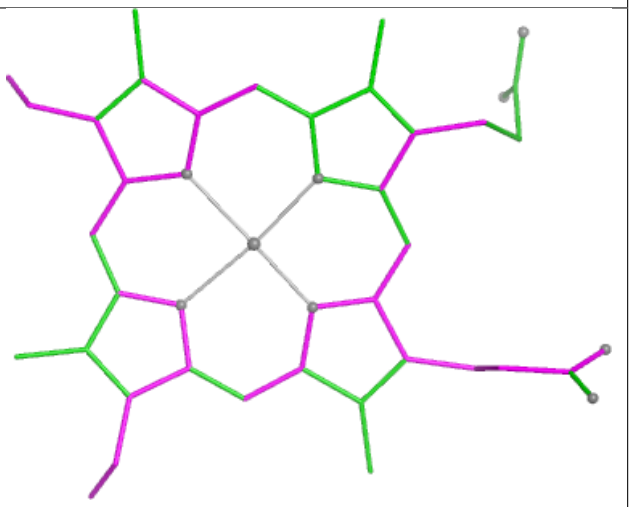

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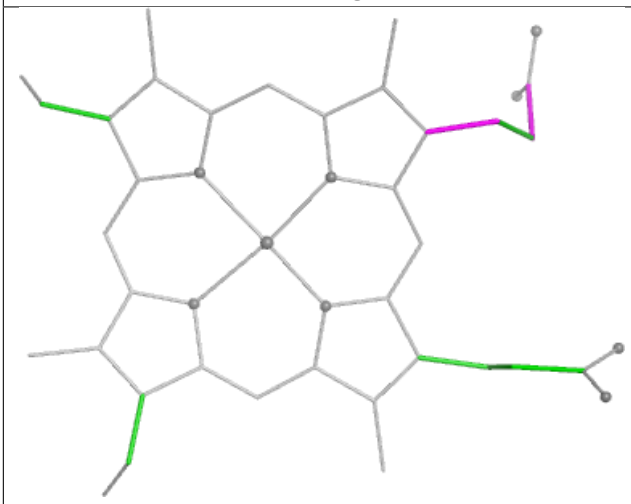

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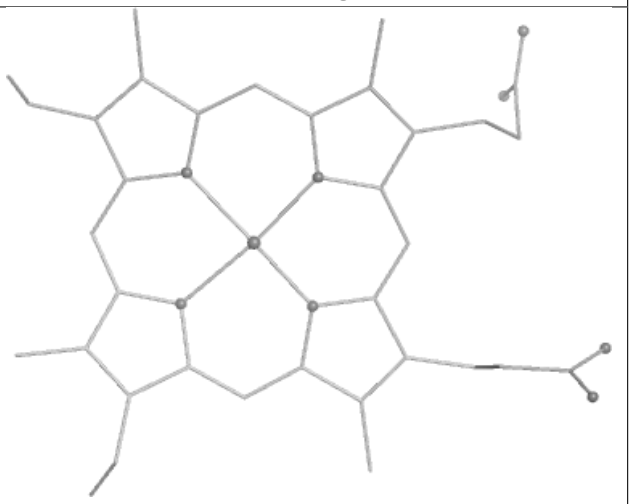

Rings

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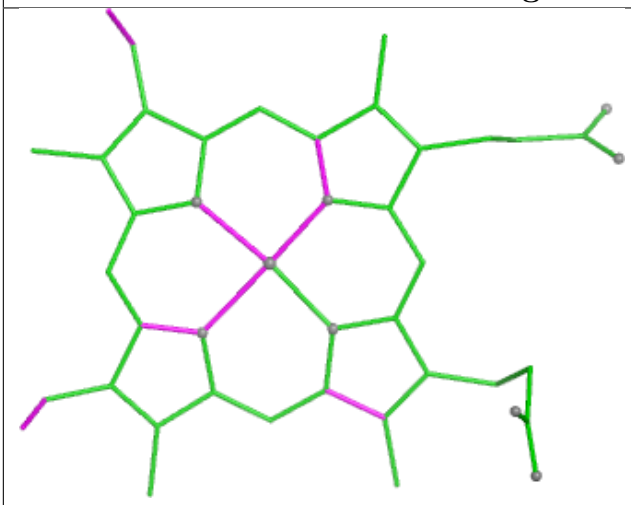

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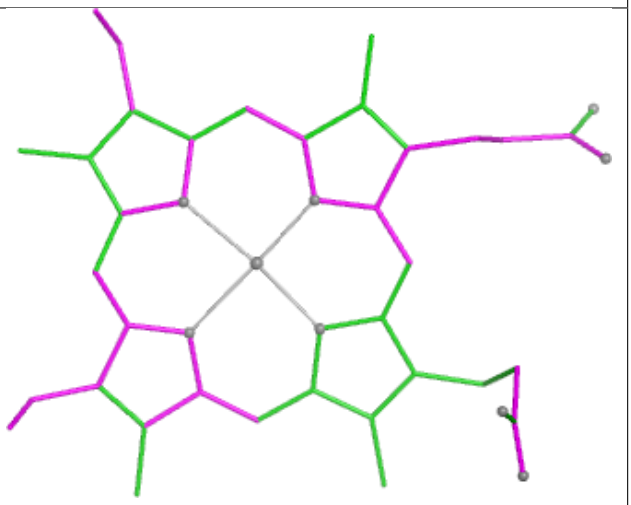

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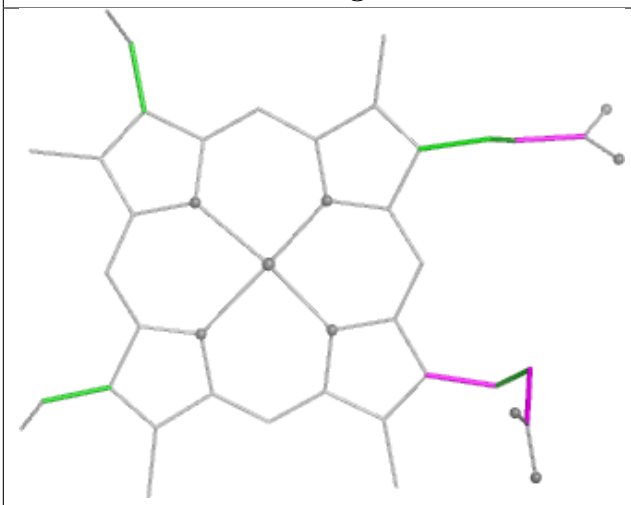

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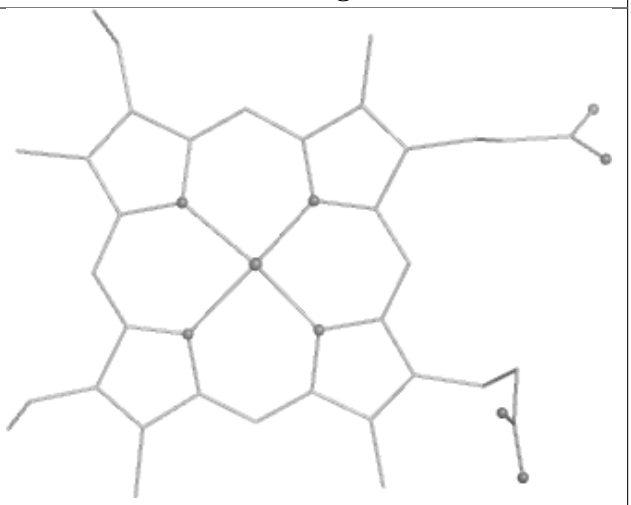
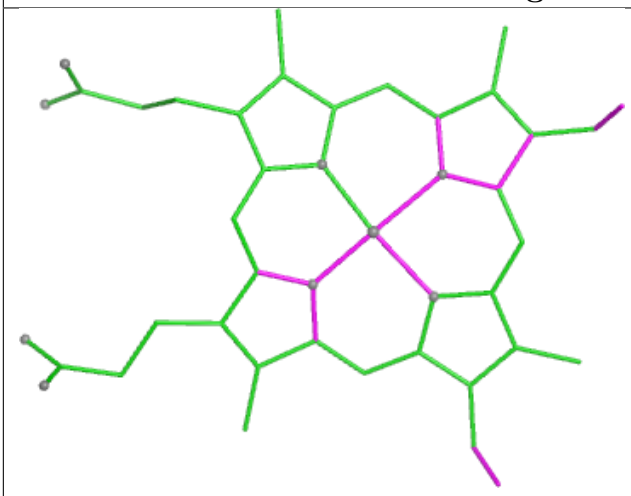


Rings

Ligand HEC J 605



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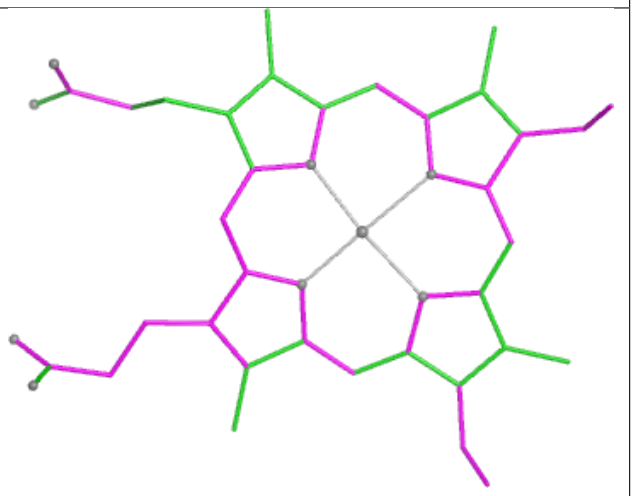

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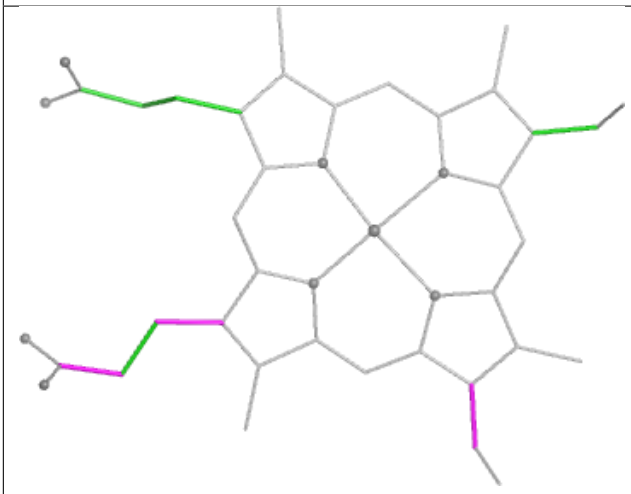

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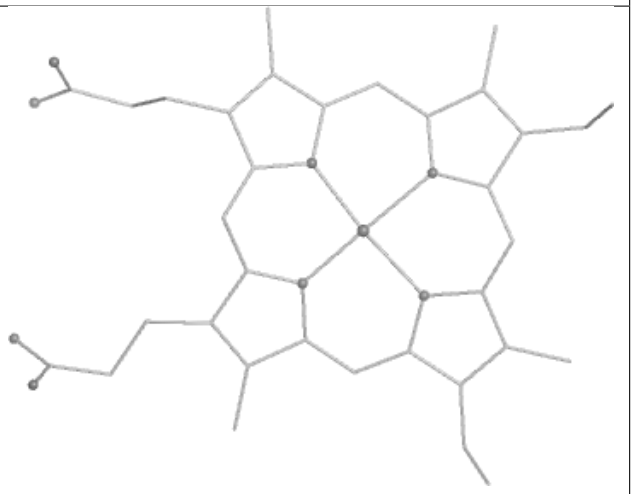
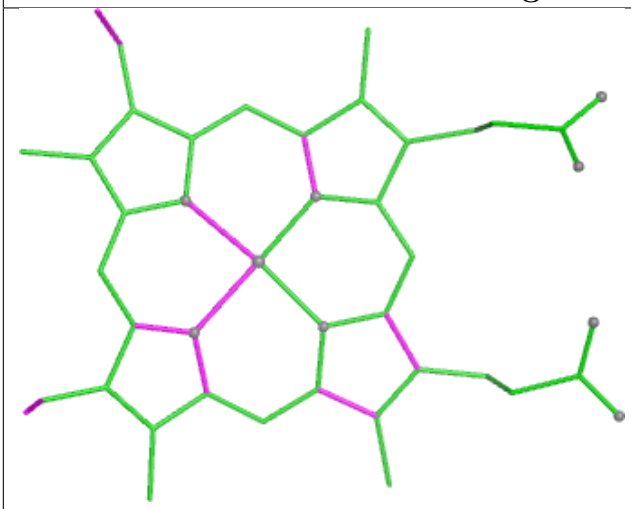


Rings

Ligand HEC Q 604



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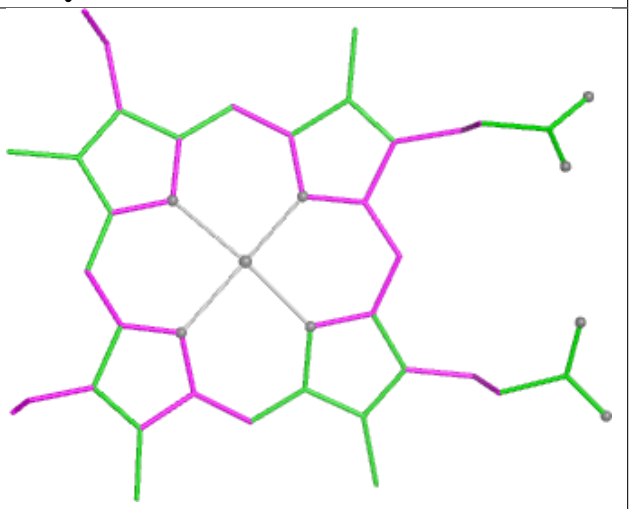
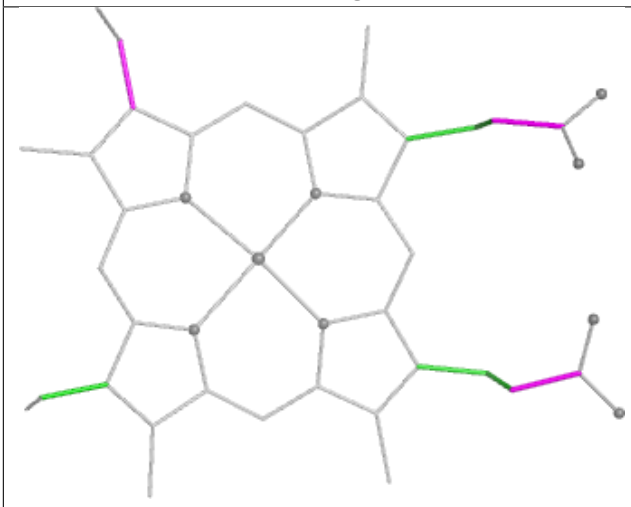


Bond angles



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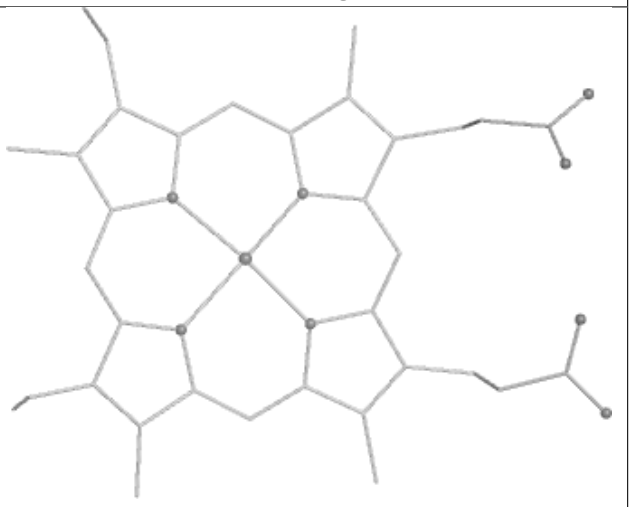
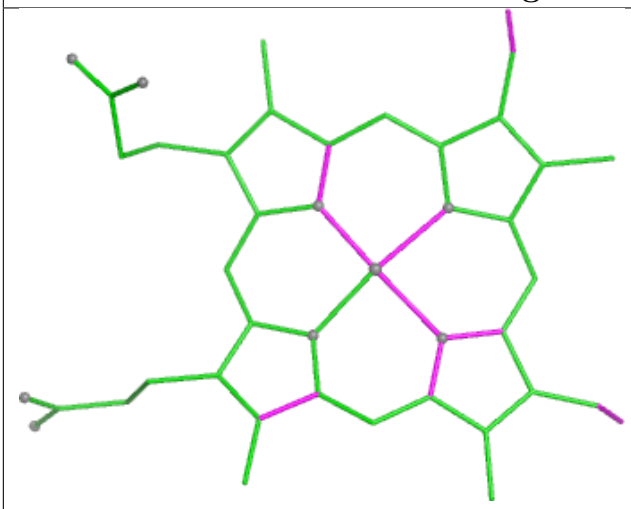


Rings

Ligand HEC V 602



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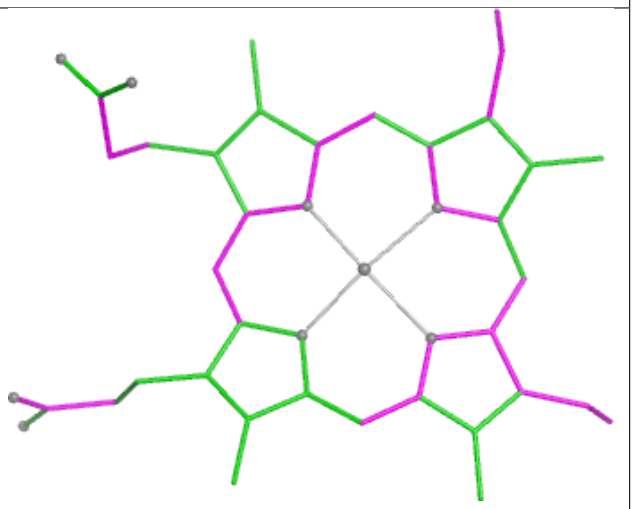

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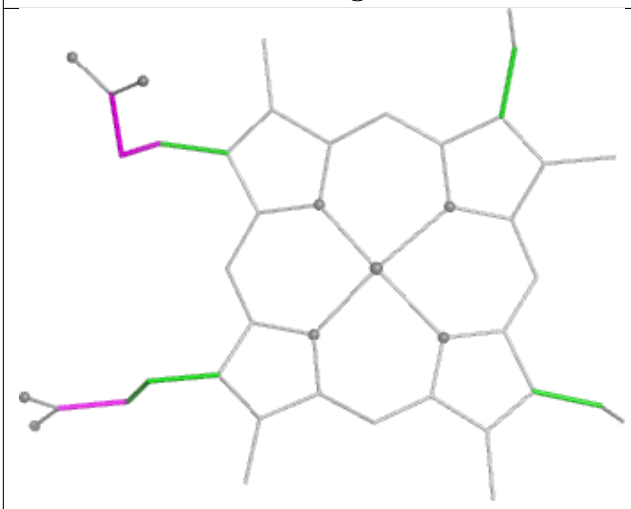
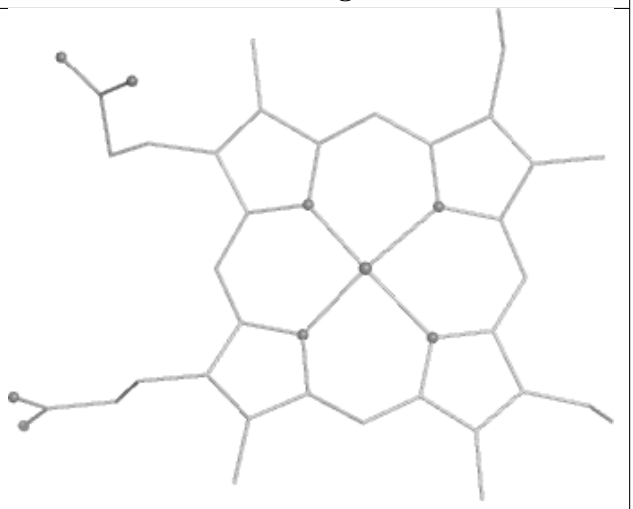
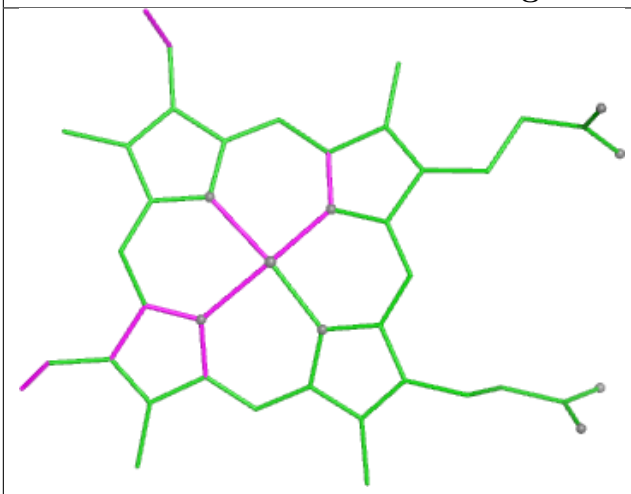


Torsions



Rings

Ligand HEC K 605



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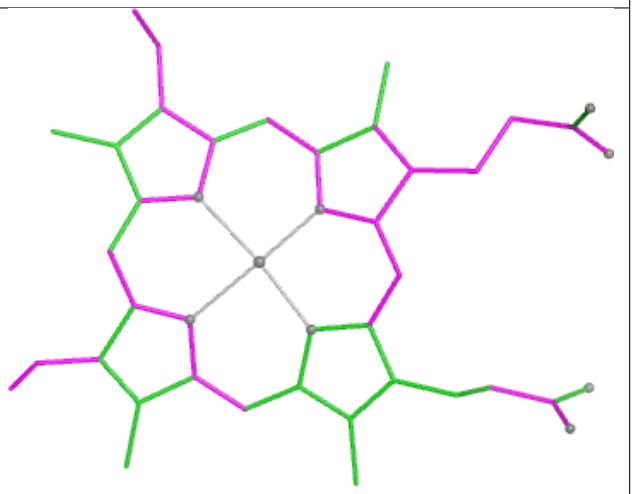

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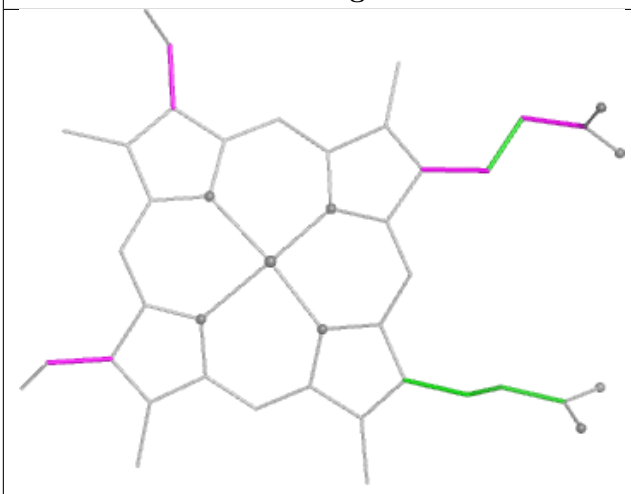

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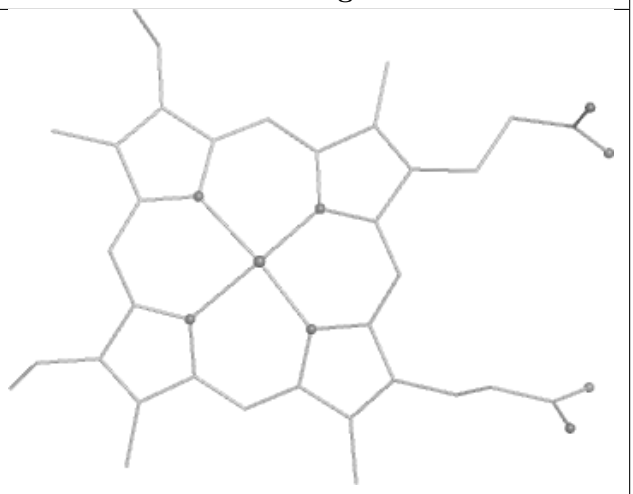
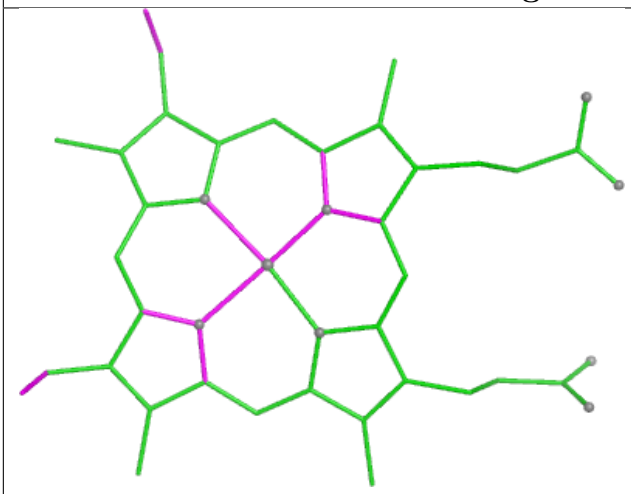


Rings

Ligand HEC X 606



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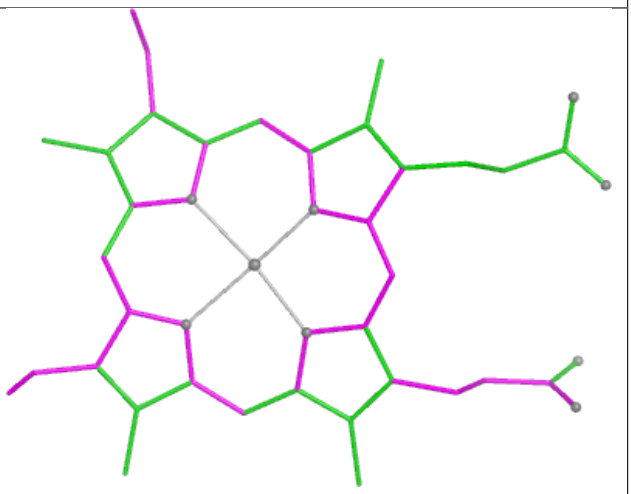

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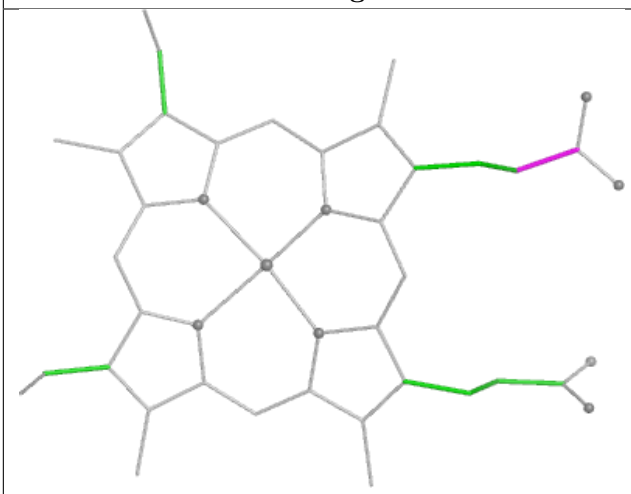

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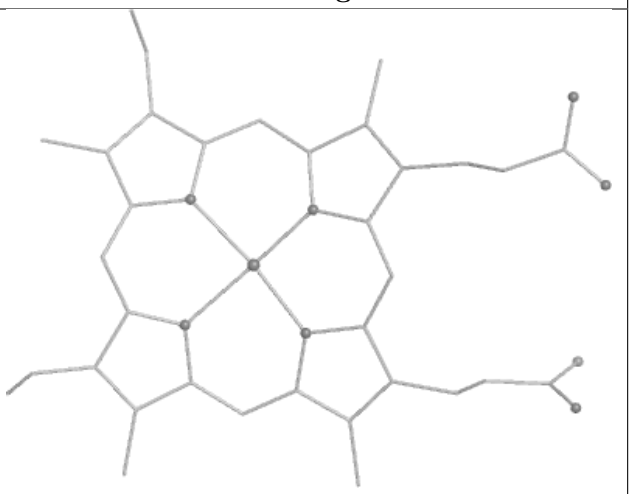

Rings

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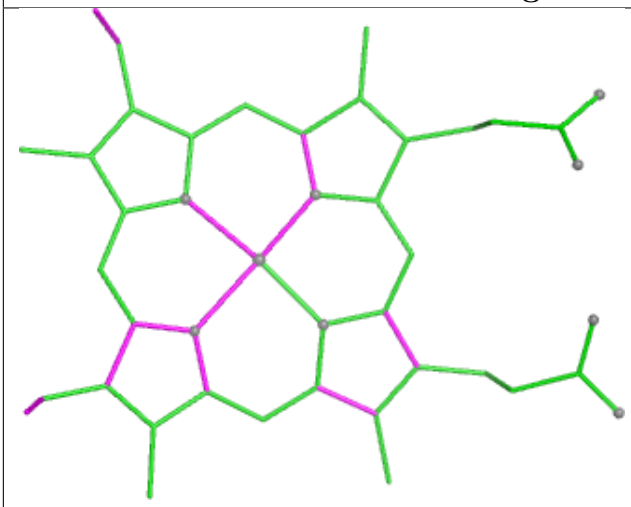

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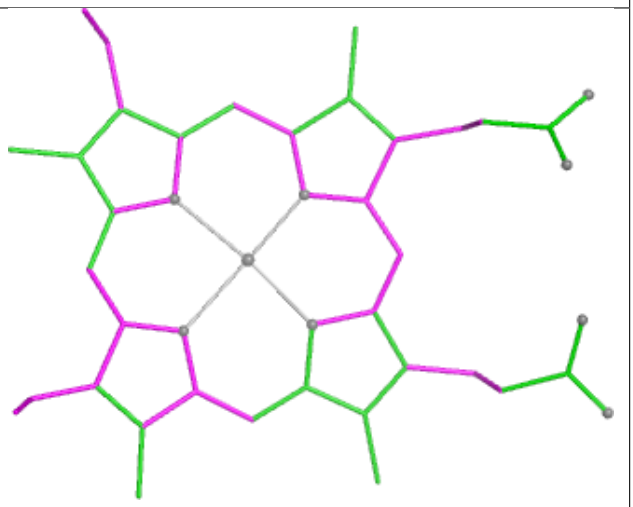

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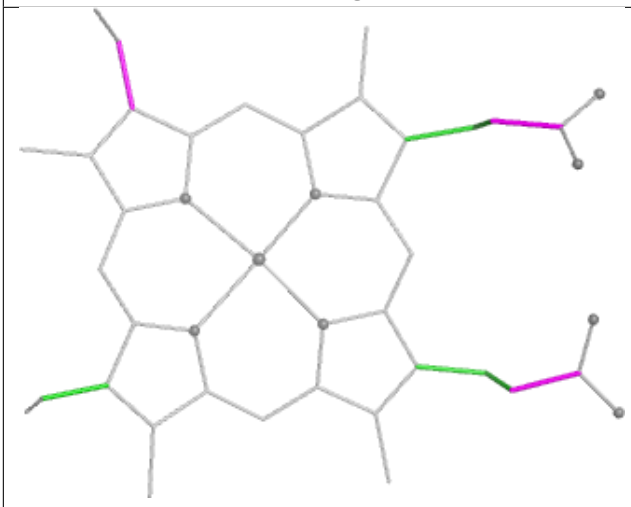

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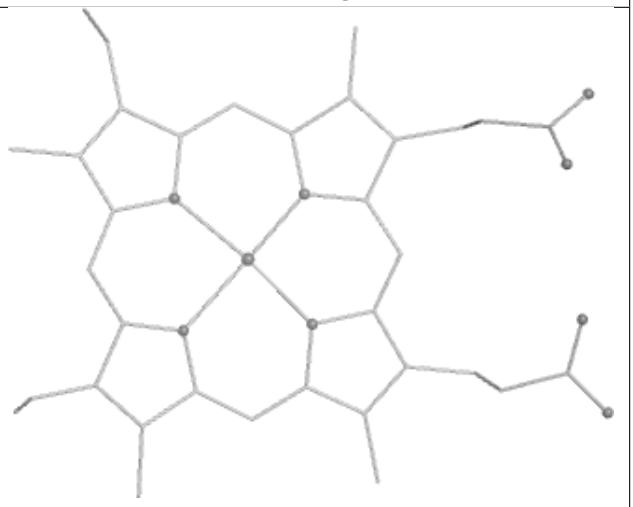

Rings

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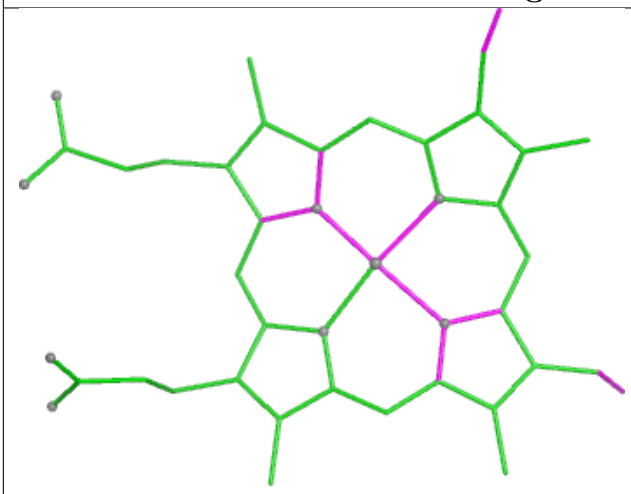

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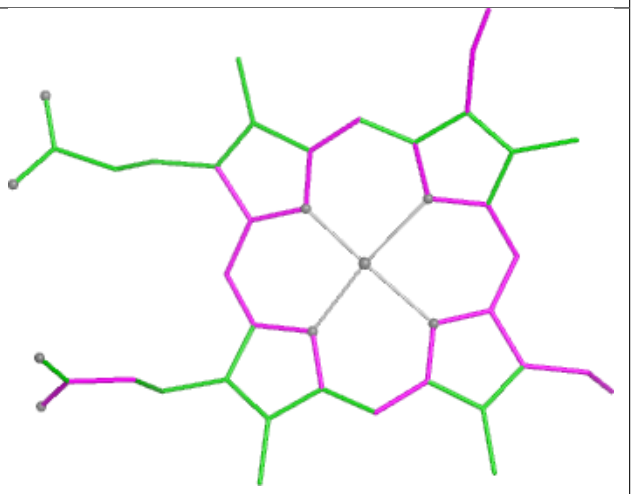

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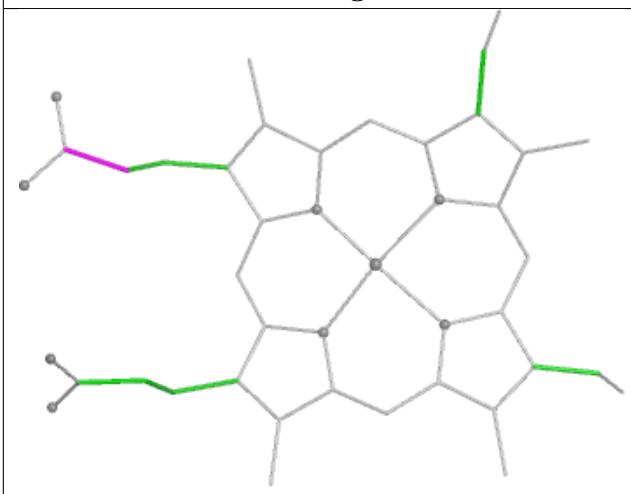

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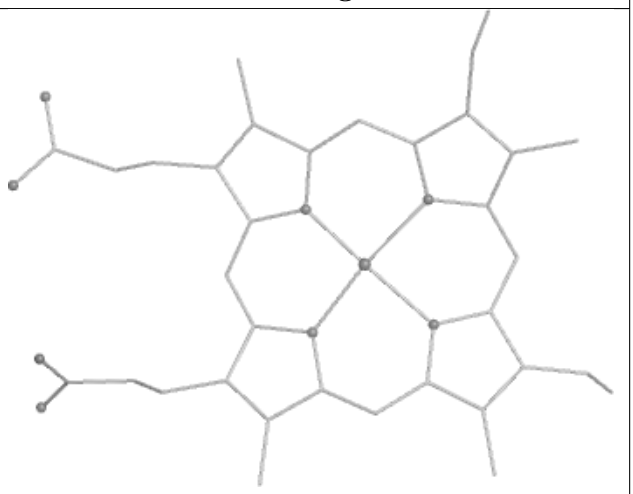
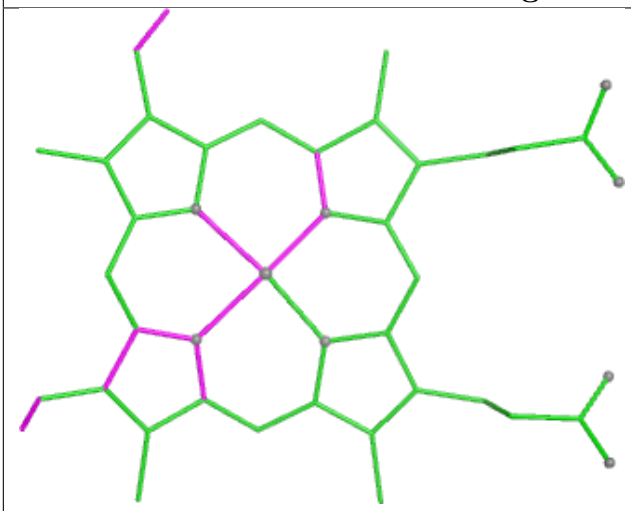


Rings

Ligand HEC N 600



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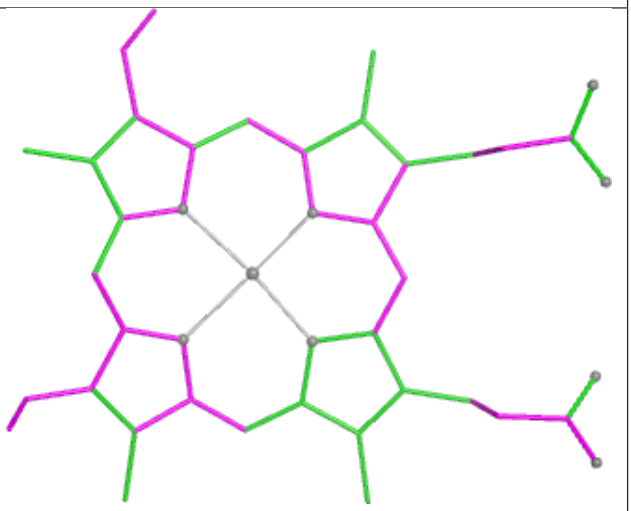

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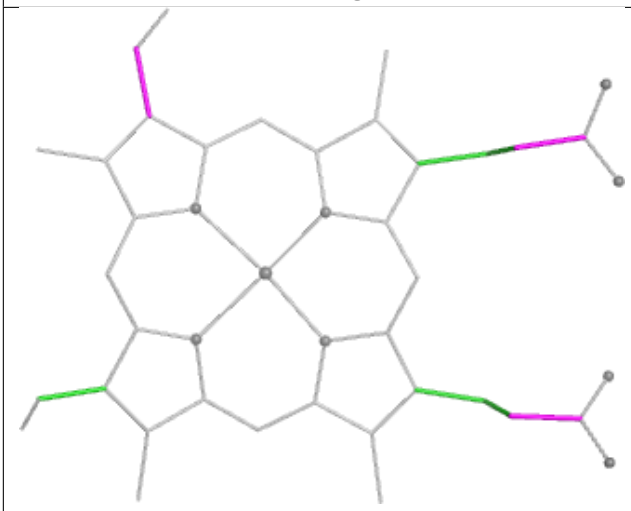

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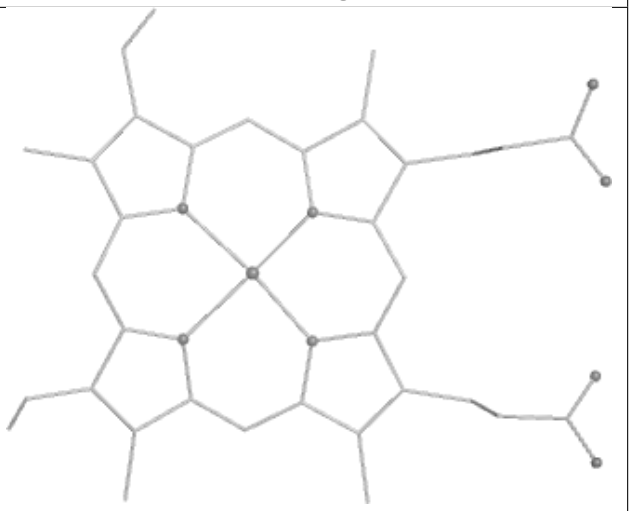

Rings

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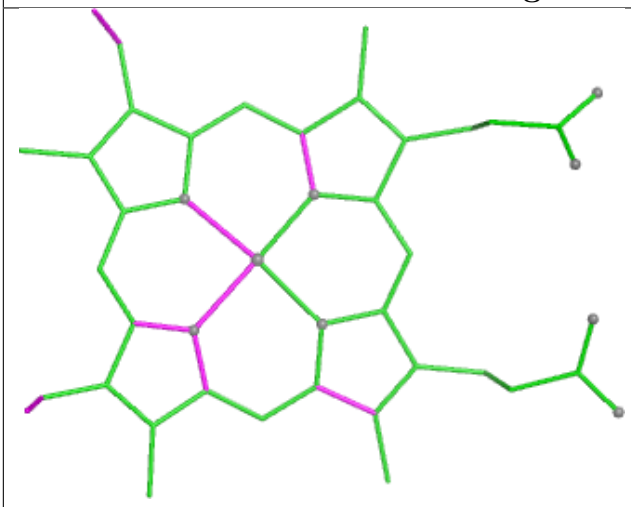

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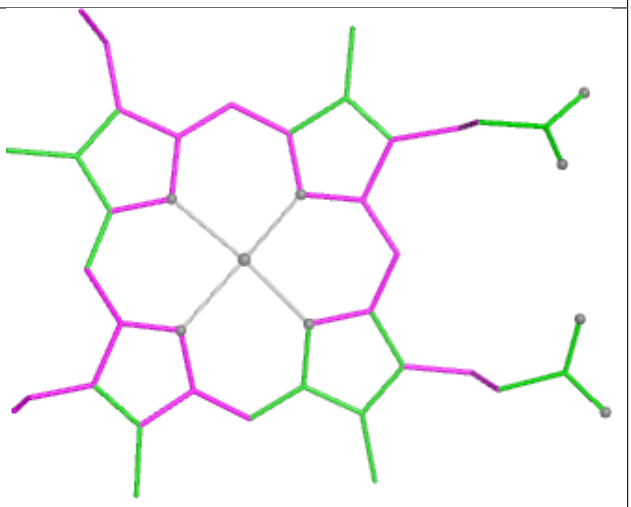

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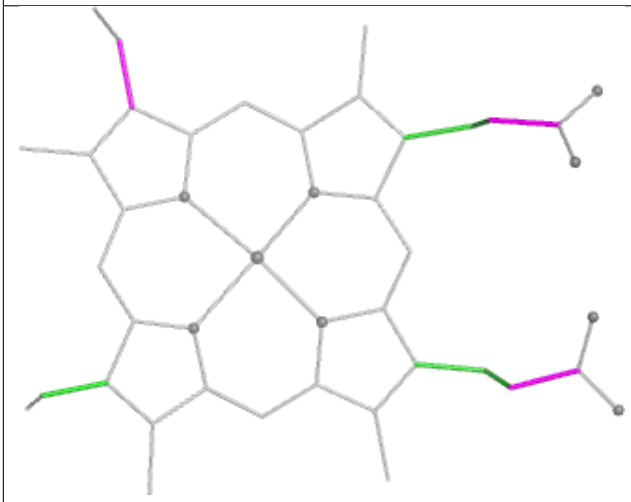

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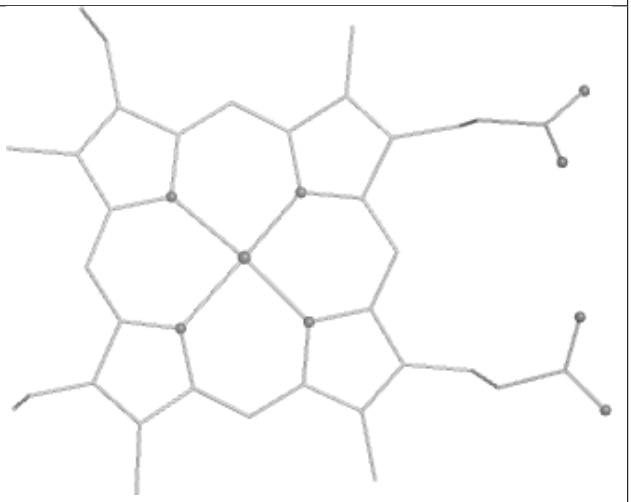
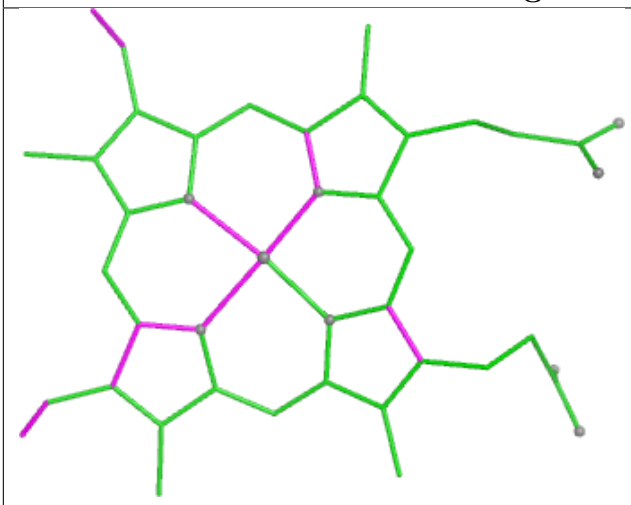


Rings

Ligand HEC F 607



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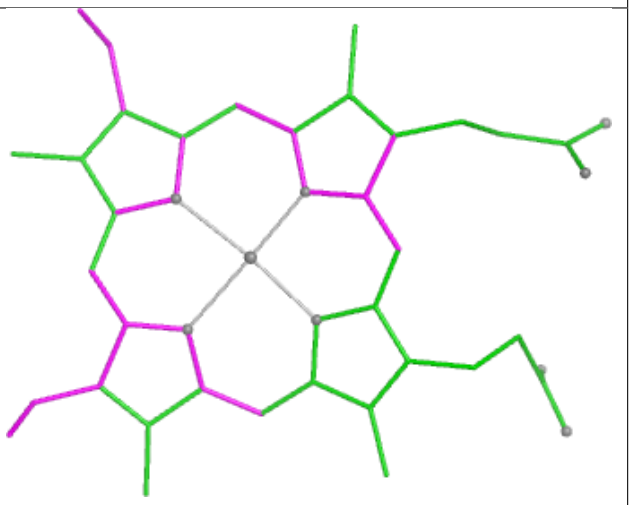

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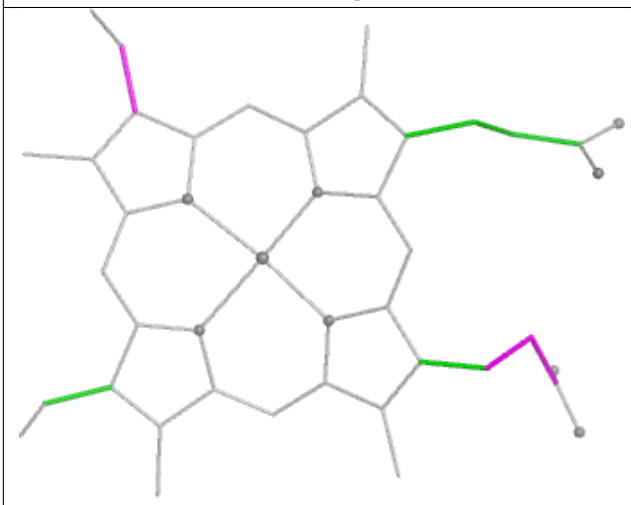

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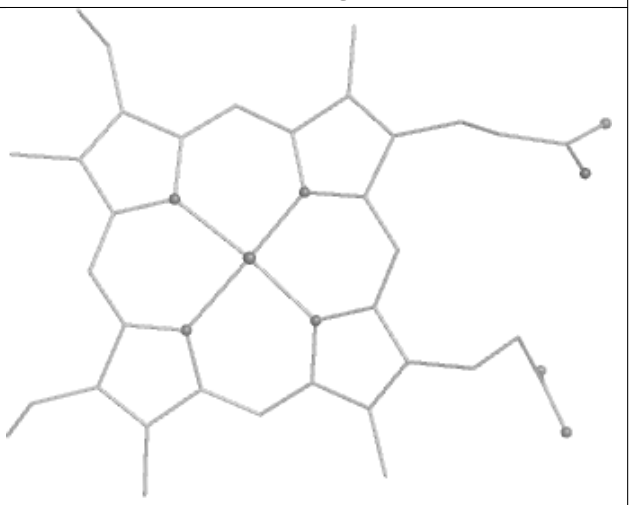
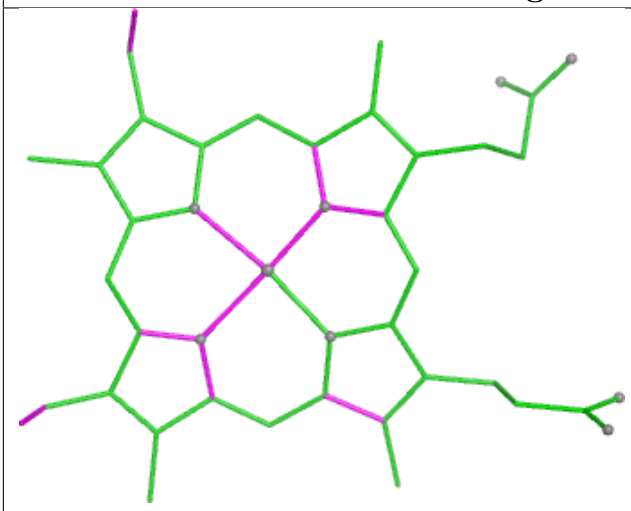


Rings

Ligand HEC J 602



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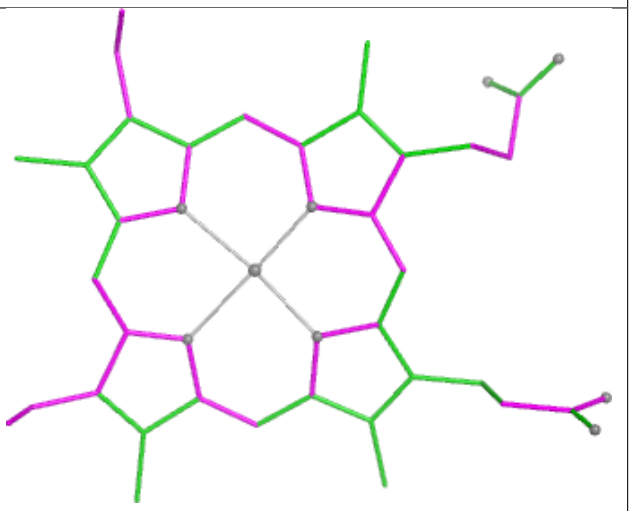

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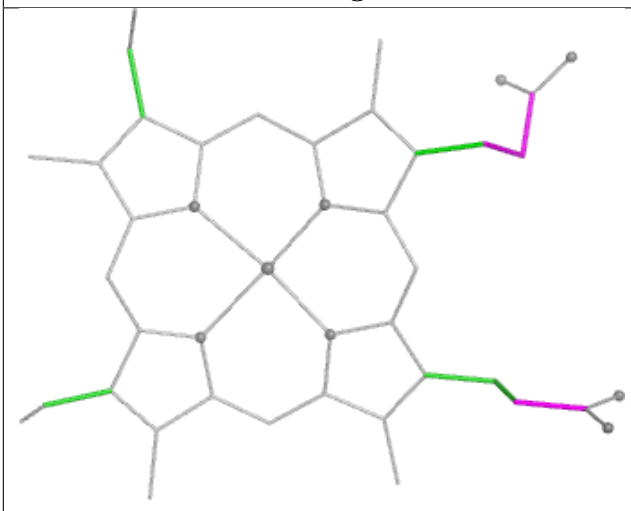

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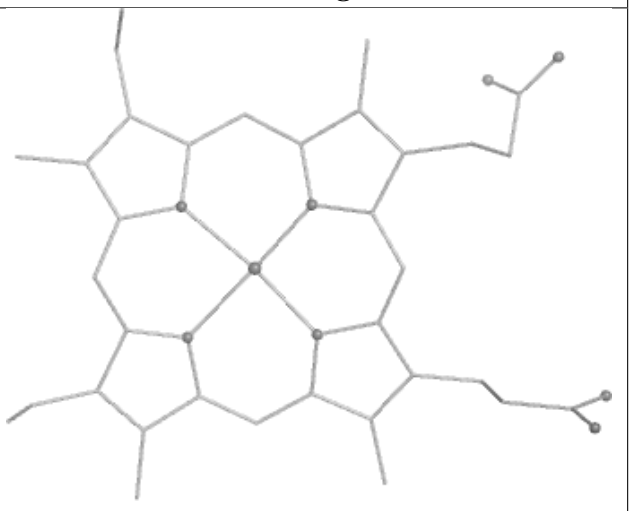
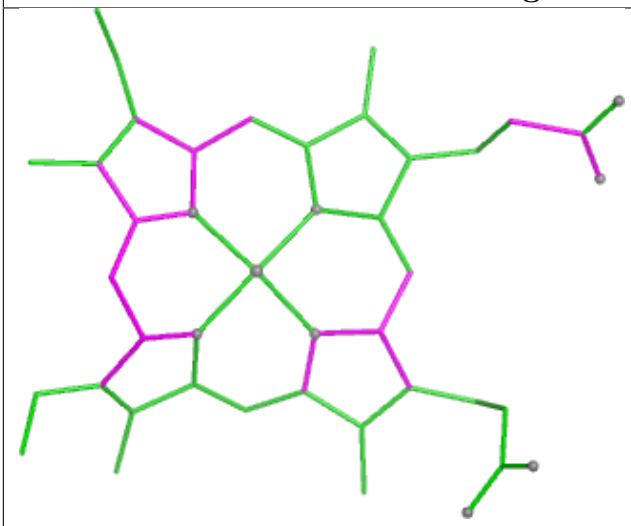


Rings

Ligand HEC C 603



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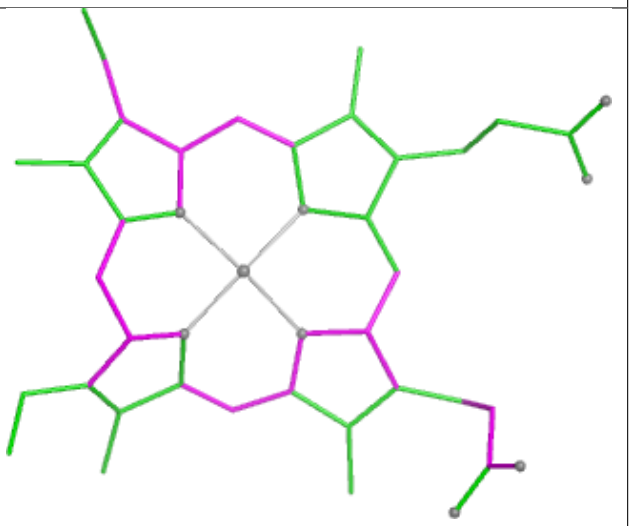

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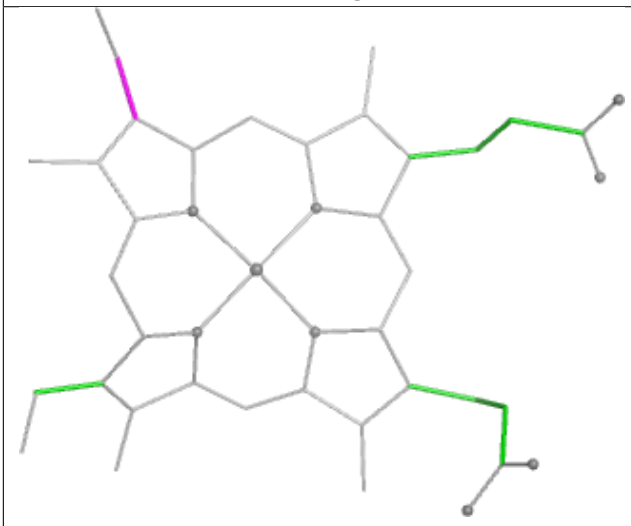

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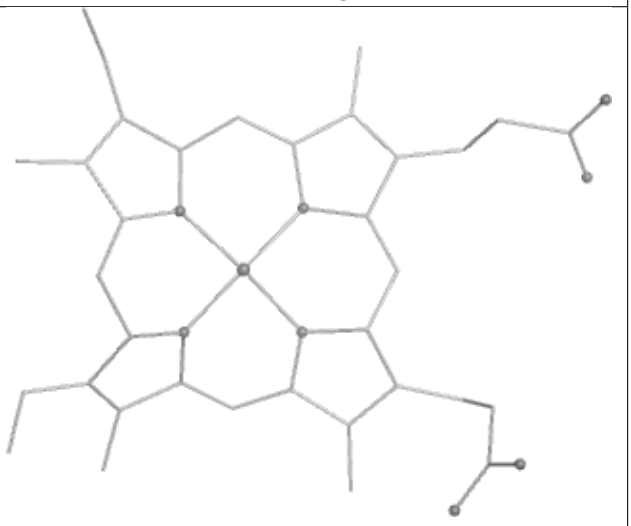
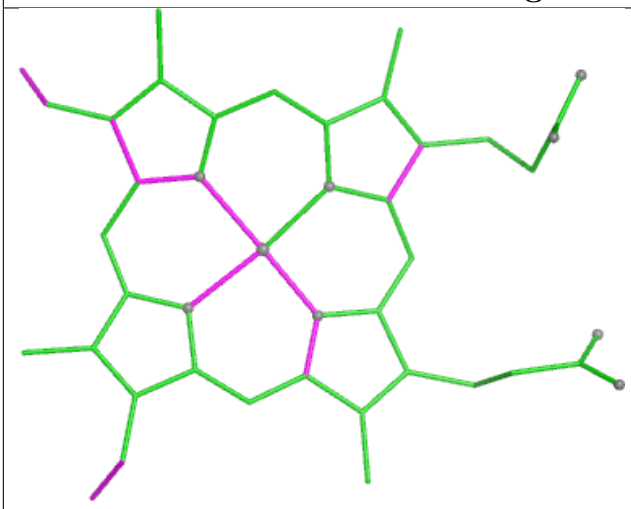


Rings

Ligand HEC L 607



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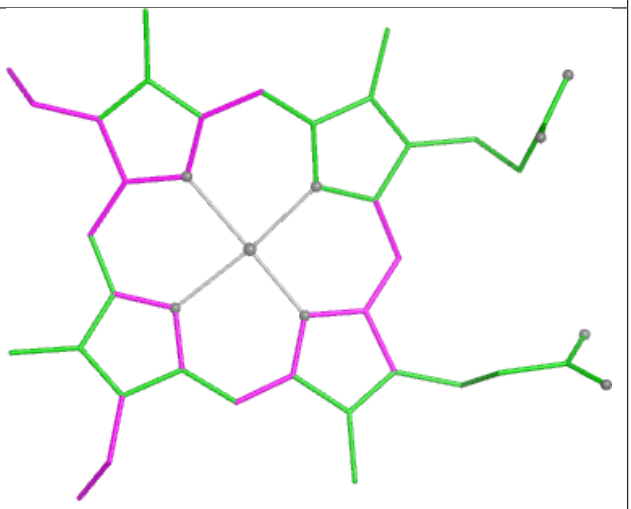

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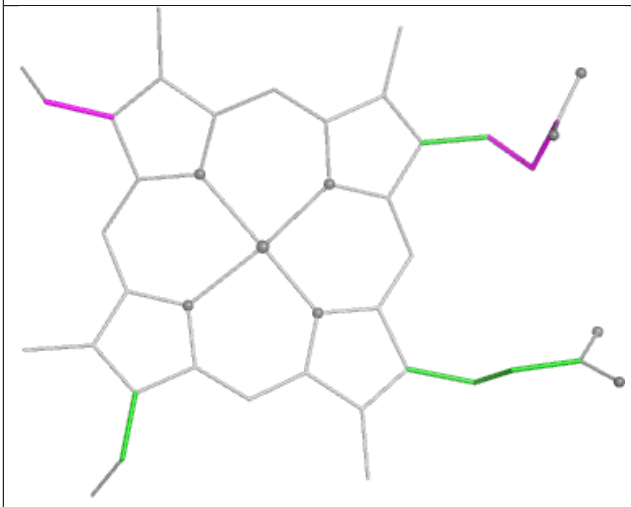

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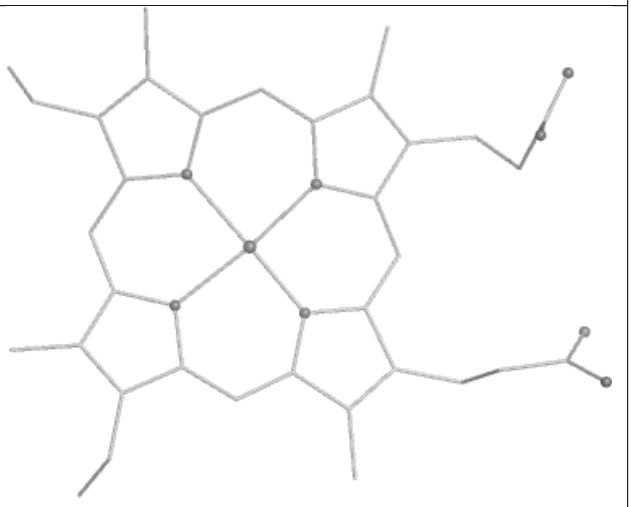
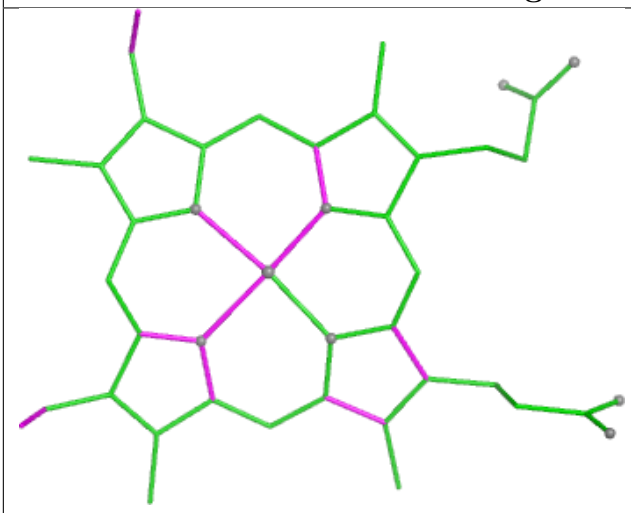


Rings

Ligand HEC L 602



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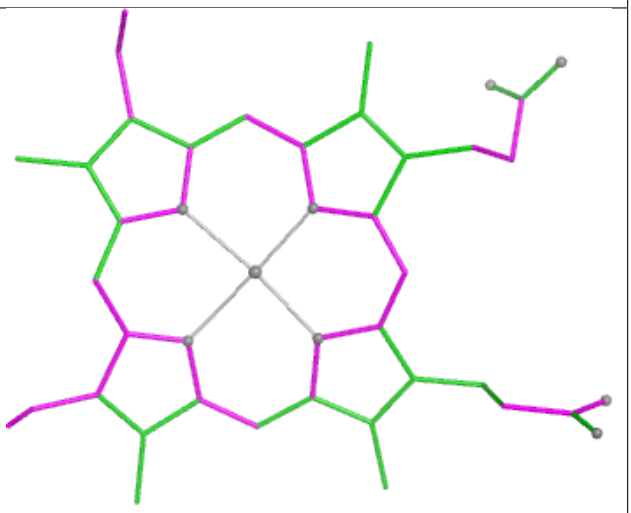

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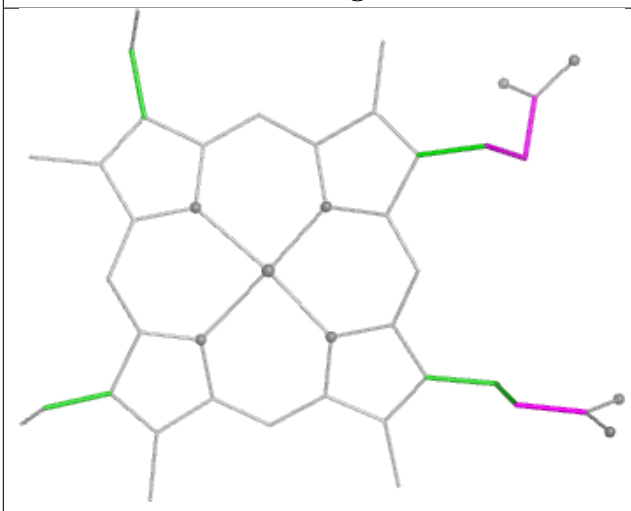

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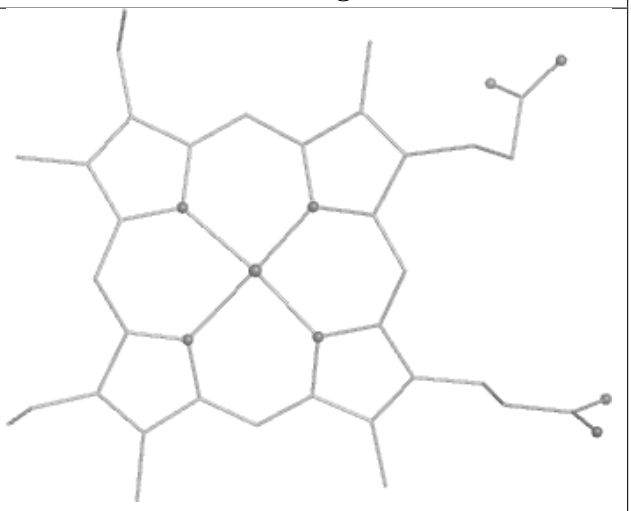
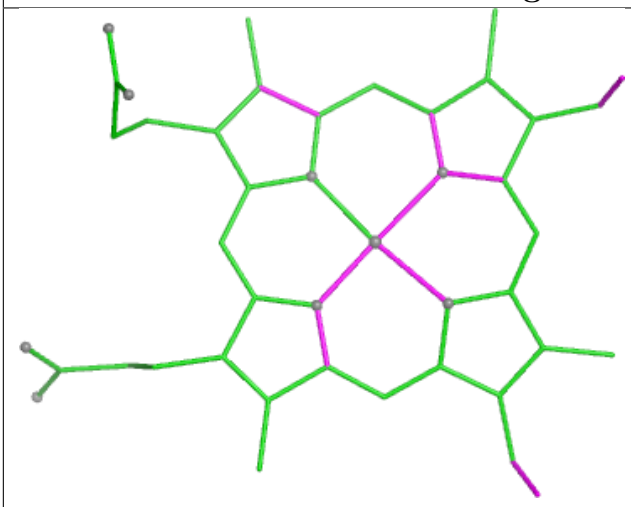


Rings

Ligand HEC T 601



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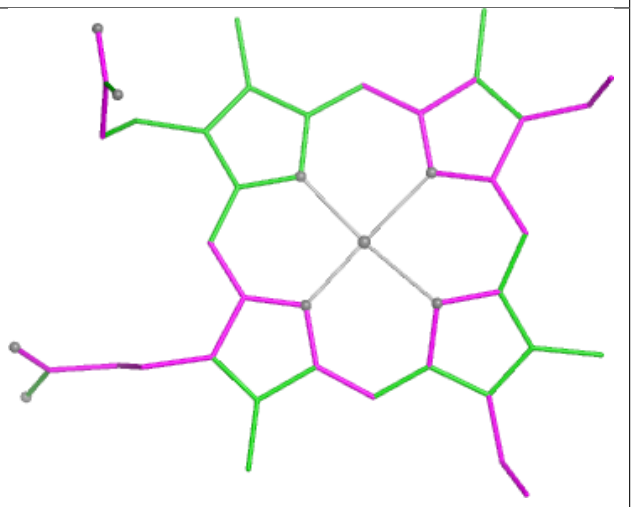
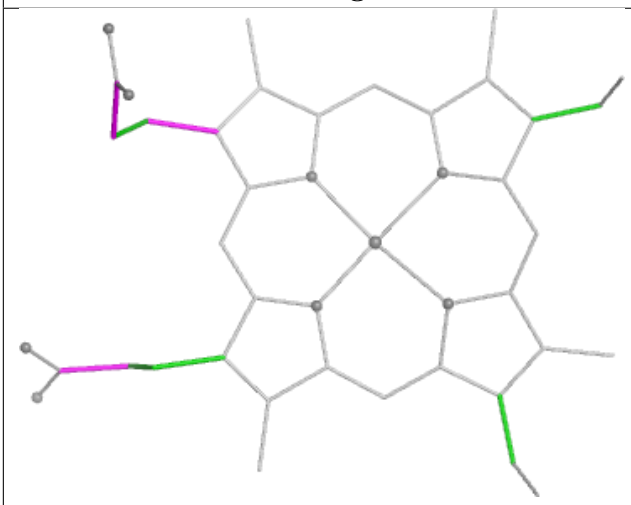


Bond angles



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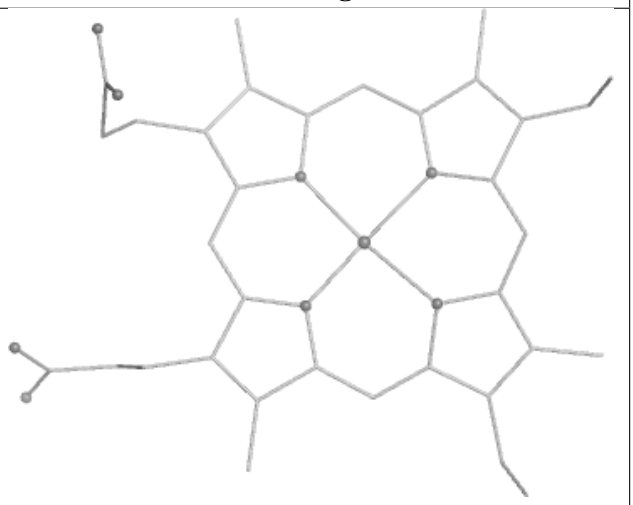
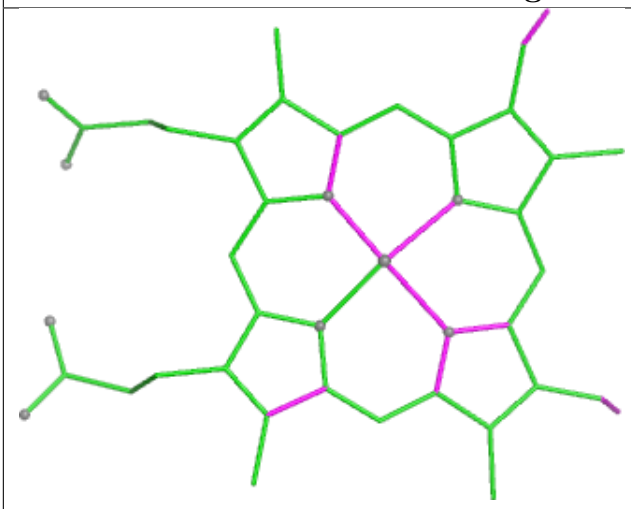


Rings

Ligand HEC F 604



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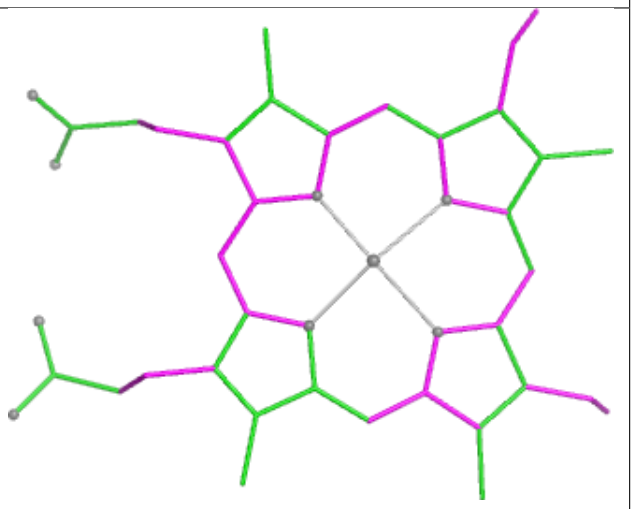
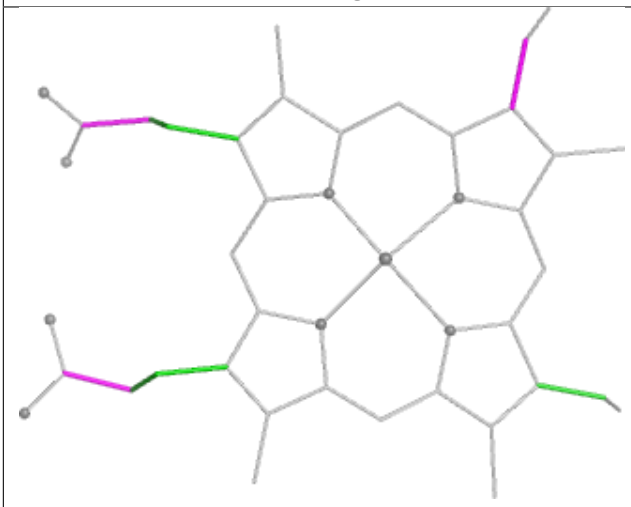


Bond angles



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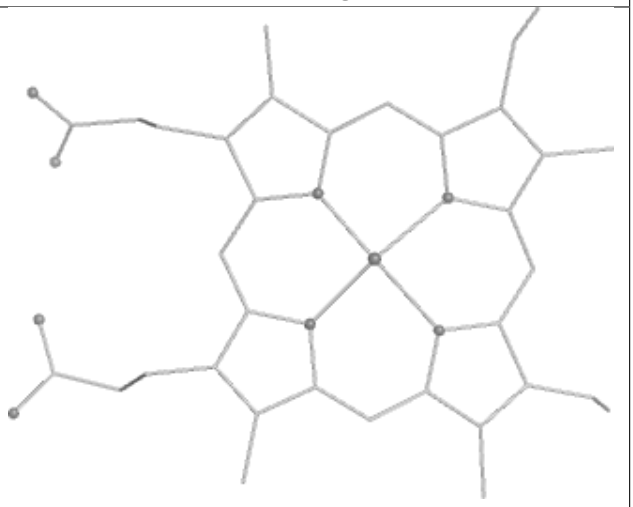
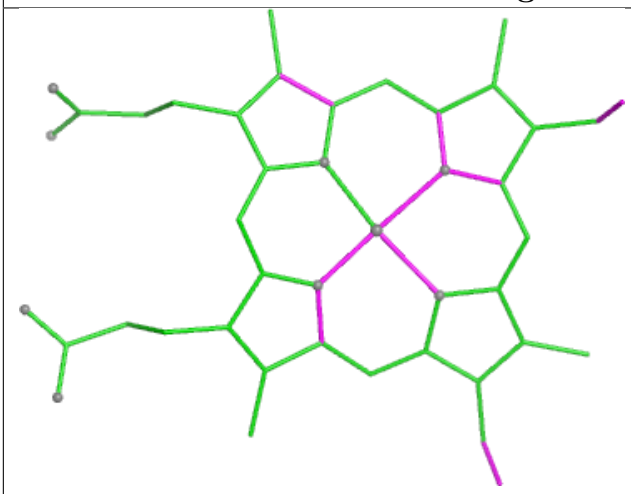


Rings

Ligand HEC W 606



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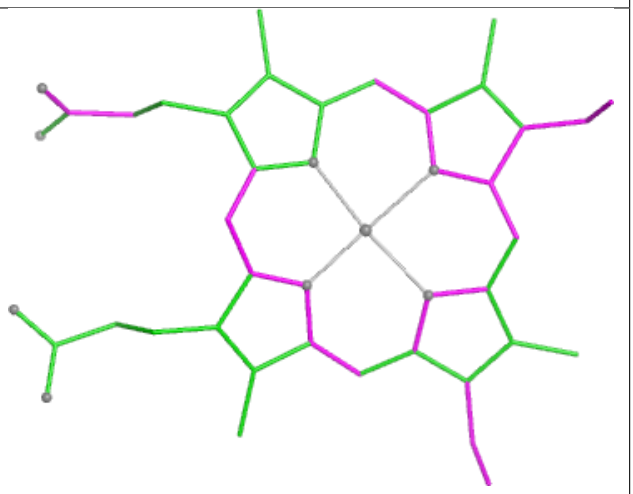
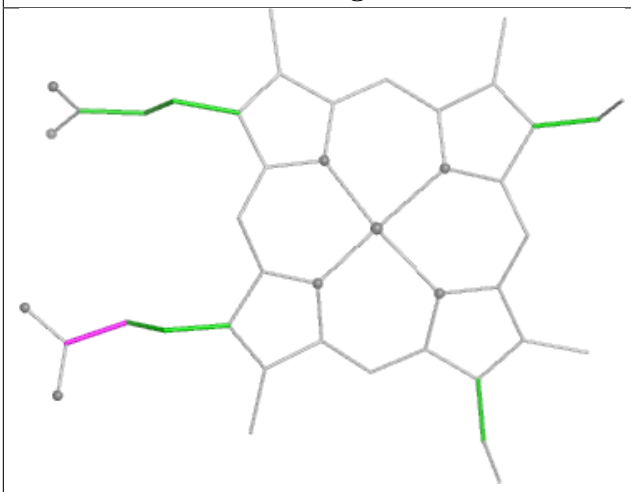
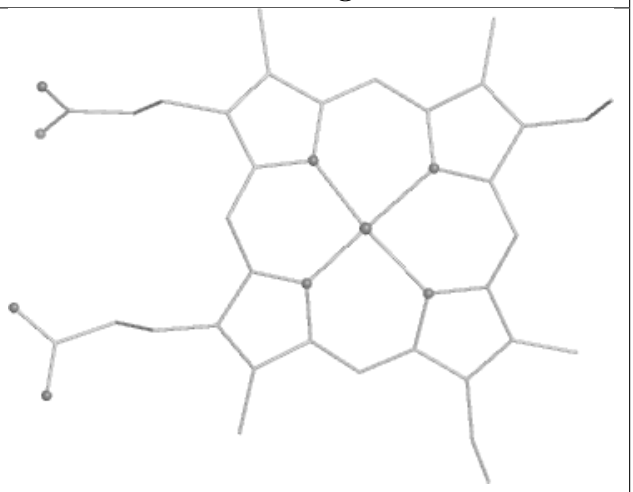


Bond angles

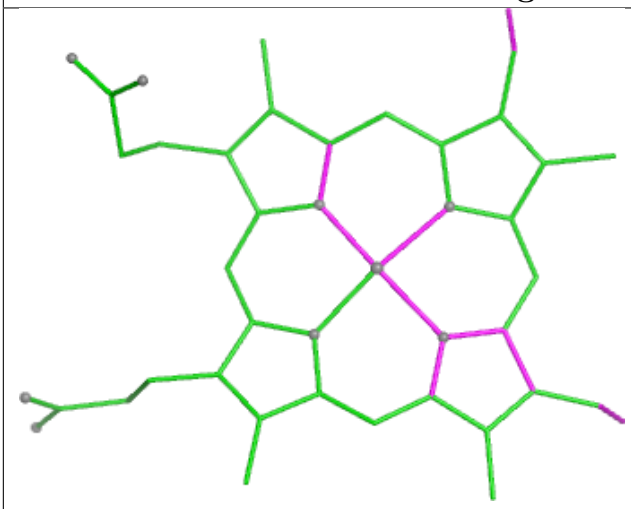


Torsions



Rings

Ligand HEC W 602



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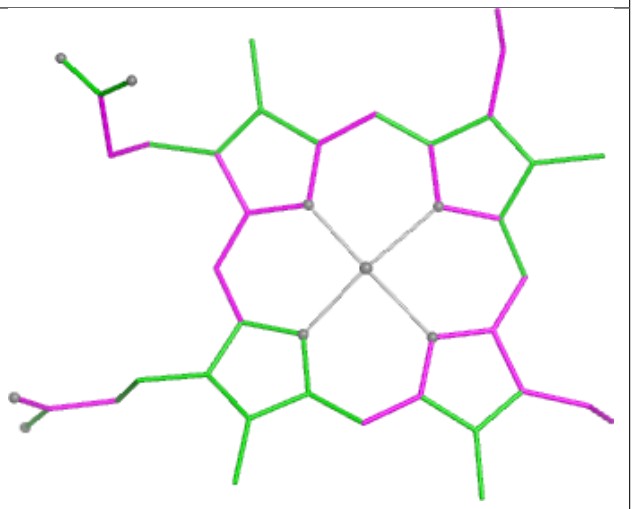

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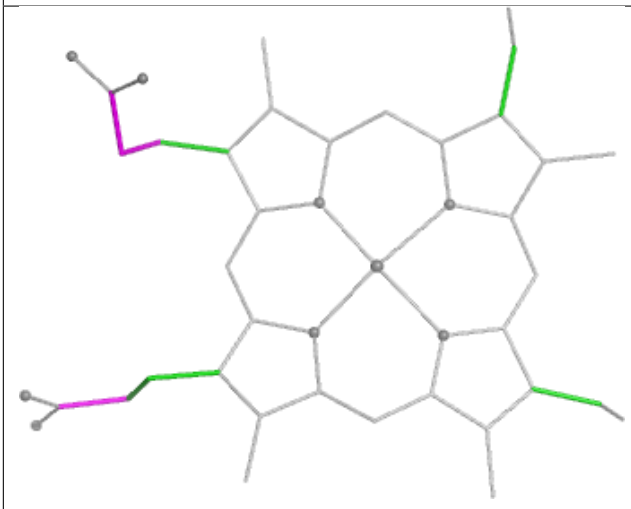

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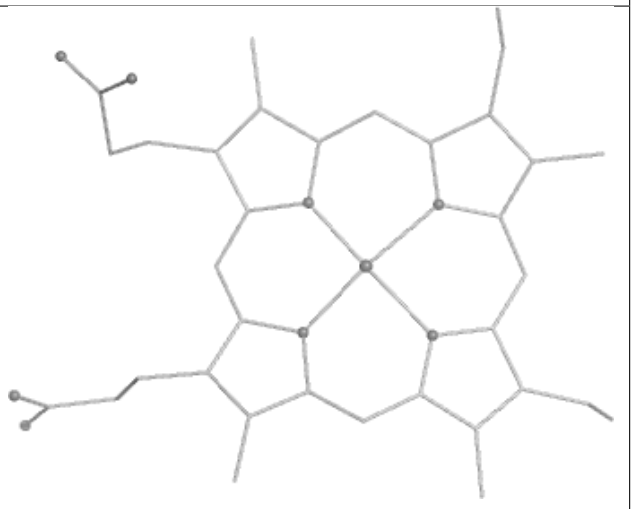
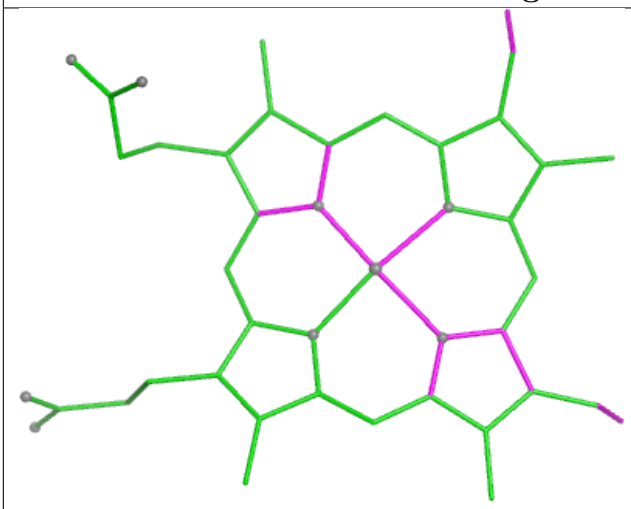


Rings

Ligand HEC A 602



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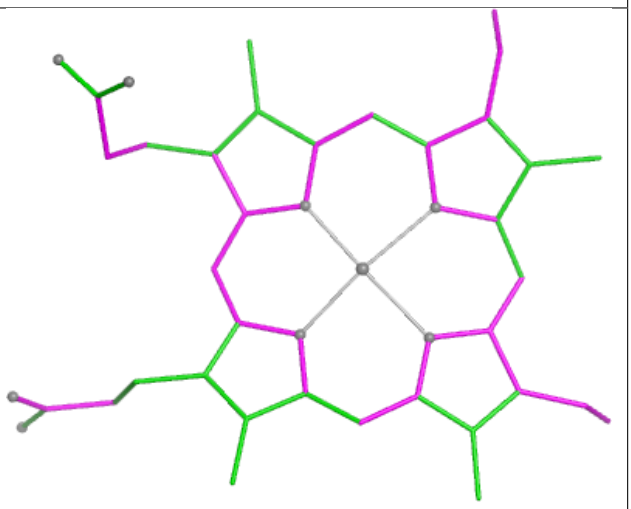

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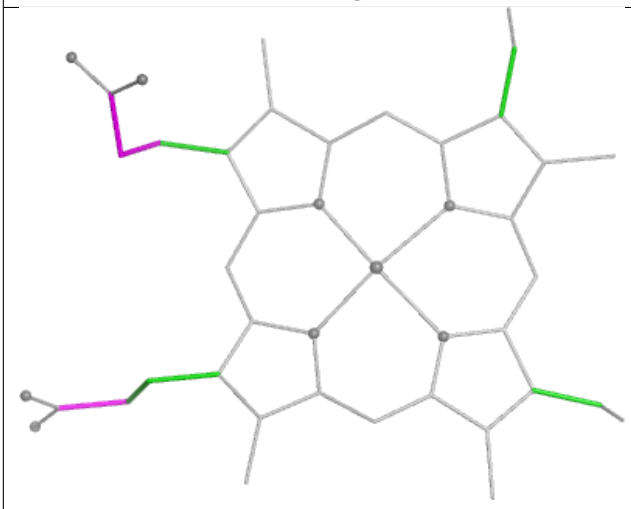

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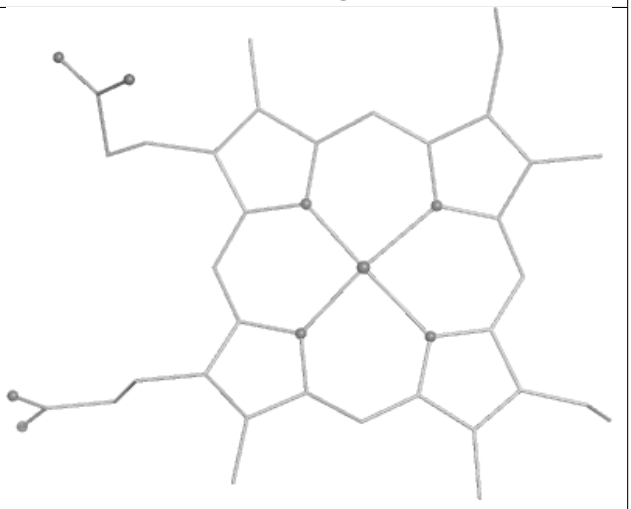

Rings

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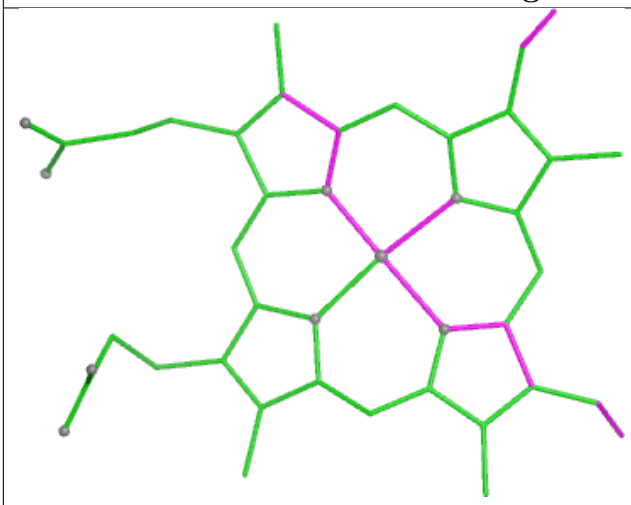

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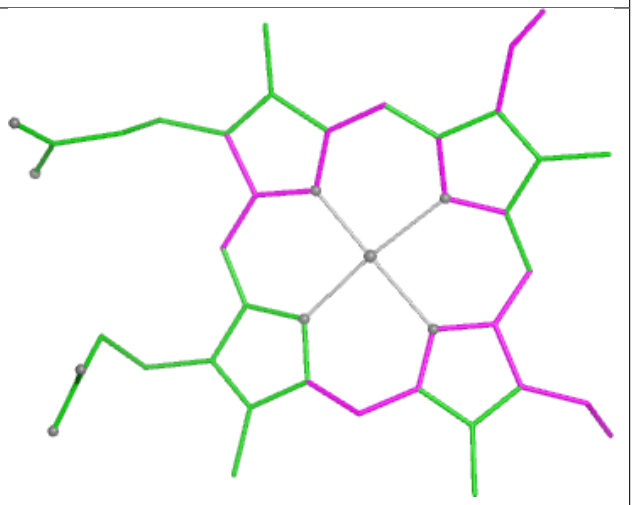

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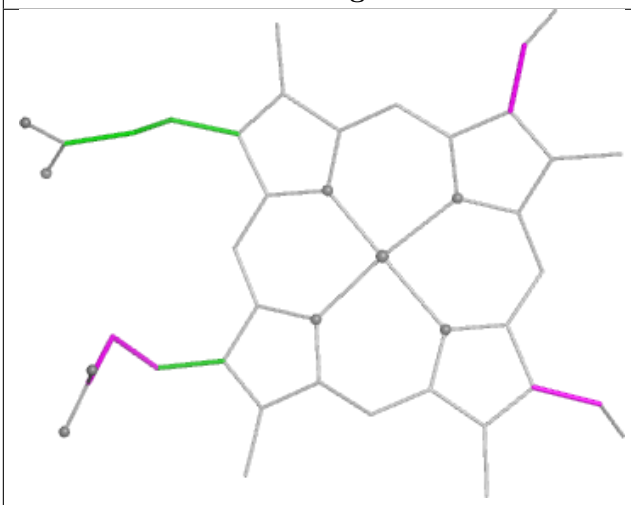

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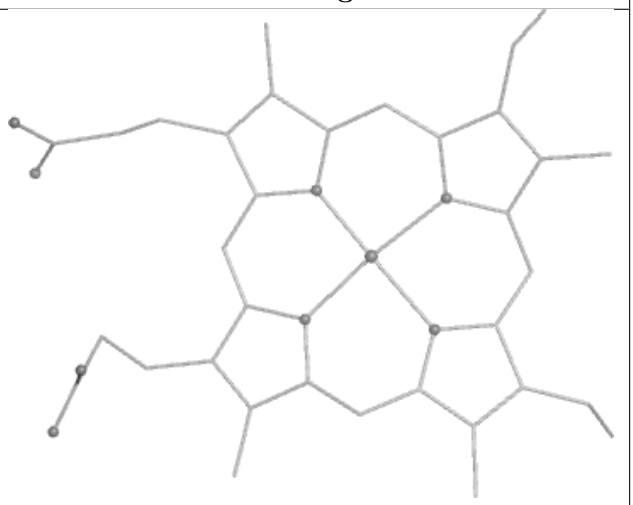
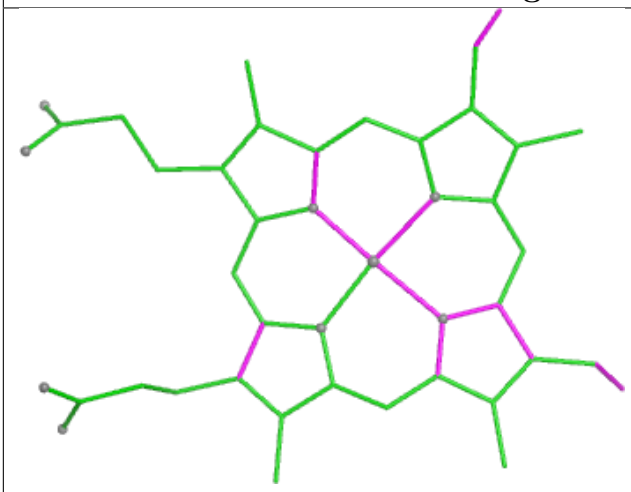


Rings

Ligand HEC P 605



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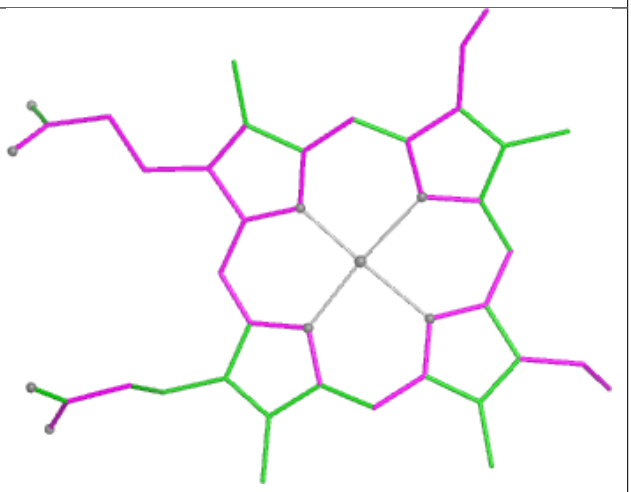

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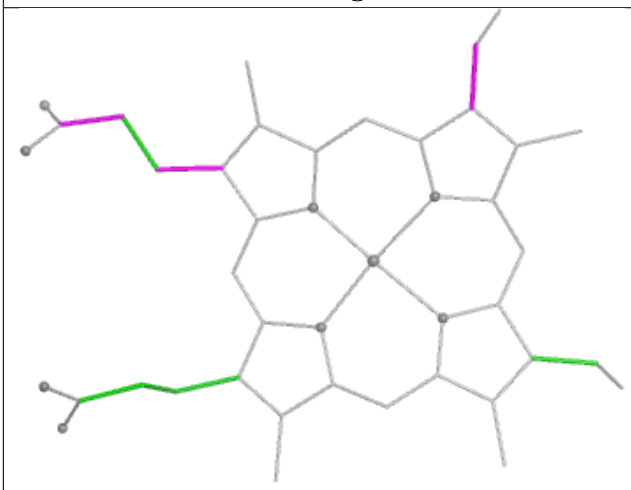

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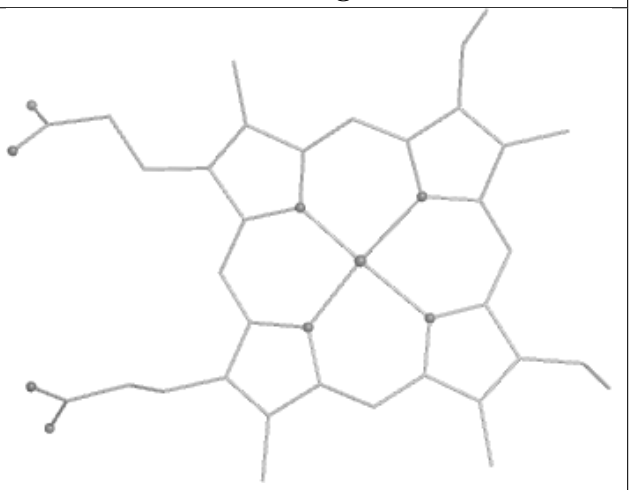
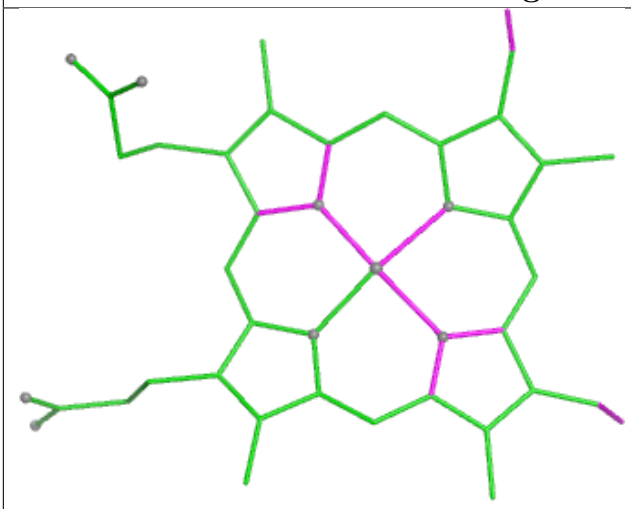


Rings

Ligand HEC C 602



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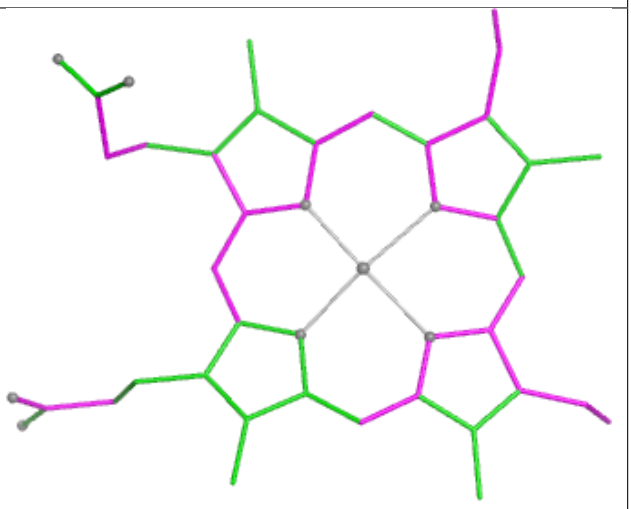

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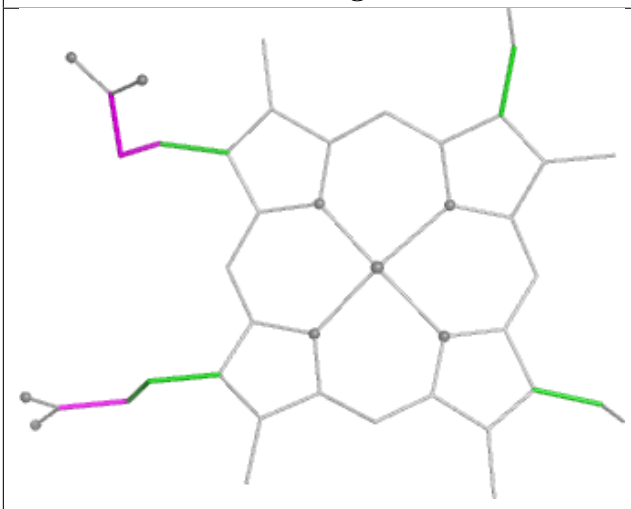

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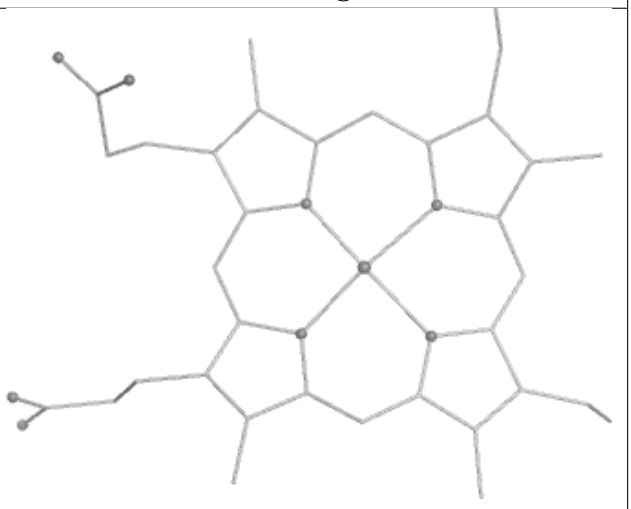
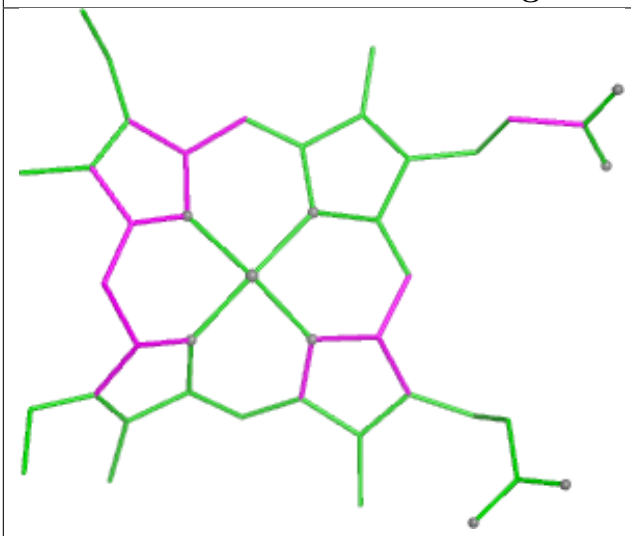


Rings

Ligand HEC D 603



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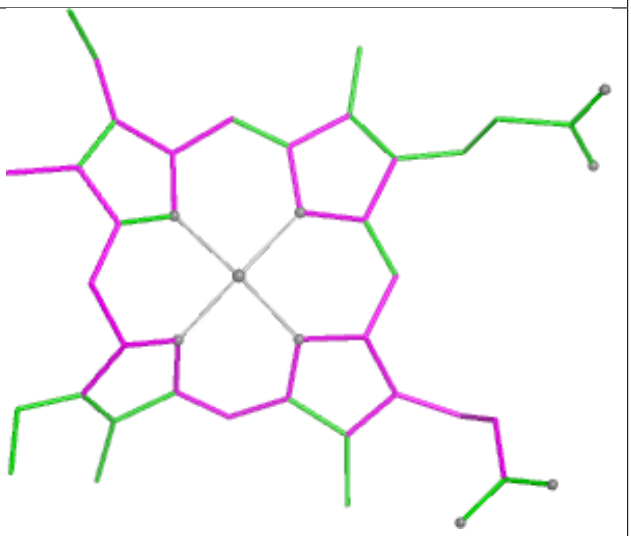

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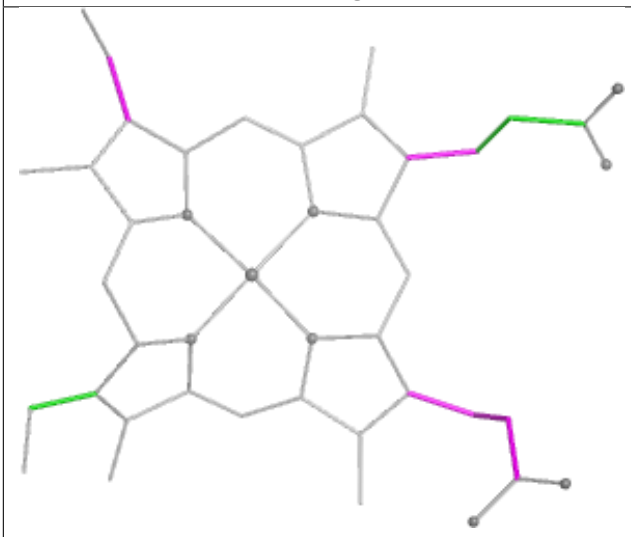

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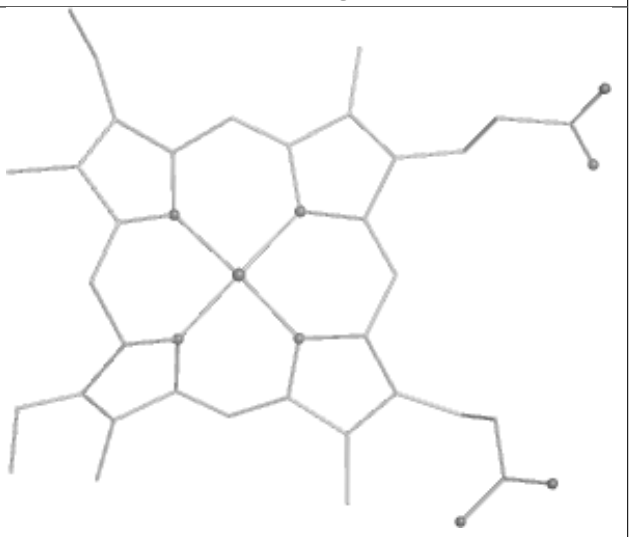
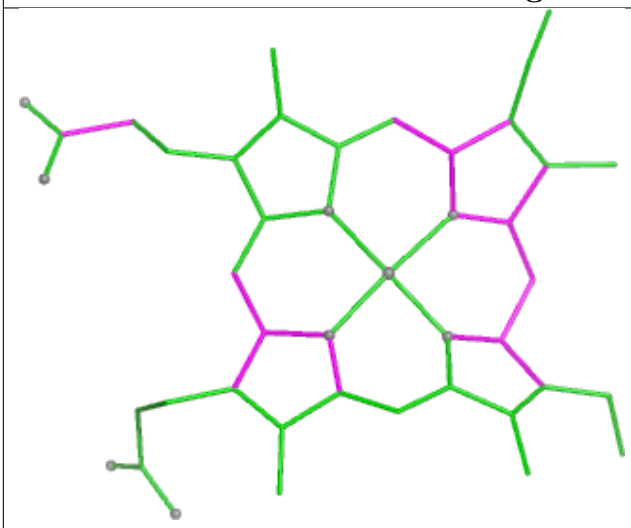


Rings

Ligand HEC S 603



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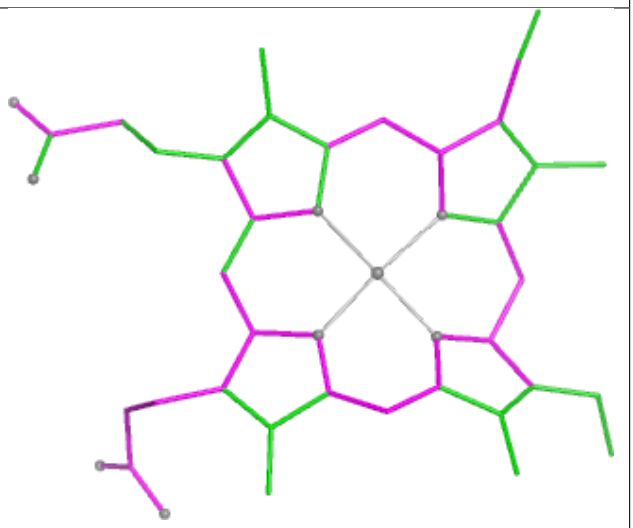

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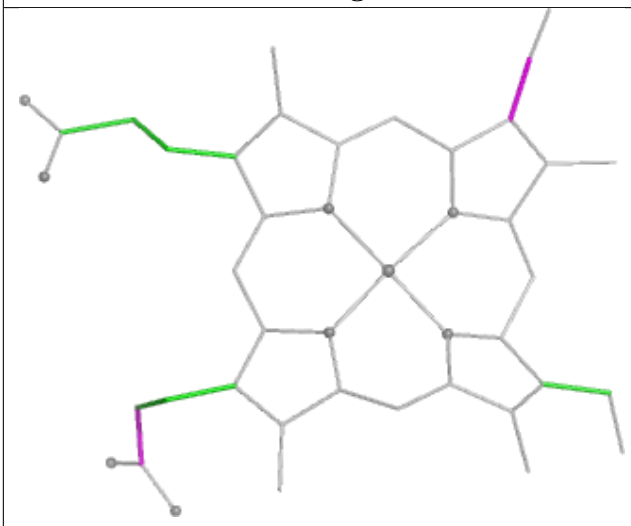

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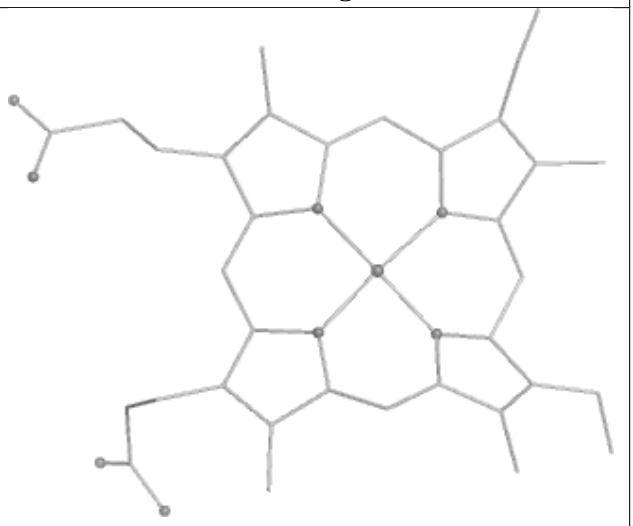
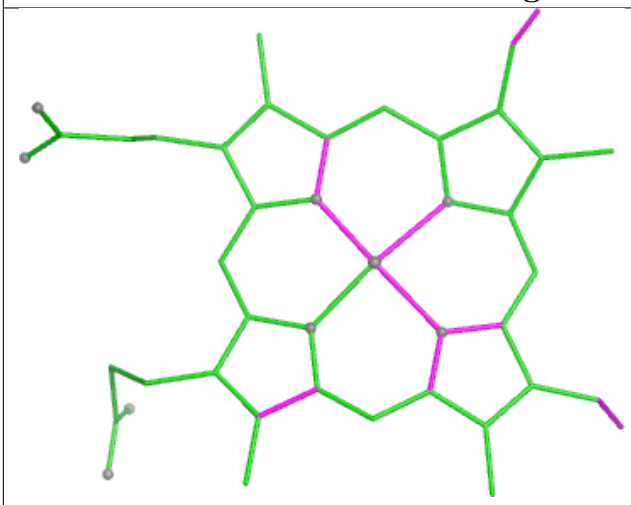


Rings

Ligand HEC B 601



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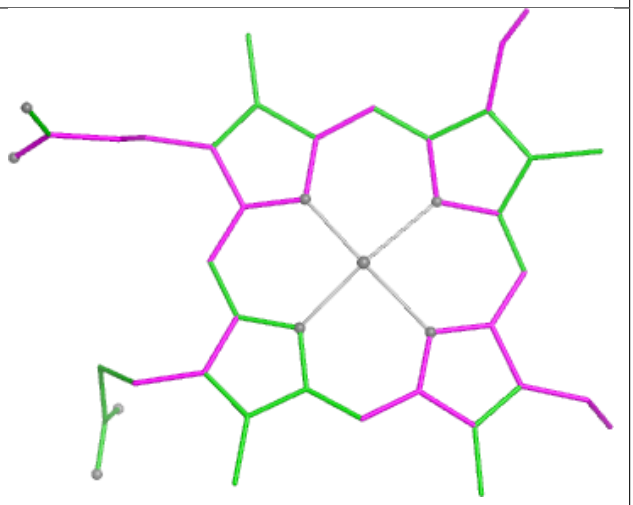

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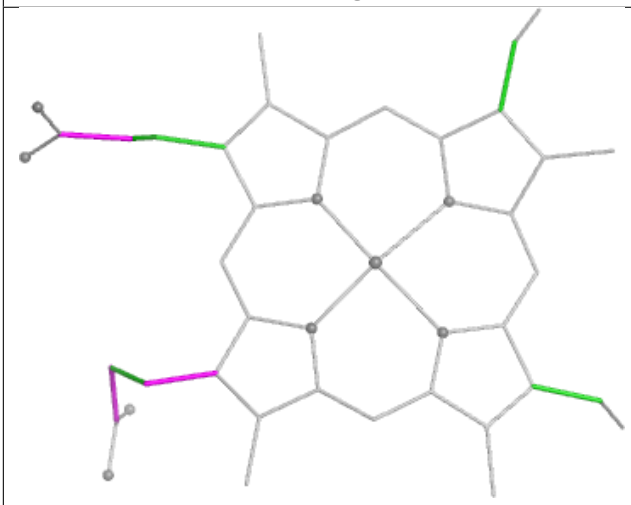

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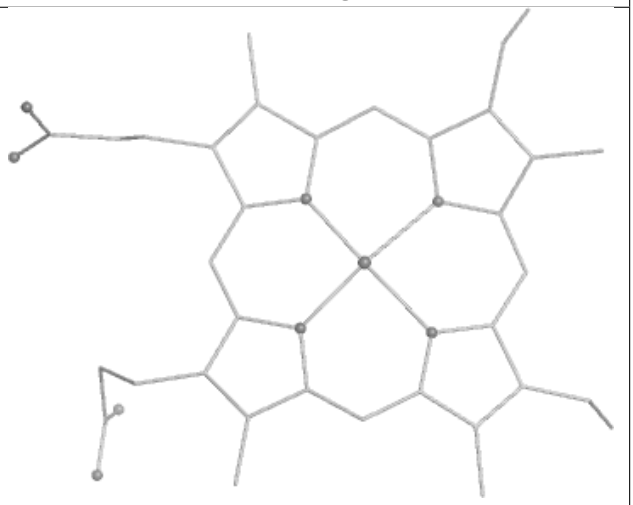

Rings

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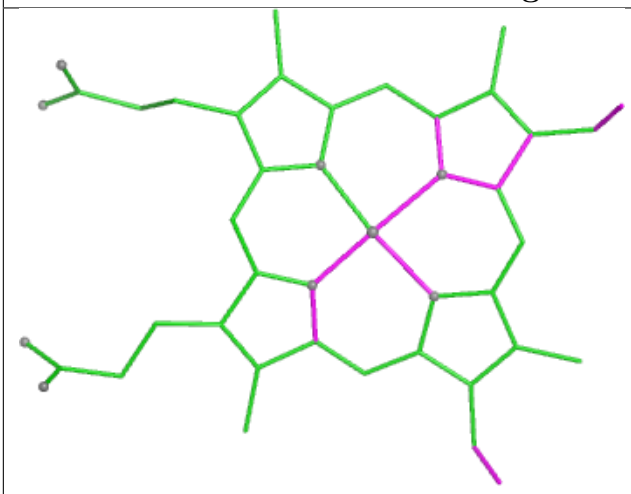

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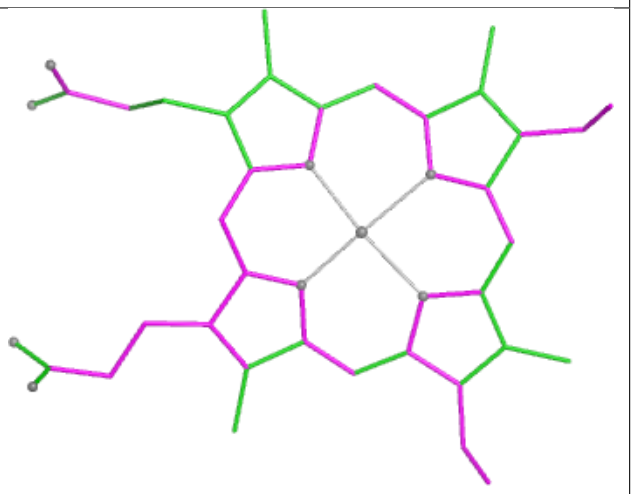

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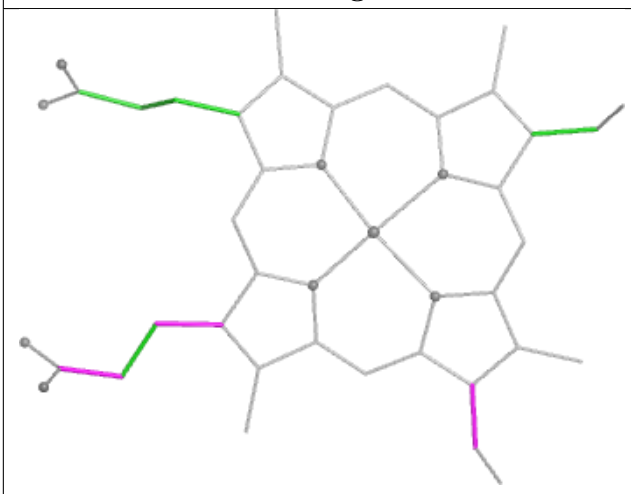

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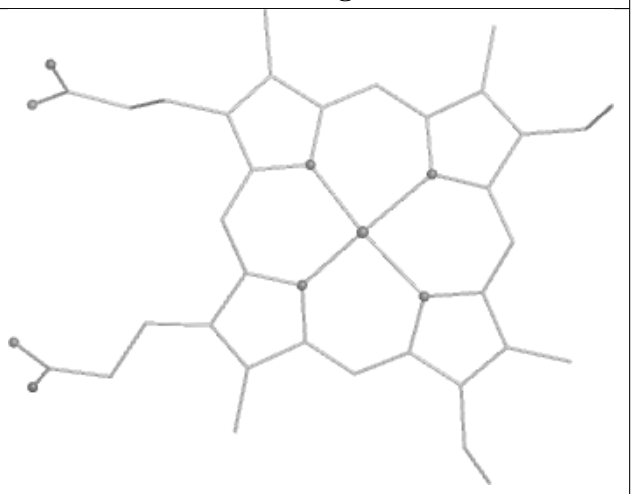

Rings

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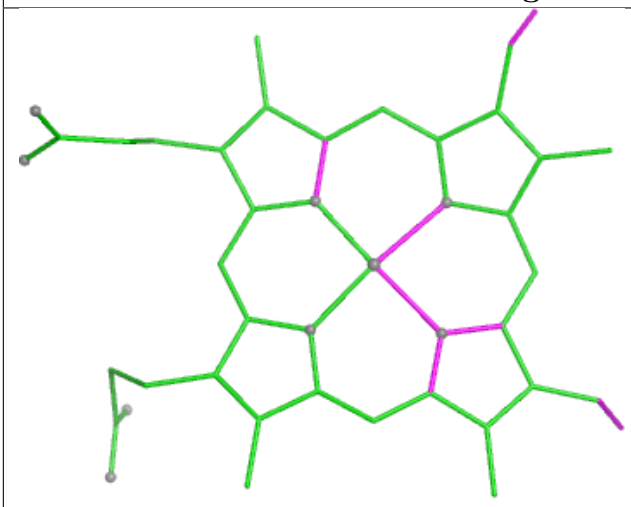

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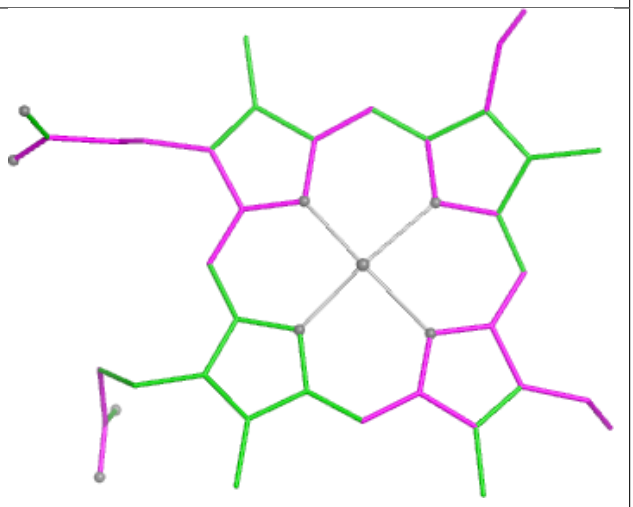

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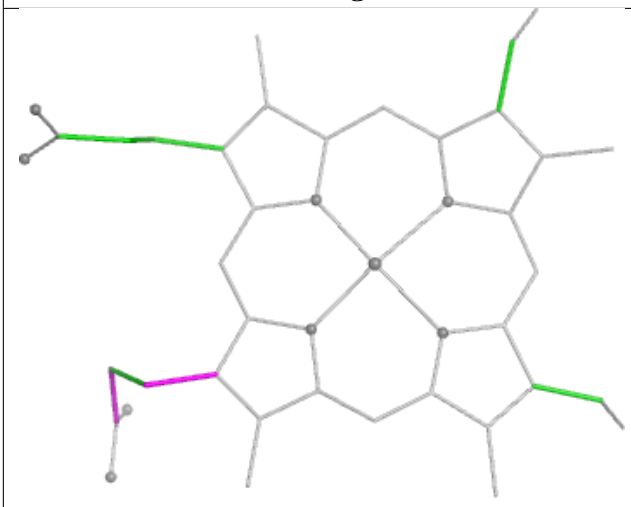

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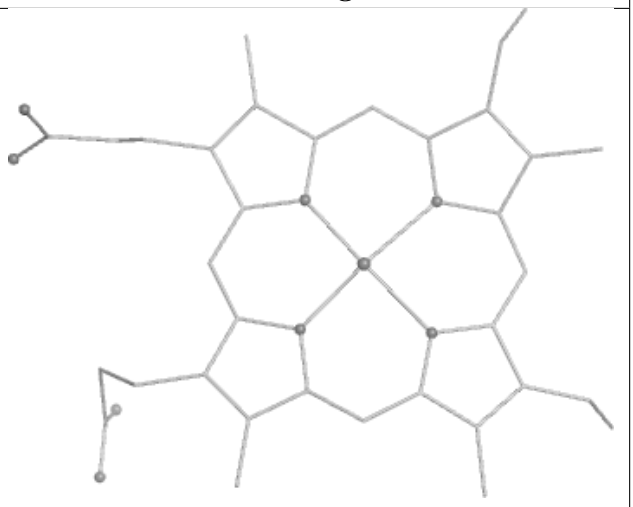
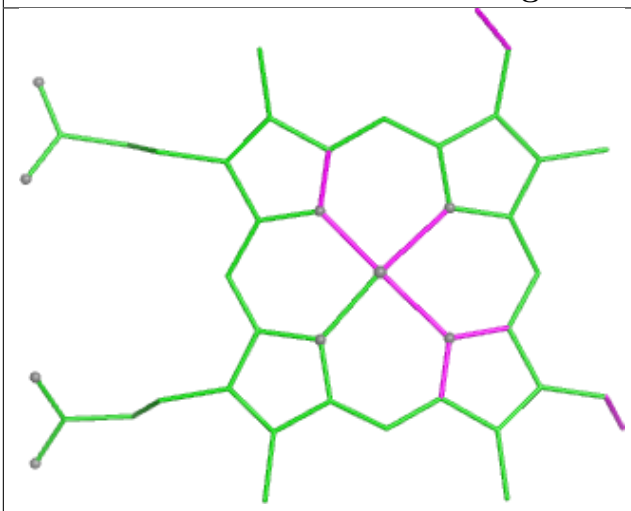


Rings

Ligand HEC K 600



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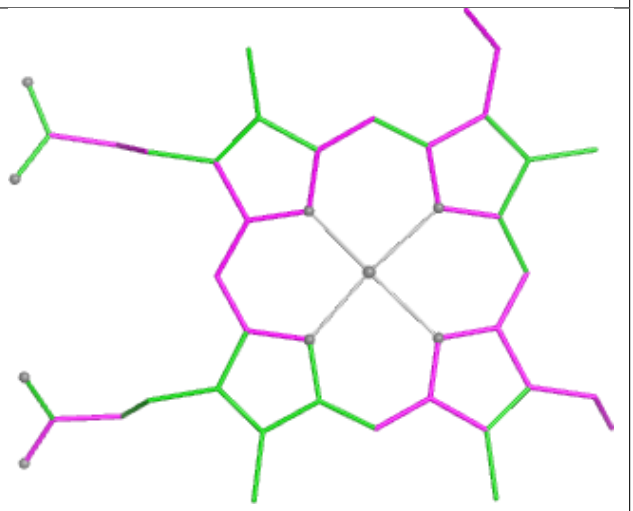

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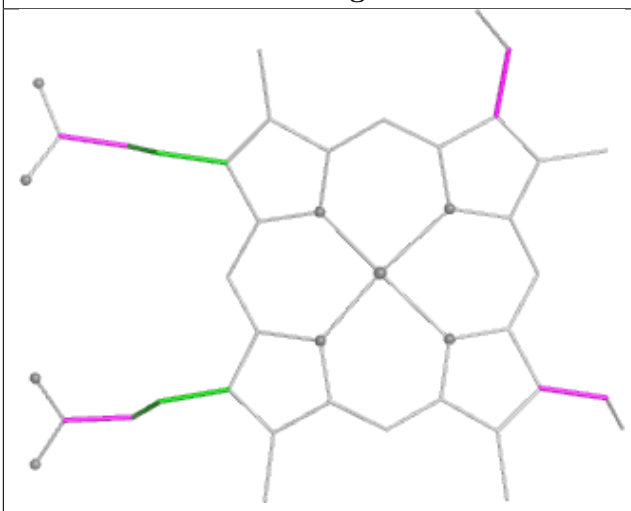

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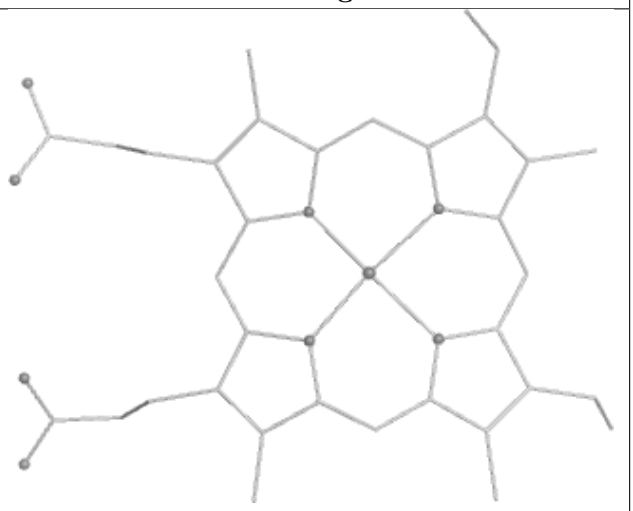

Rings

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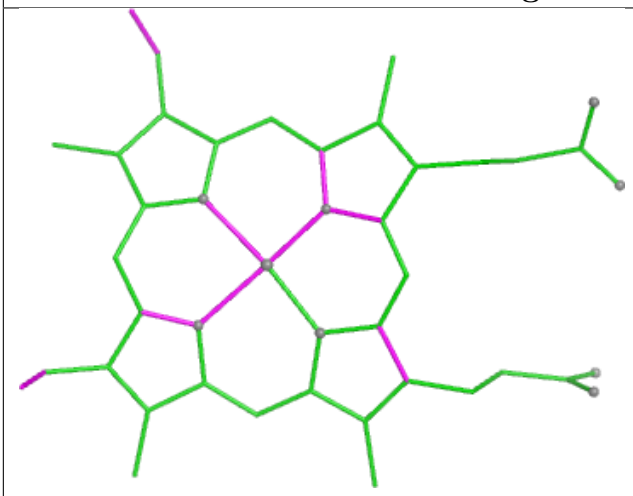

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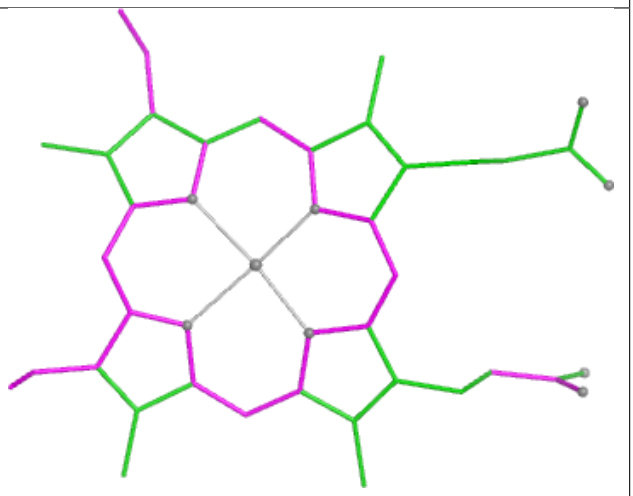

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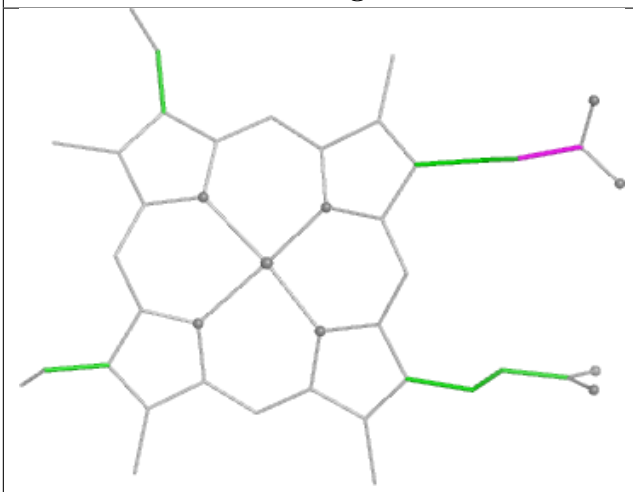

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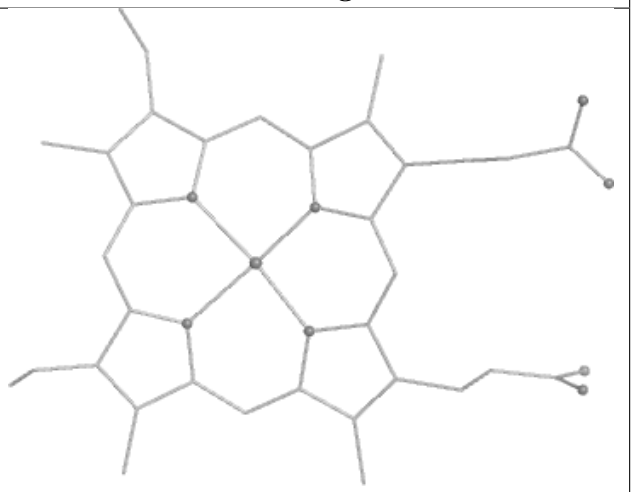

Rings

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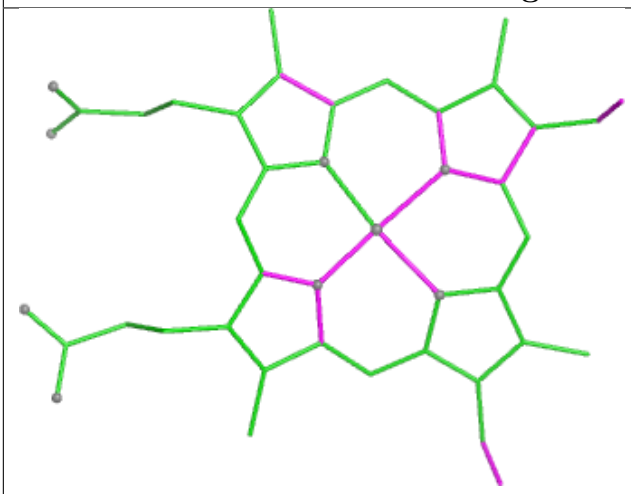

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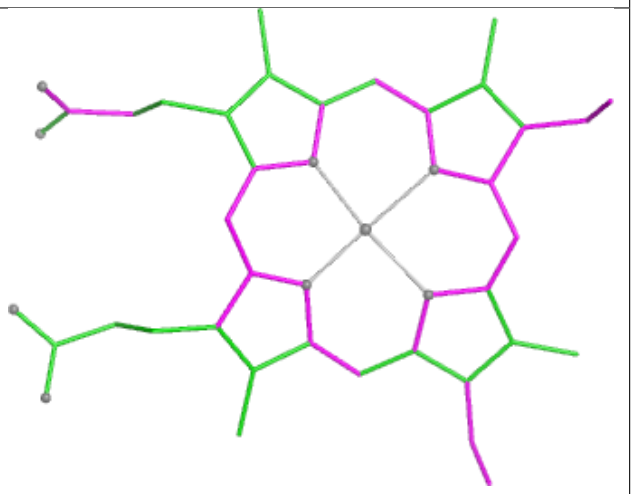

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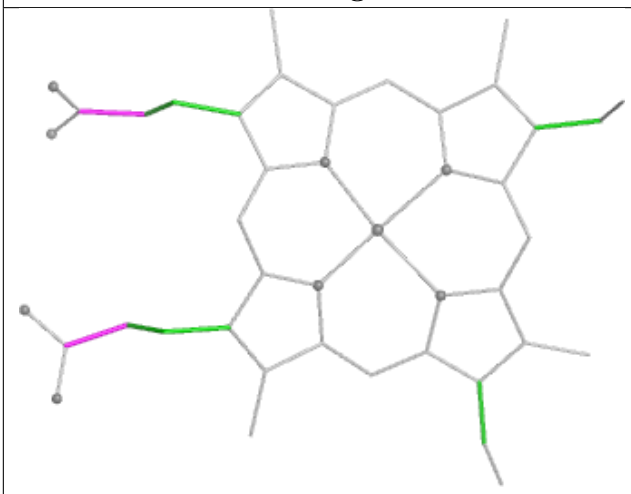

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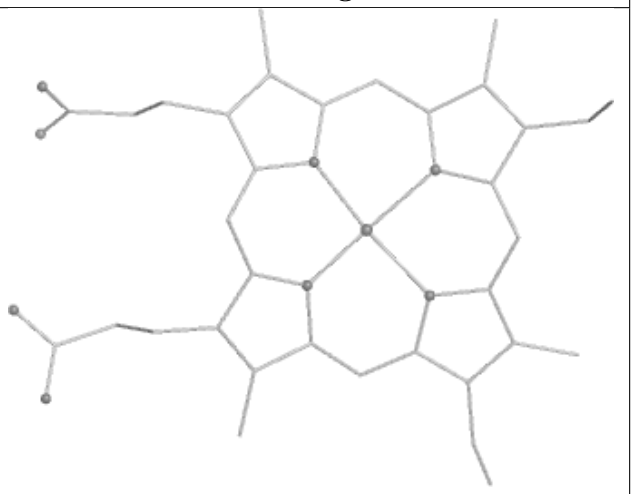

Rings

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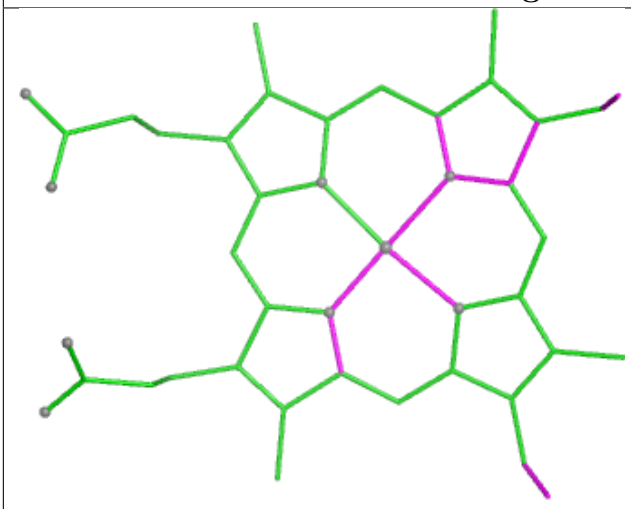

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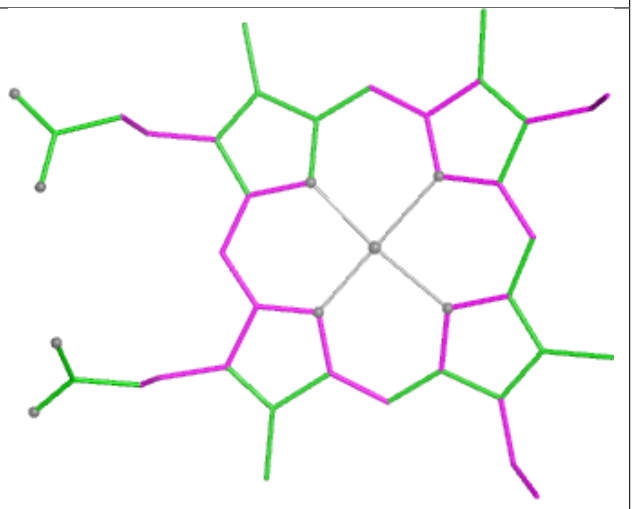

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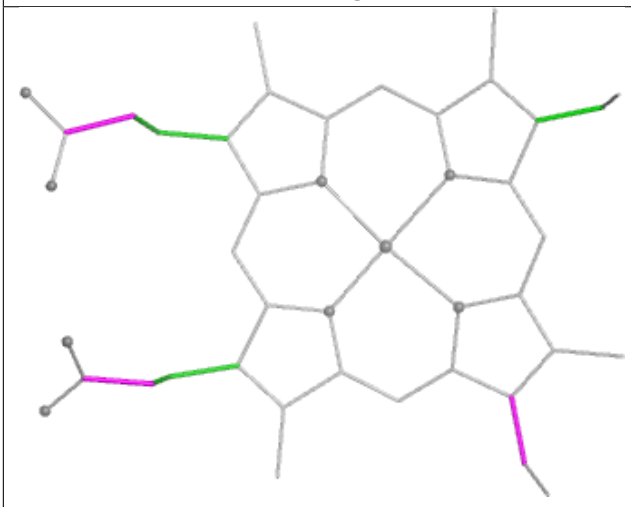

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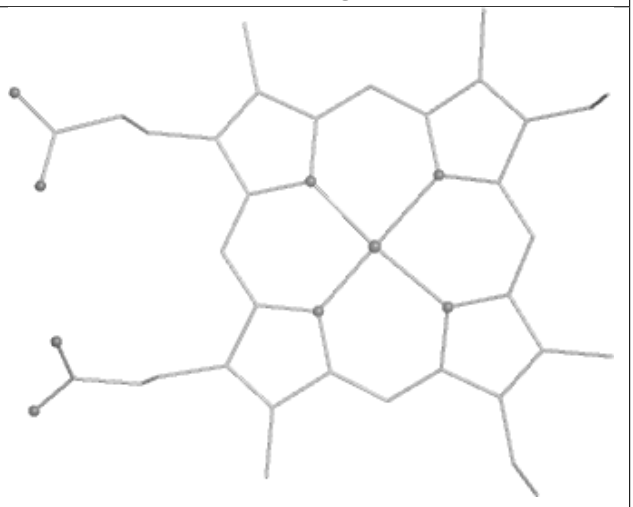

Rings

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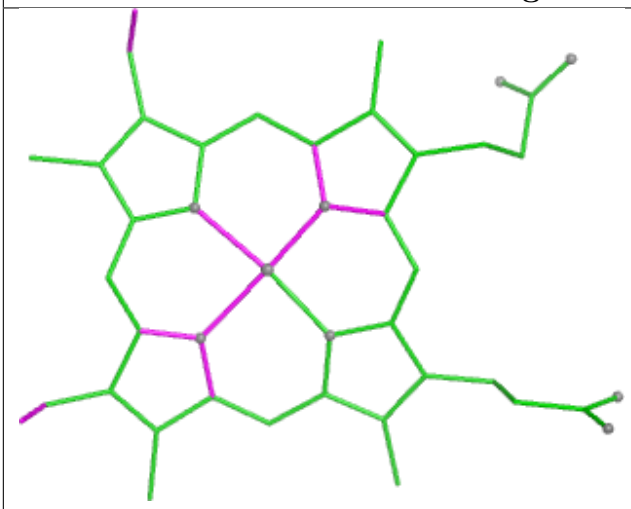
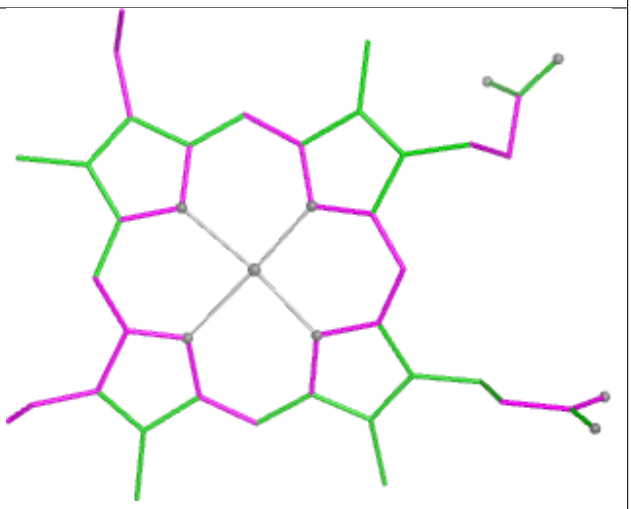


Bond lengths



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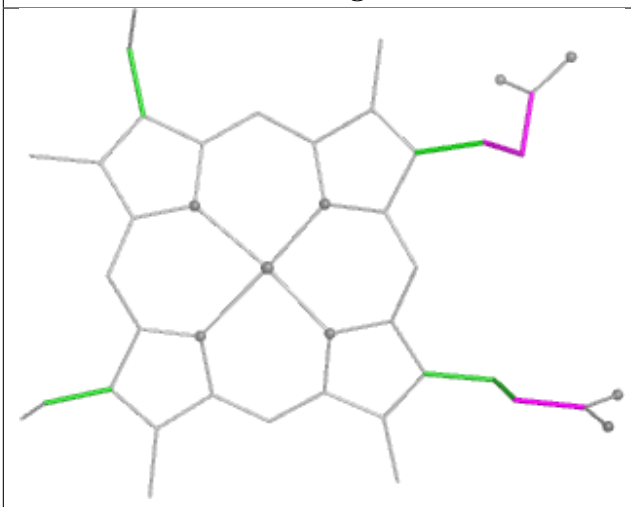
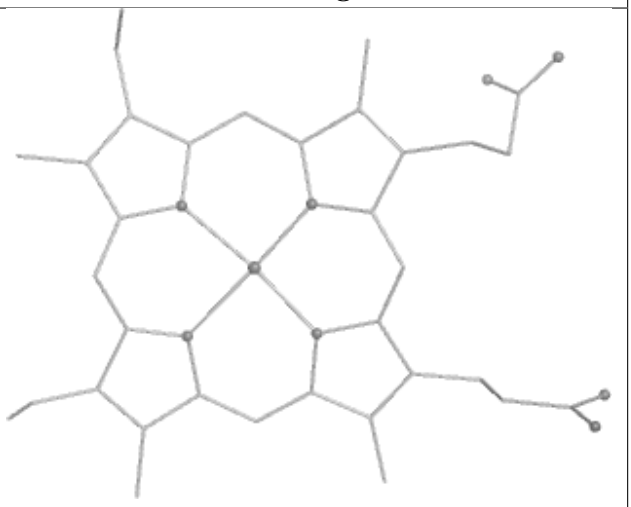
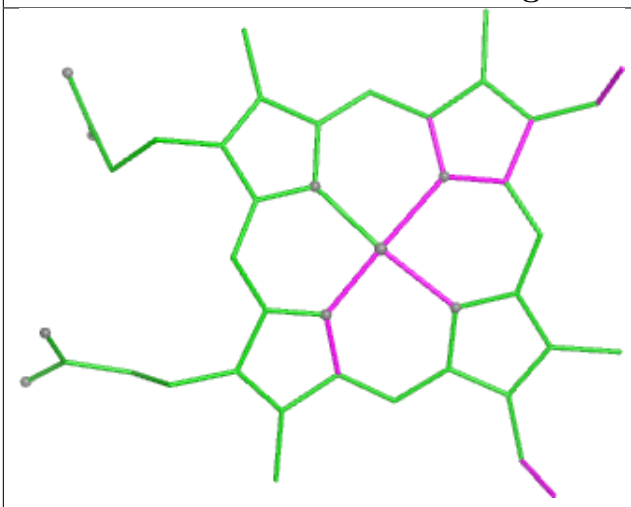


Torsions



Rings

Ligand HEC R 607



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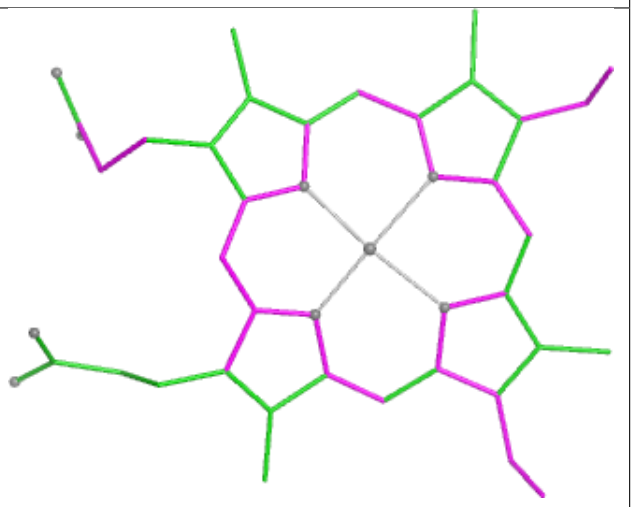

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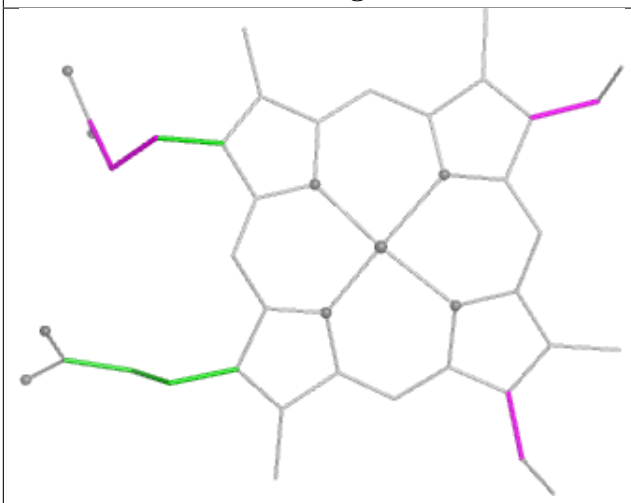

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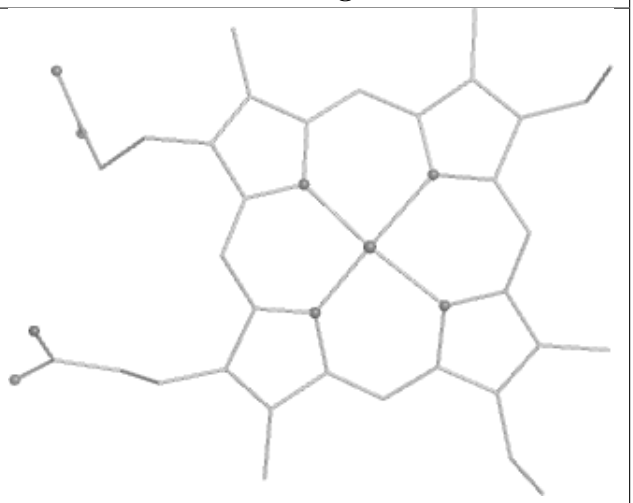
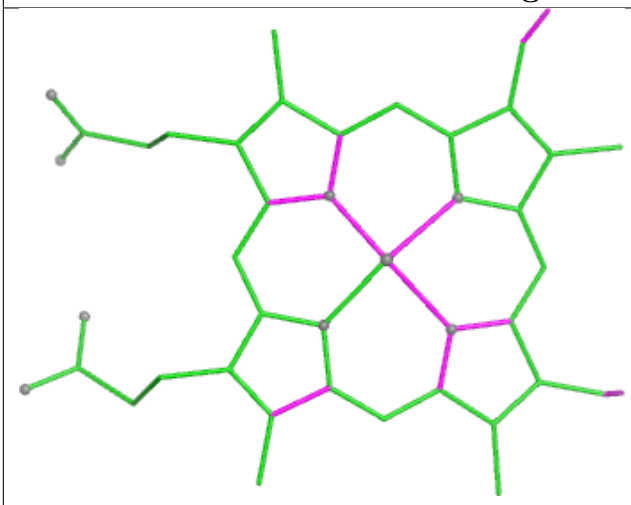


Rings

Ligand HEC D 604



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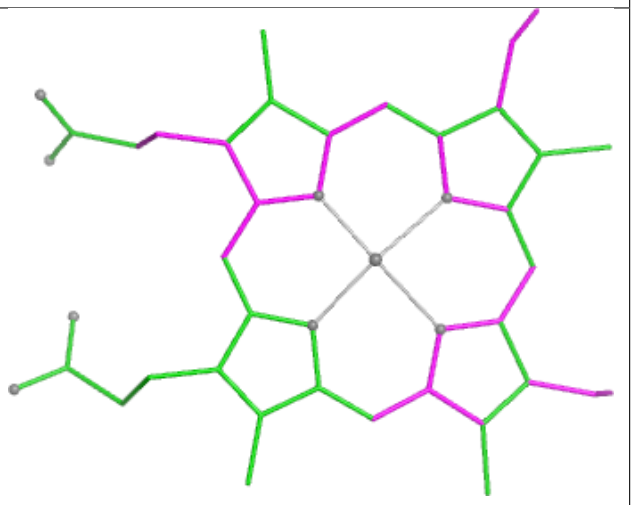

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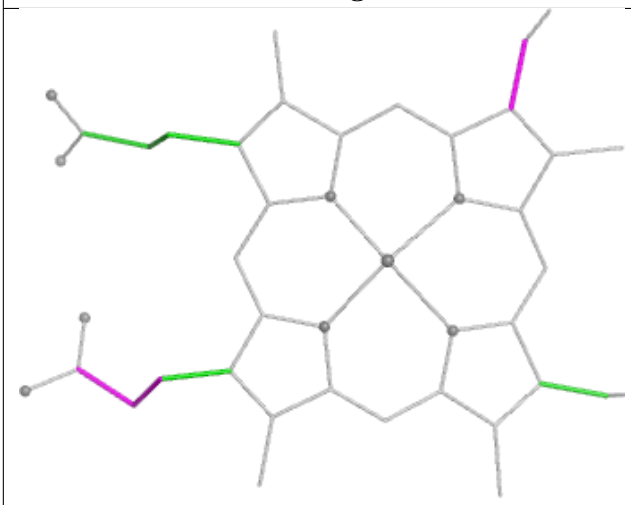

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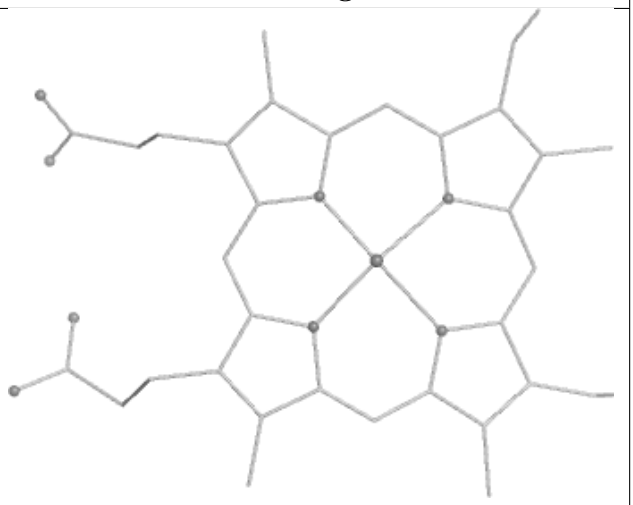

Rings

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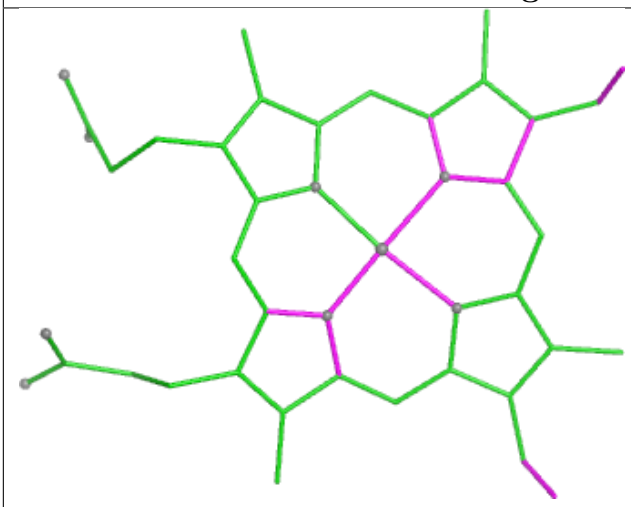

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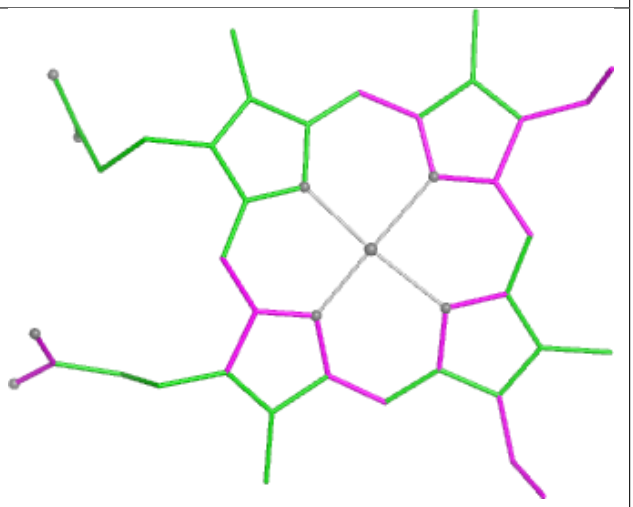

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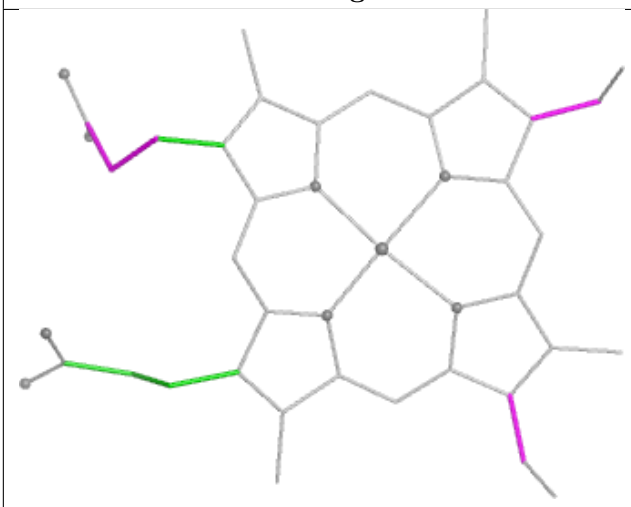

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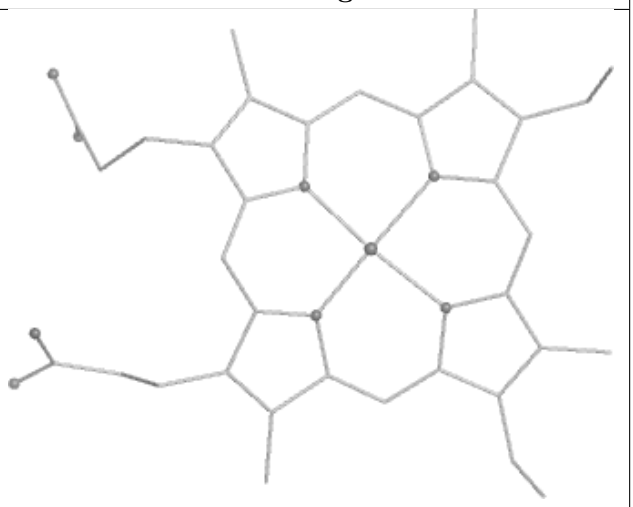
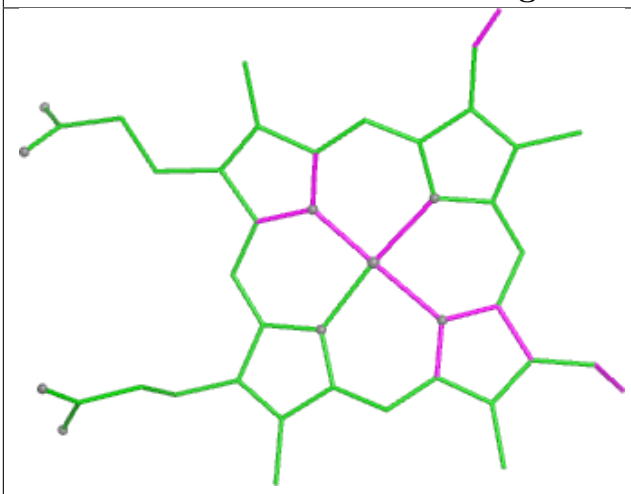


Rings

Ligand HEC M 605



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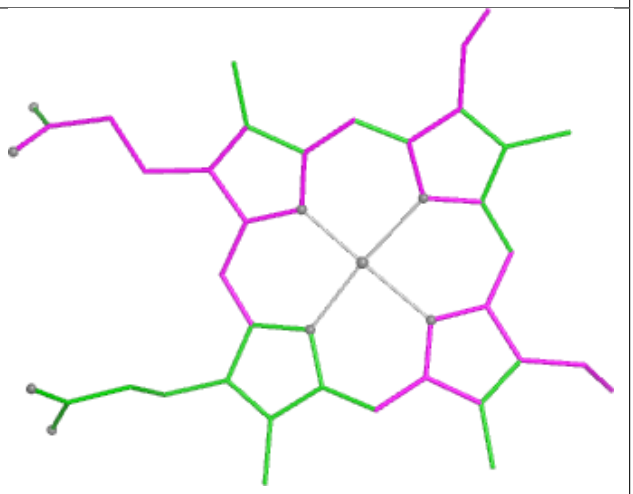

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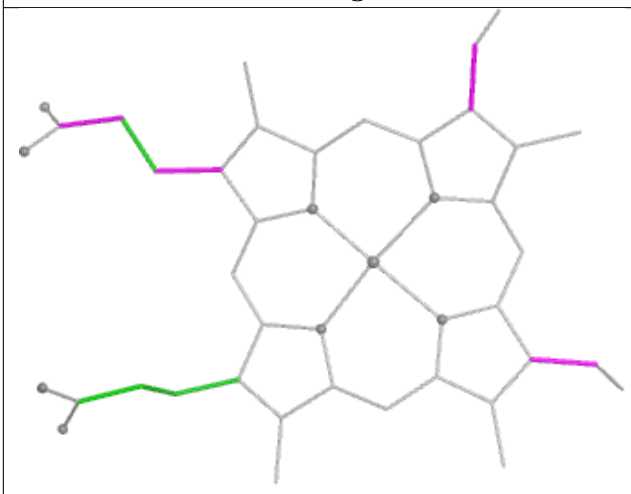

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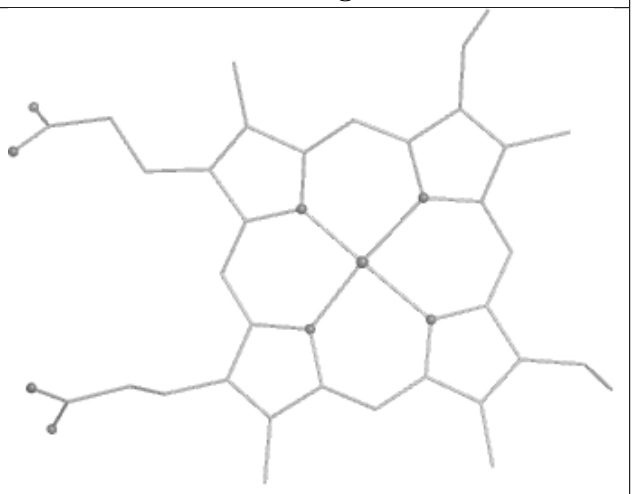

Rings

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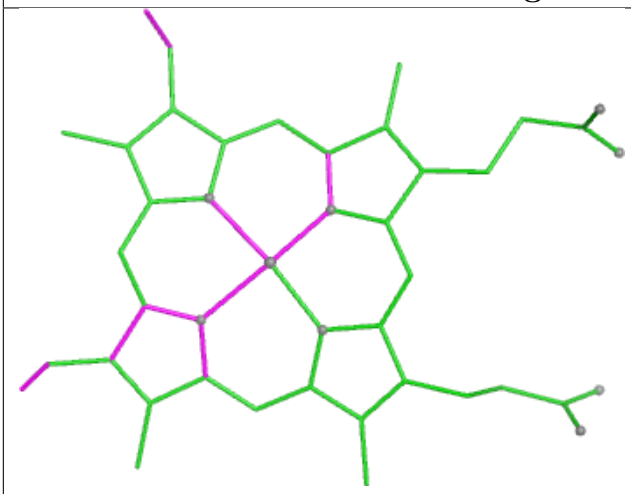

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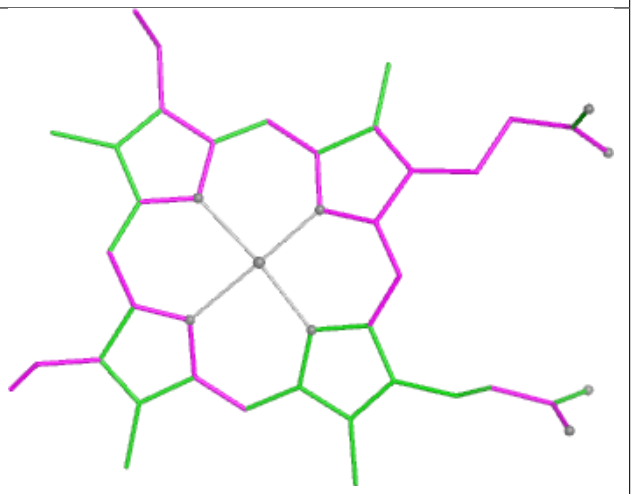

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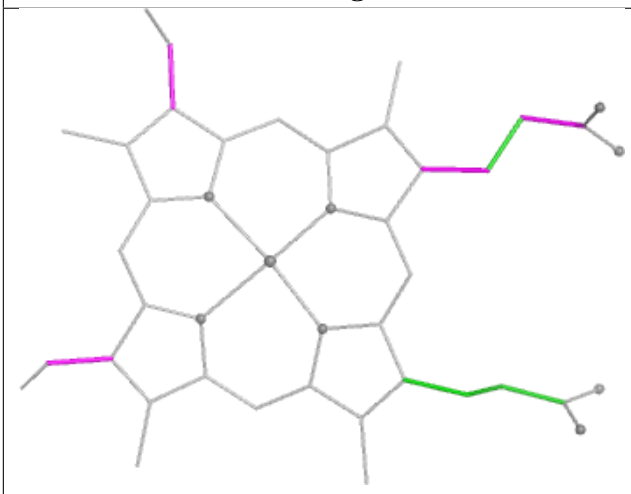

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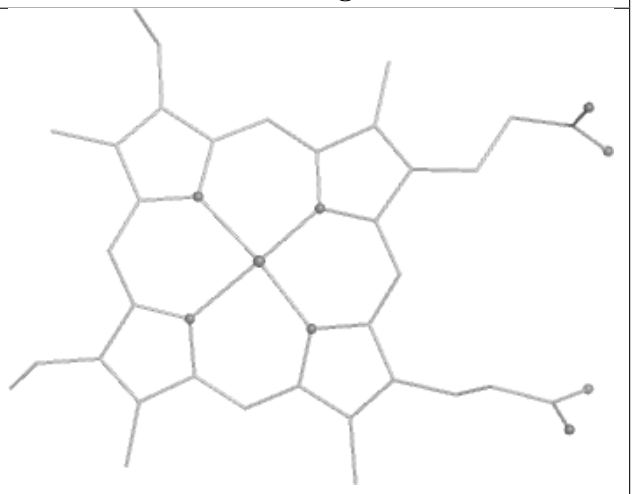

Rings

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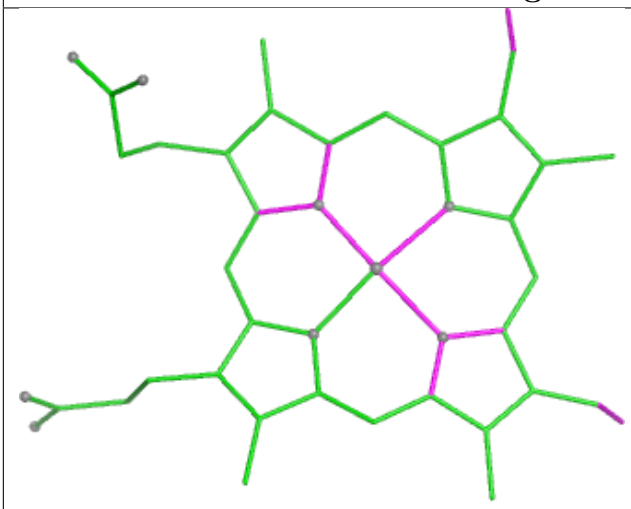

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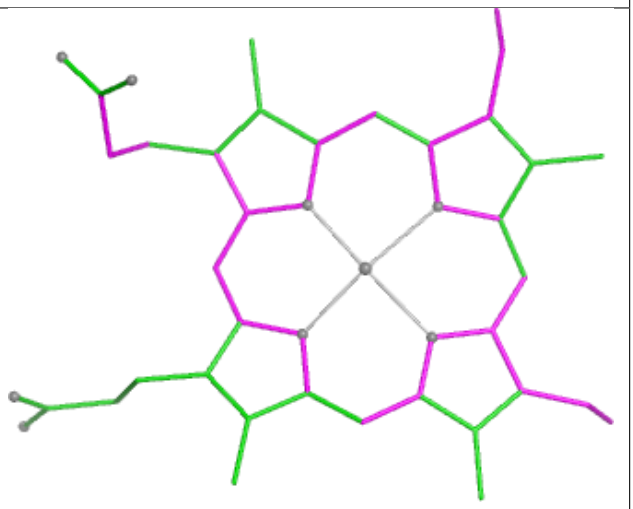

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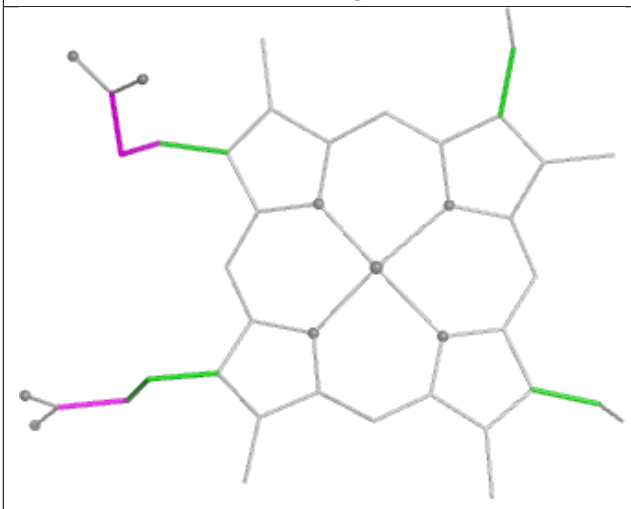

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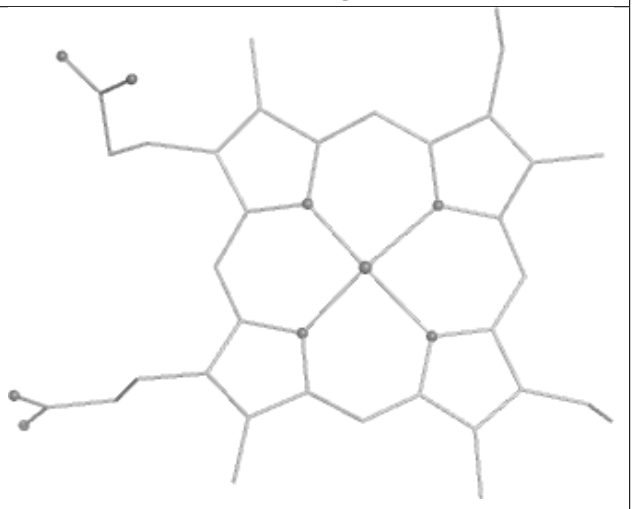

Rings

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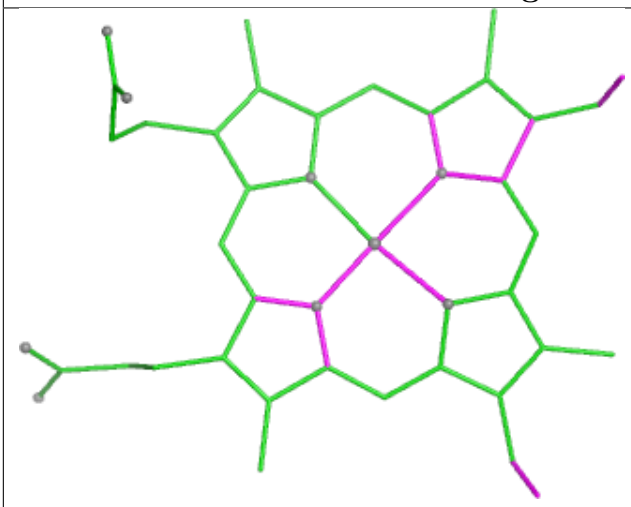

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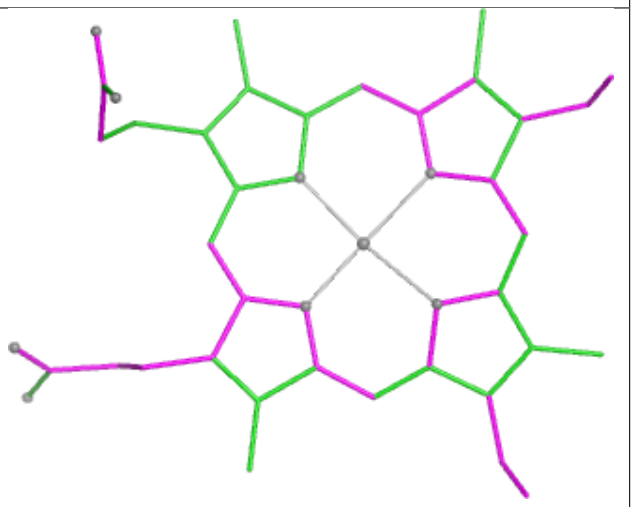

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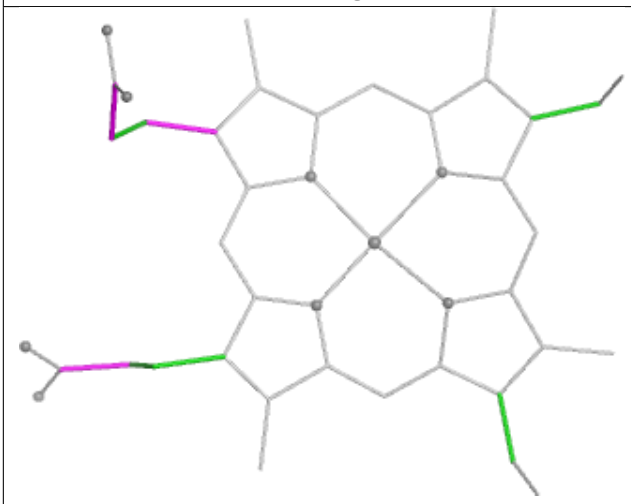

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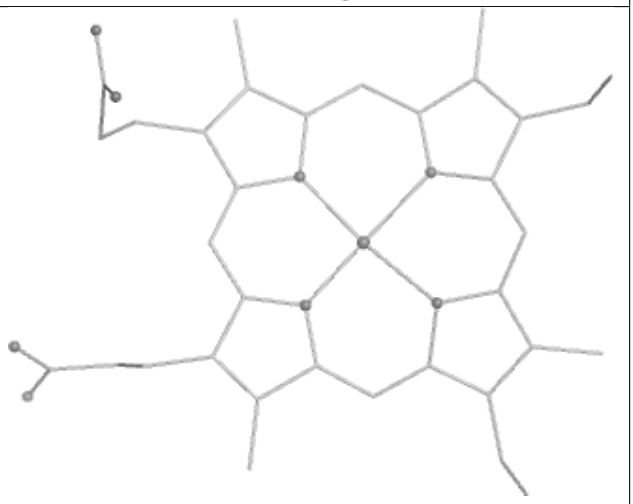

Rings

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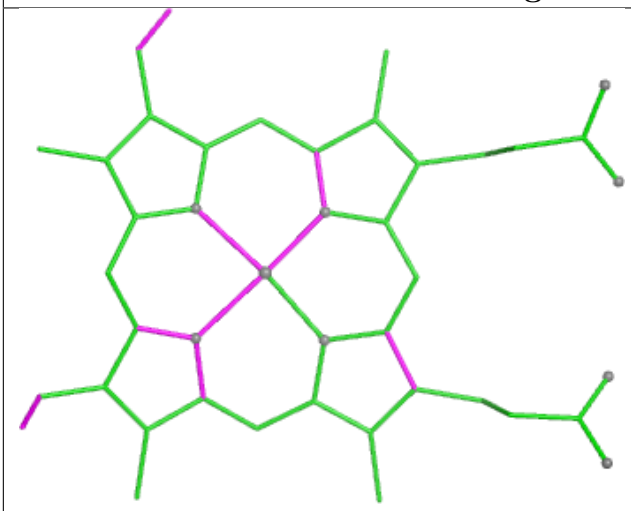

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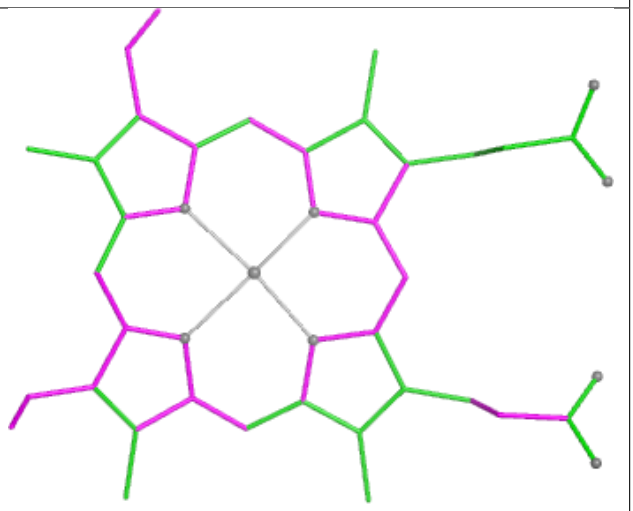

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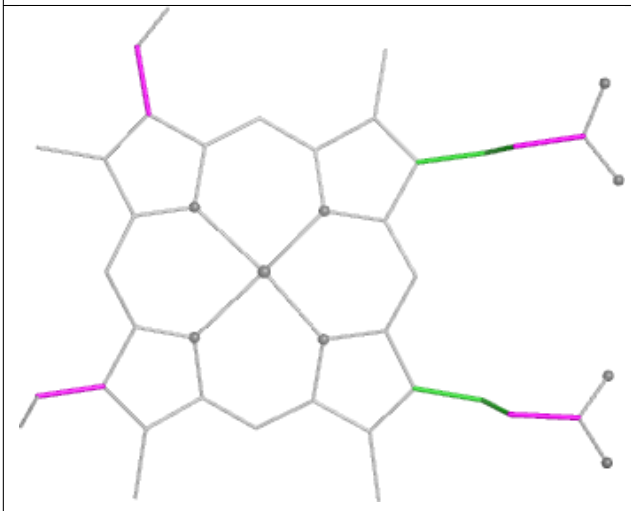

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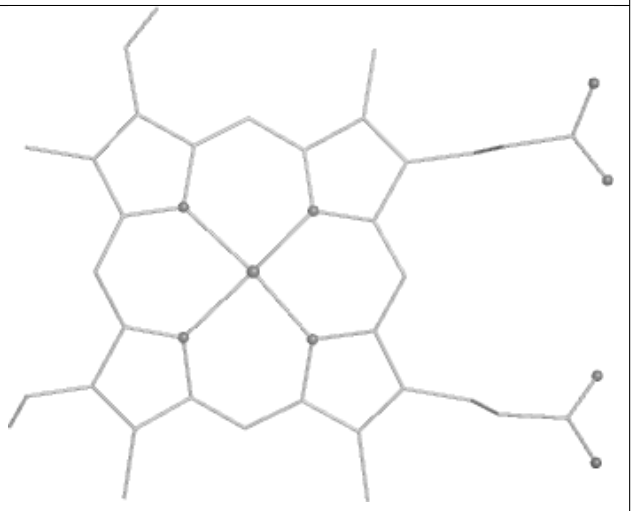
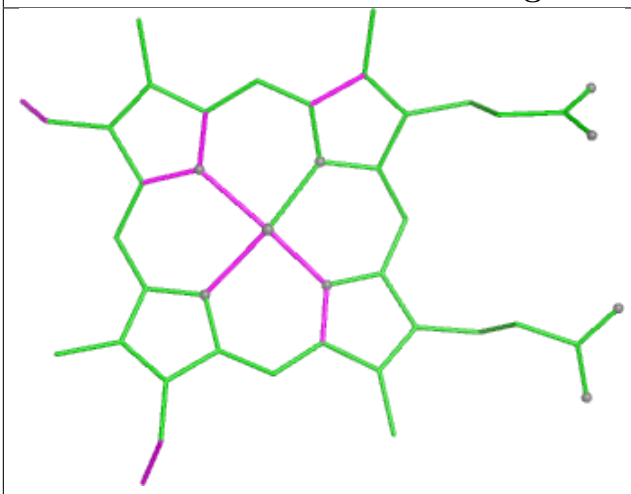


Rings

Ligand HEC E 606



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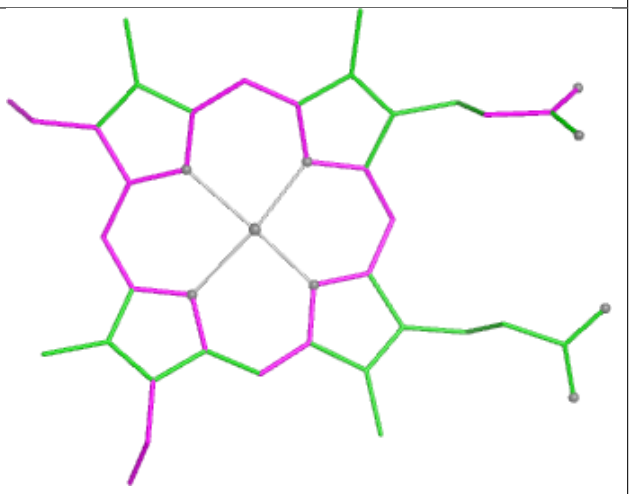

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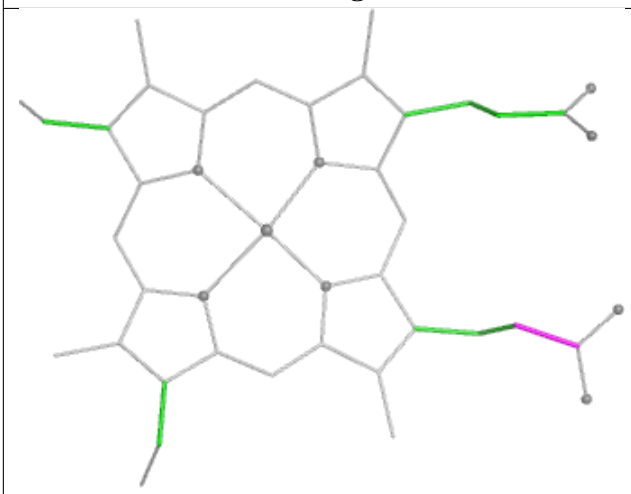

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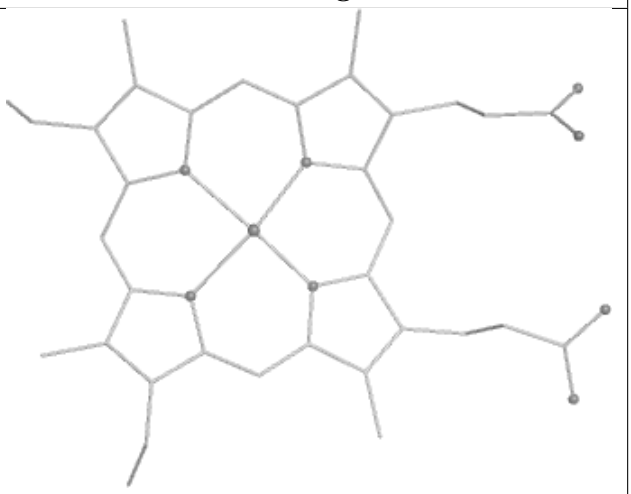
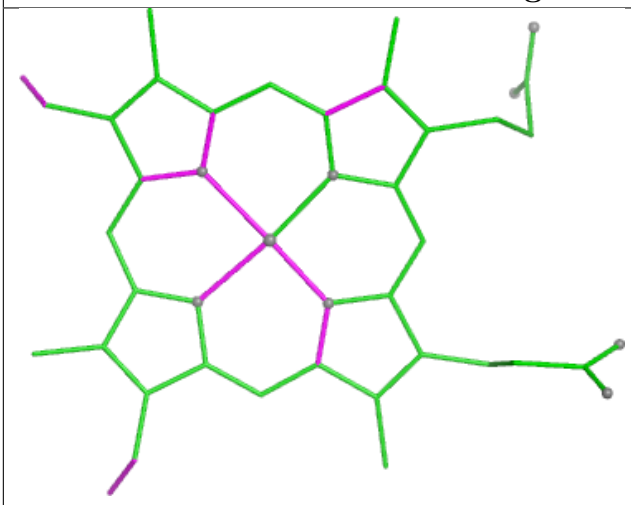


Rings

Ligand HEC F 601



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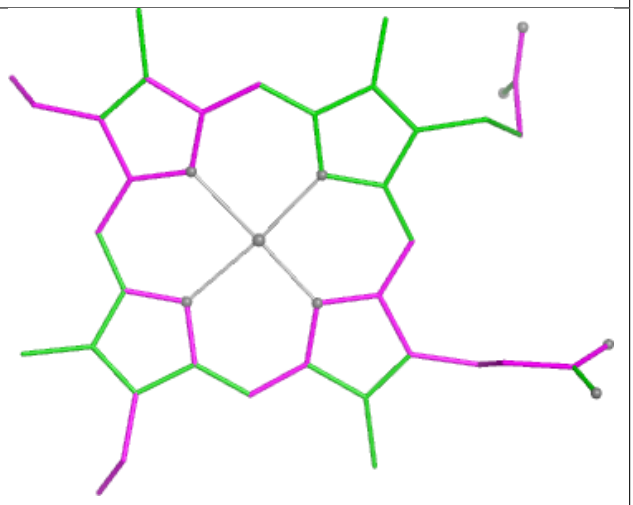

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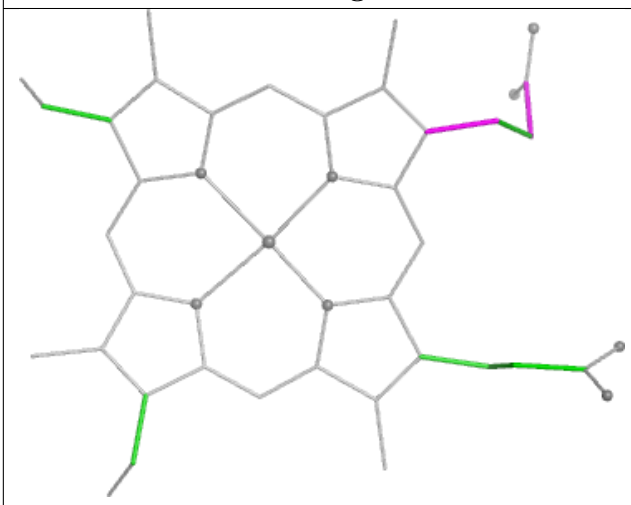

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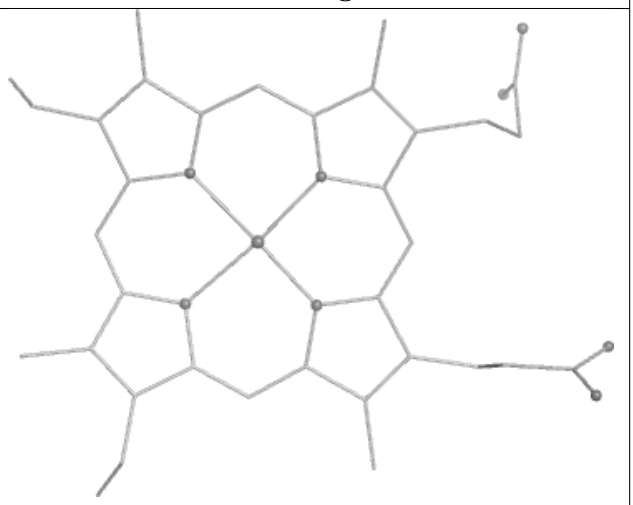
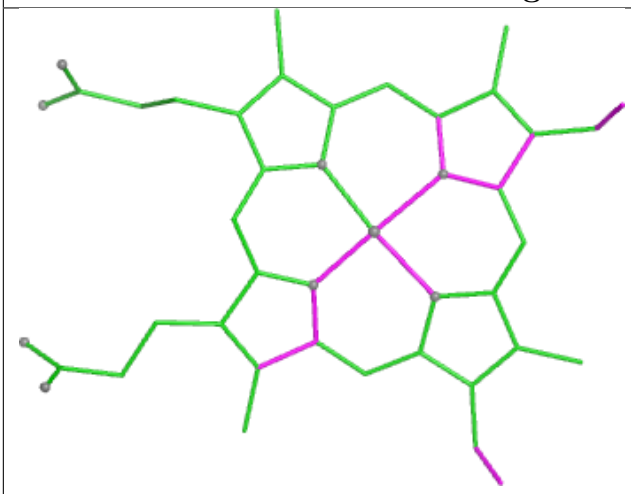


Rings

Ligand HEC B 605



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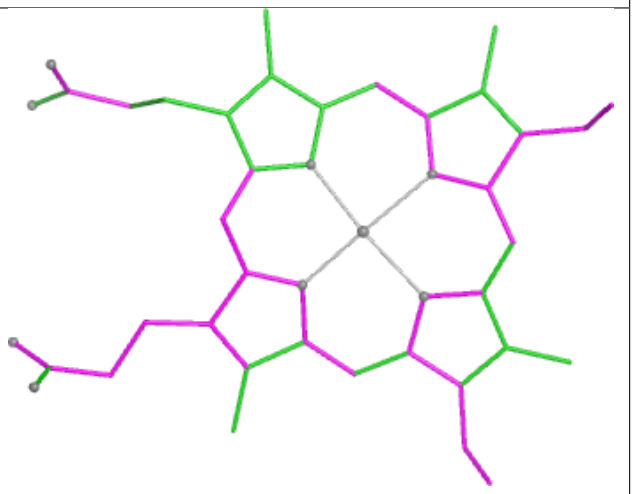

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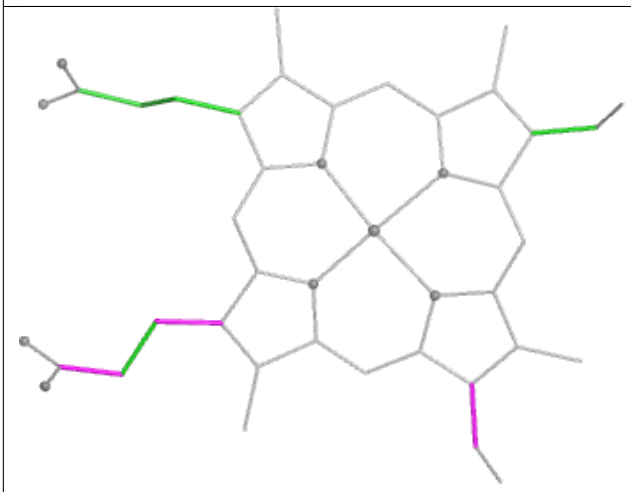

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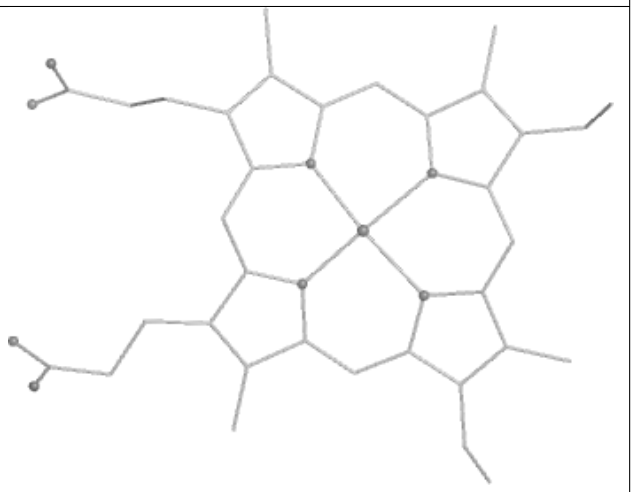
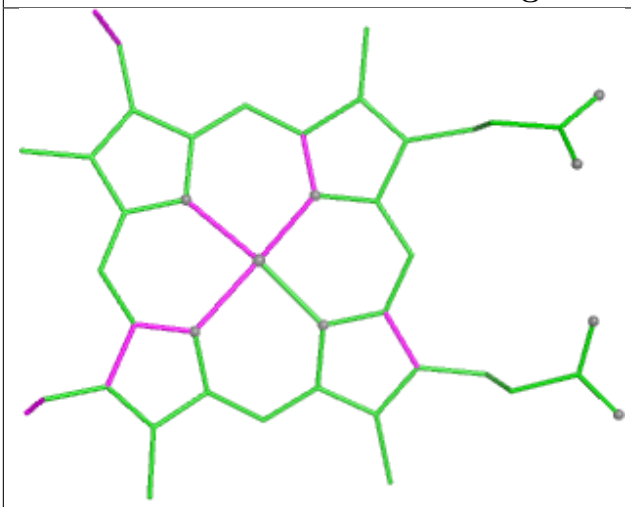


Rings

Ligand HEC N 604



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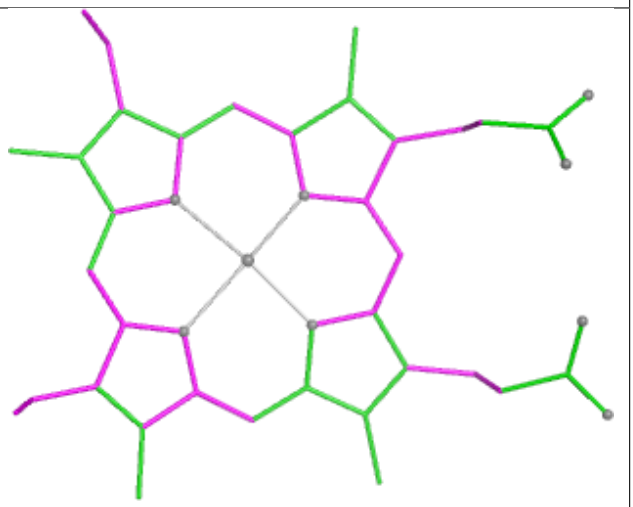

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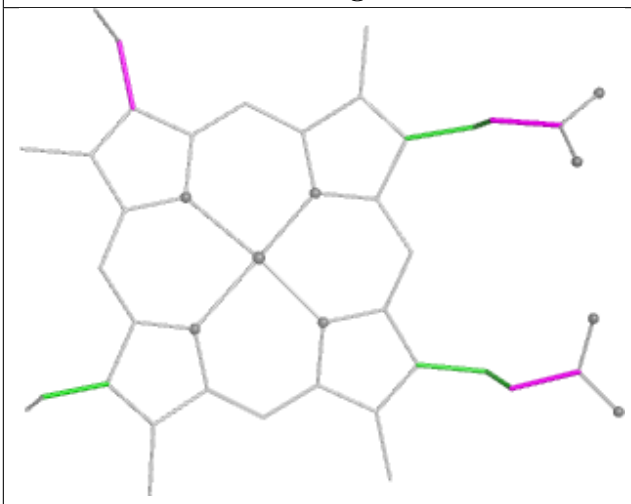

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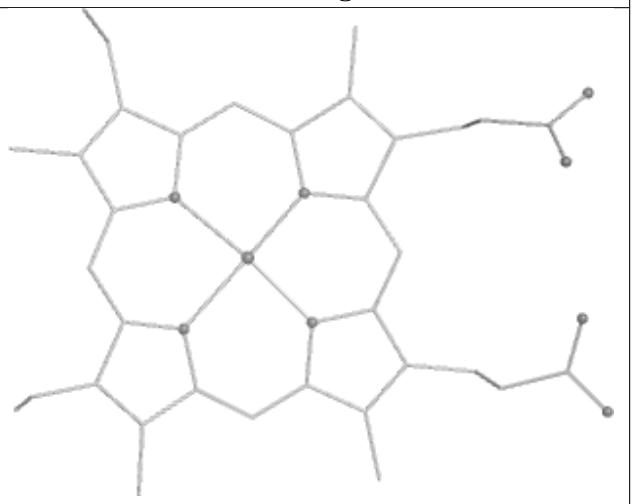
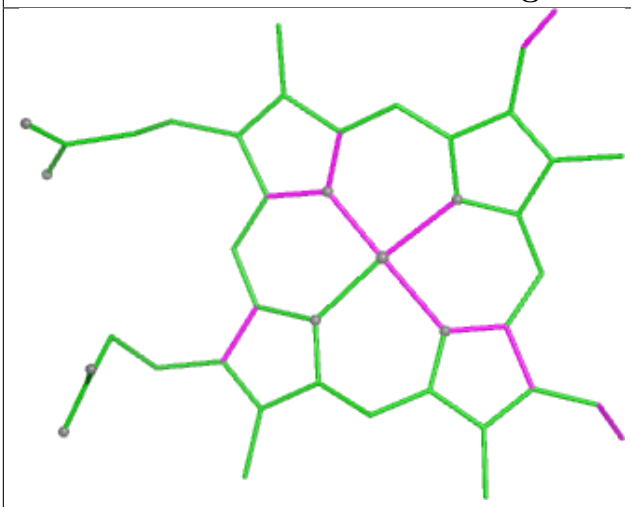


Rings

Ligand HEC K 607



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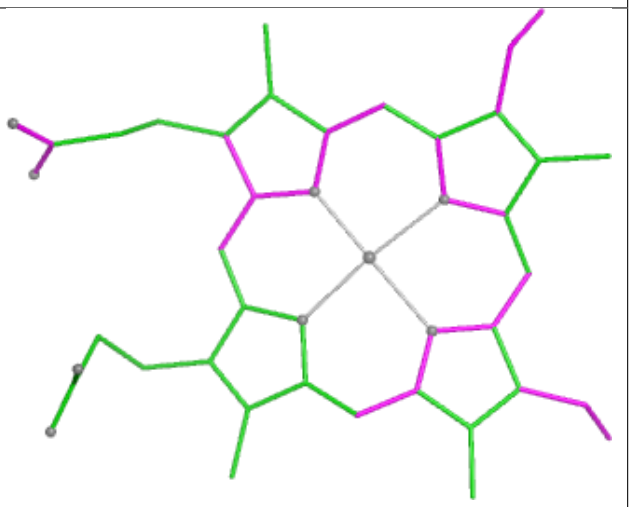

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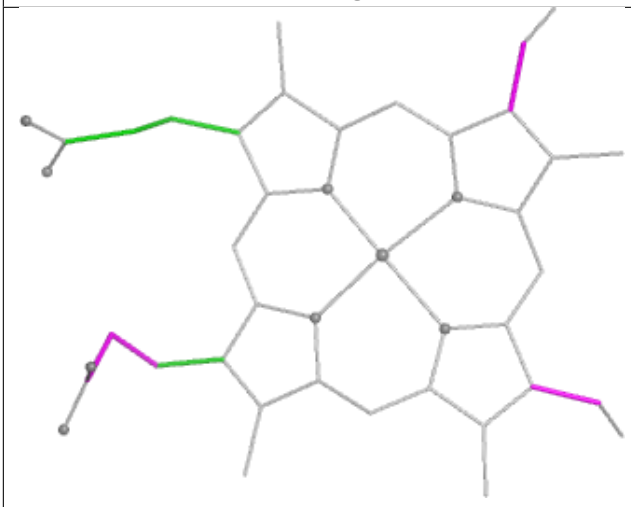

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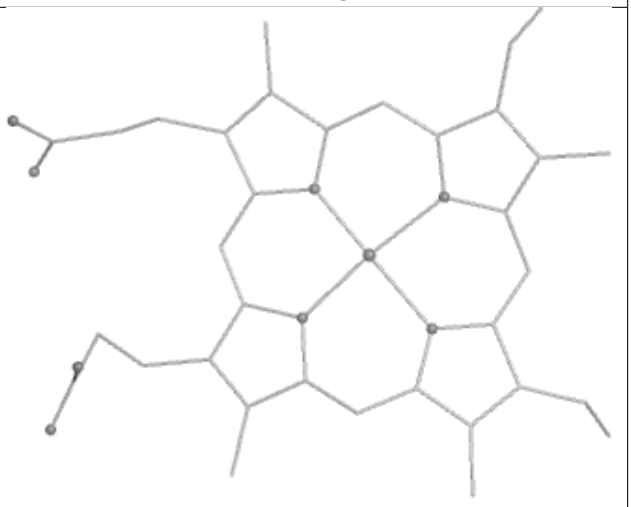
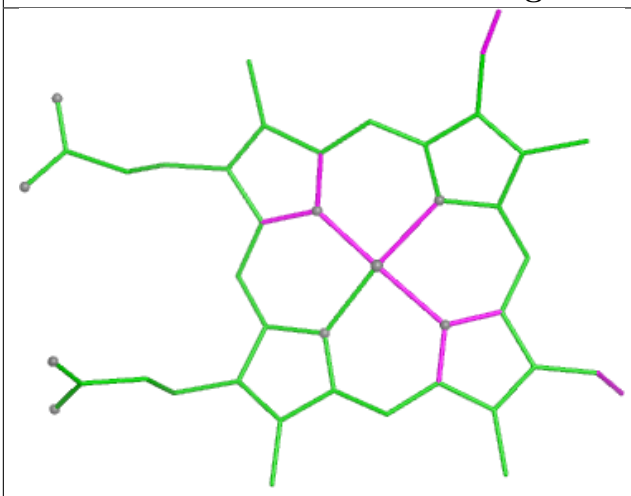


Rings

Ligand HEC L 606



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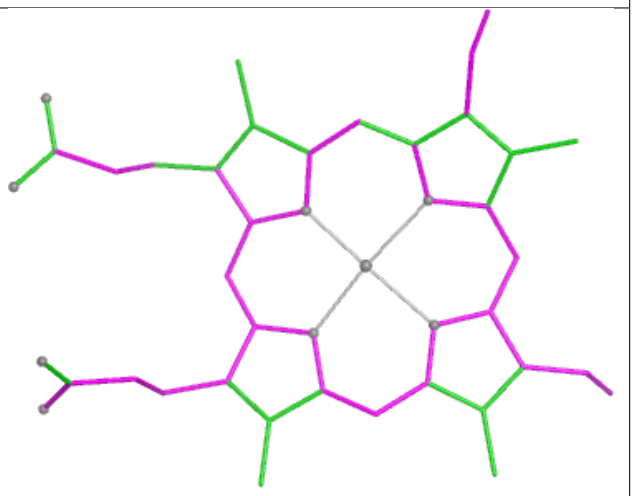
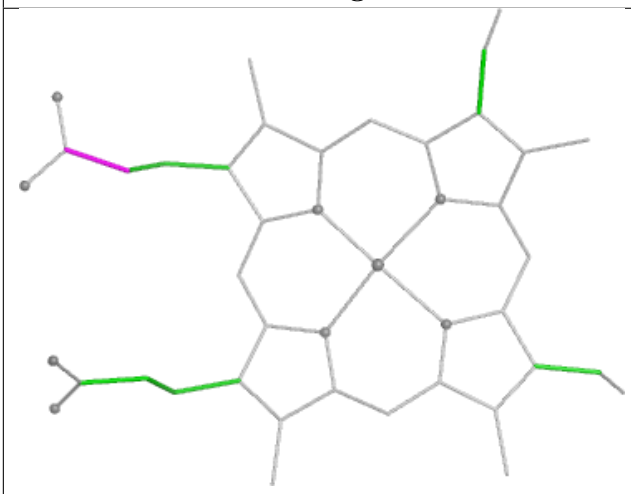


Bond angles



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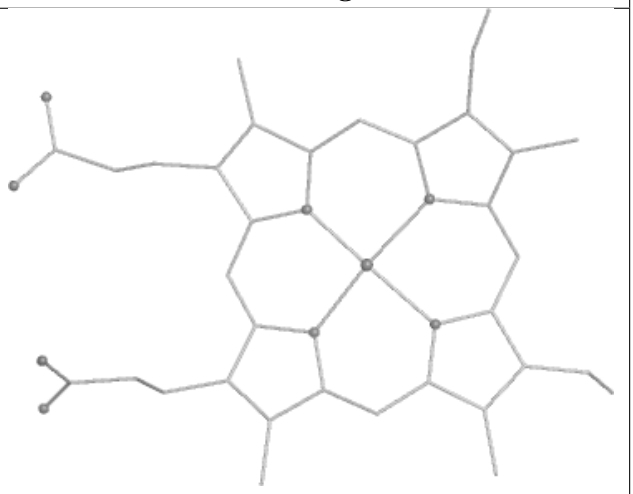
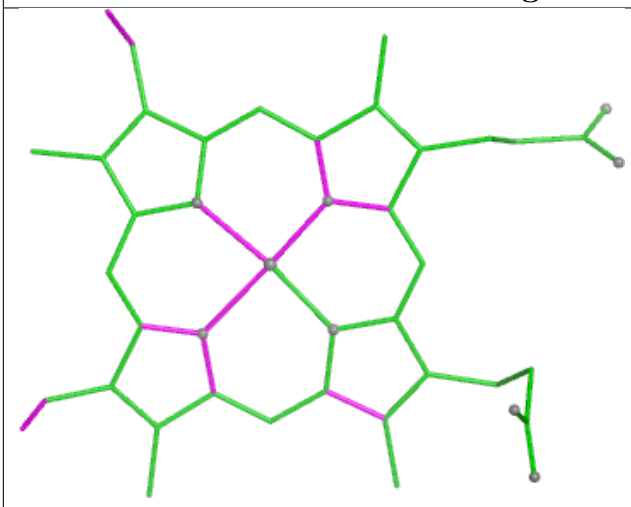


Rings

Ligand HEC H 601



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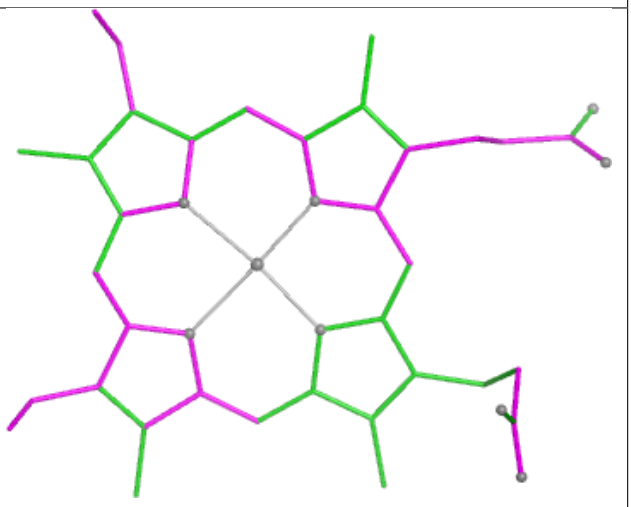

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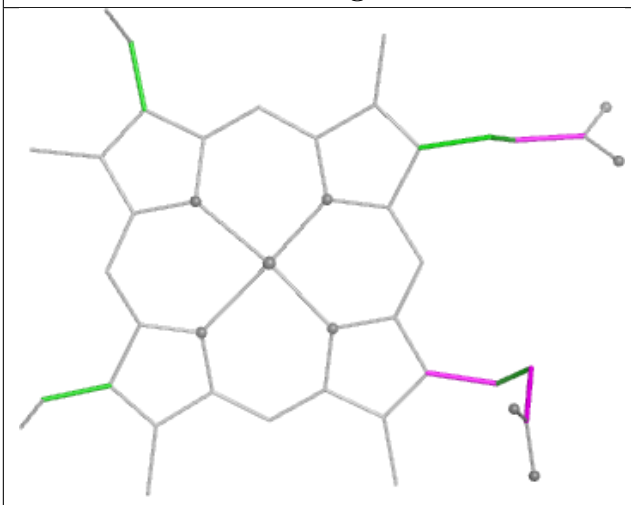

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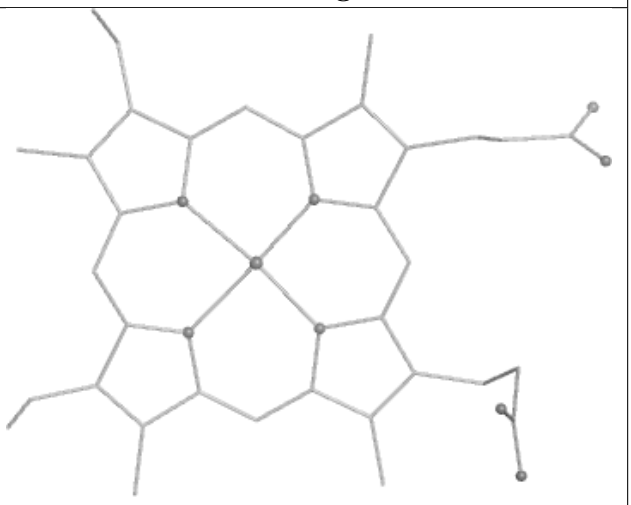
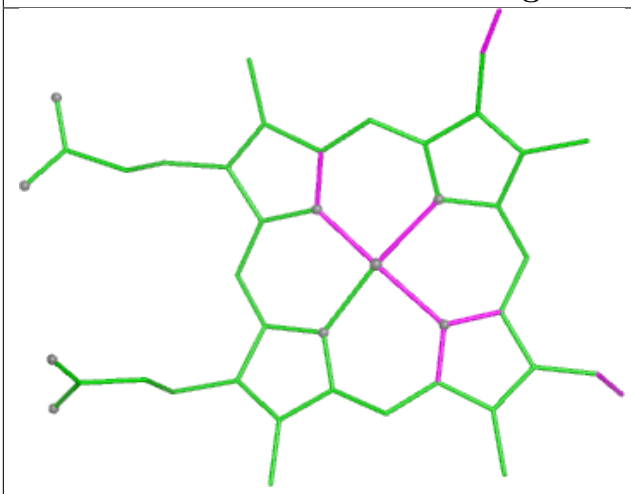


Rings

Ligand HEC A 606



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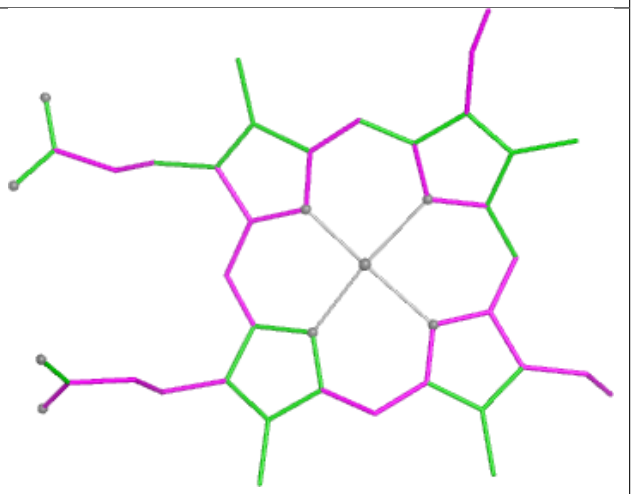

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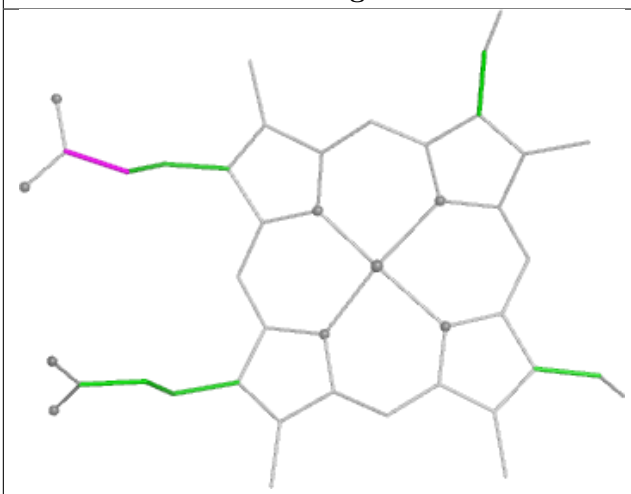

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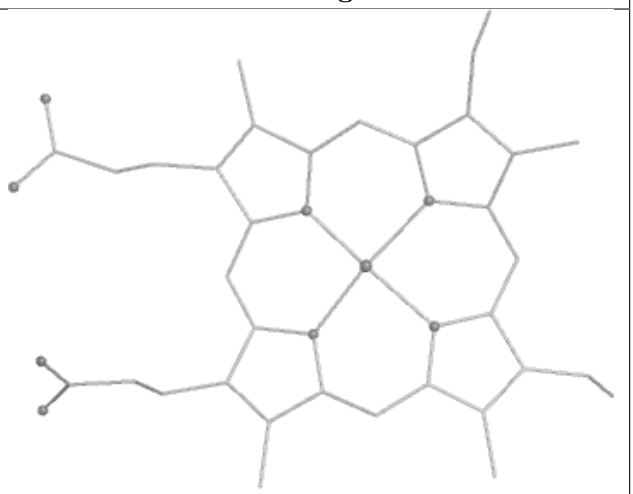
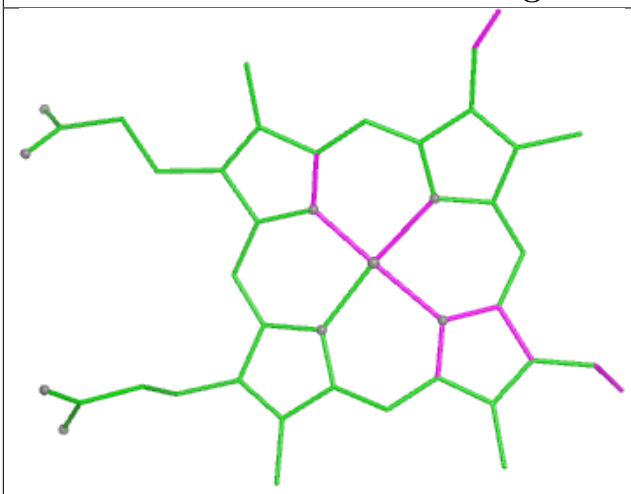


Rings

Ligand HEC T 605



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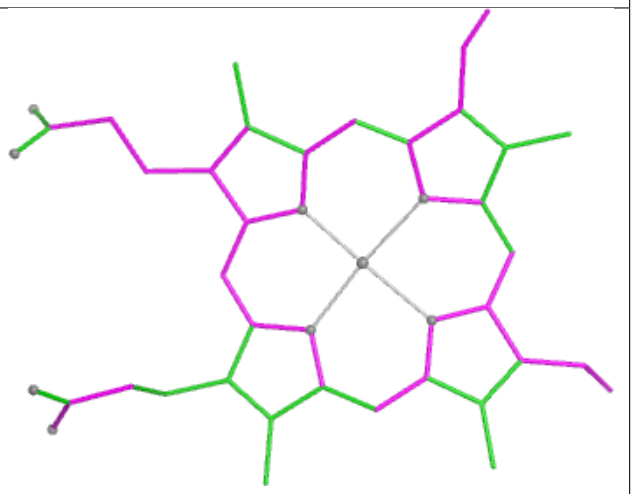

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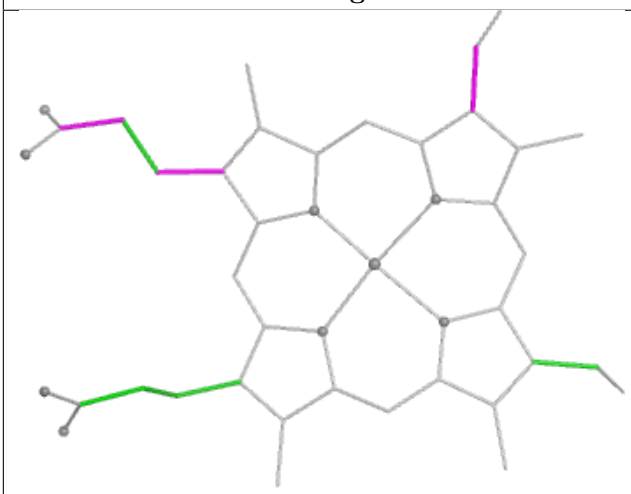

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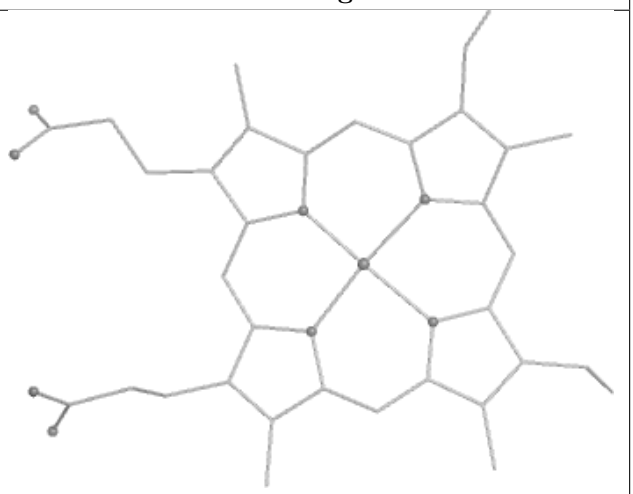
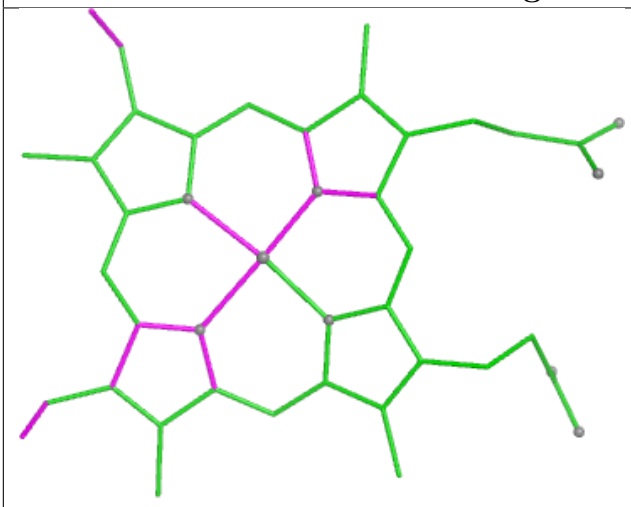


Rings

Ligand HEC T 607



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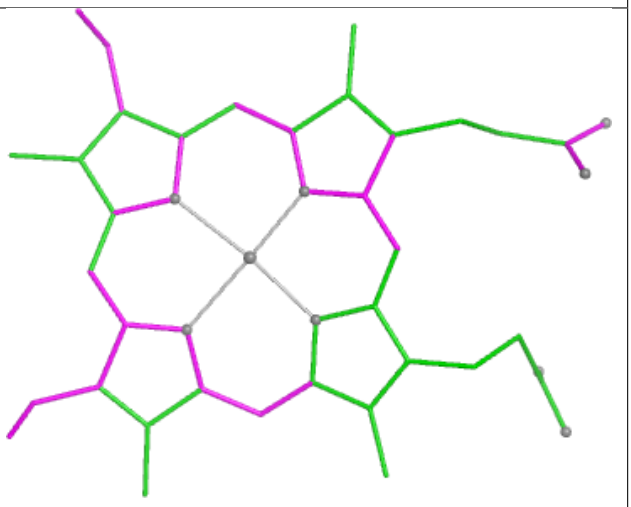

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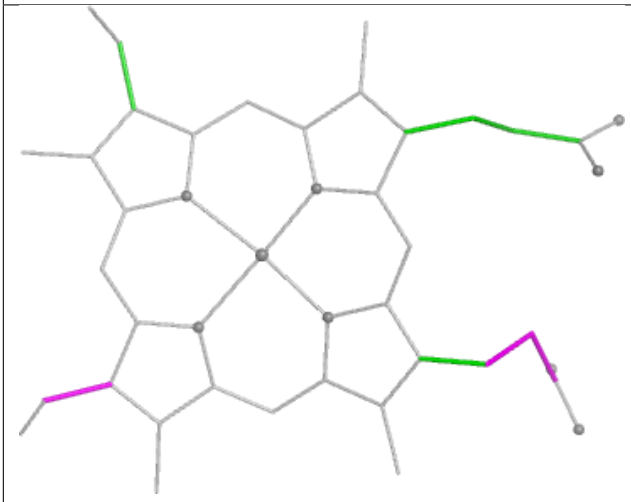

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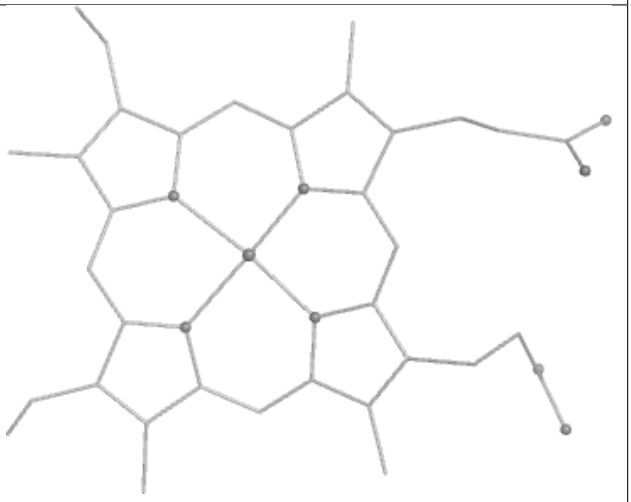
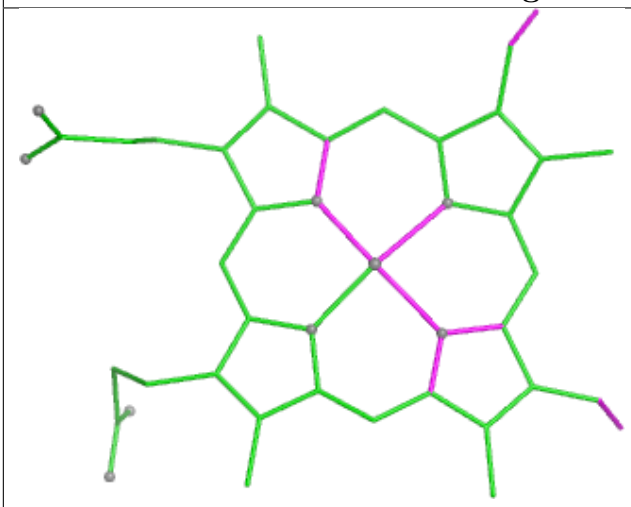


Rings

Ligand HEC V 601



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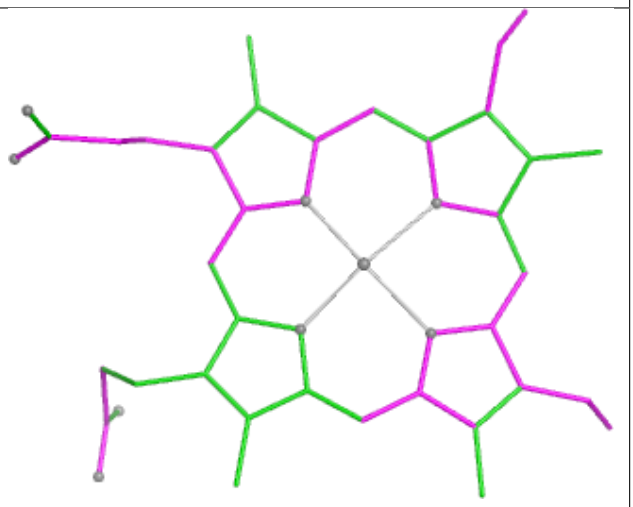

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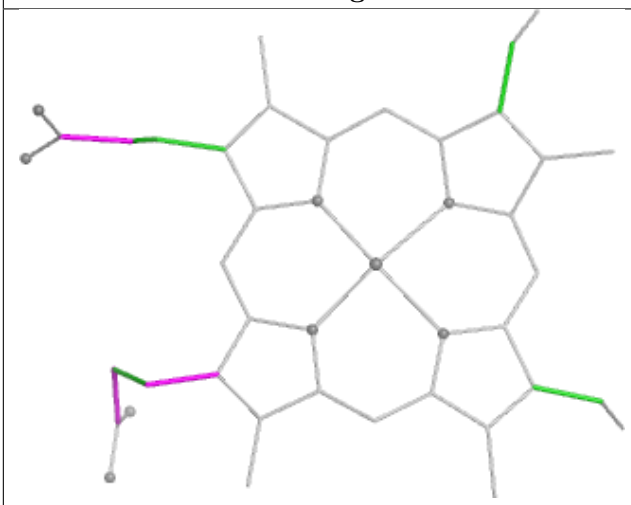

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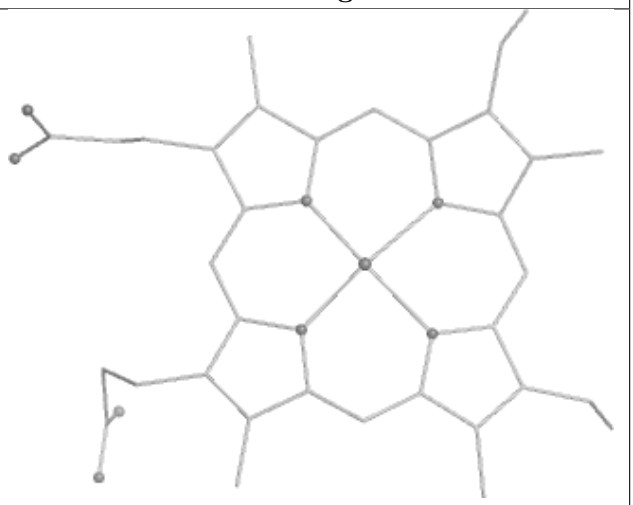
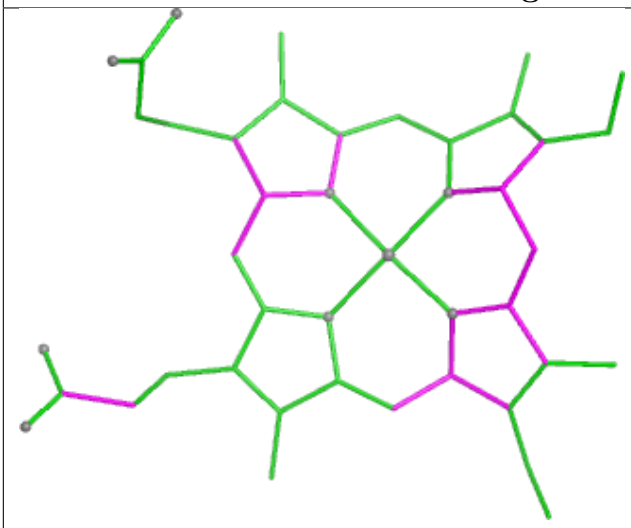


Rings

Ligand HEC H 603



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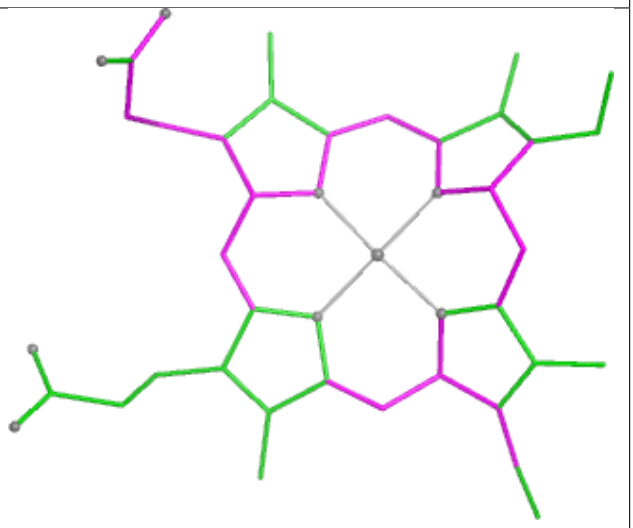

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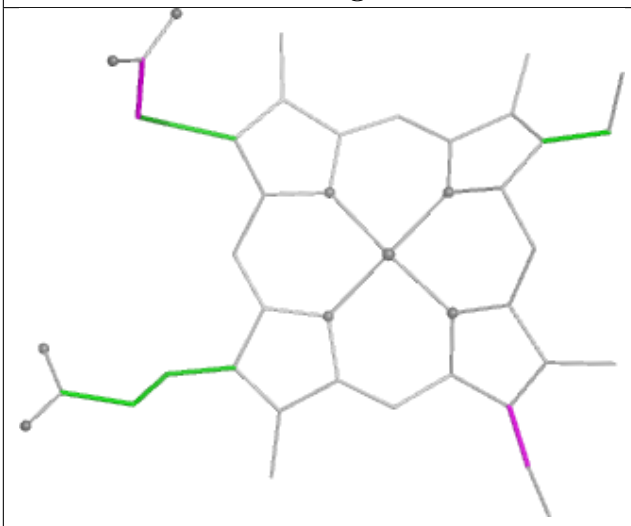

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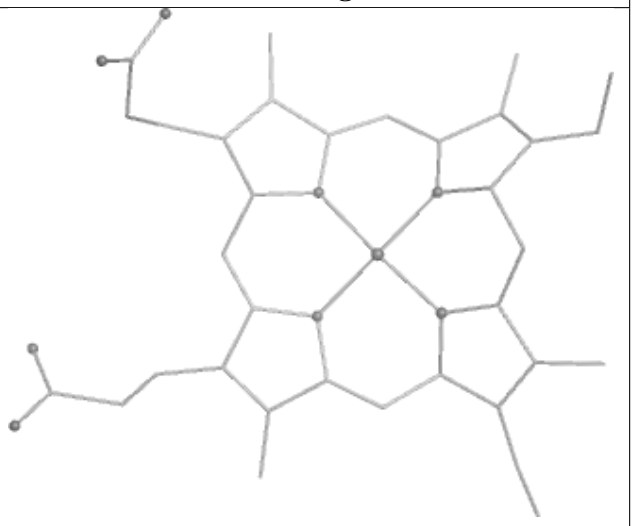
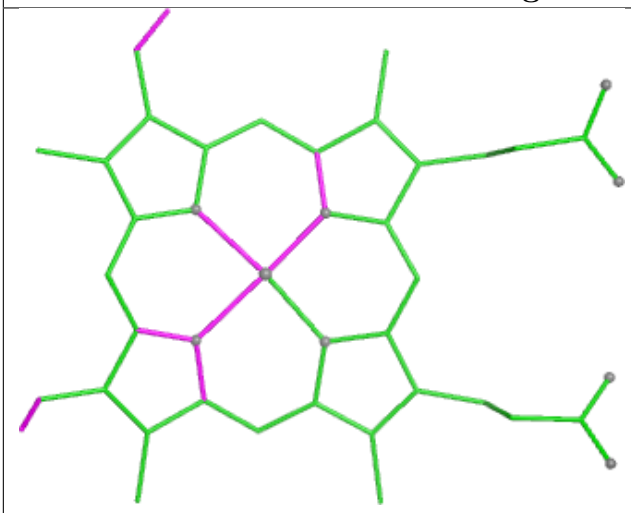


Rings

Ligand HEC A 600



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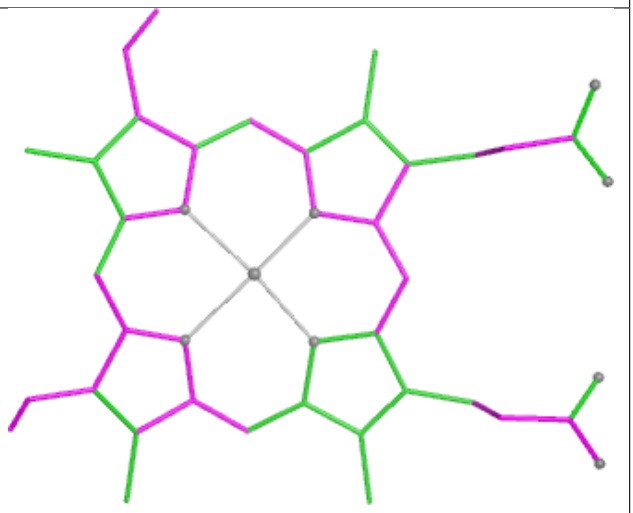

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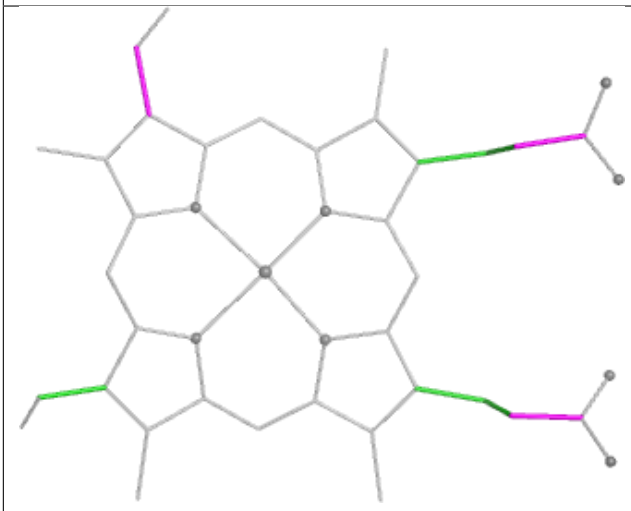

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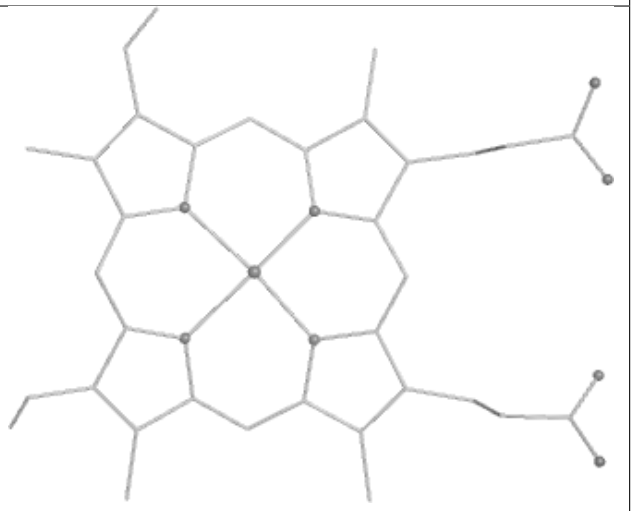

Rings

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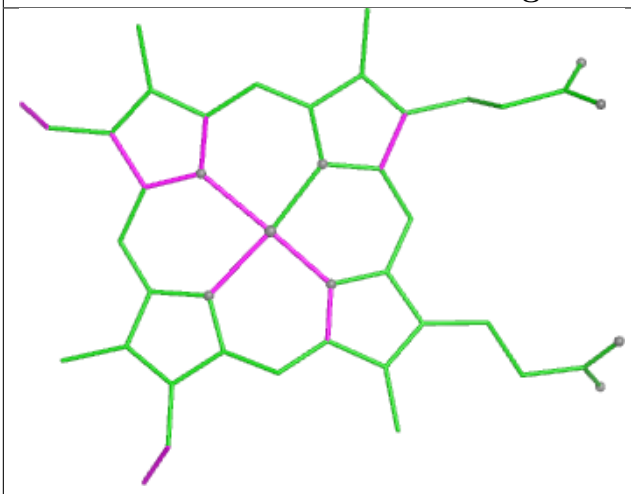

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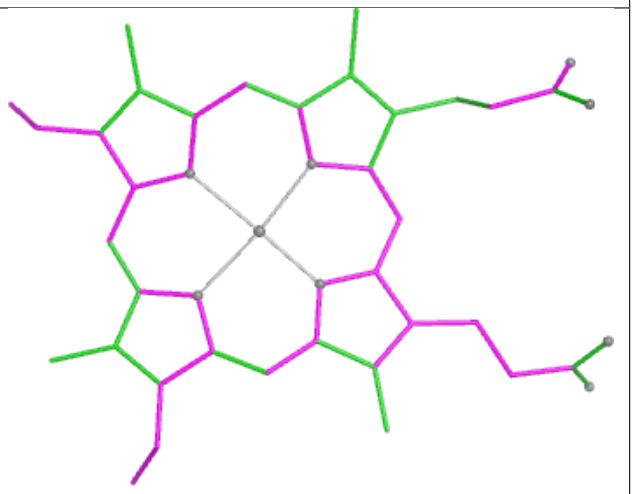

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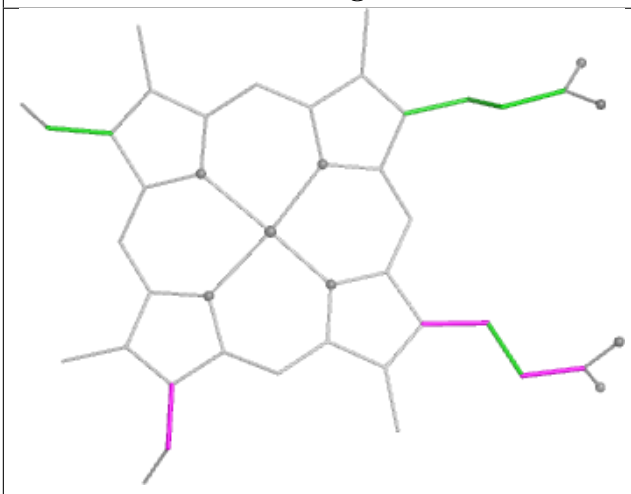

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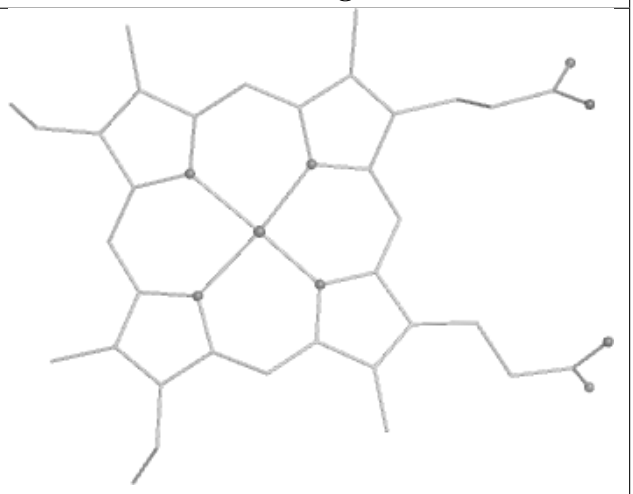
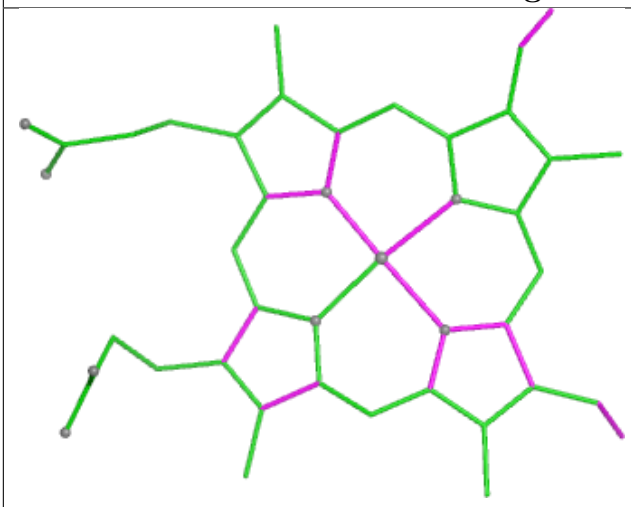


Rings

Ligand HEC E 607



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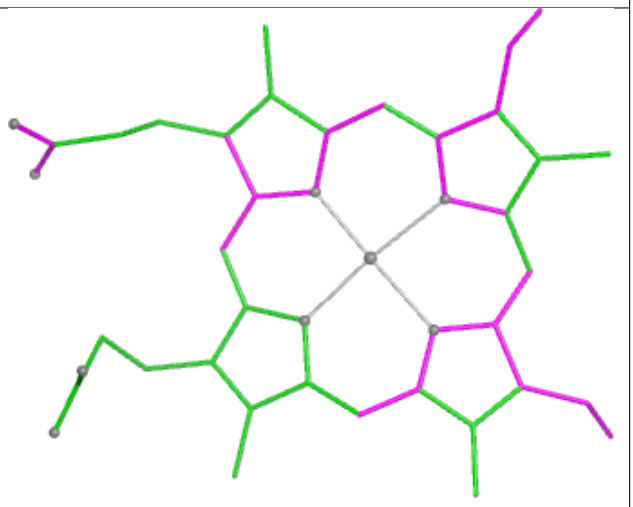

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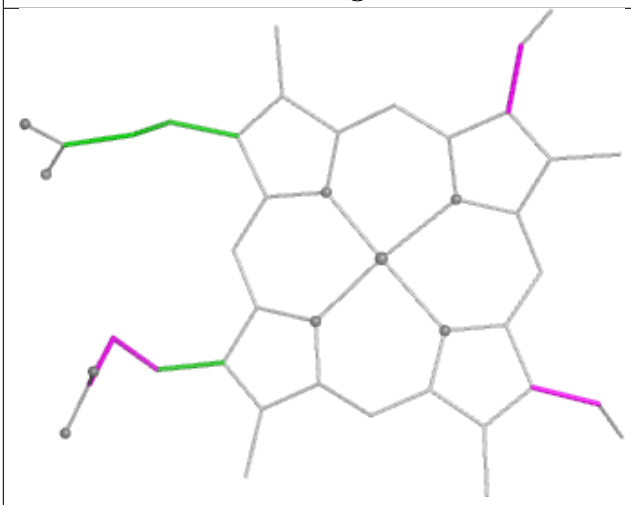

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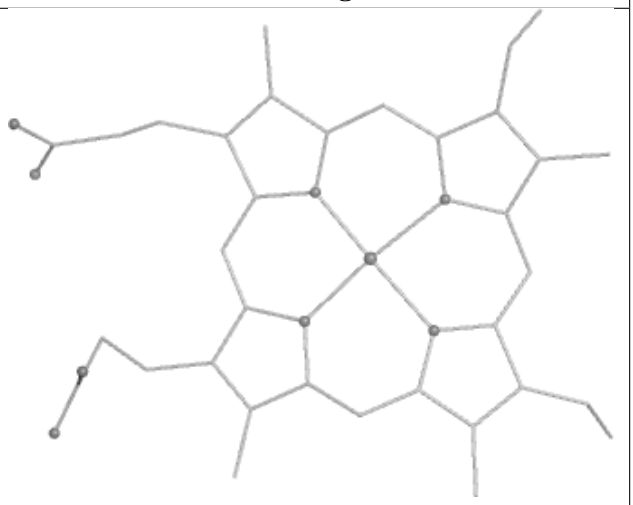
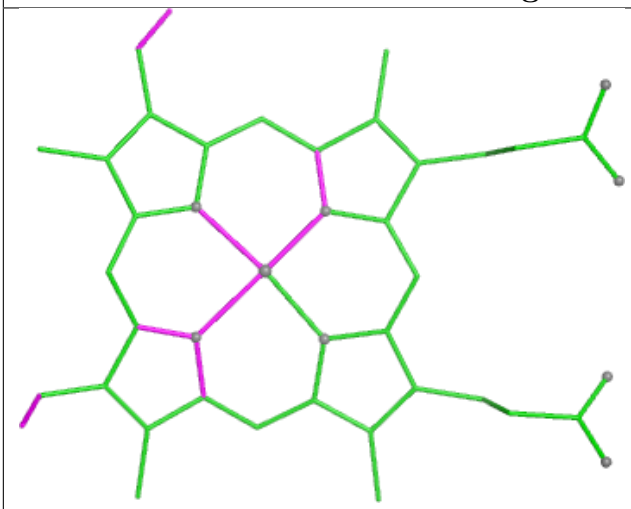


Rings

Ligand HEC G 600



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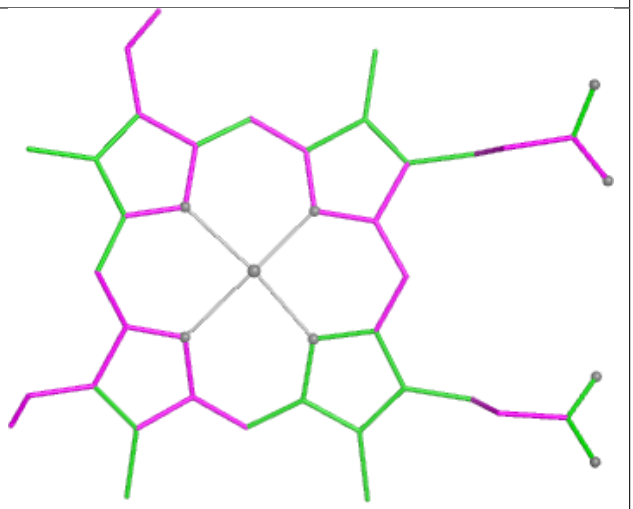

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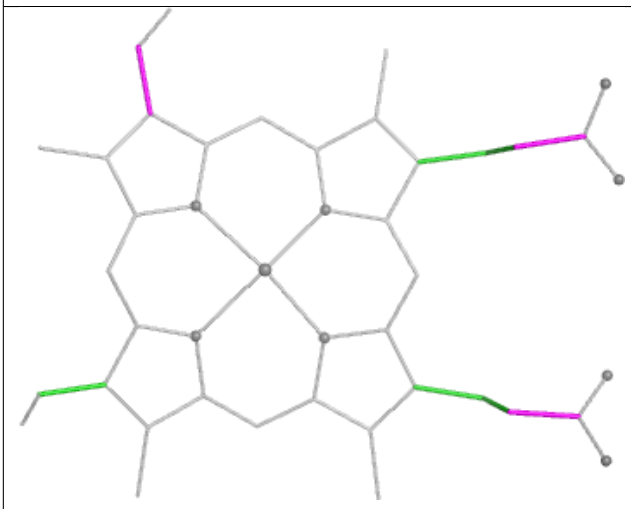

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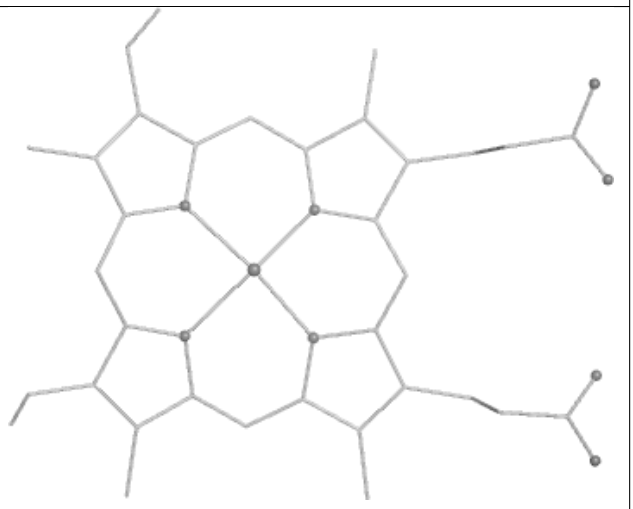
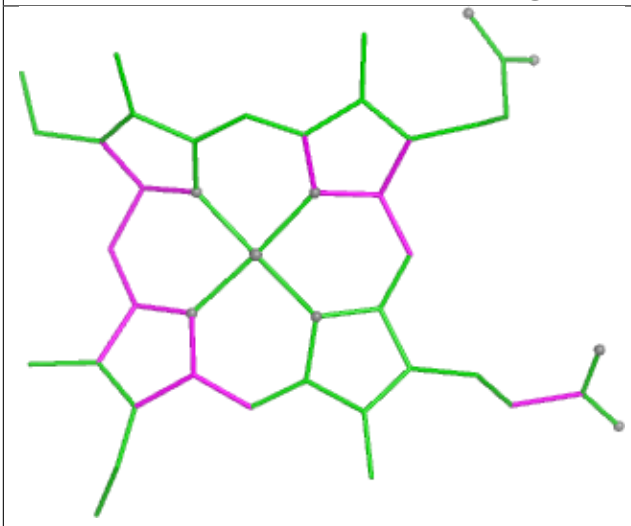


Rings

Ligand HEC J 603



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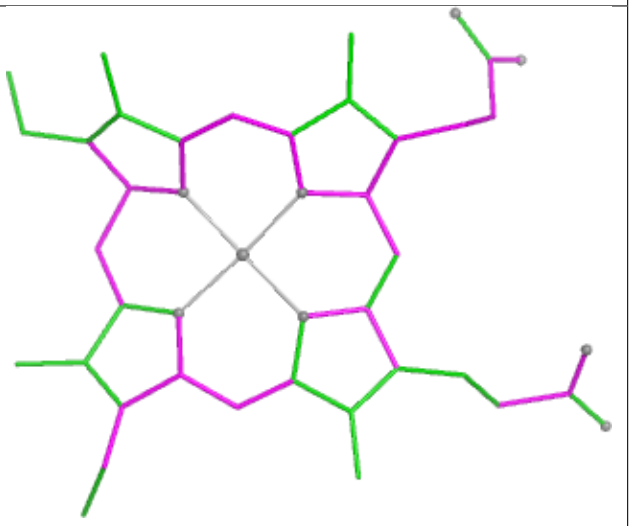

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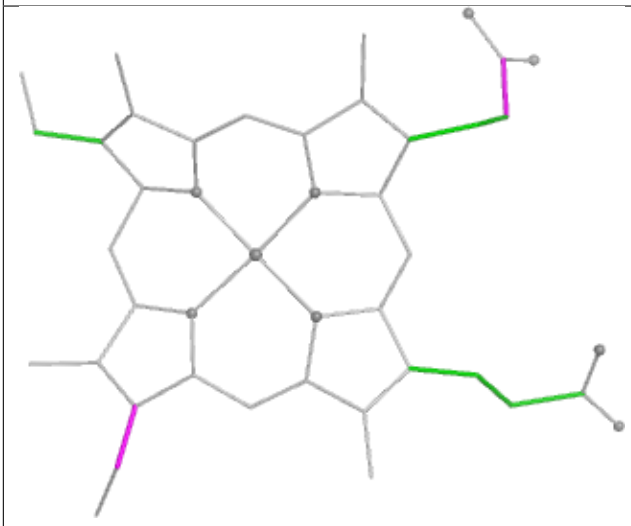

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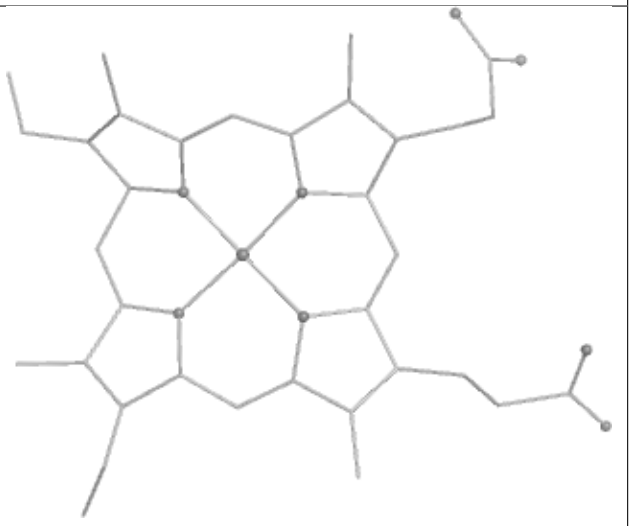
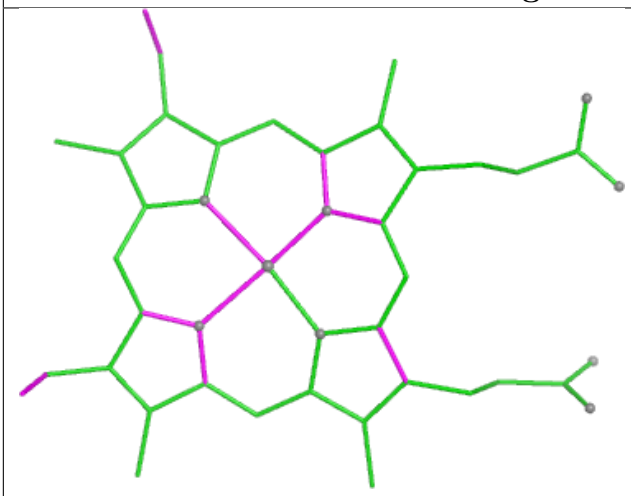


Rings

Ligand HEC V 606



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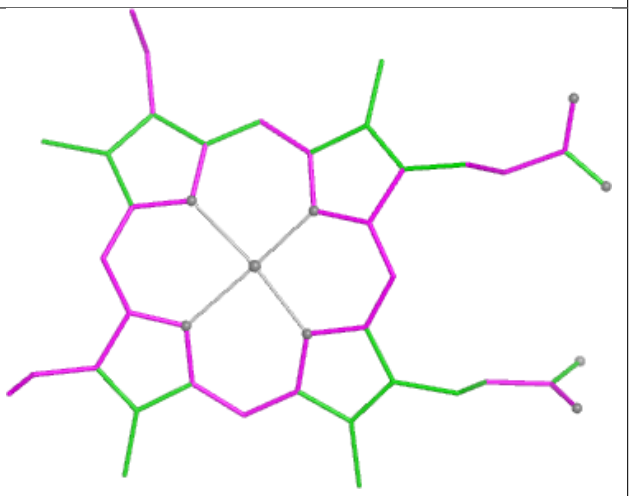

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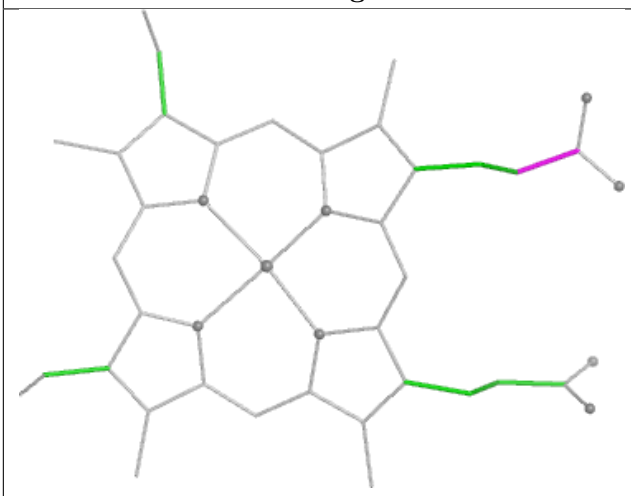

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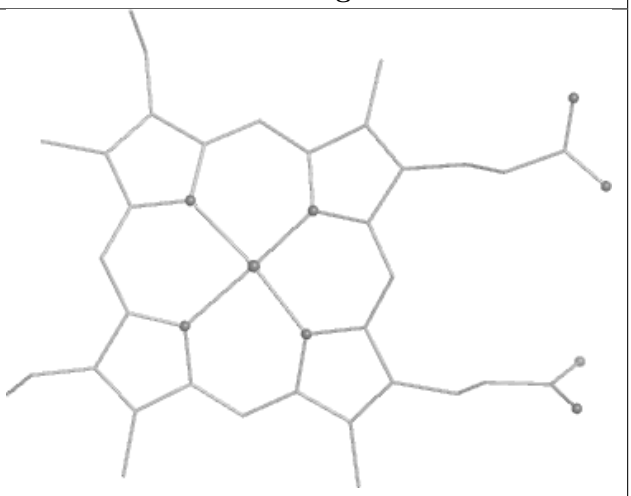
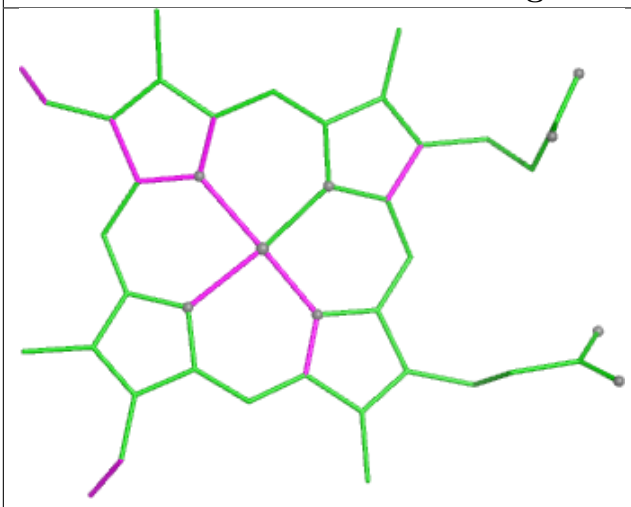


Rings

Ligand HEC J 607



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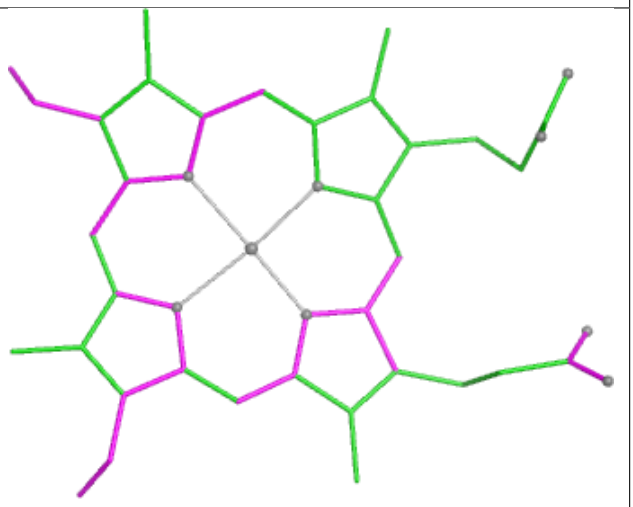

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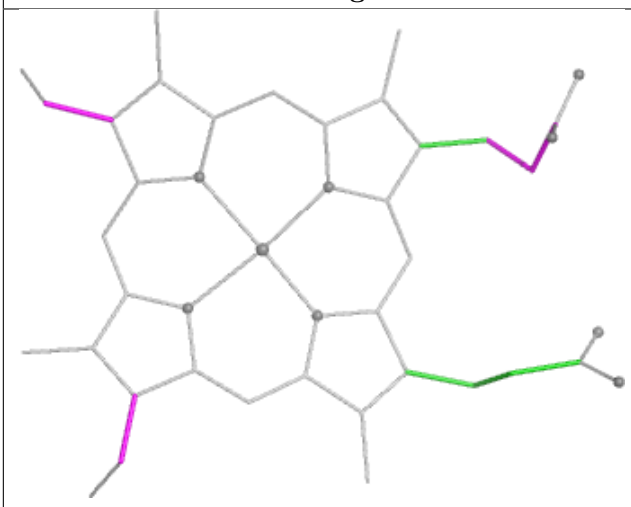

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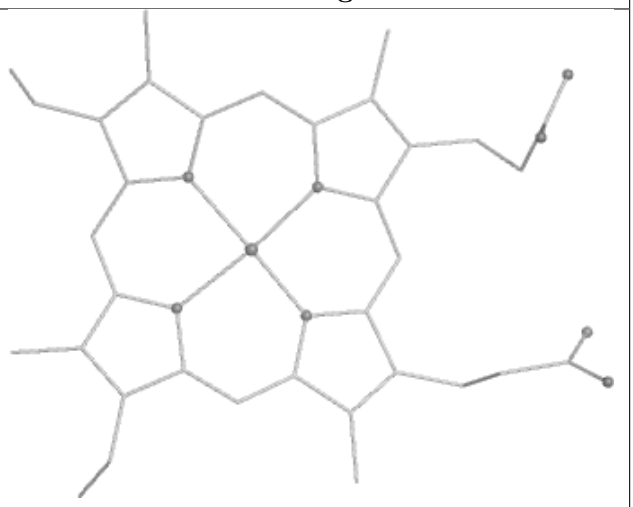
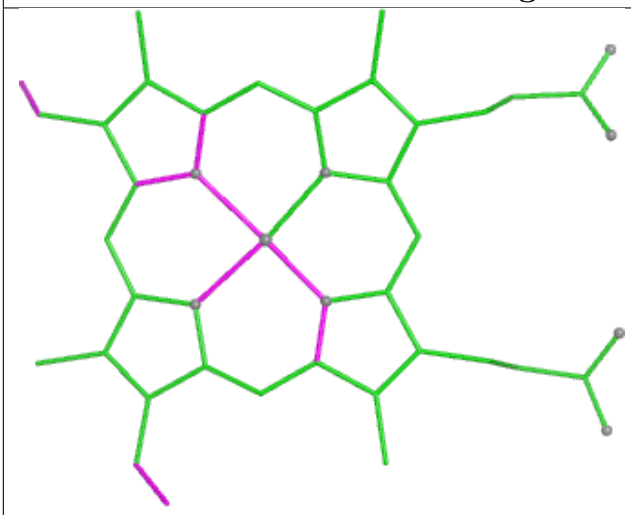


Rings

Ligand HEC M 600



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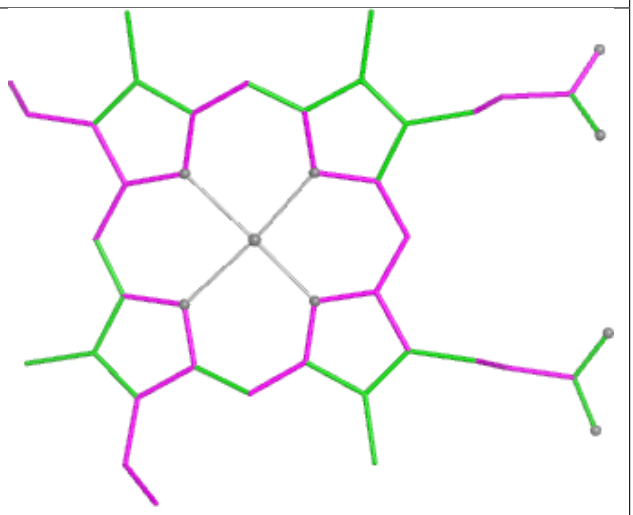
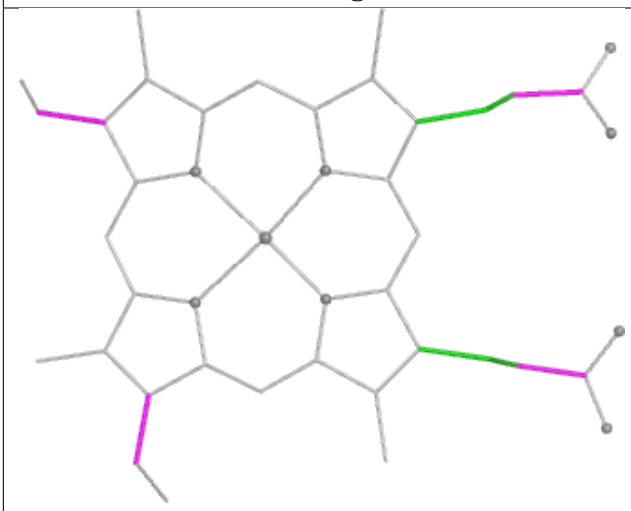


Bond angles



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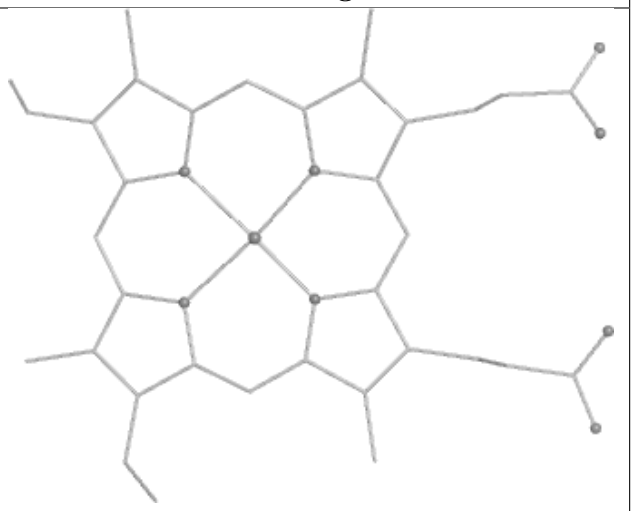
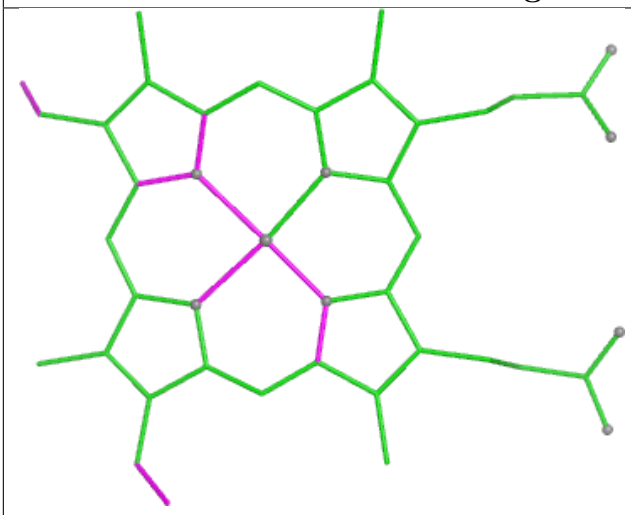


Rings

Ligand HEC E 600



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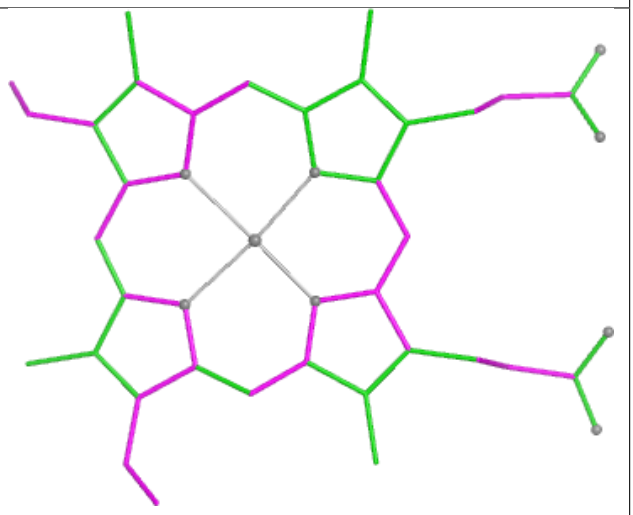
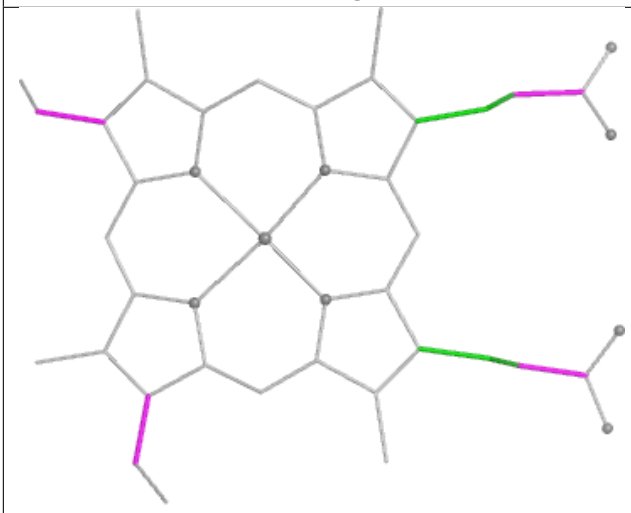


Bond angles



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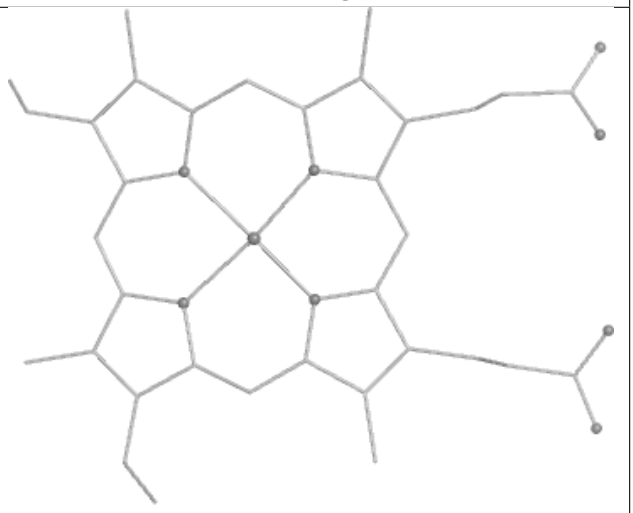
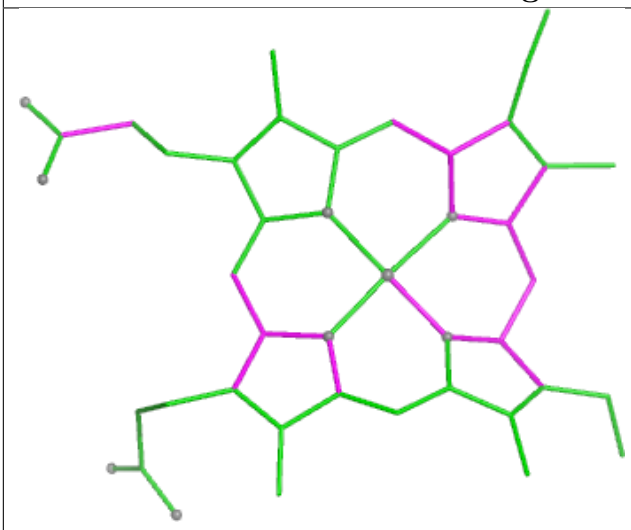


Rings

Ligand HEC K 603



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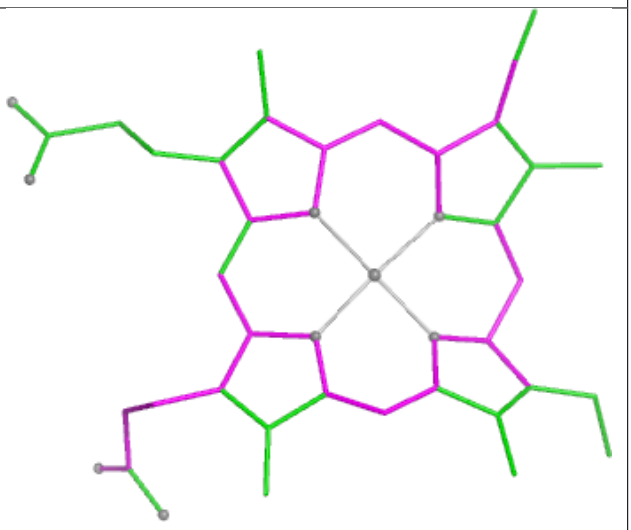

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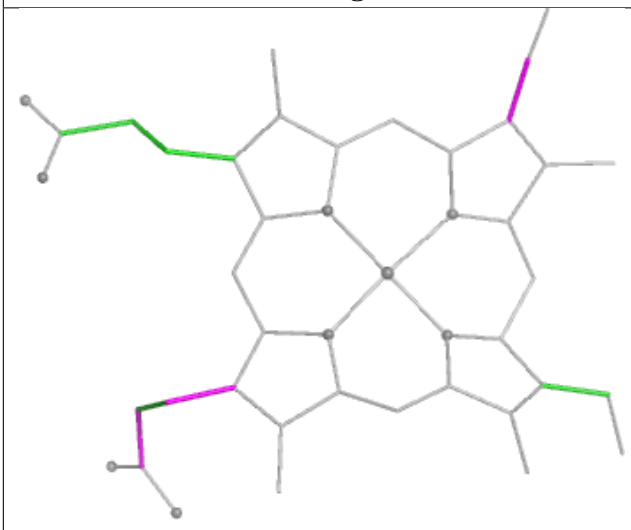

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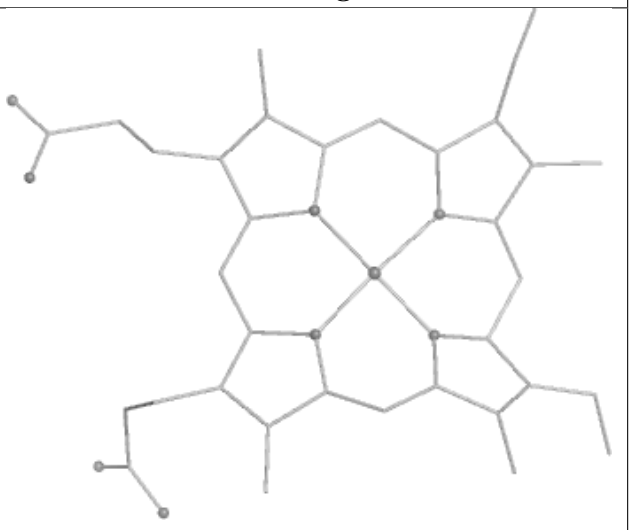

Rings

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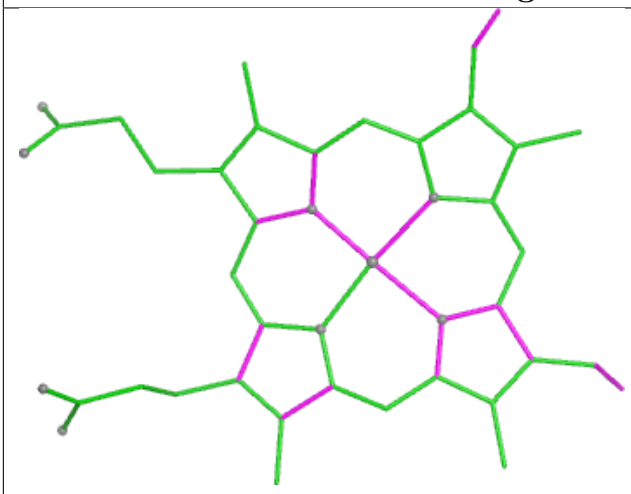

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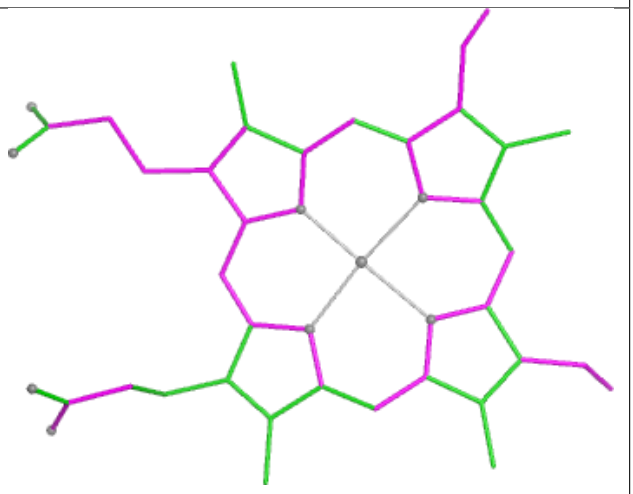

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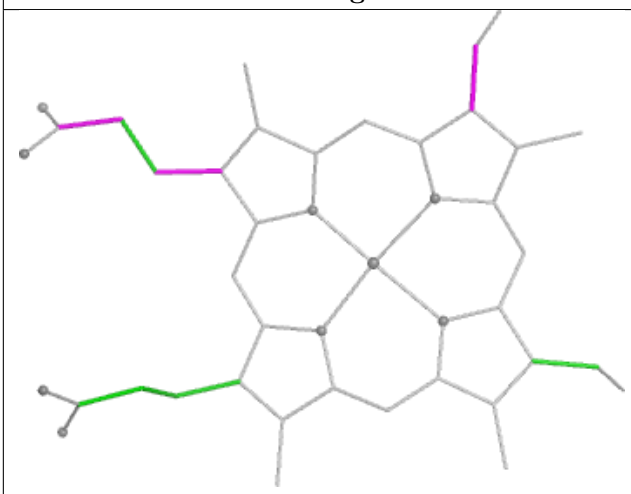

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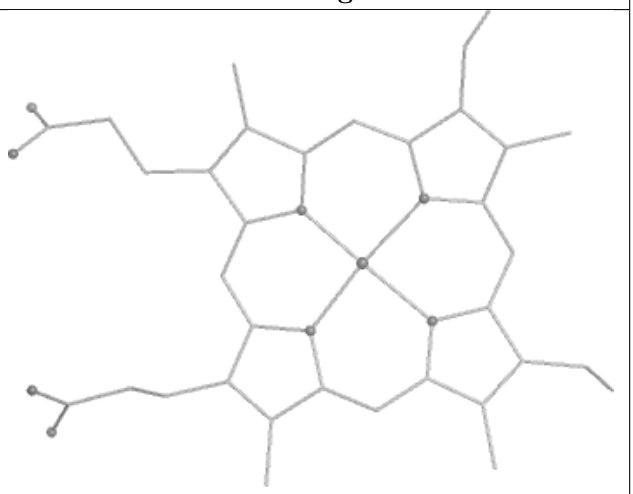

Rings

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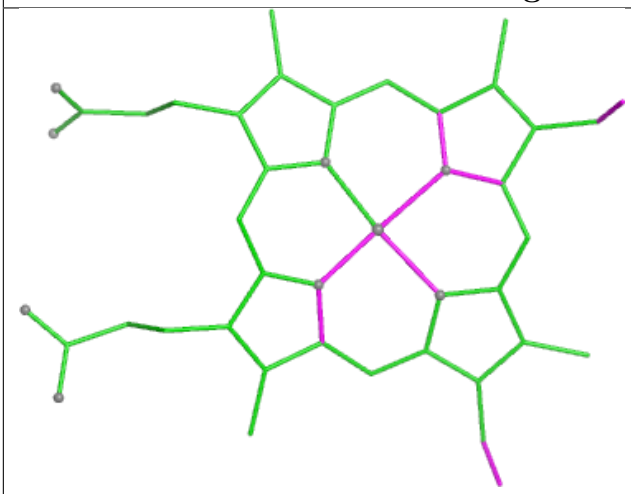

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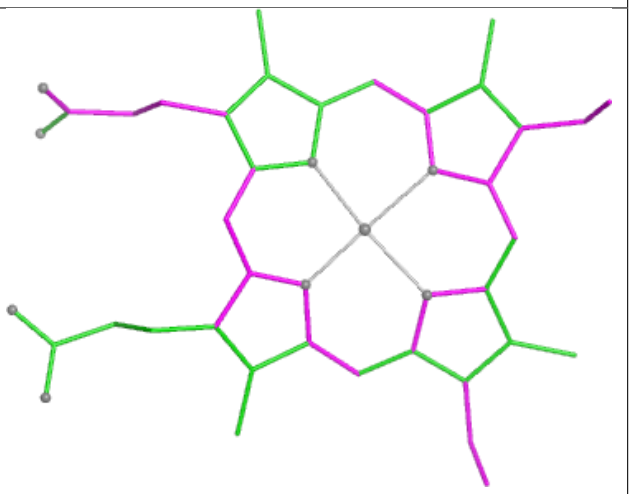

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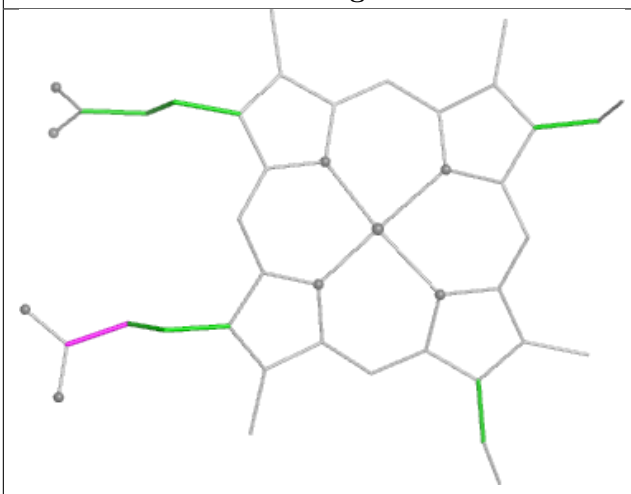

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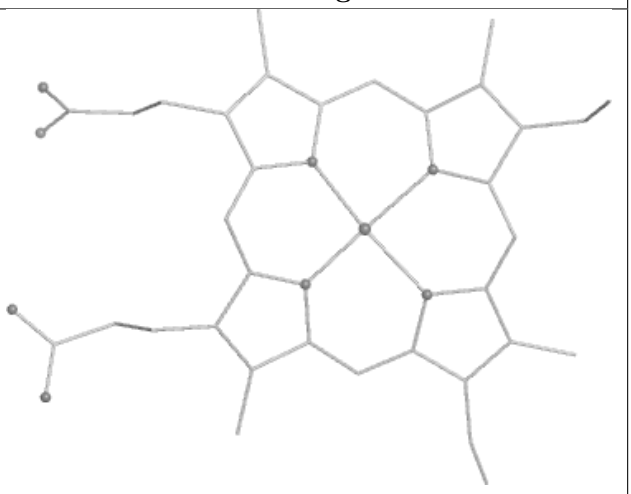

Rings

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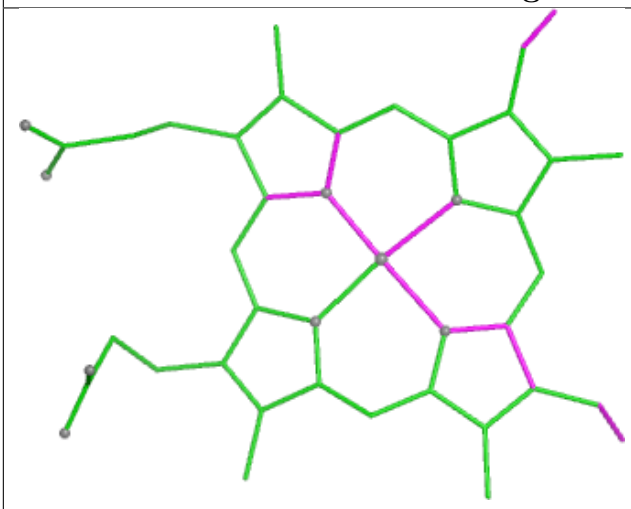

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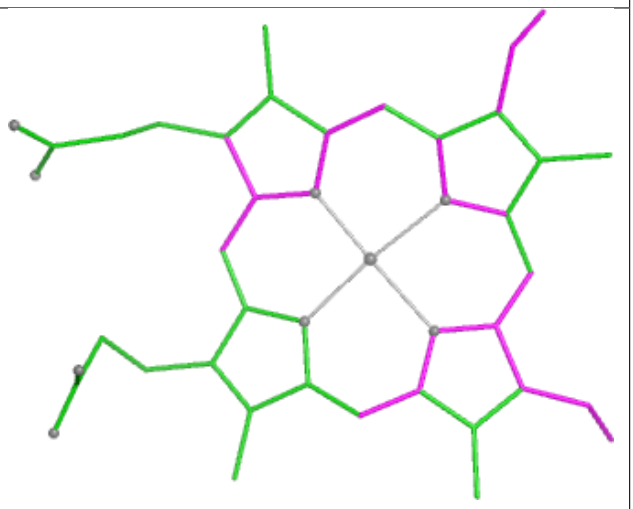

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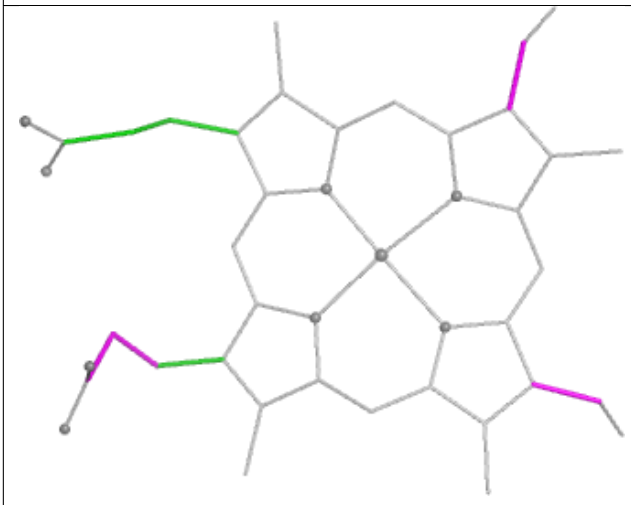

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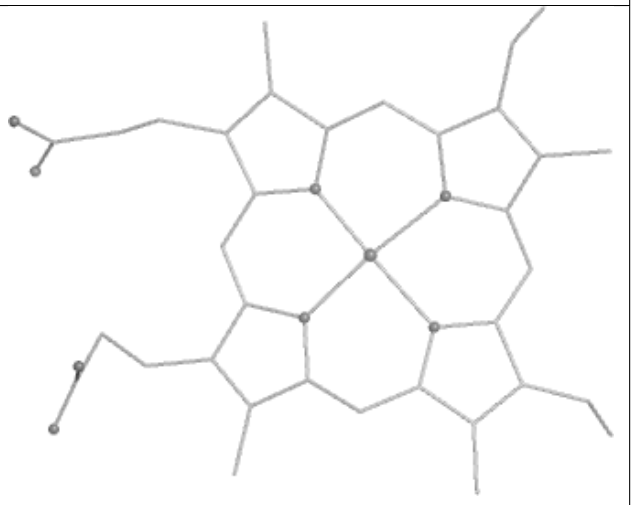

Rings

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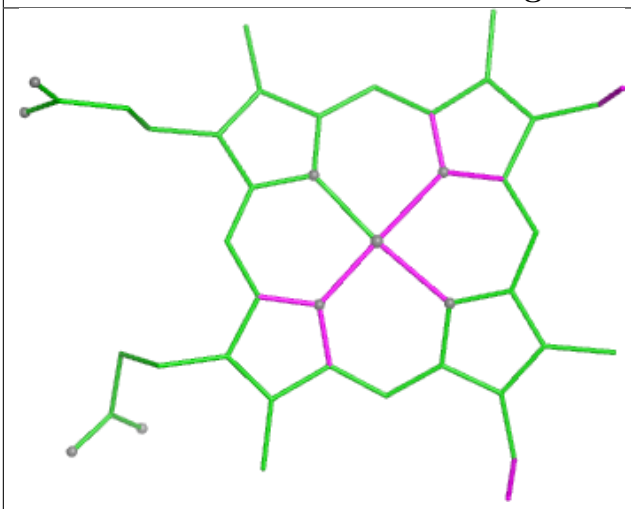

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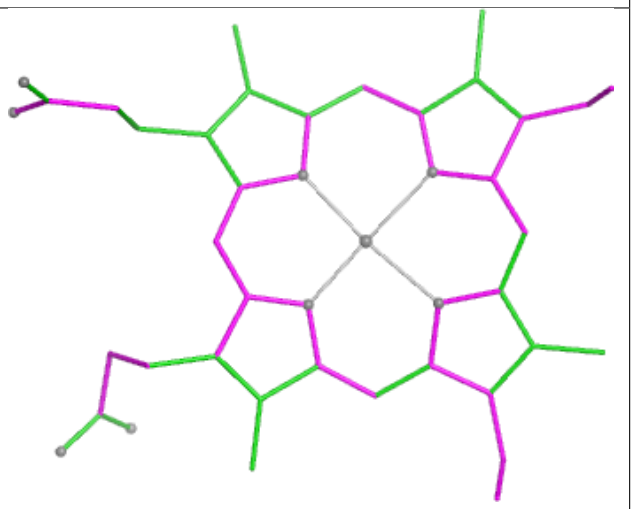

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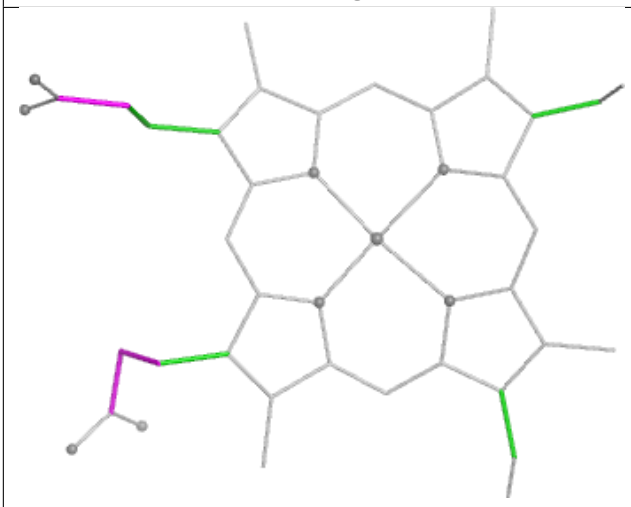

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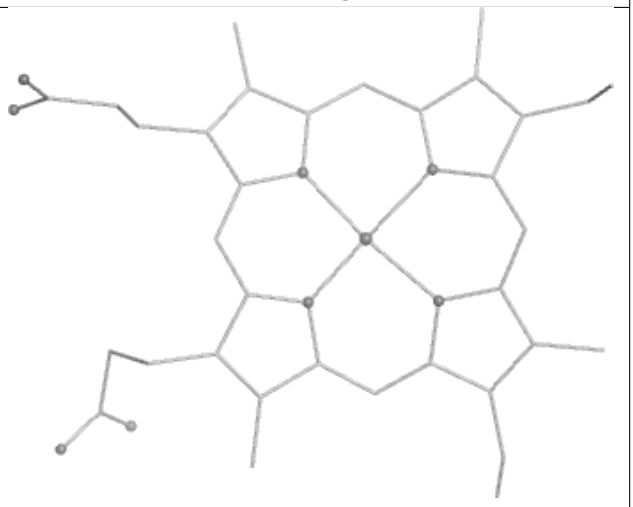

Rings

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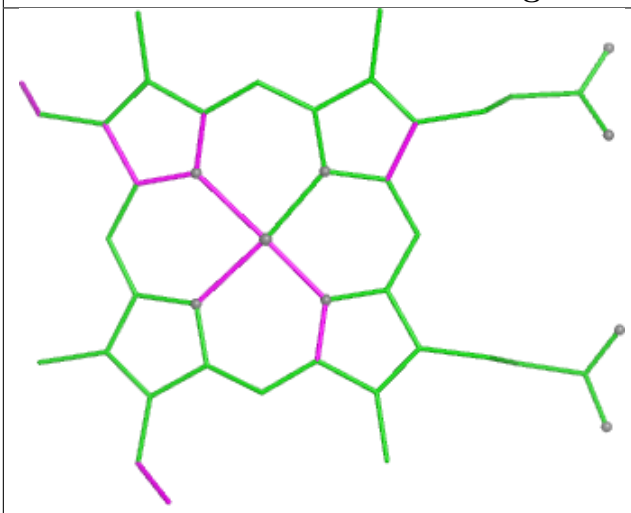

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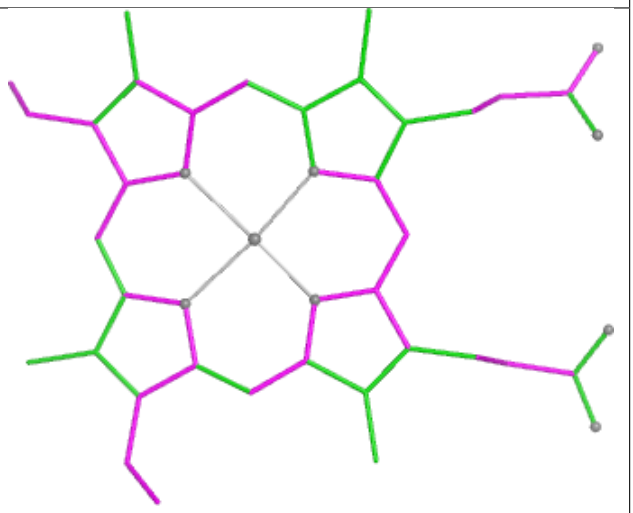
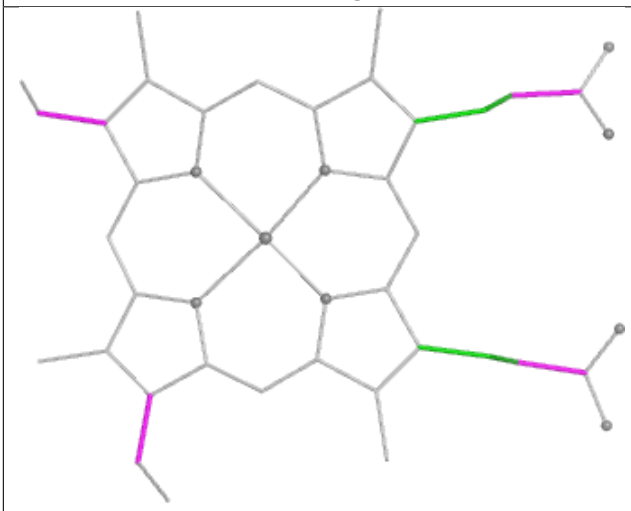


Bond angles



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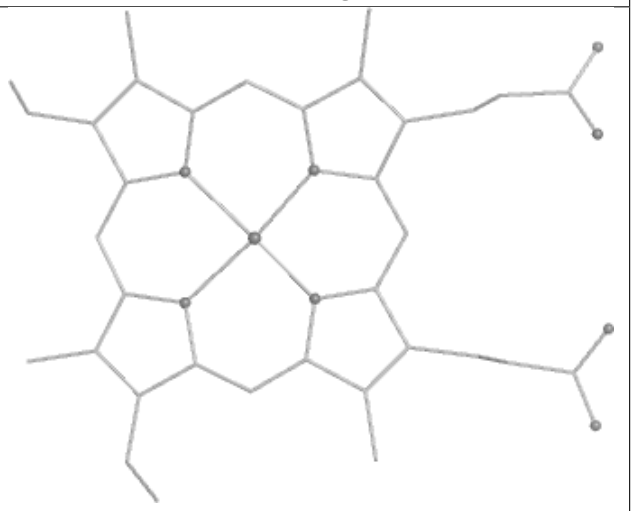

Rings

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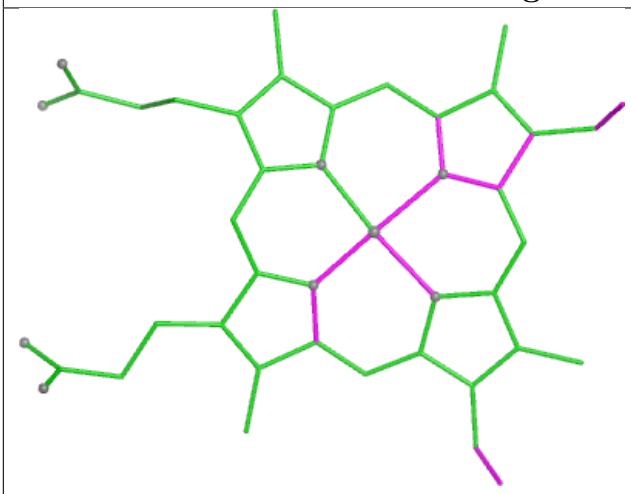

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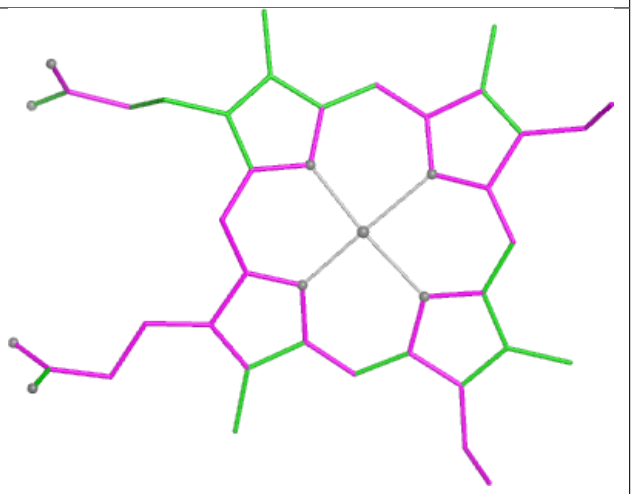

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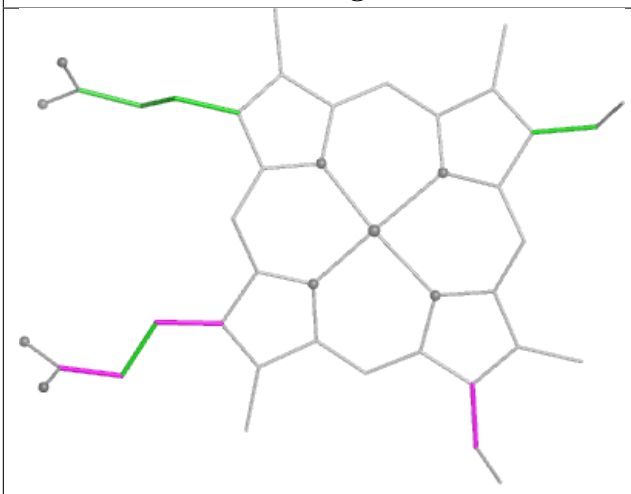

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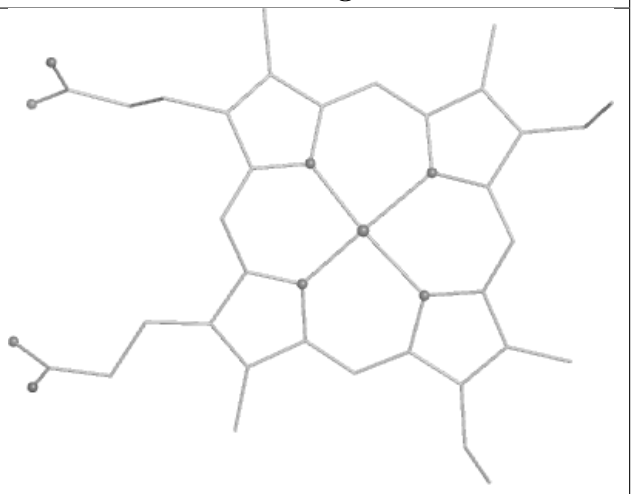

Rings

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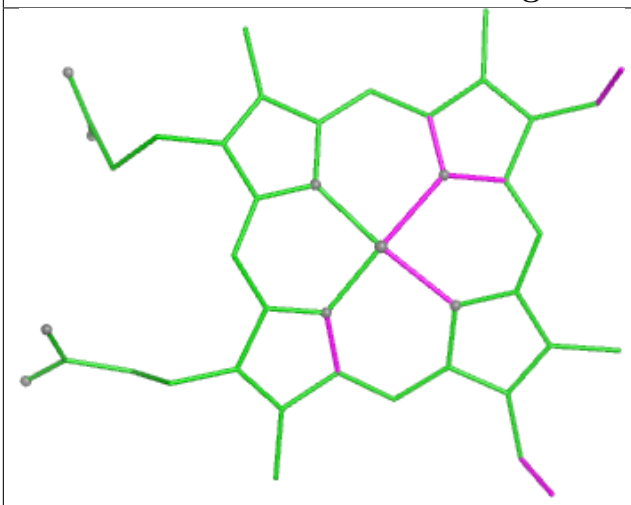

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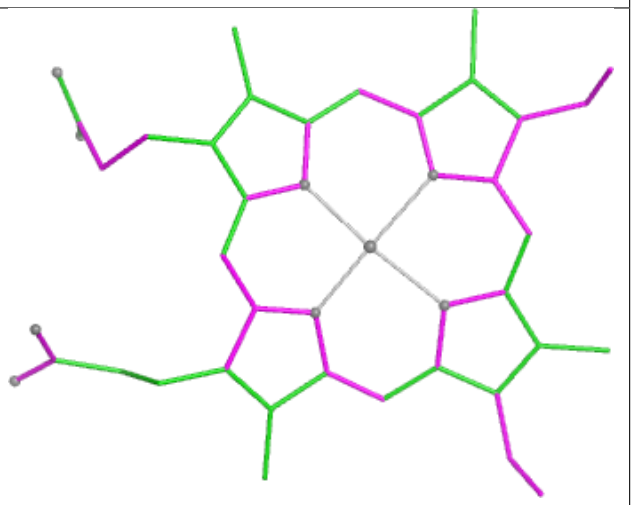

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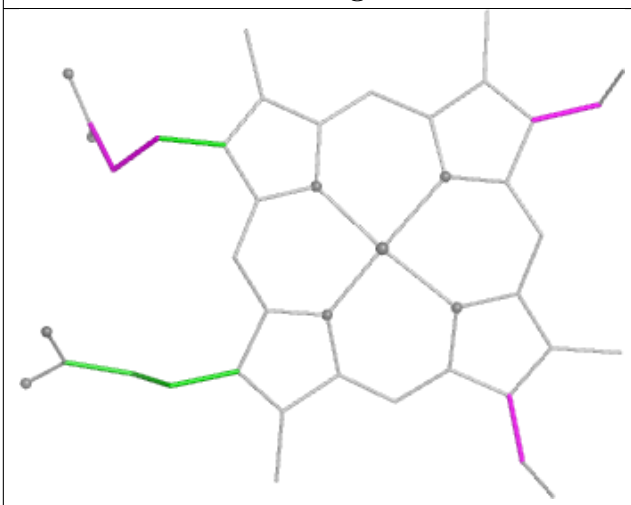

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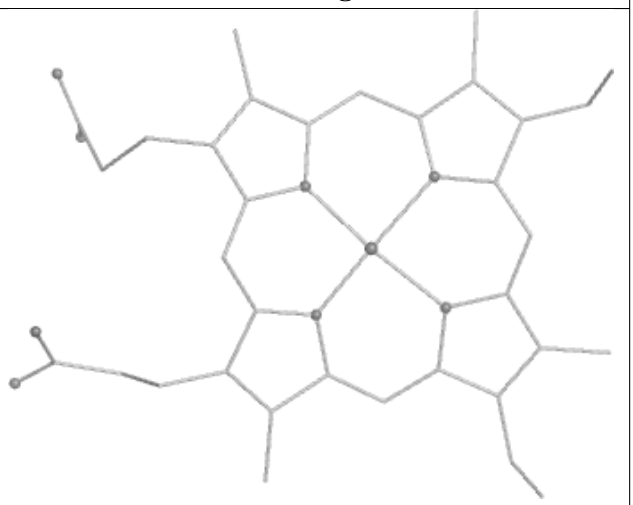
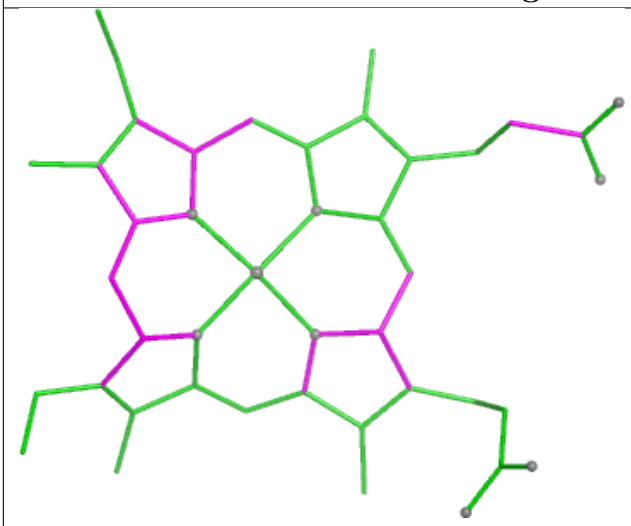


Rings

Ligand HEC U 603



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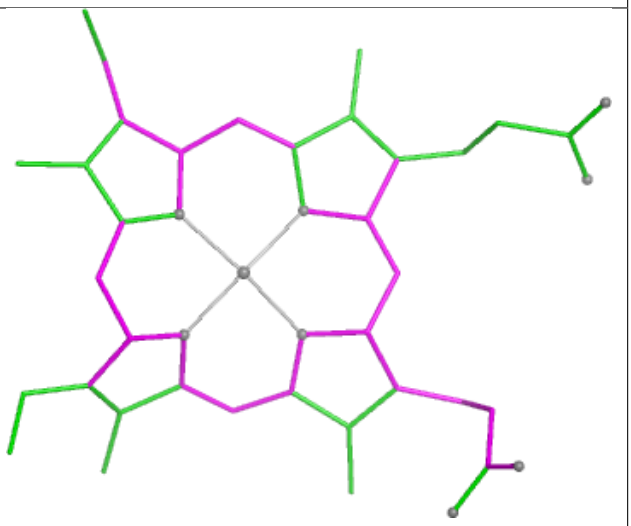

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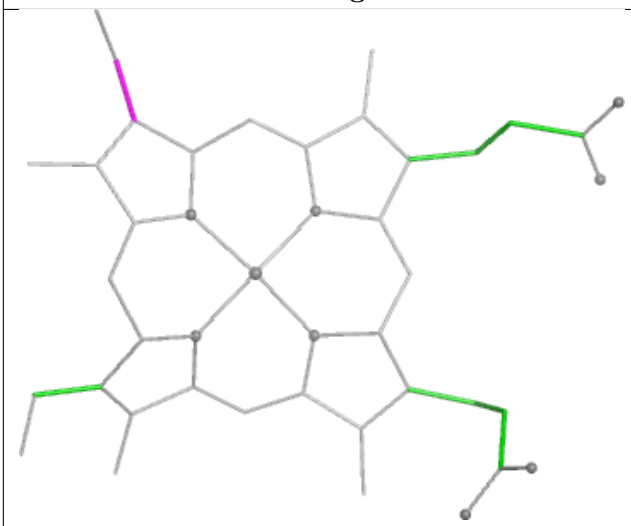

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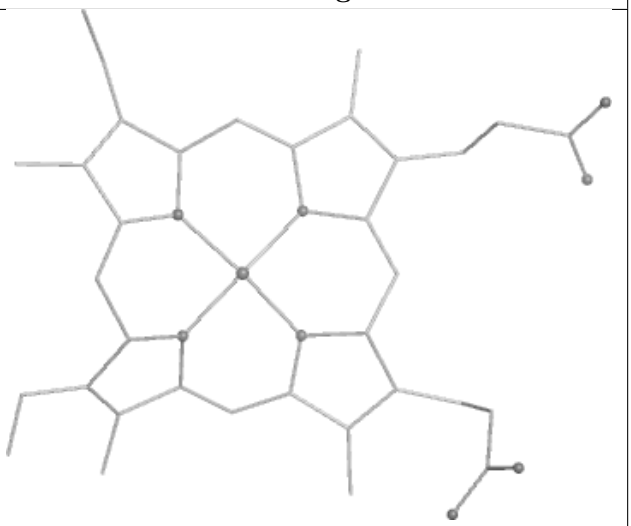

Rings

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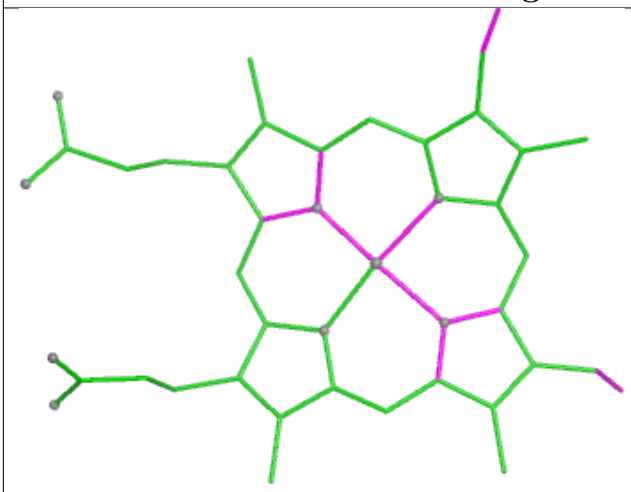

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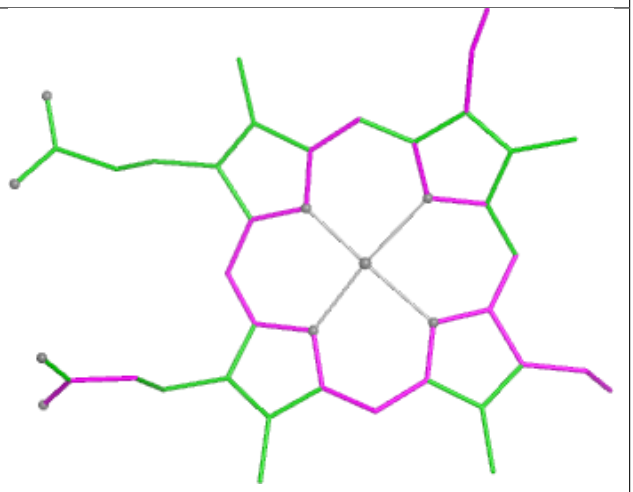

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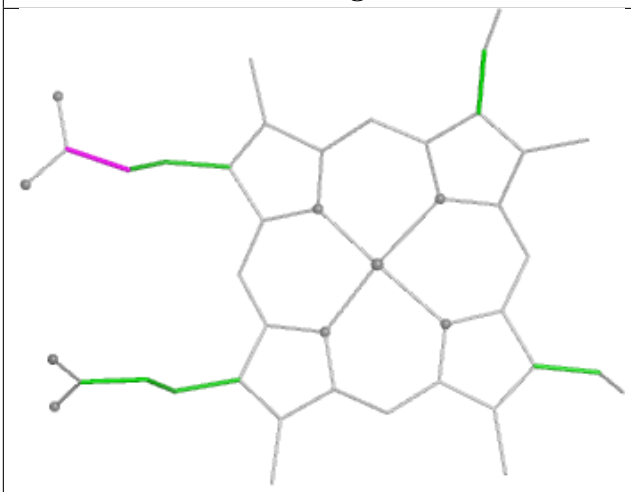

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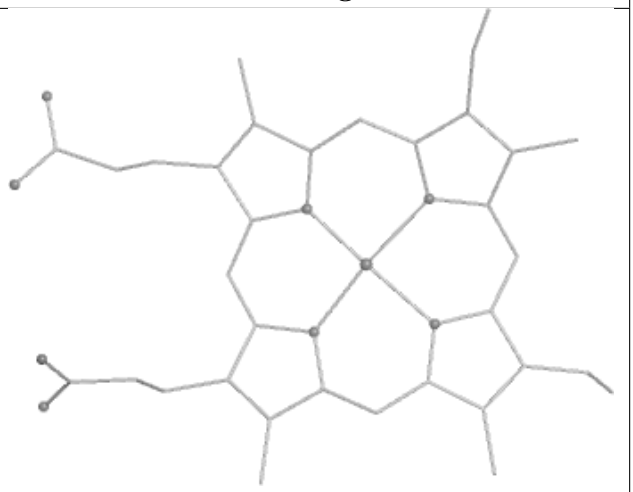
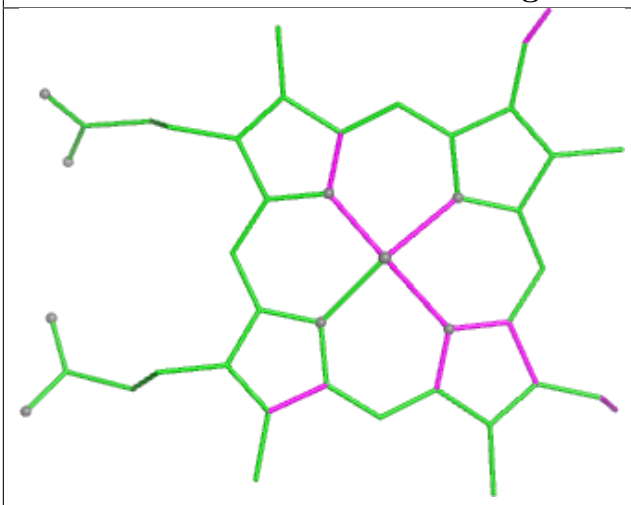


Rings

Ligand HEC H 604



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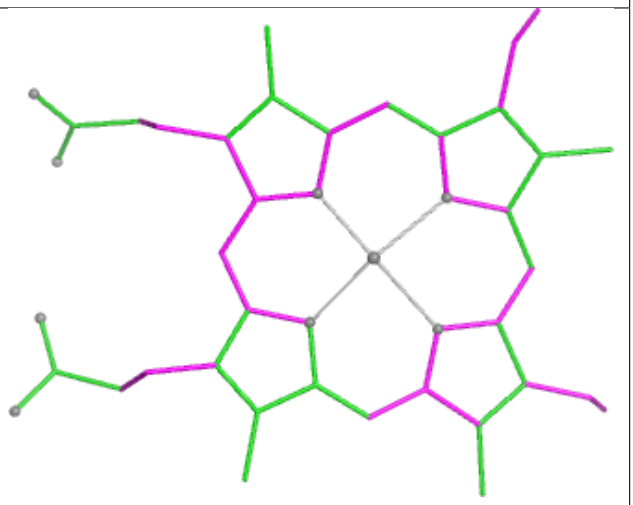

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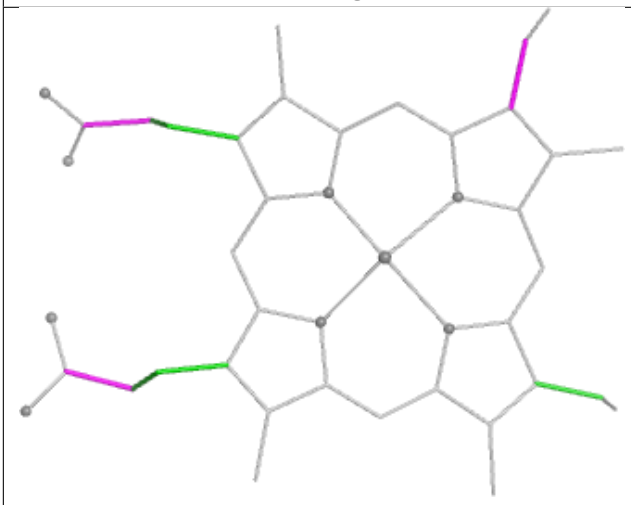

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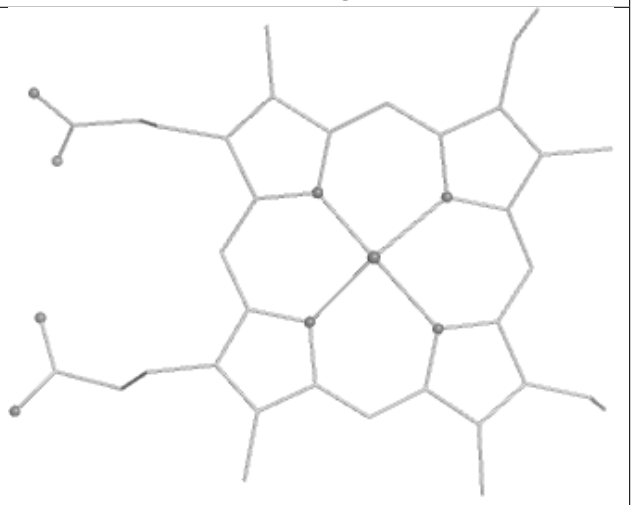
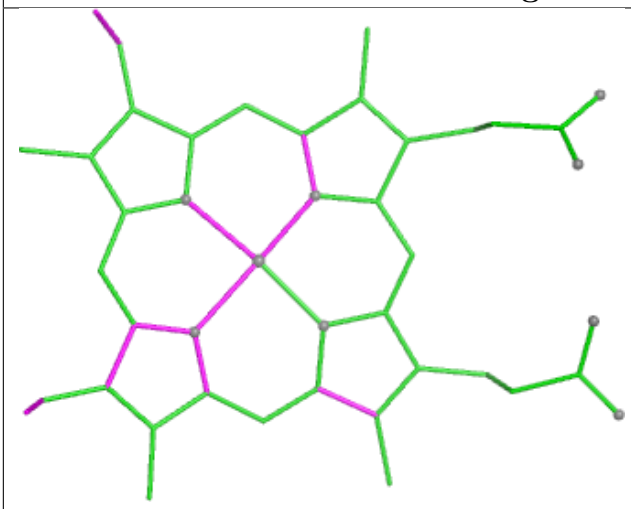


Rings

Ligand HEC K 604



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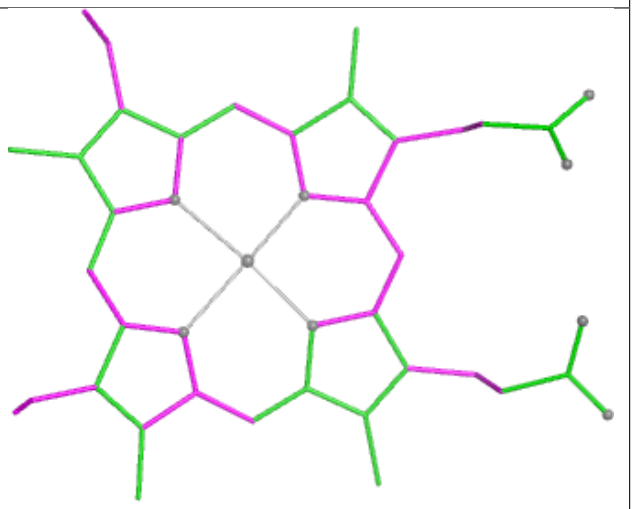
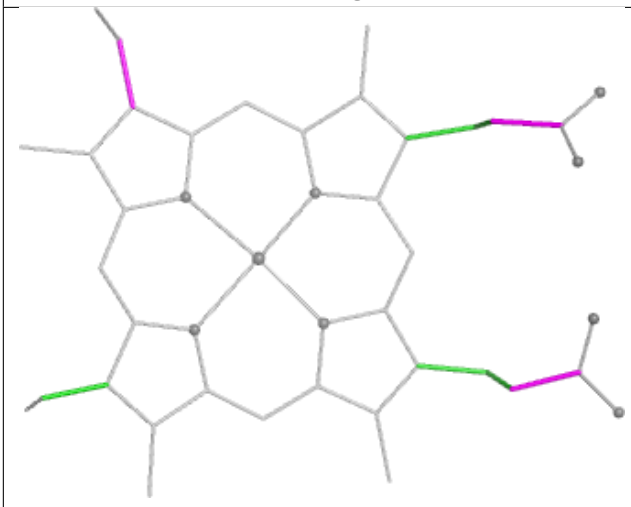


Bond angles



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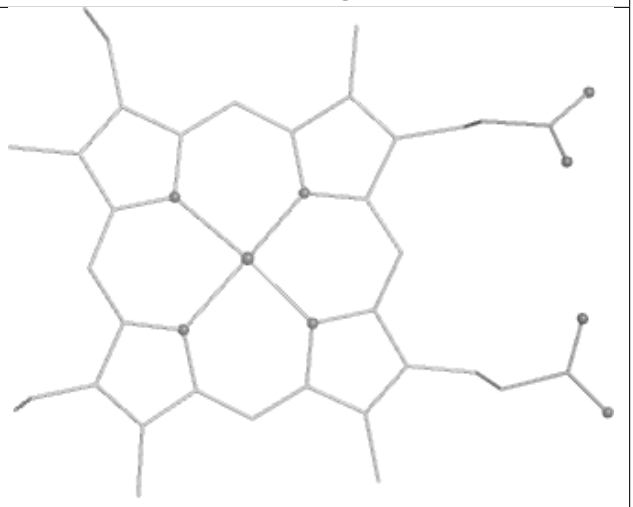
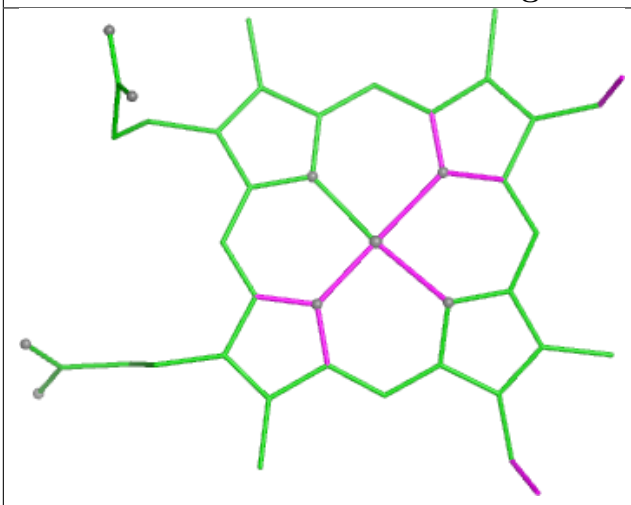


Rings

Ligand HEC N 601



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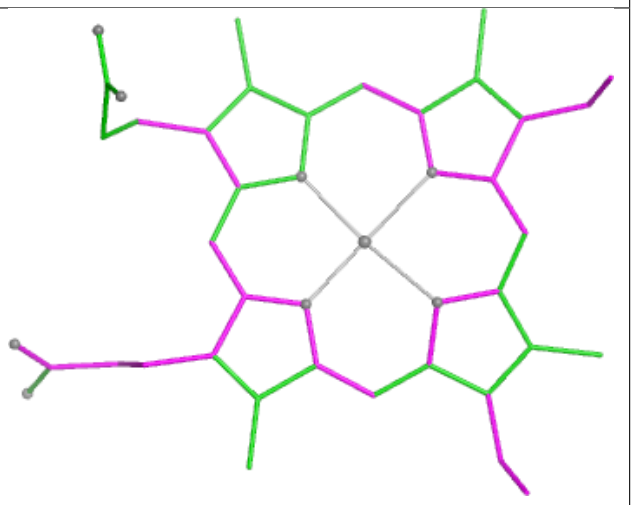

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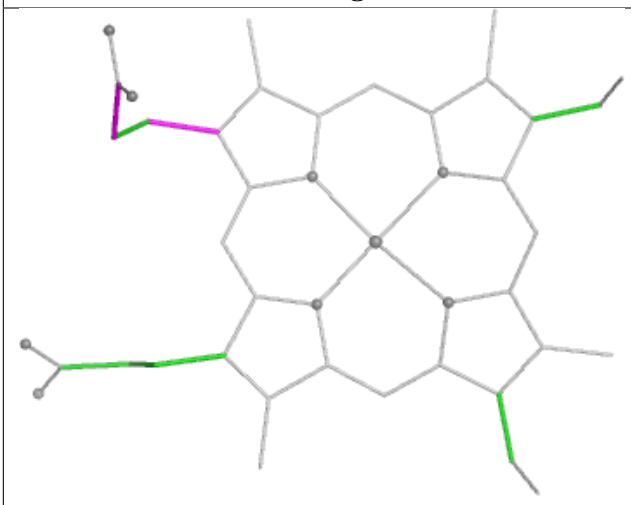

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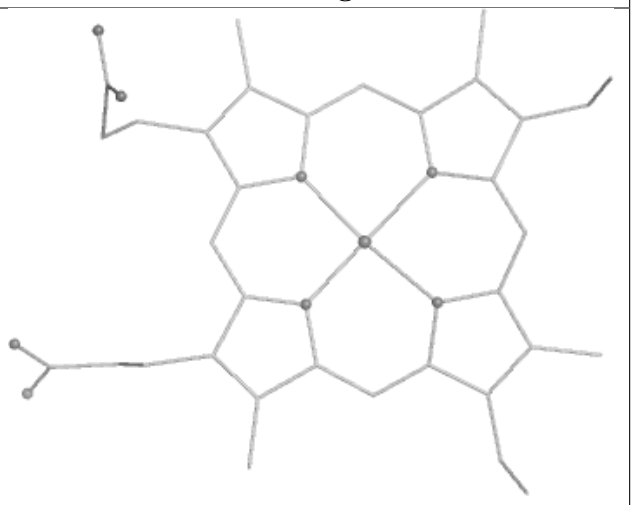
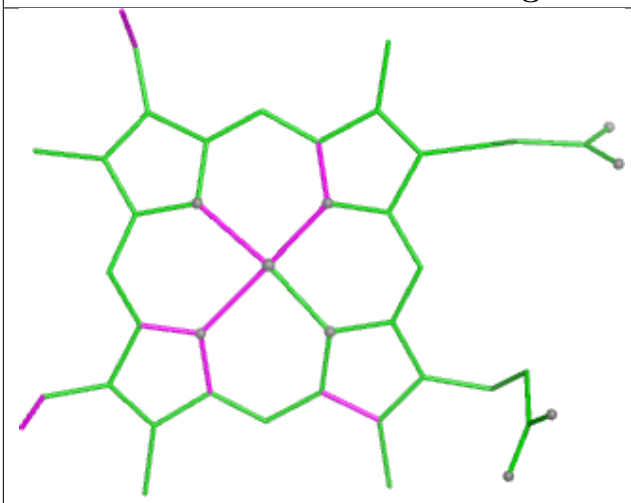


Rings

Ligand HEC D 601



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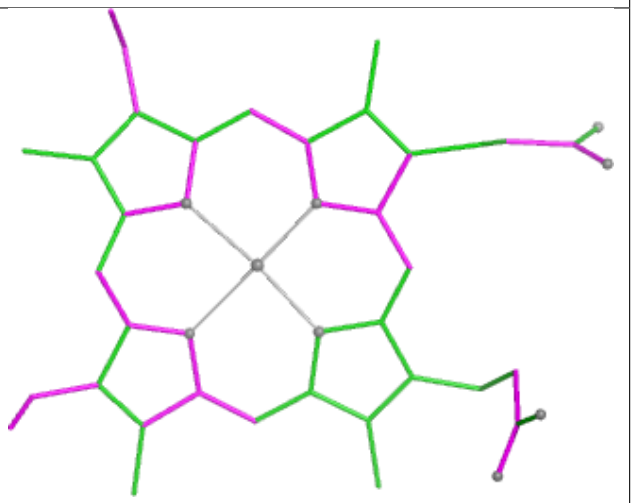
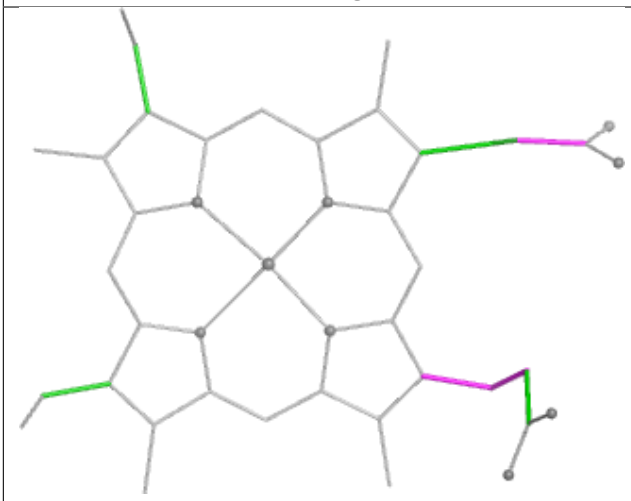


Bond angles



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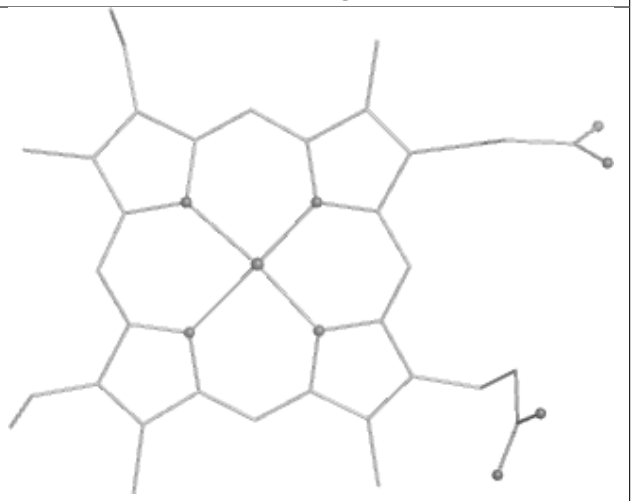
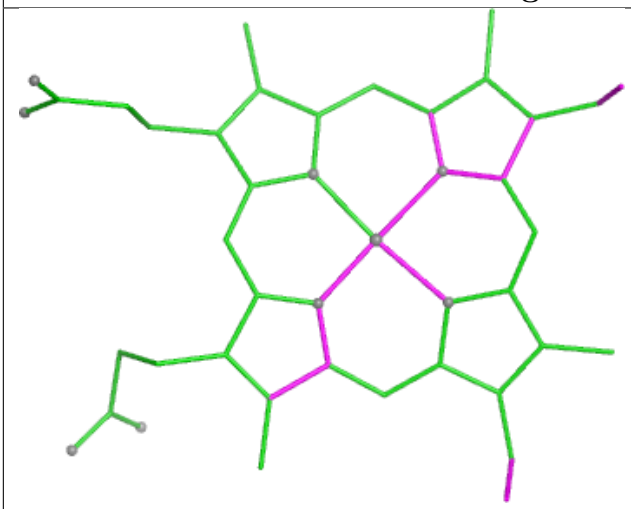


Rings

Ligand HEC G 602



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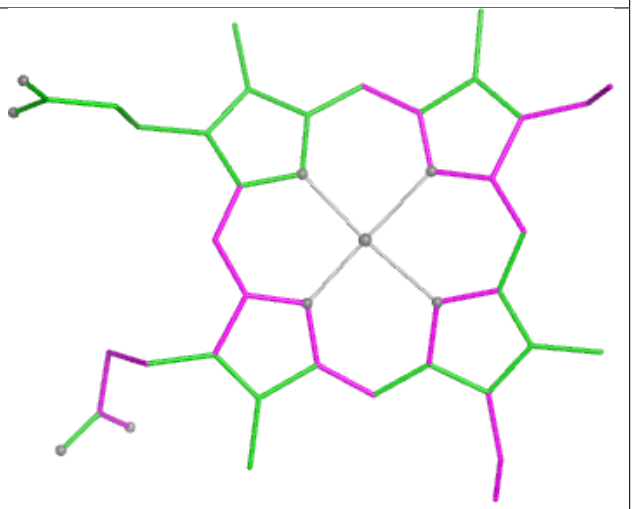

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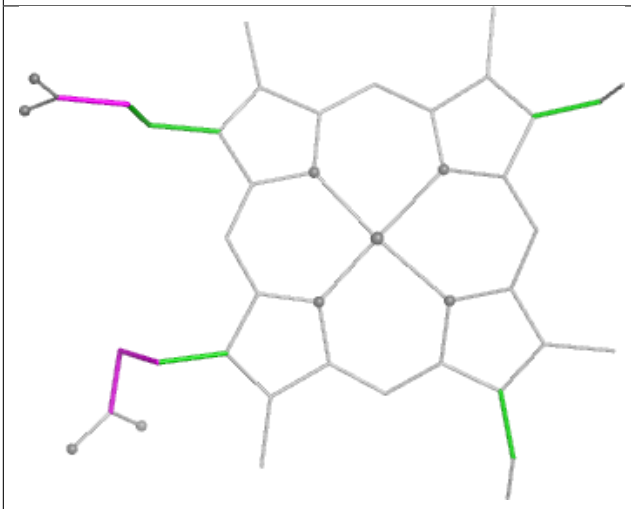
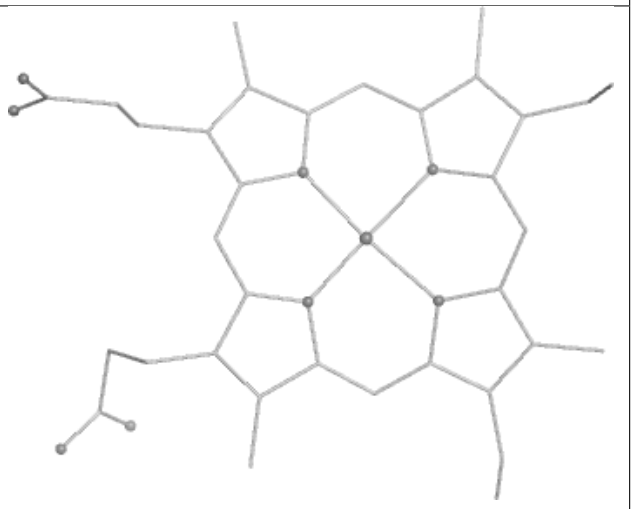
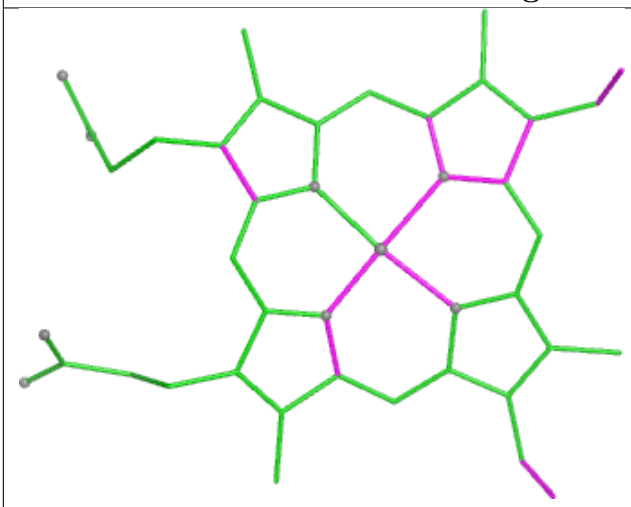


Torsions



Rings

Ligand HEC V 607



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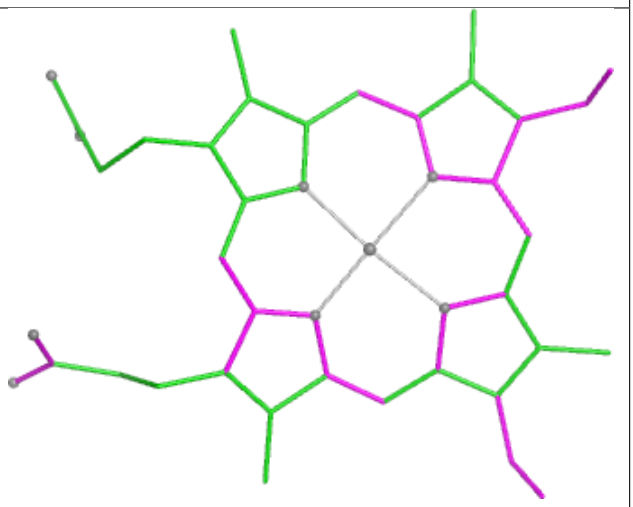

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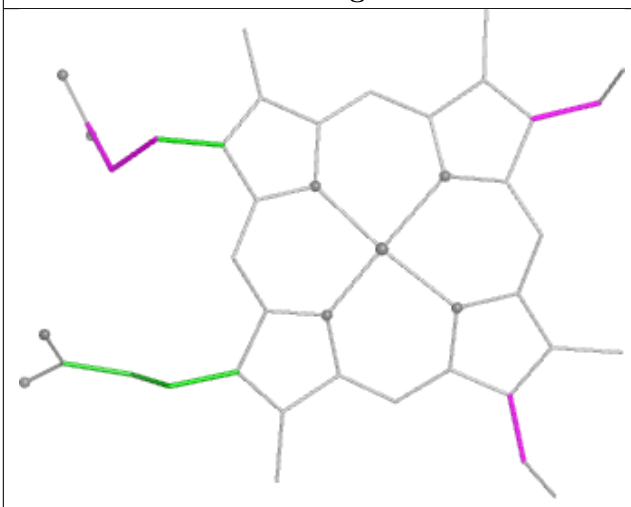

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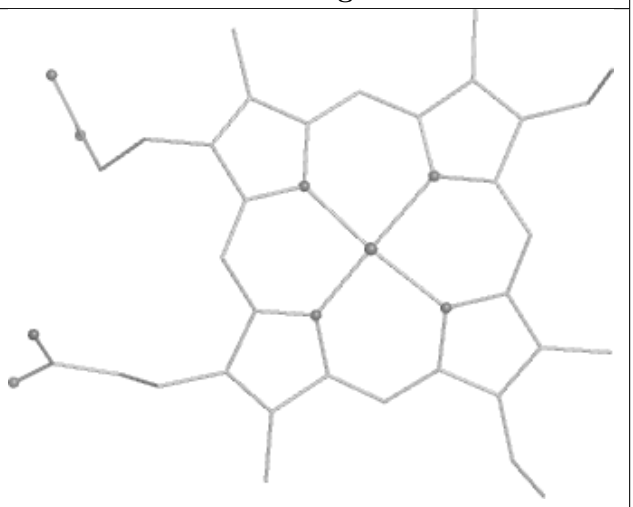
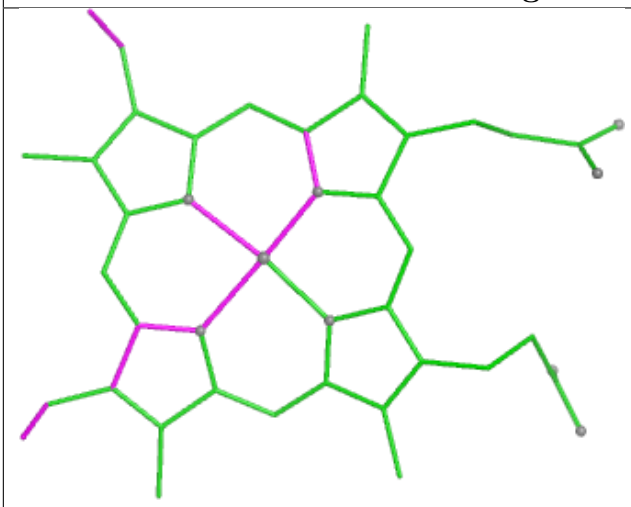


Rings

Ligand HEC X 607



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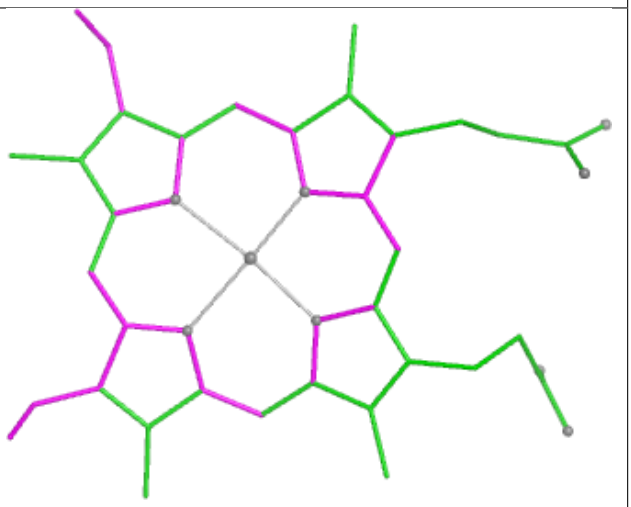

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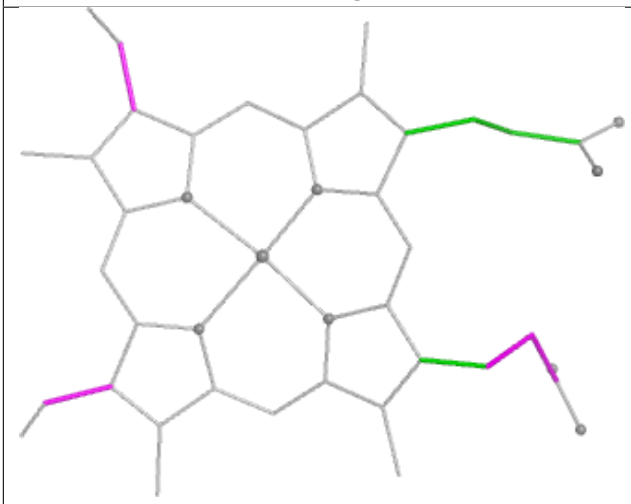

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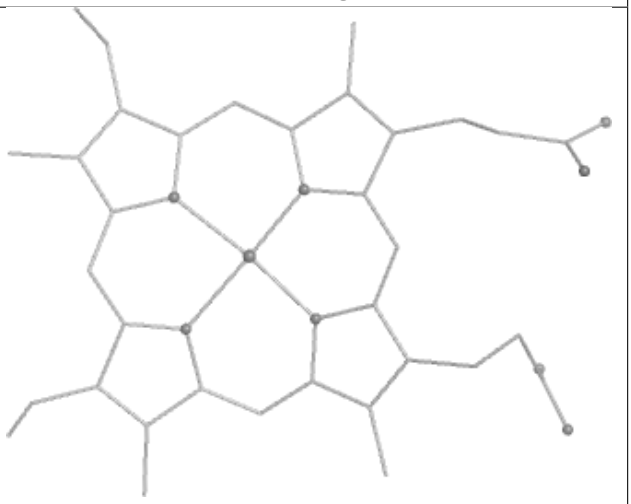
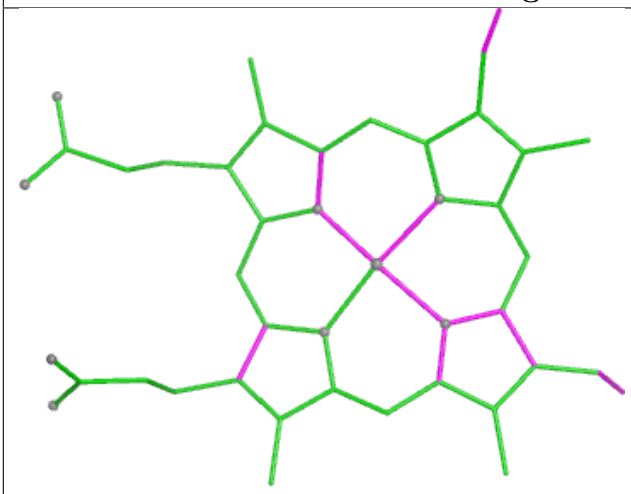


Rings

Ligand HEC Q 606



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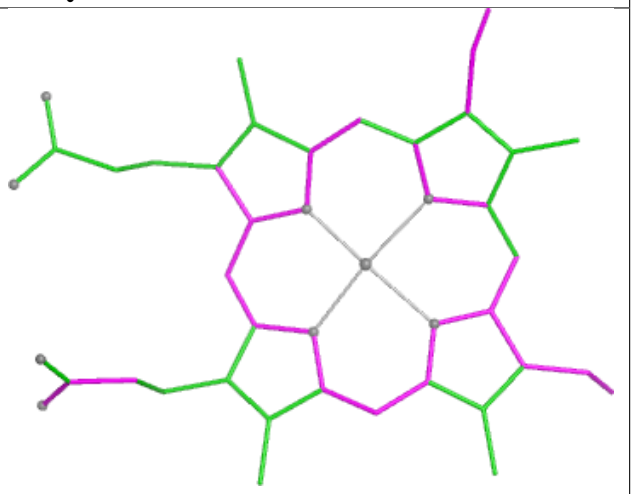

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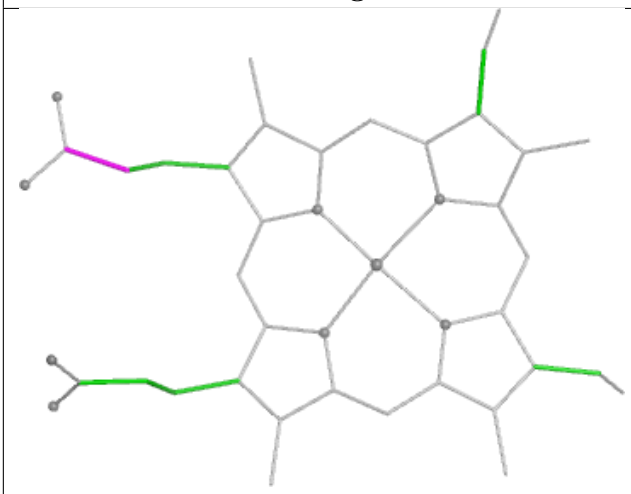

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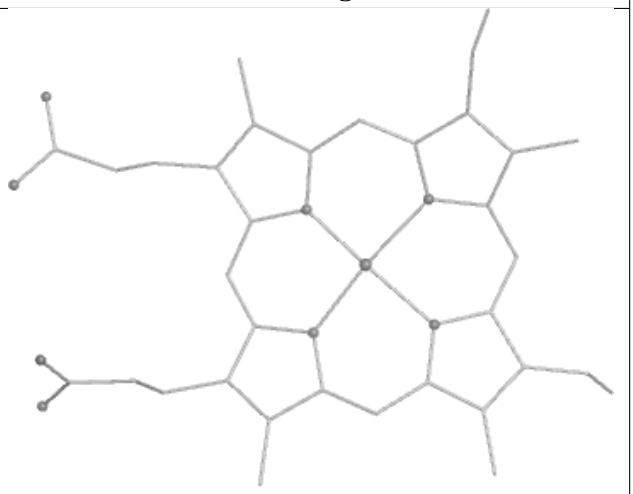
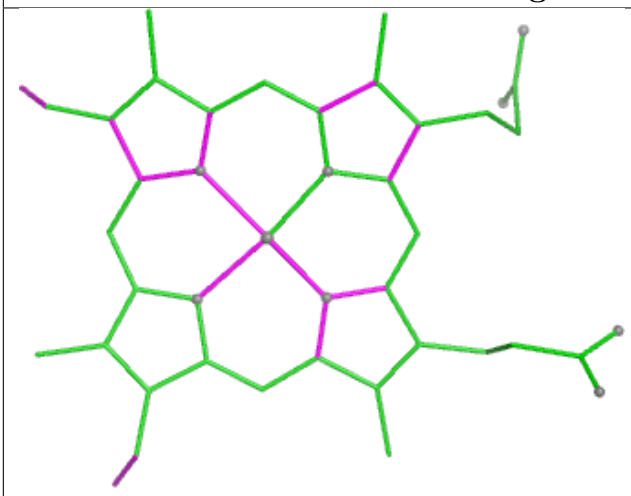


Rings

Ligand HEC I 601



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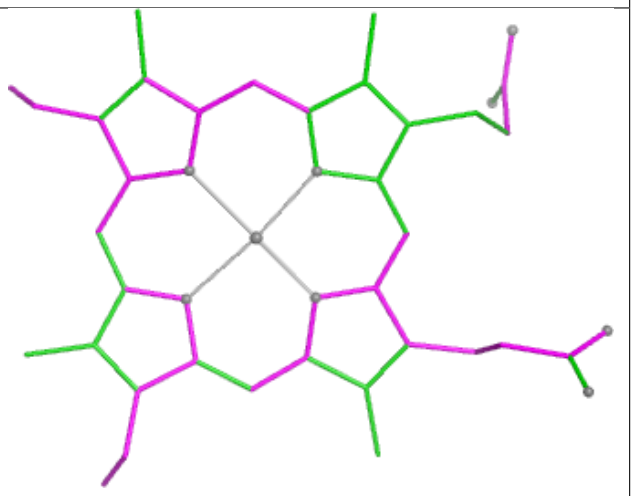

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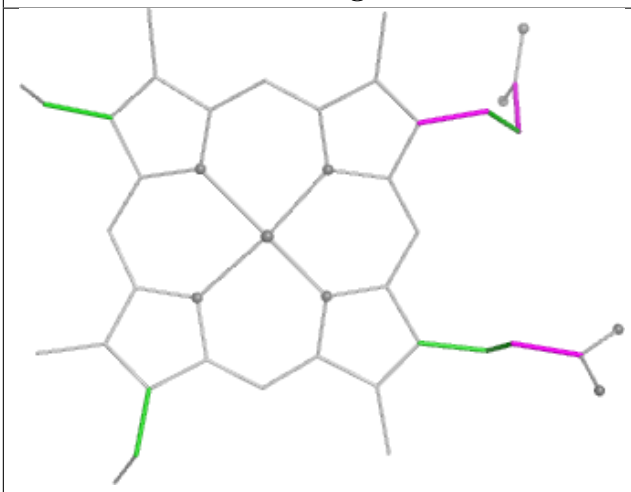

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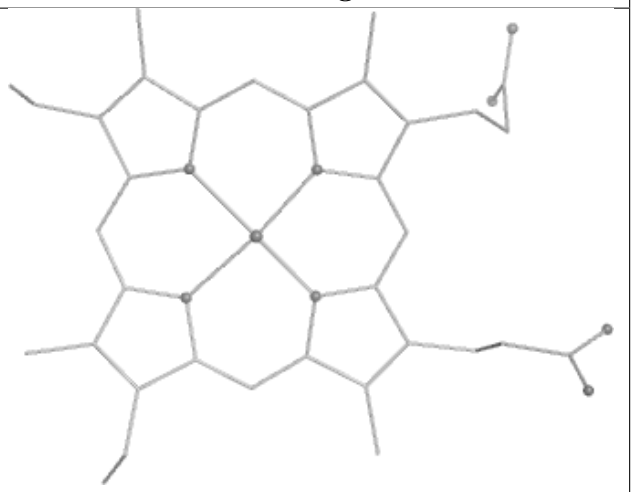
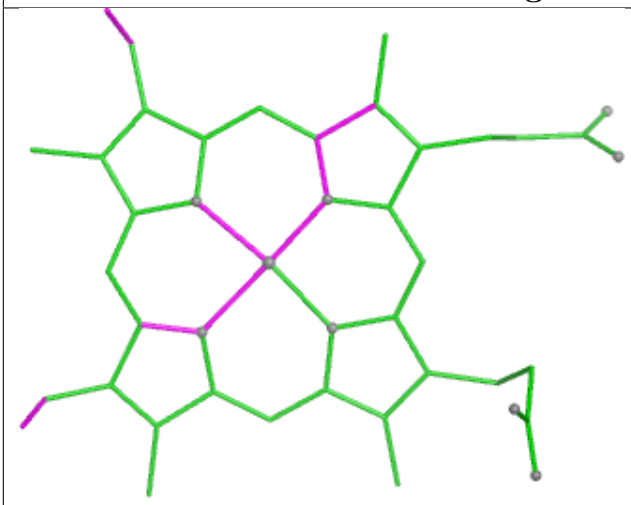


Rings

Ligand HEC L 601



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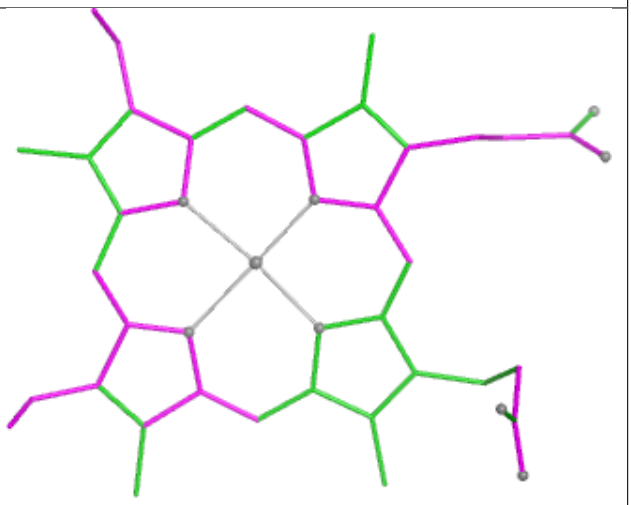

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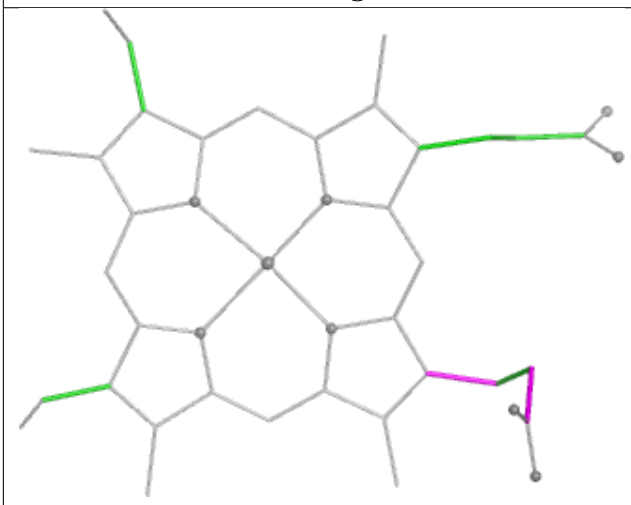

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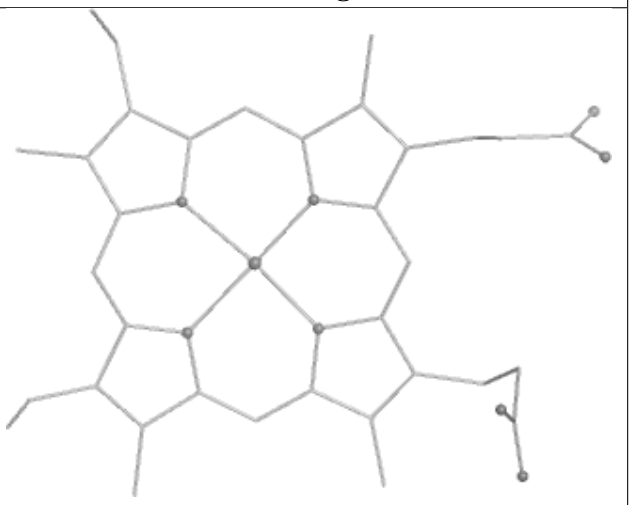
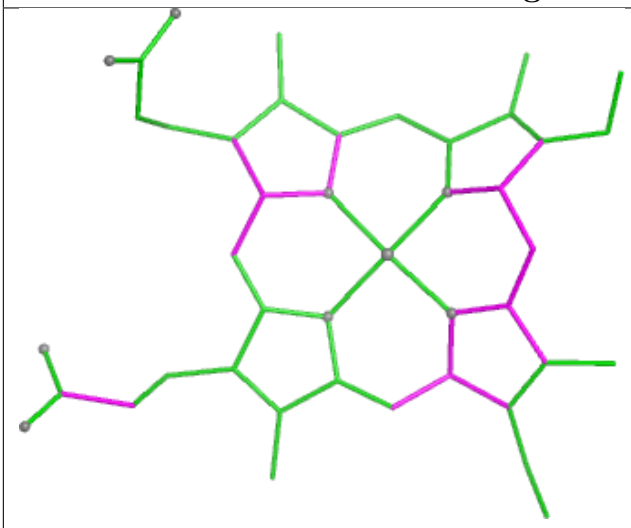


Rings

Ligand HEC P 603



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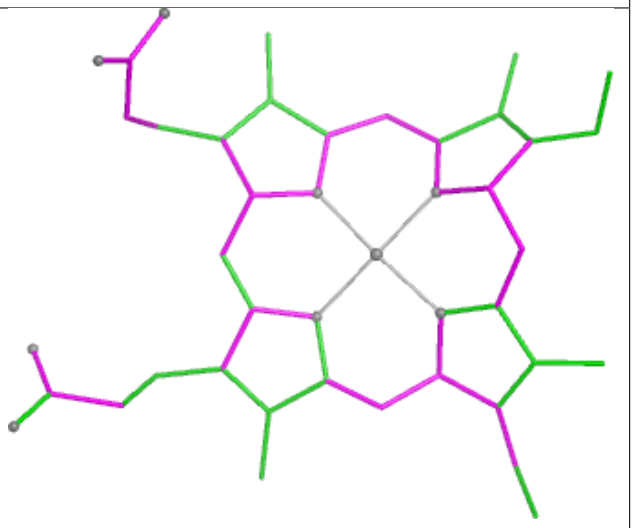

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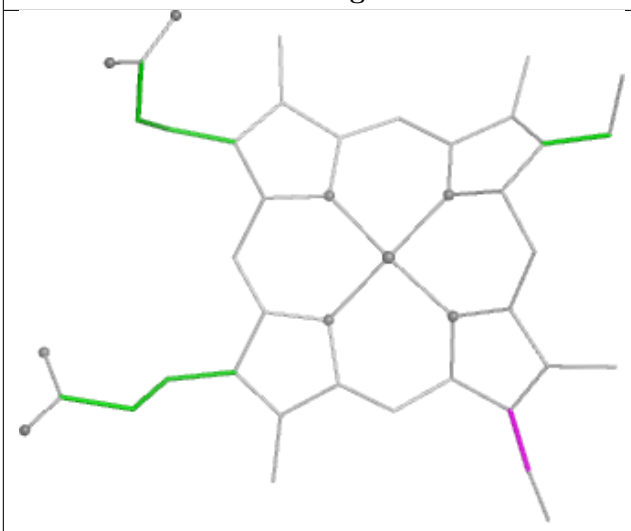

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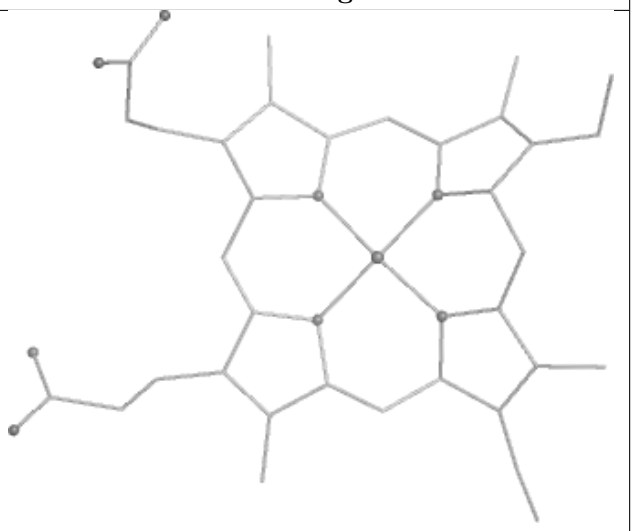
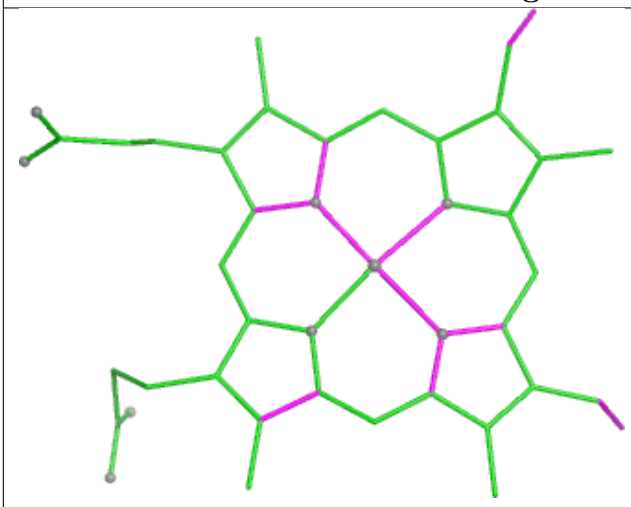


Rings

Ligand HEC O 601



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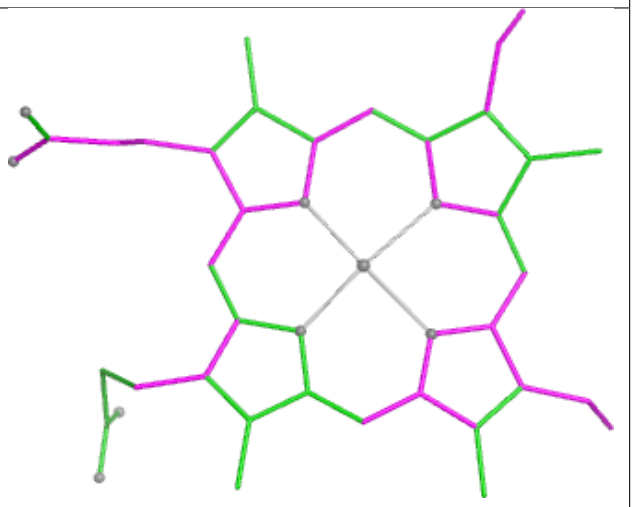

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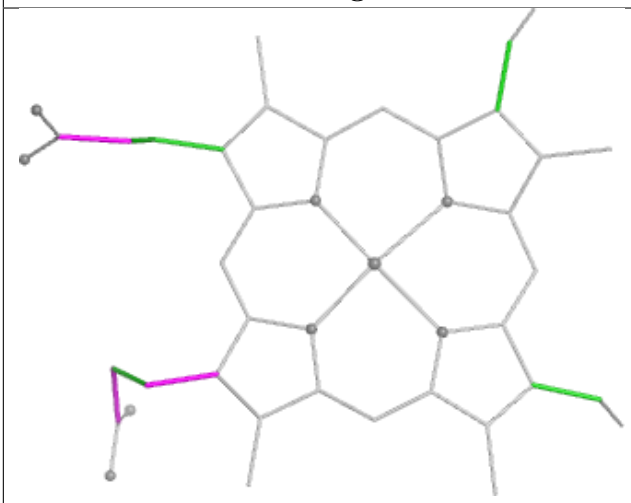

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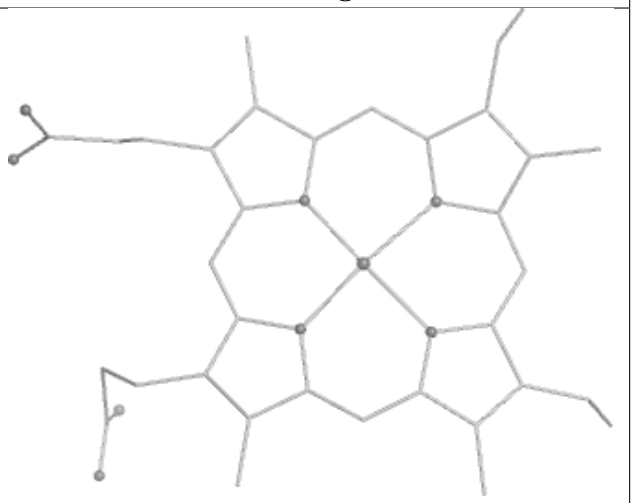
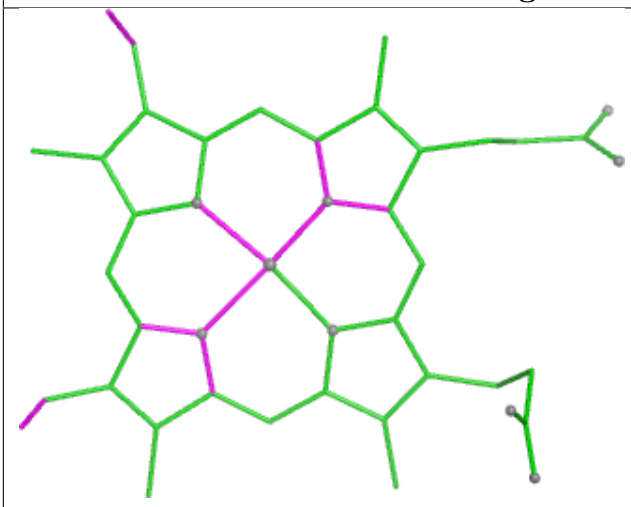


Rings

Ligand HEC M 601



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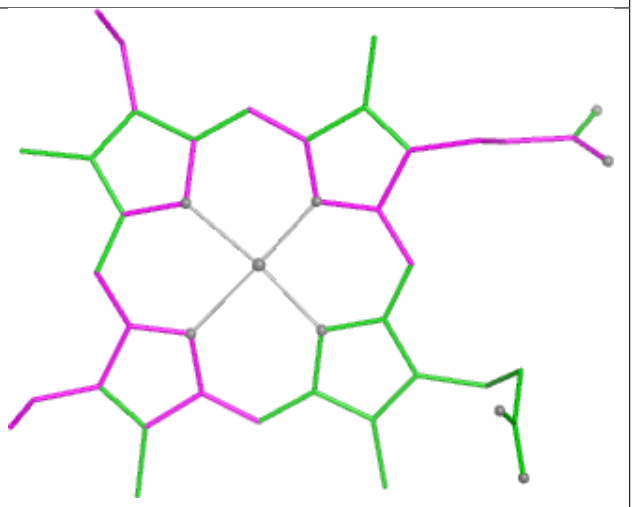

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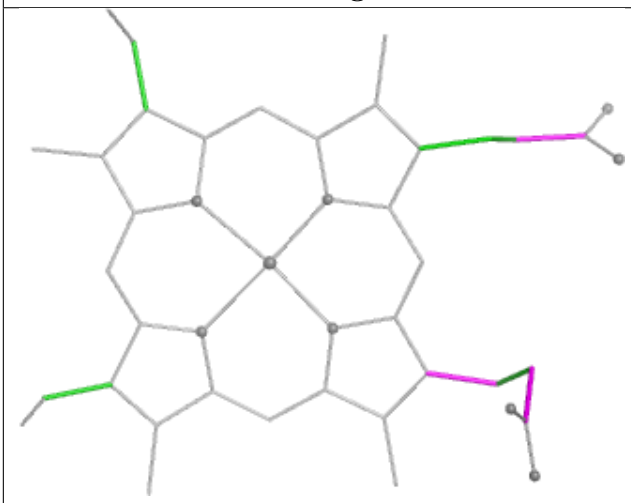

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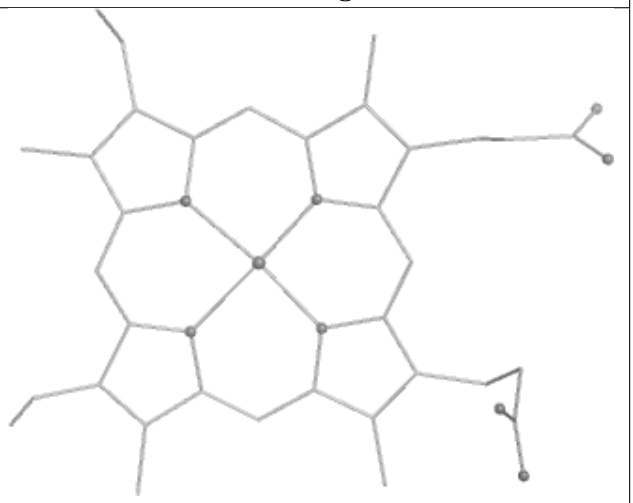
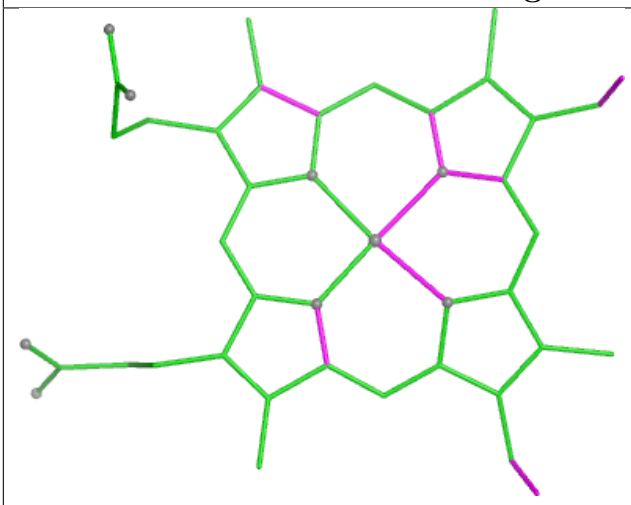


Rings

Ligand HEC E 601



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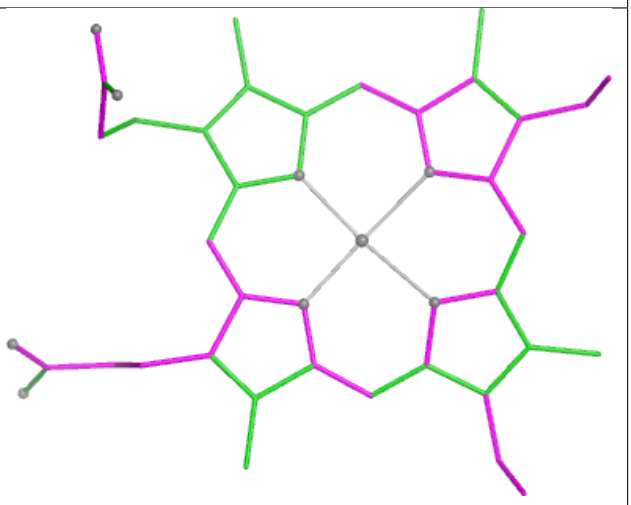

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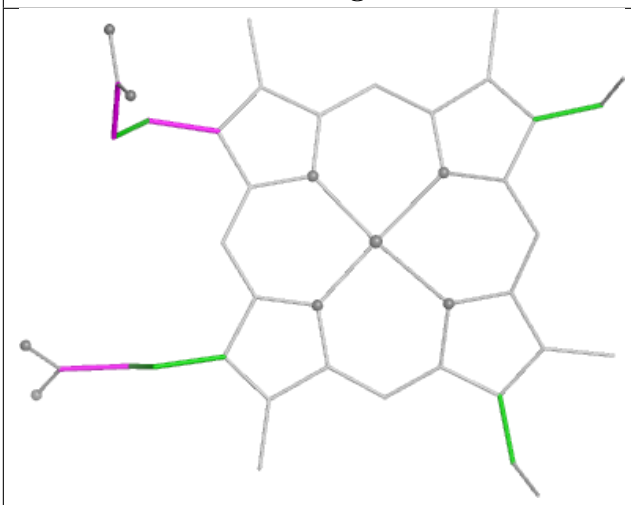

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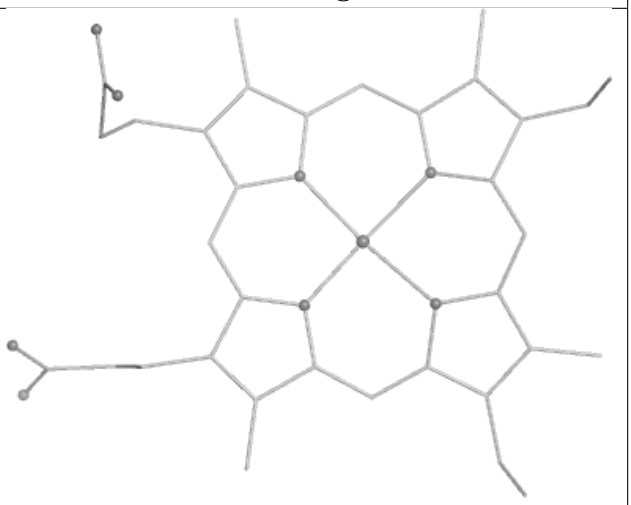
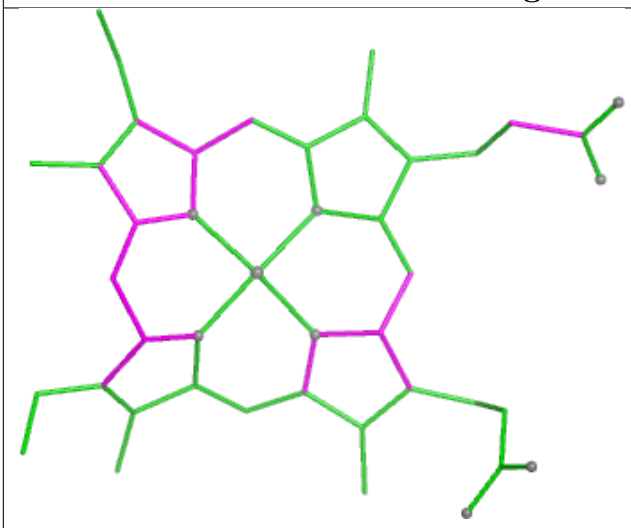


Rings

Ligand HEC T 603



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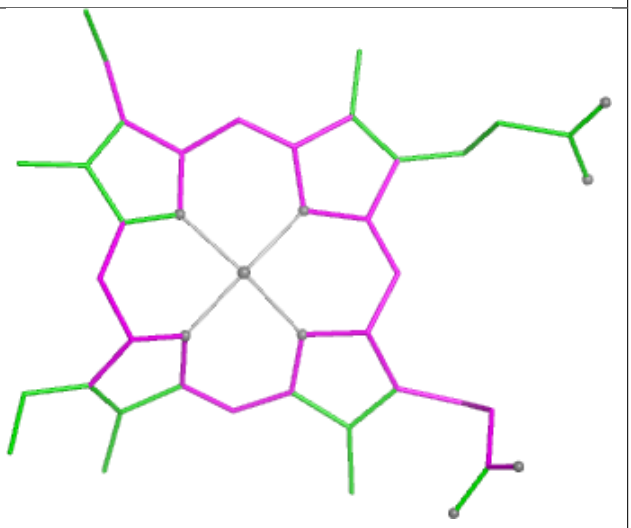

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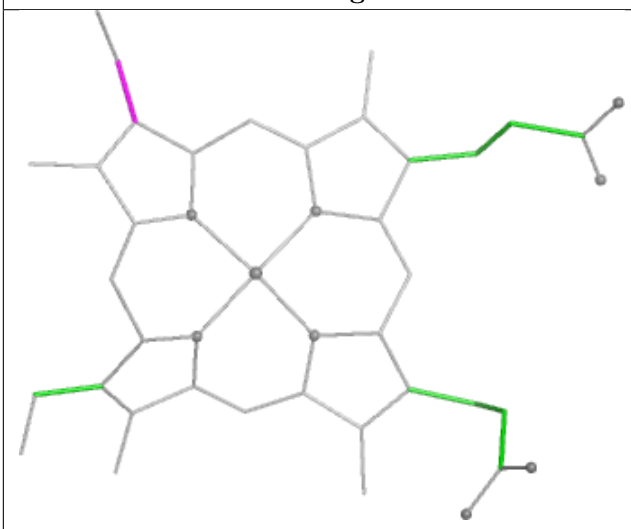

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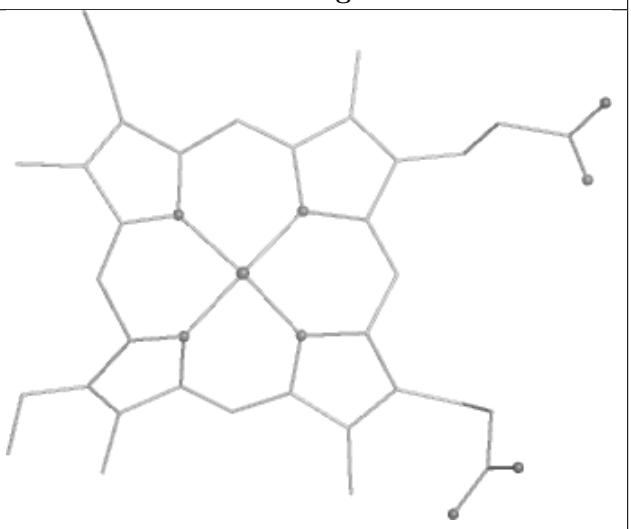
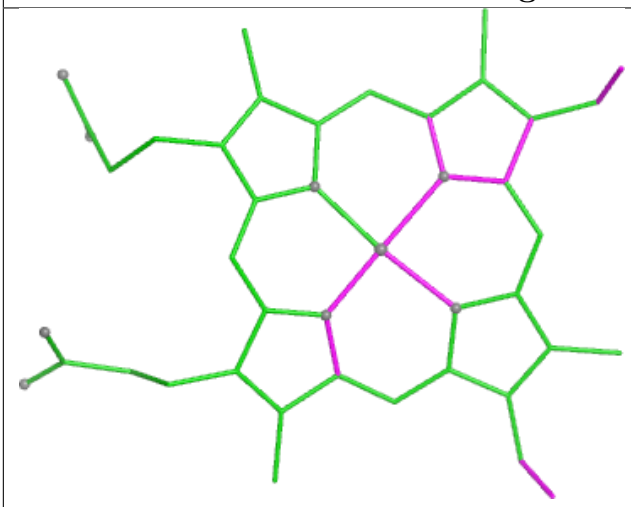


Rings

Ligand HEC M 607



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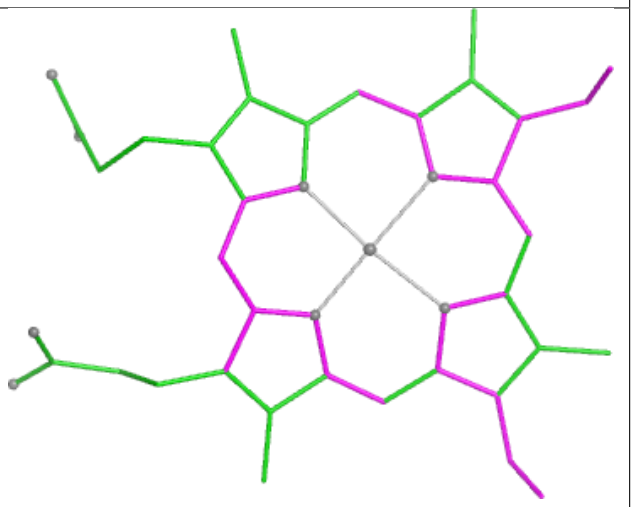

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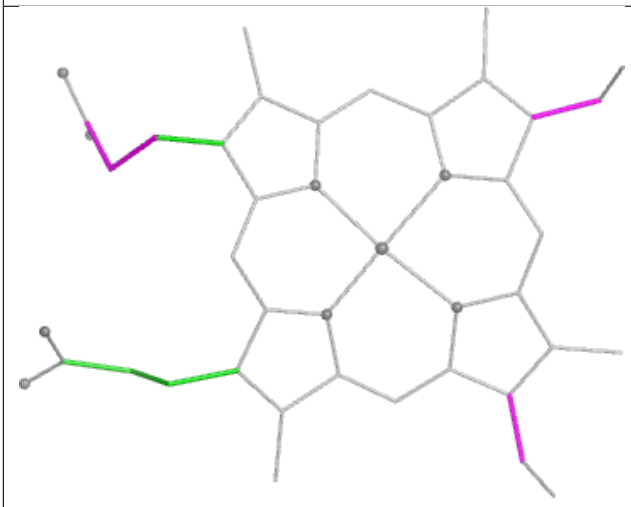

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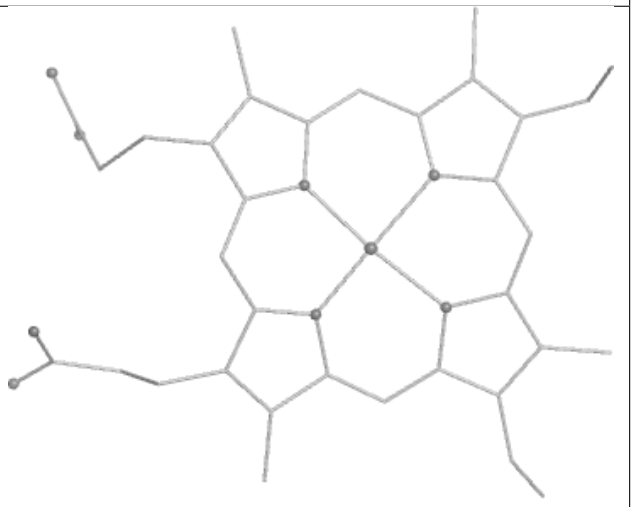
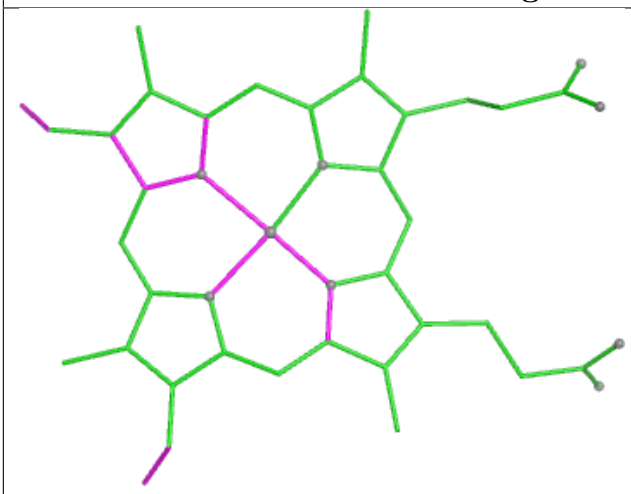


Rings

Ligand HEC H 605



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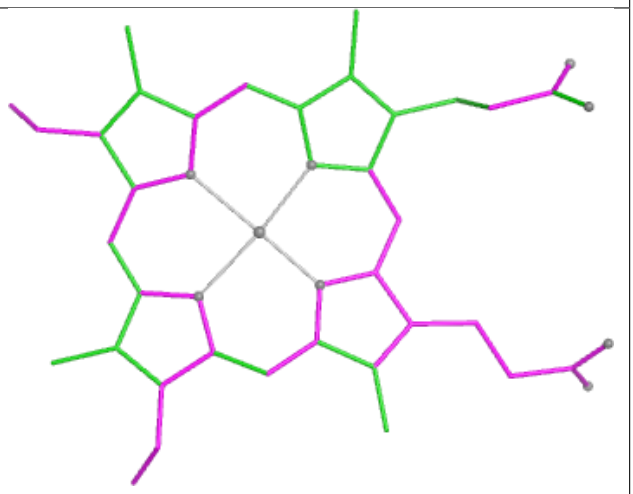
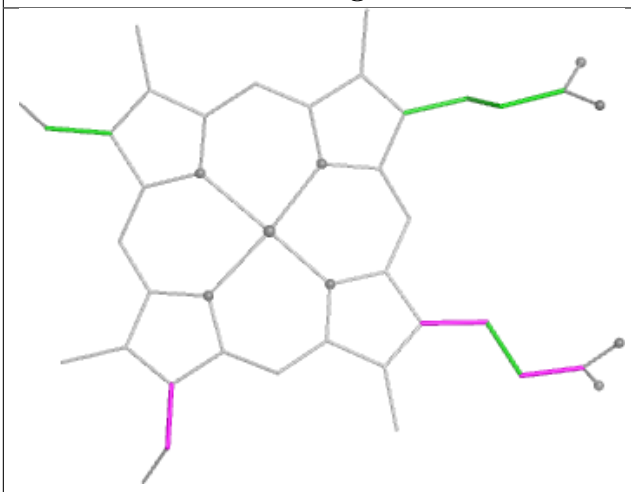


Bond angles



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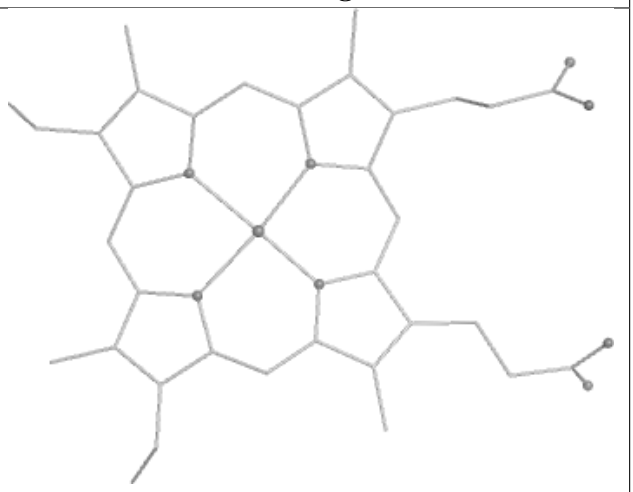
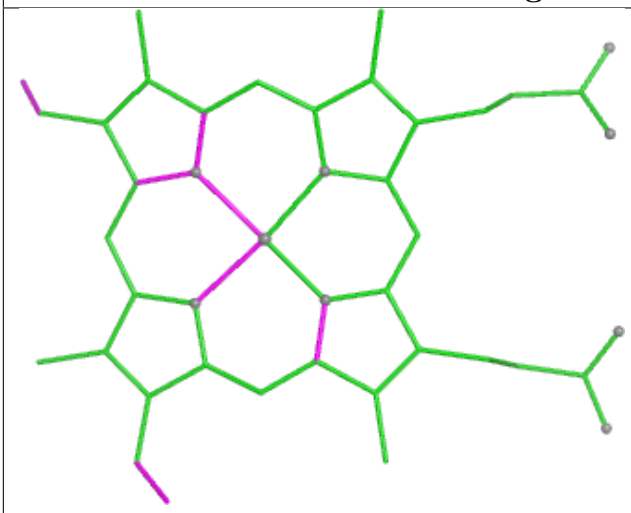


Rings

Ligand HEC L 600



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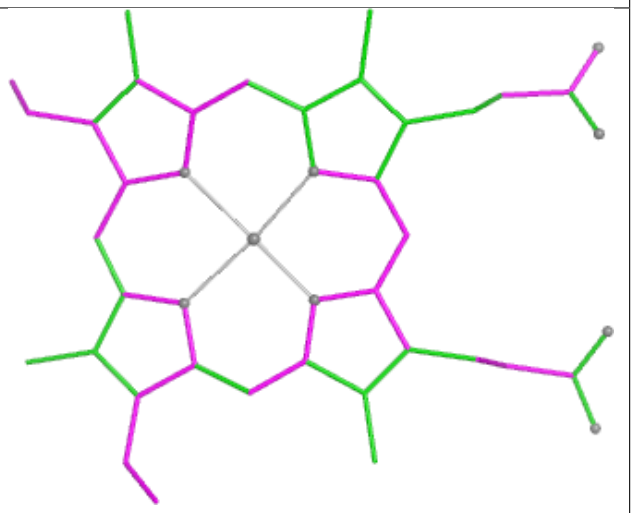
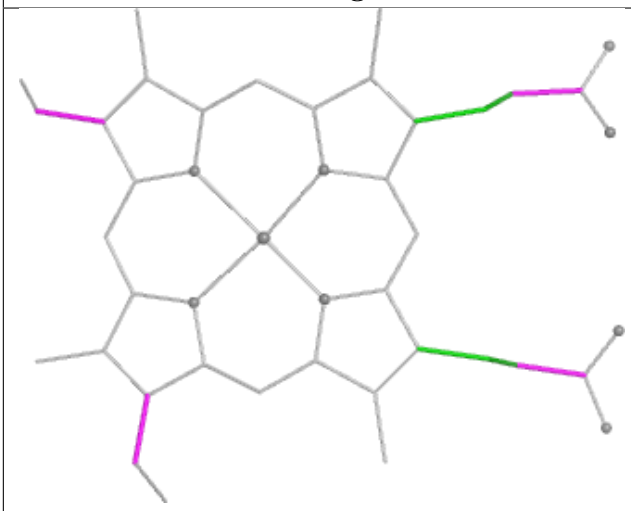


Bond angles



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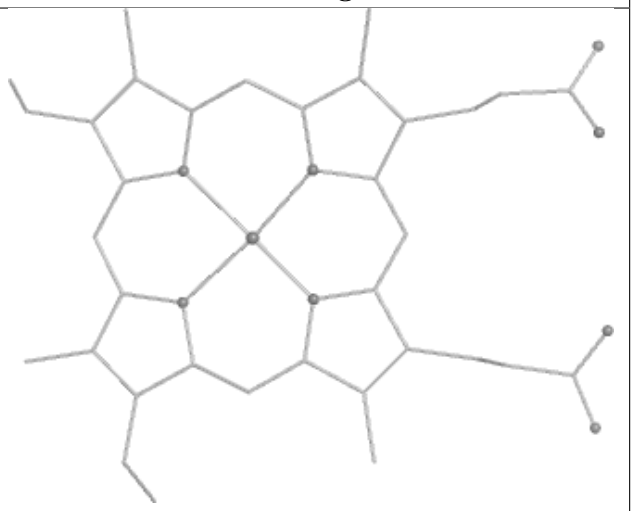
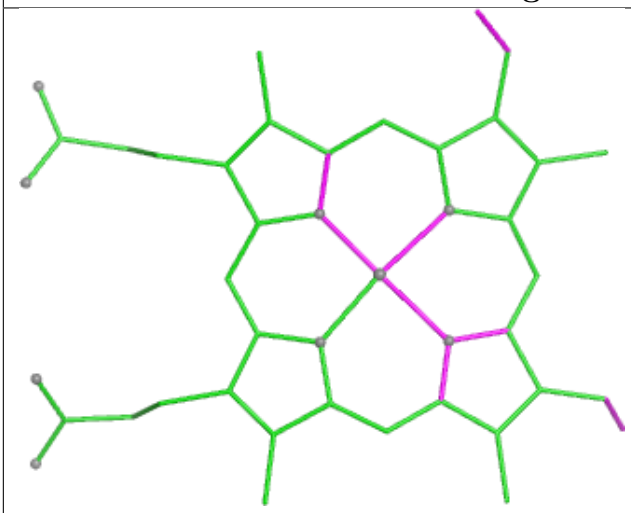


Rings

Ligand HEC C 600



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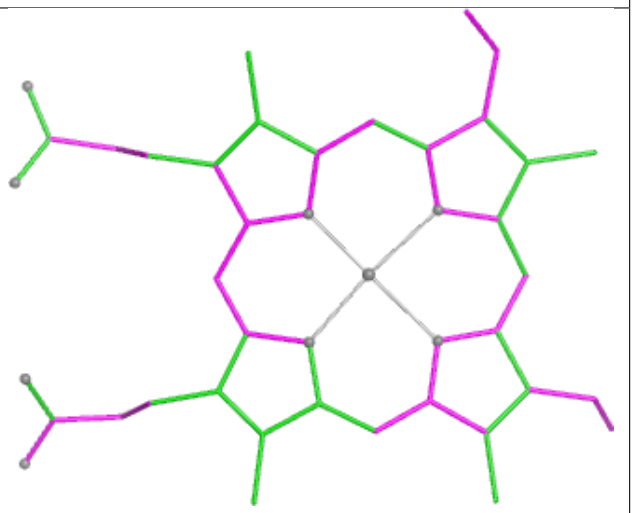
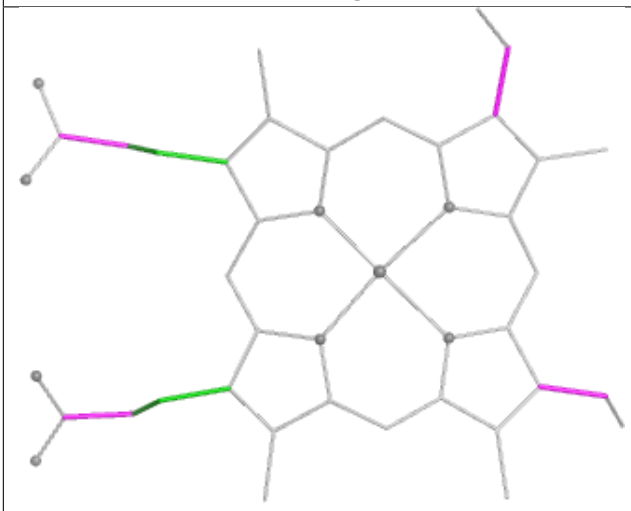
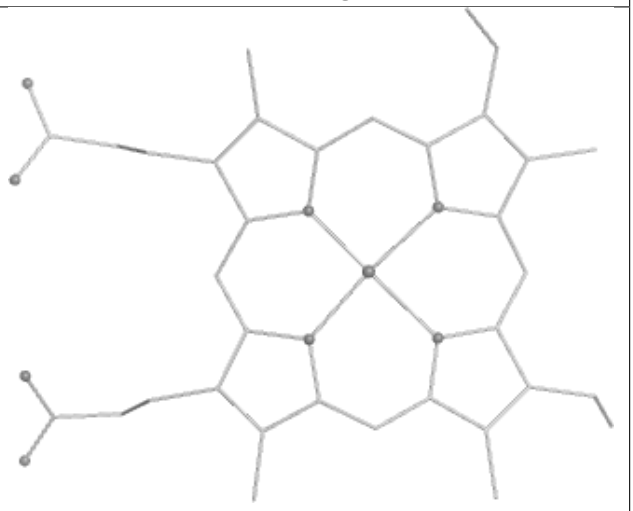


Bond angles

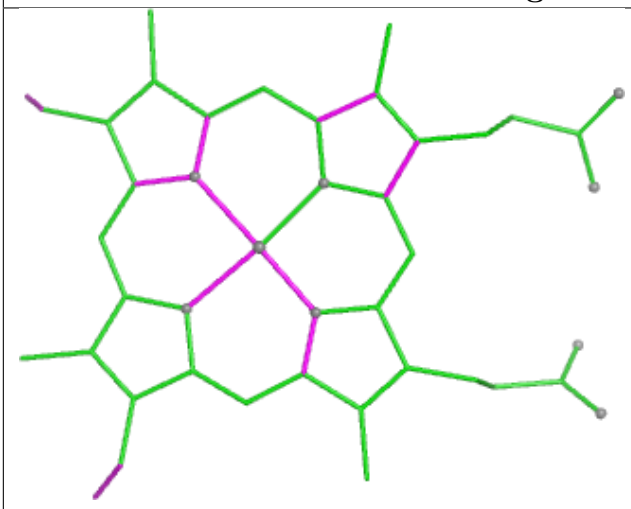


Torsions



Rings

Ligand HEC J 604



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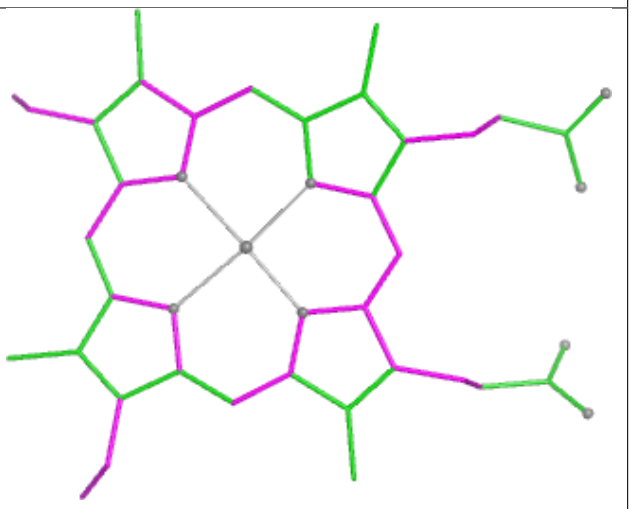

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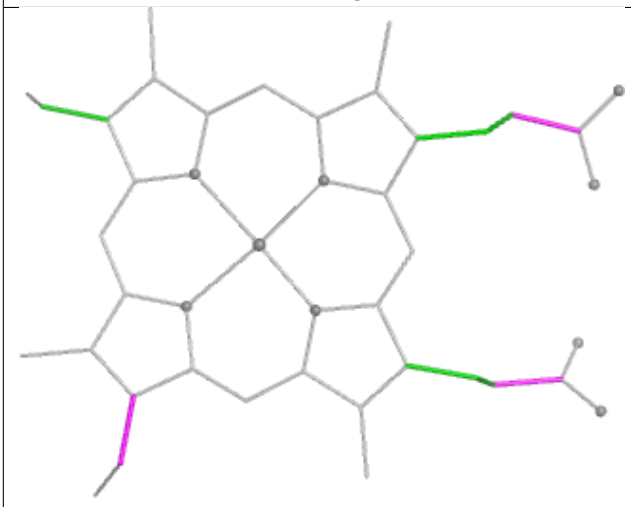

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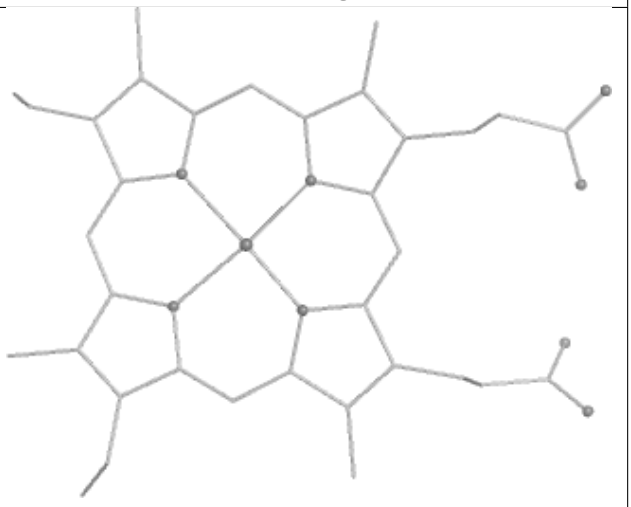
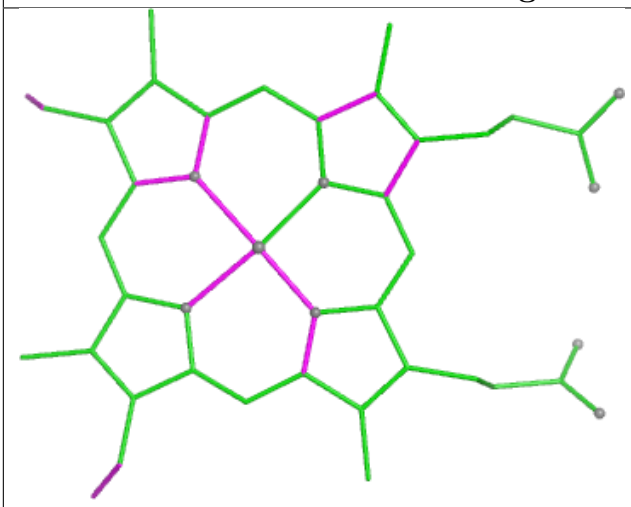


Rings

Ligand HEC M 604



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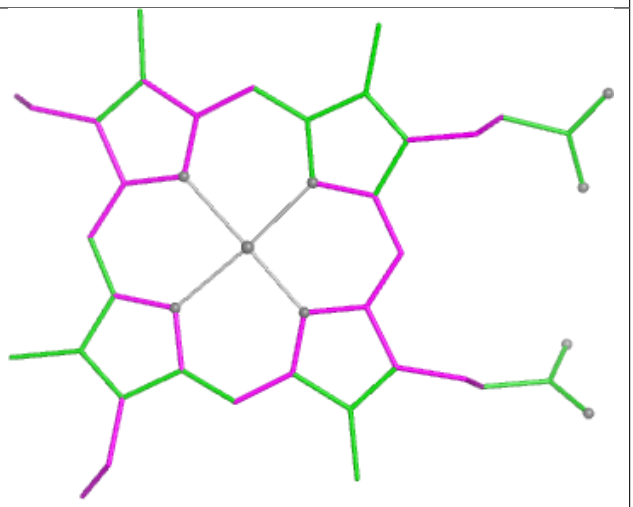

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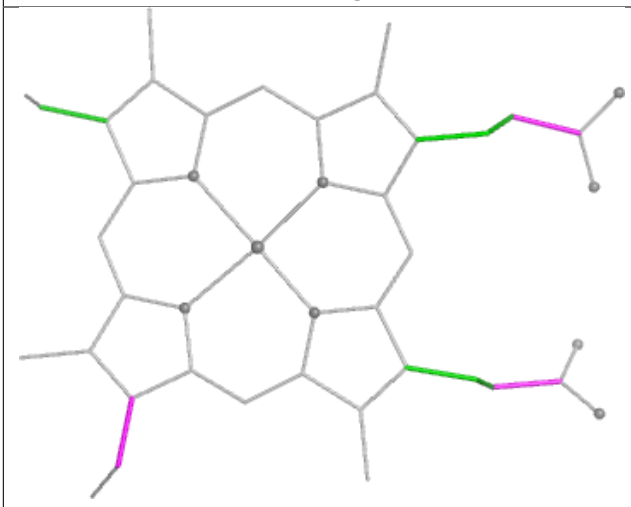

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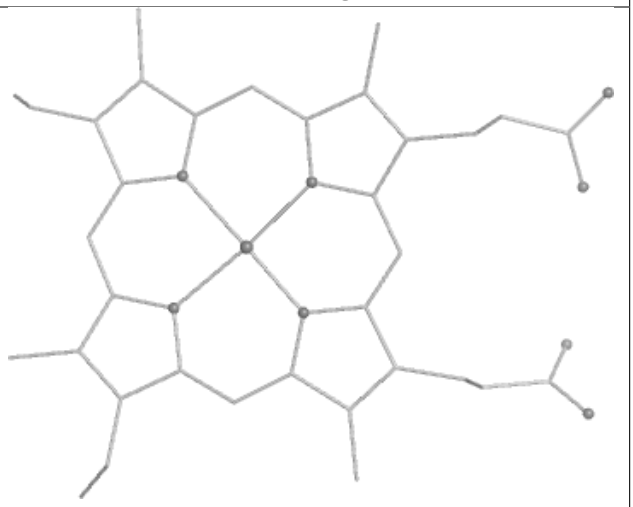
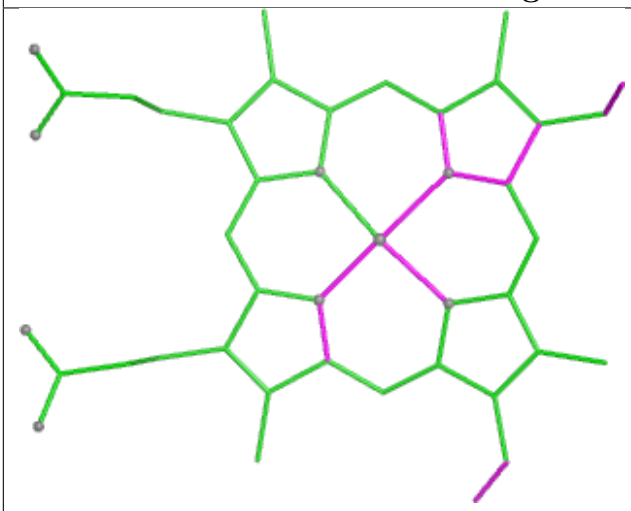


Rings

Ligand HEC O 600



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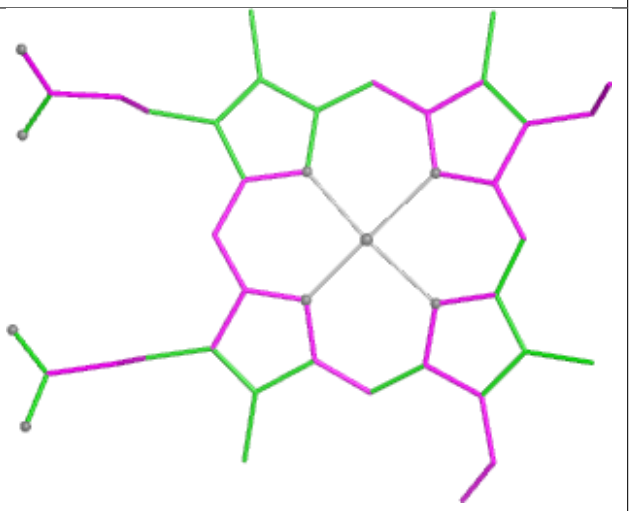

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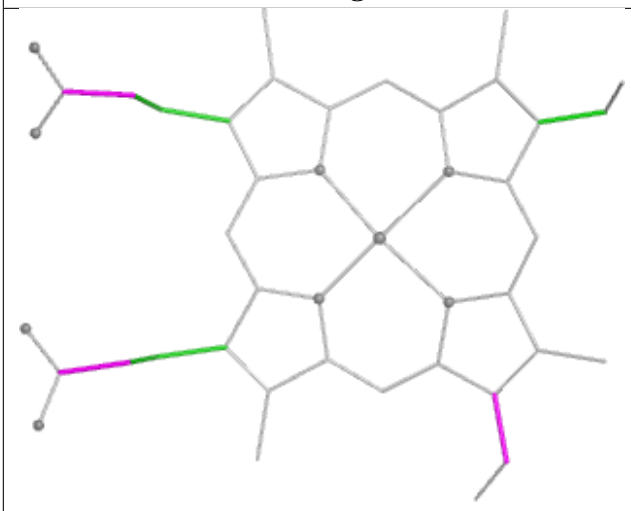

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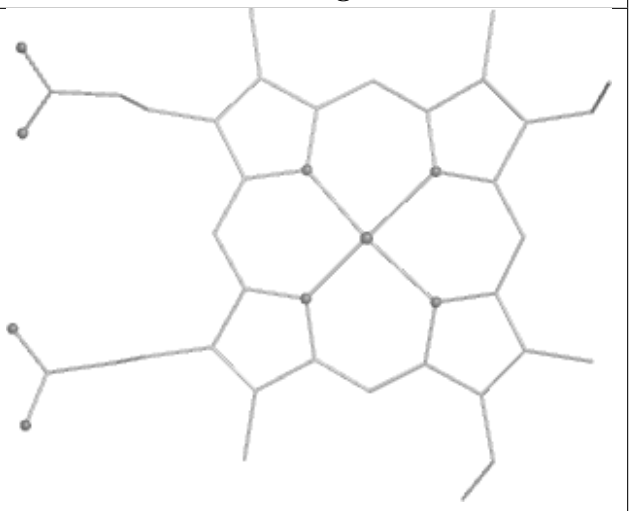

Rings

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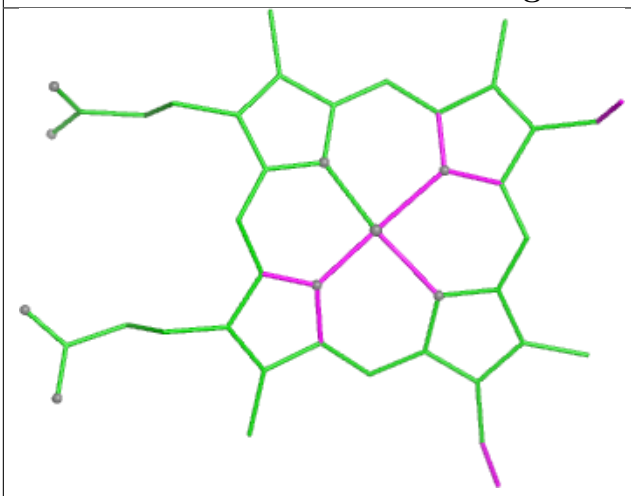

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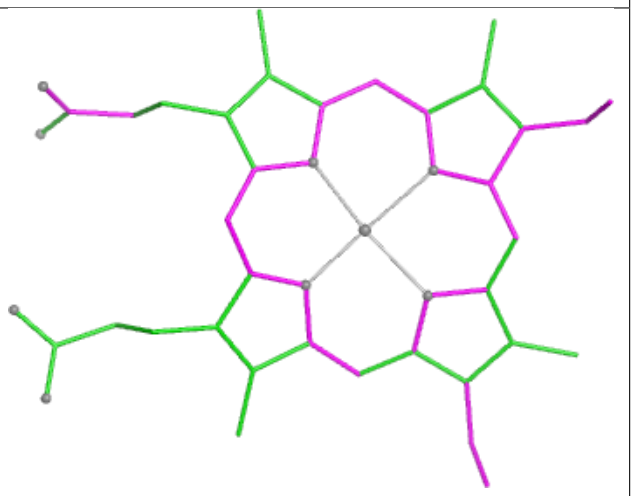

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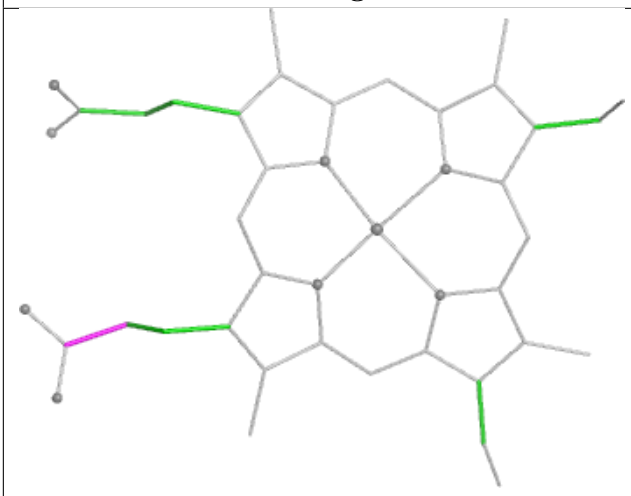

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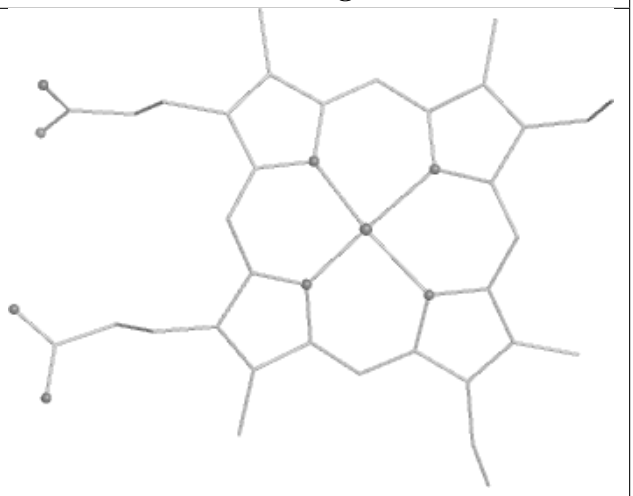
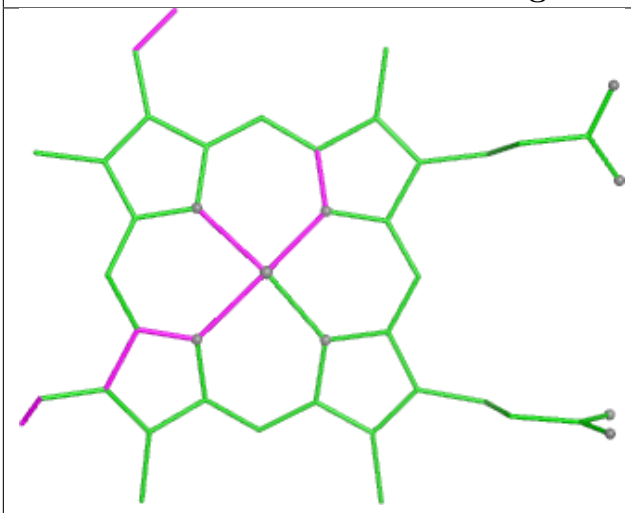


Rings

Ligand HEC I 600



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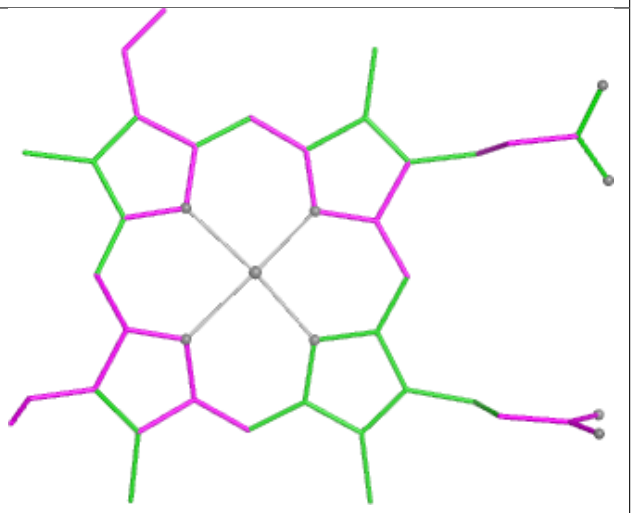

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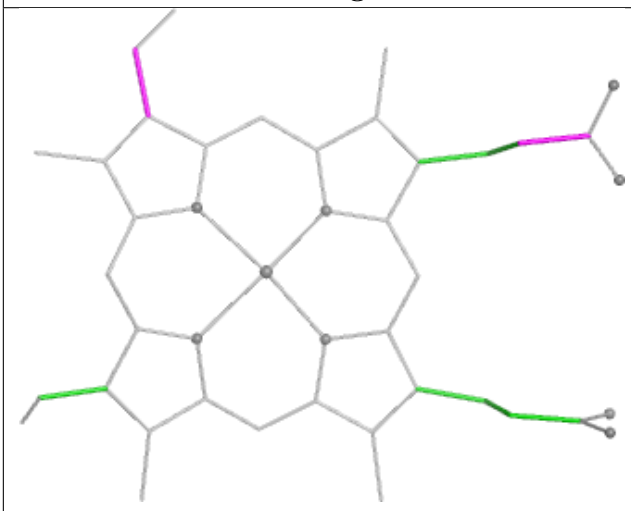

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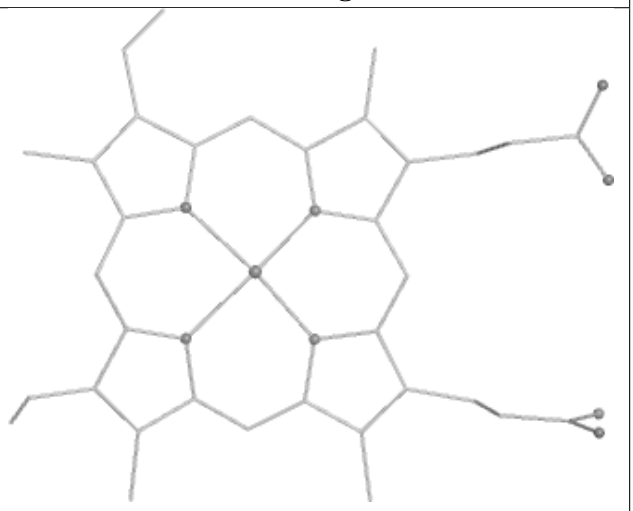

Rings

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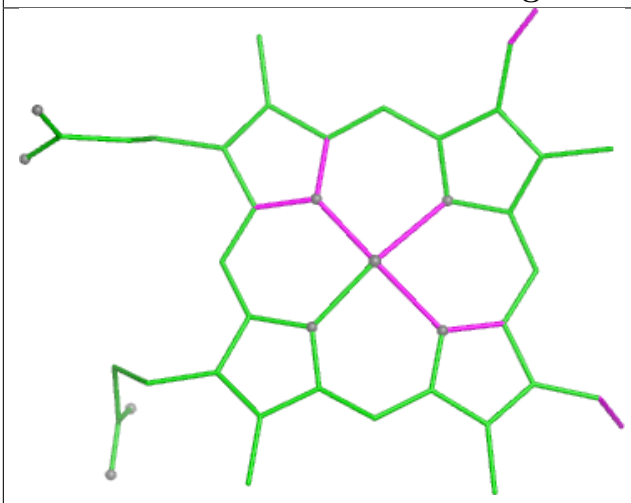

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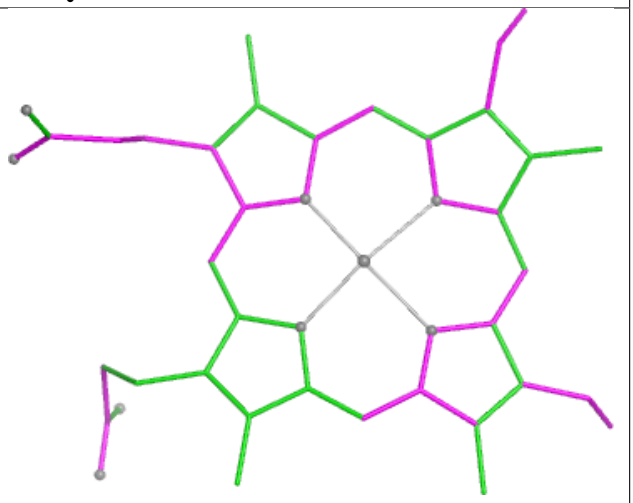

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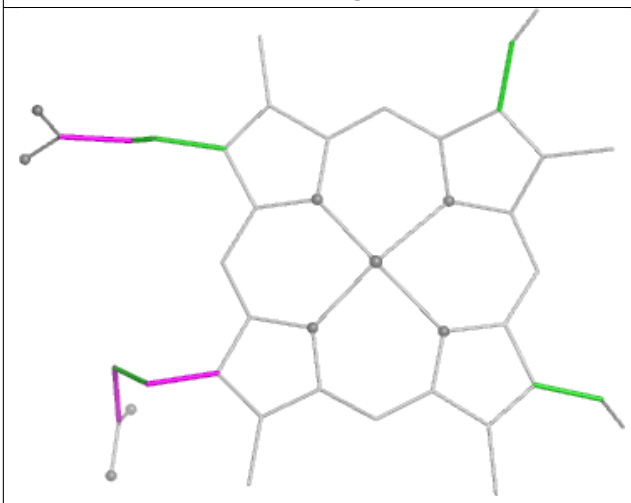

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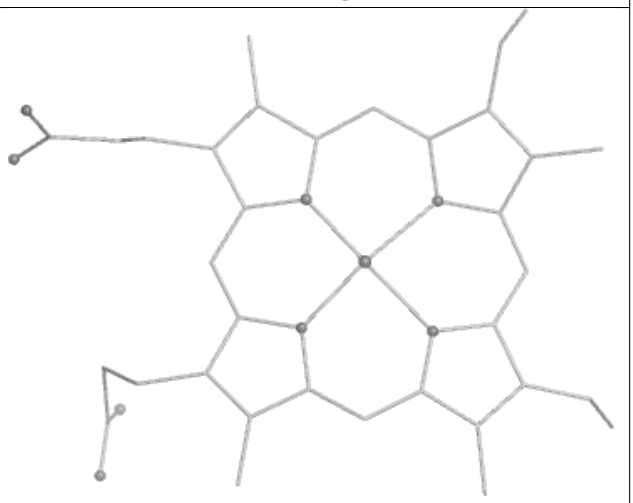

Rings

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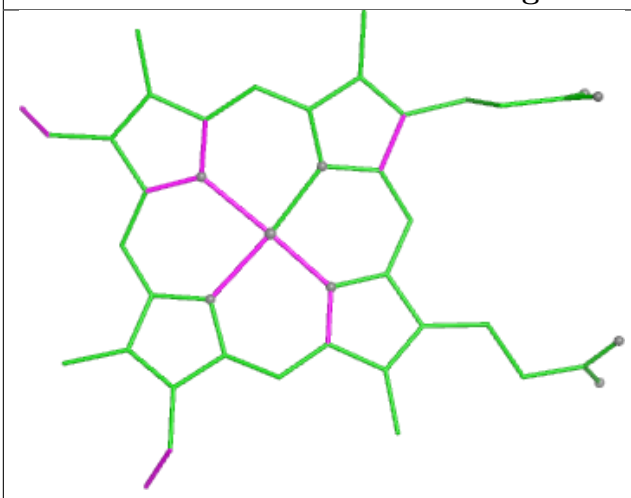

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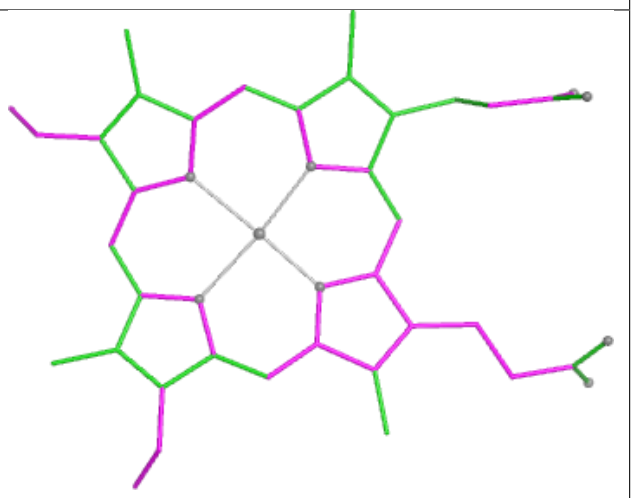

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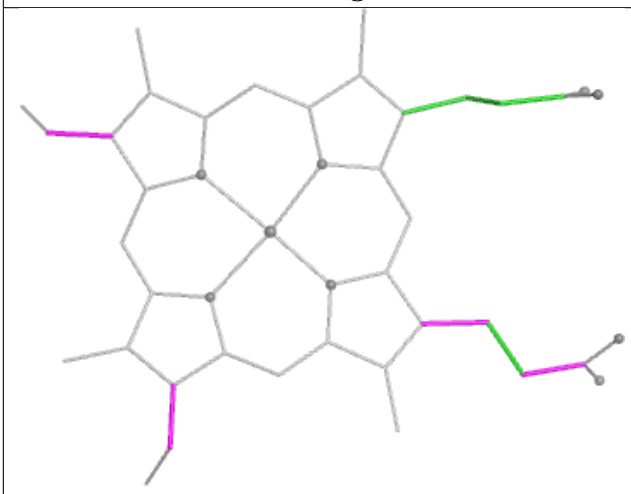

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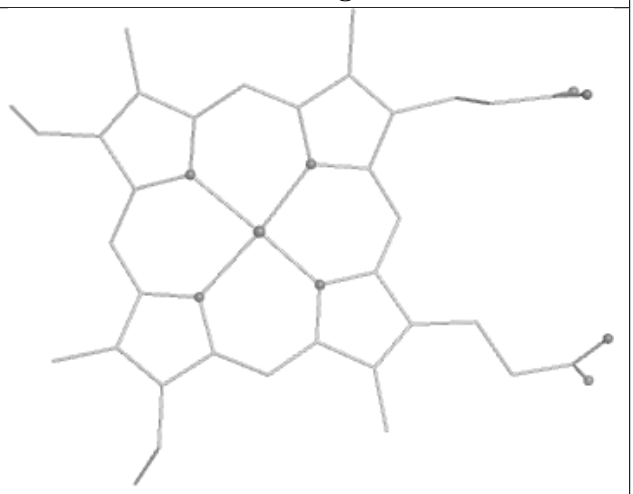
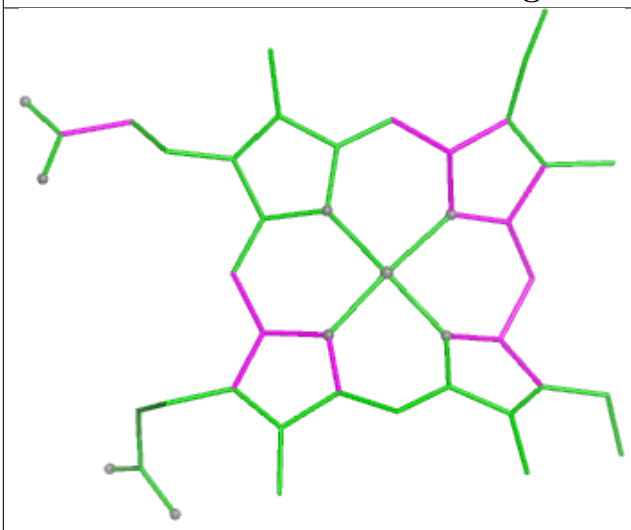


Rings

Ligand HEC B 603



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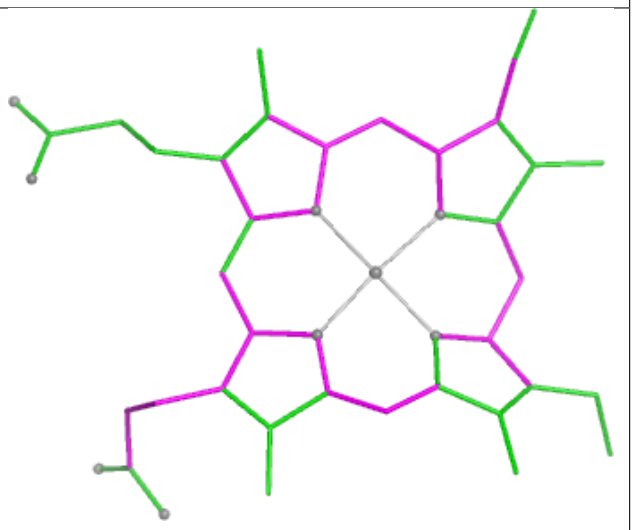

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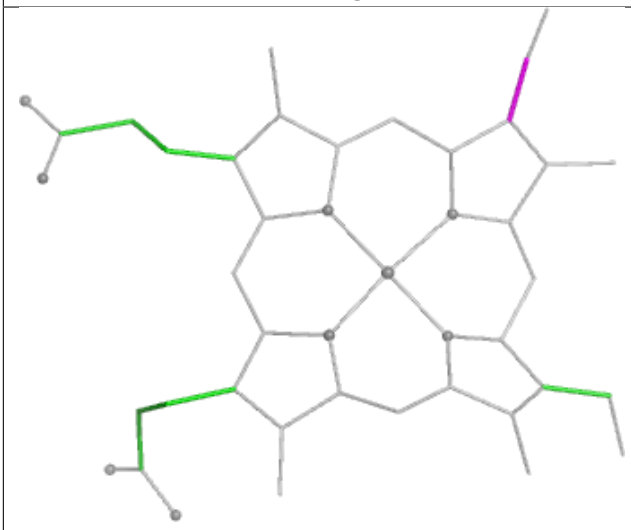

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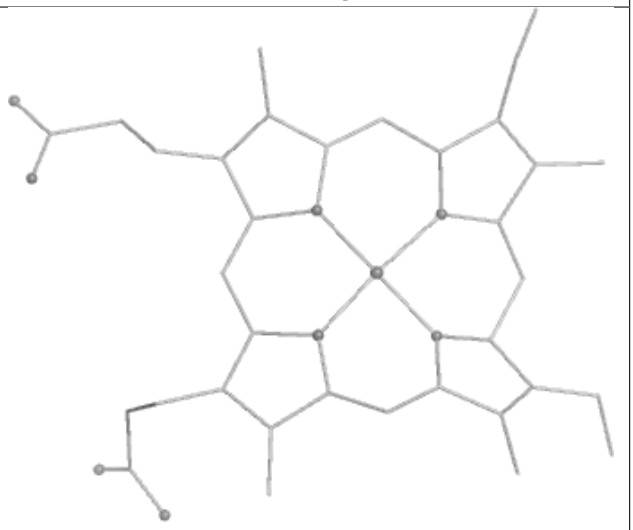
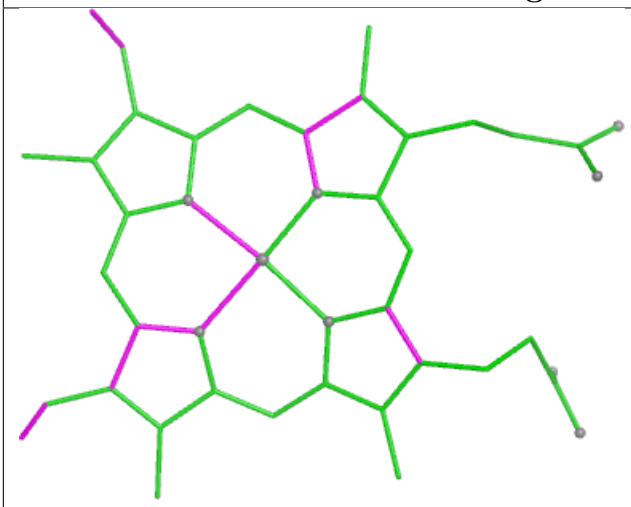


Rings

Ligand HEC S 607



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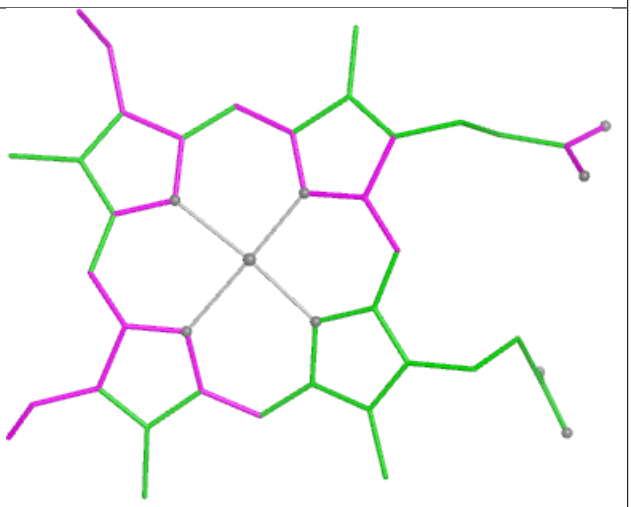

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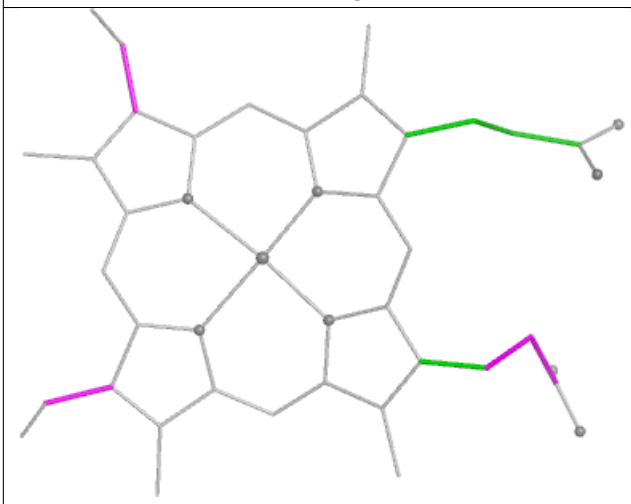

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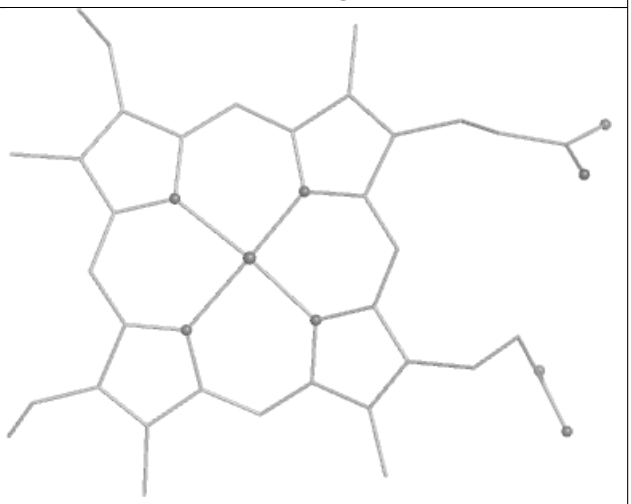

Rings

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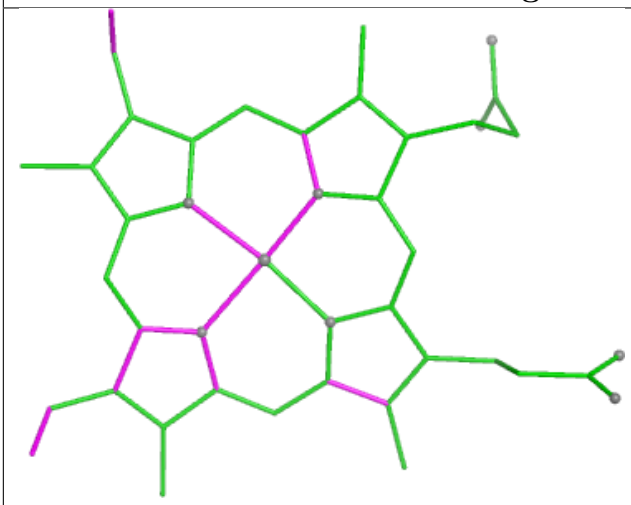

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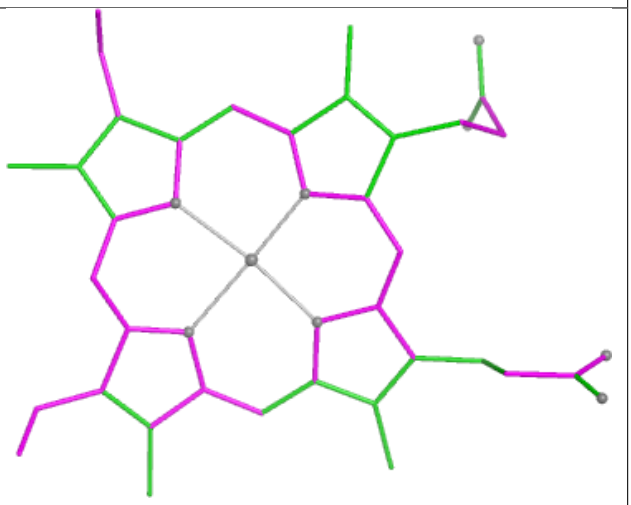

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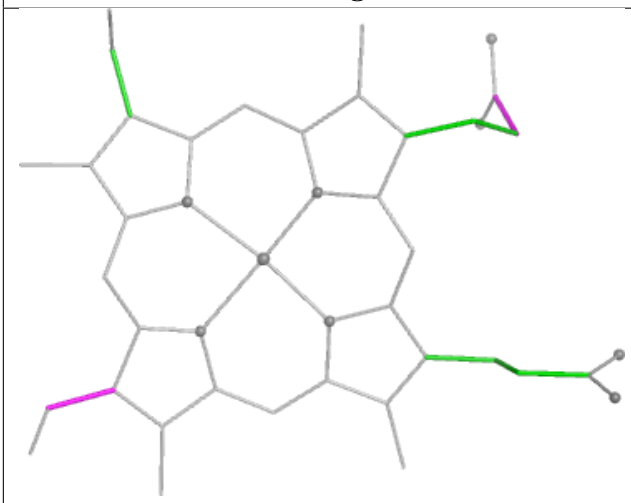

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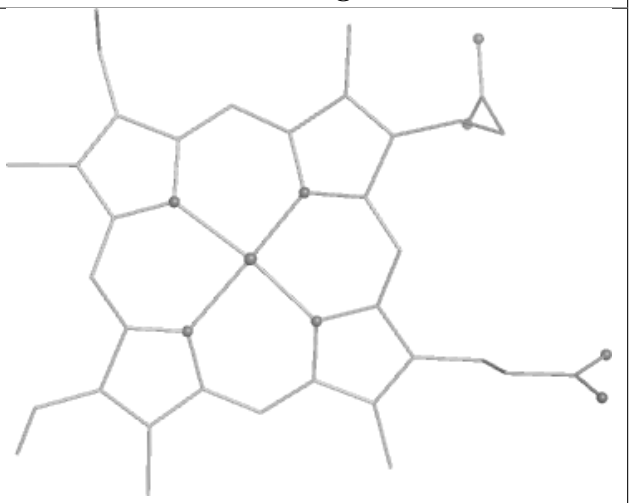
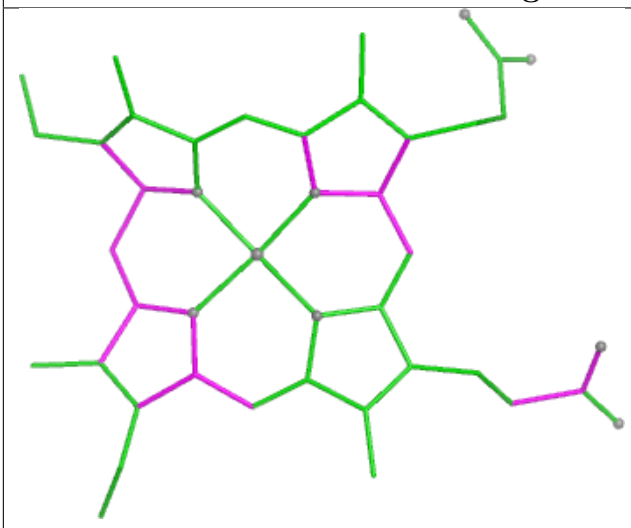


Rings

Ligand HEC R 603



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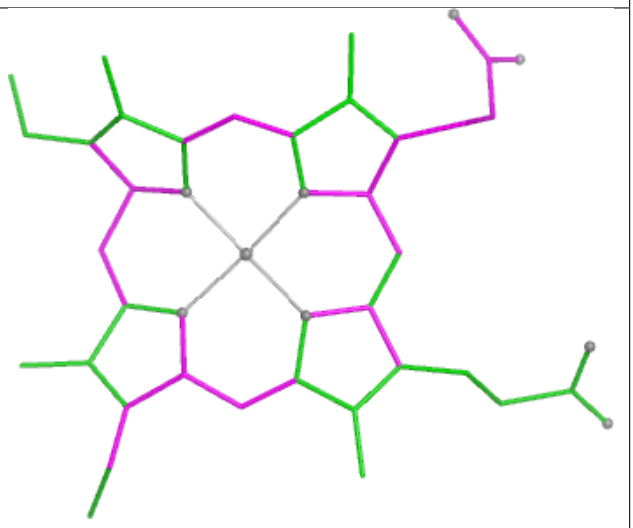

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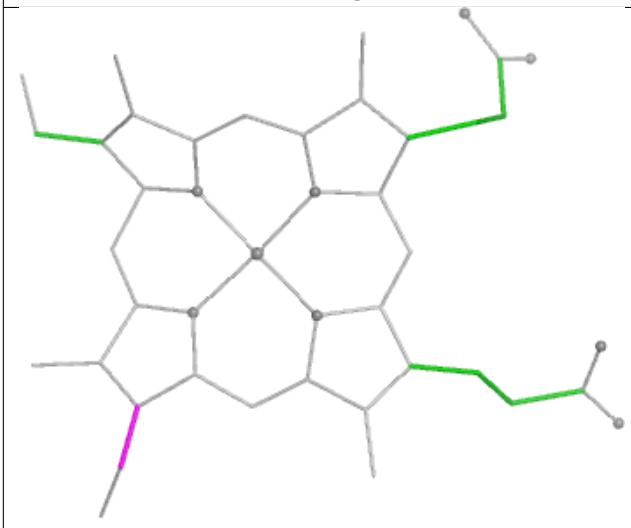

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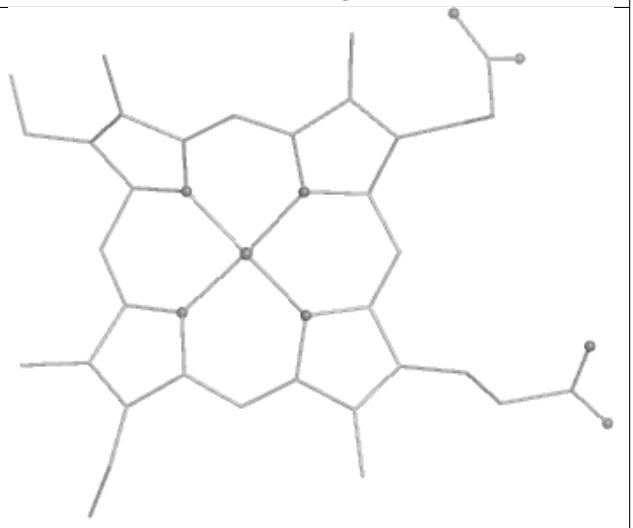

Rings

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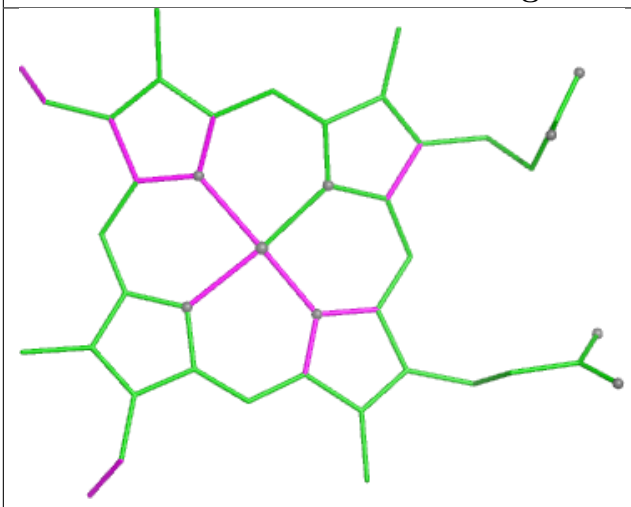

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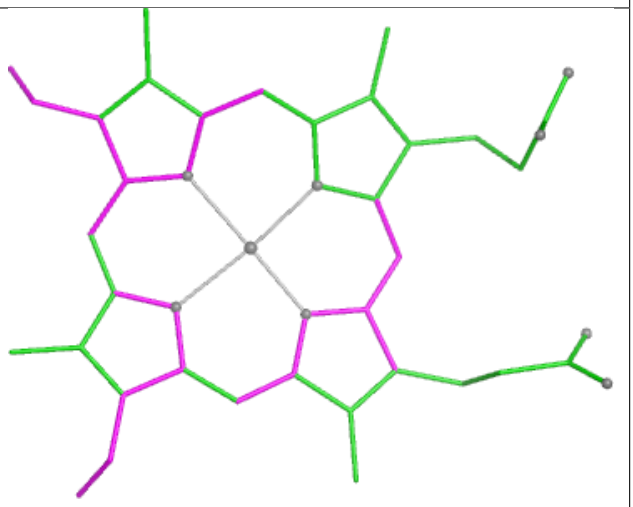

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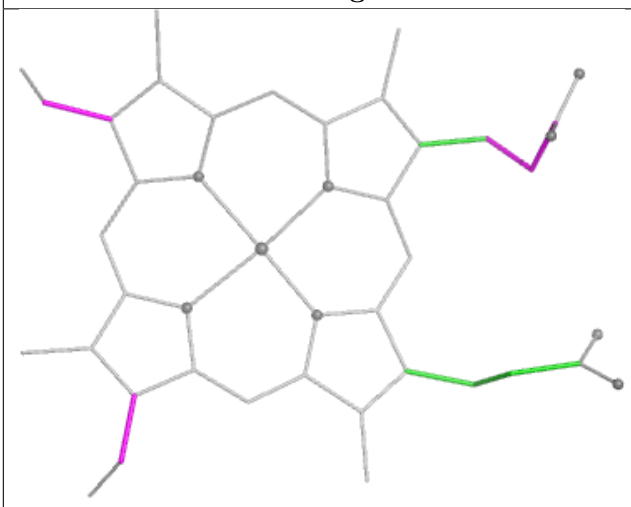

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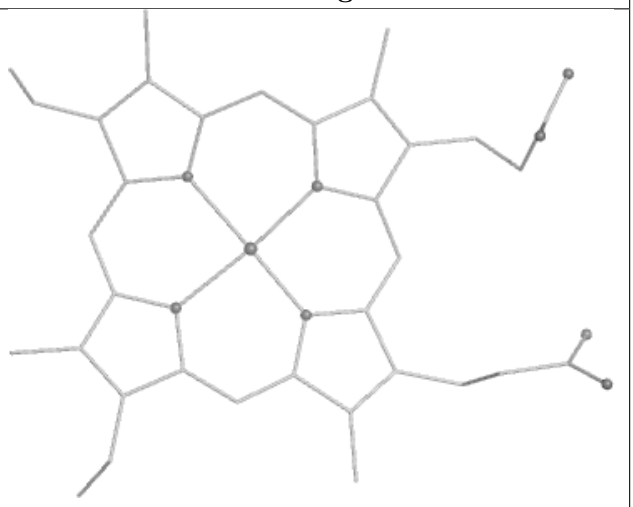
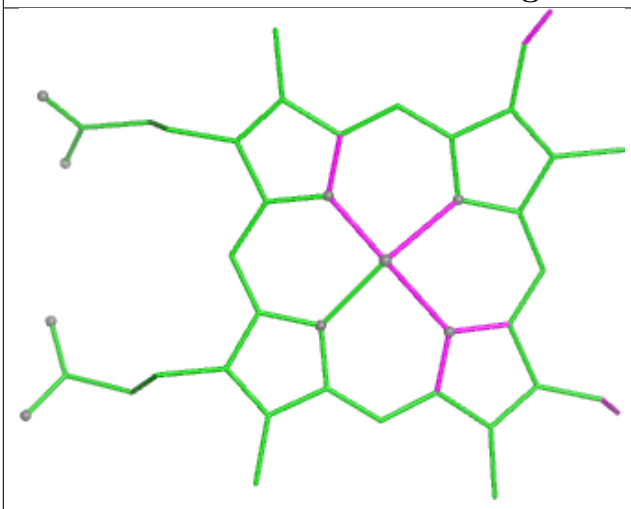


Rings

Ligand HEC G 604



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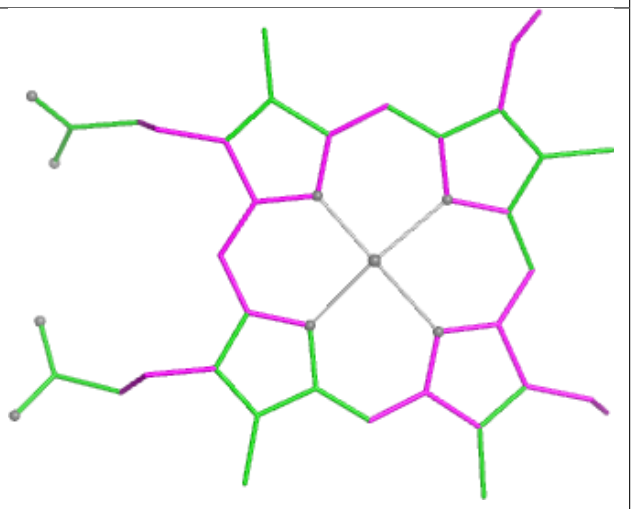

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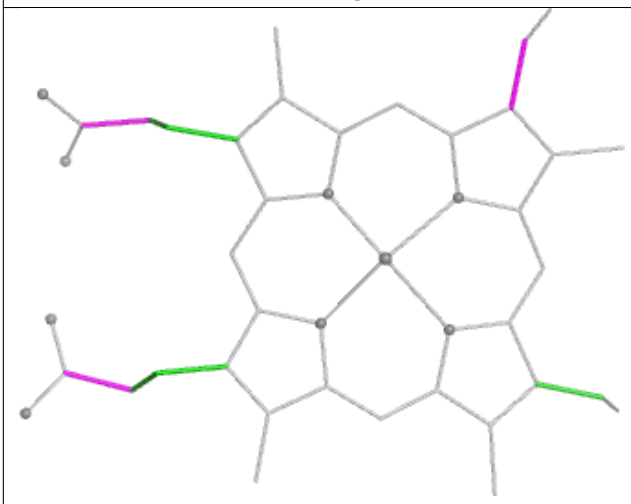

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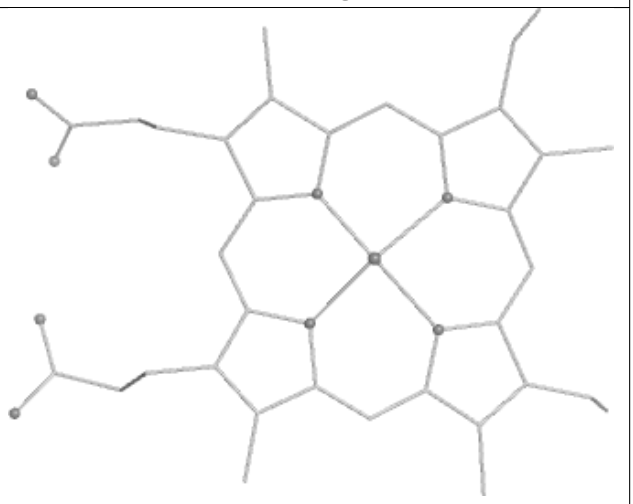
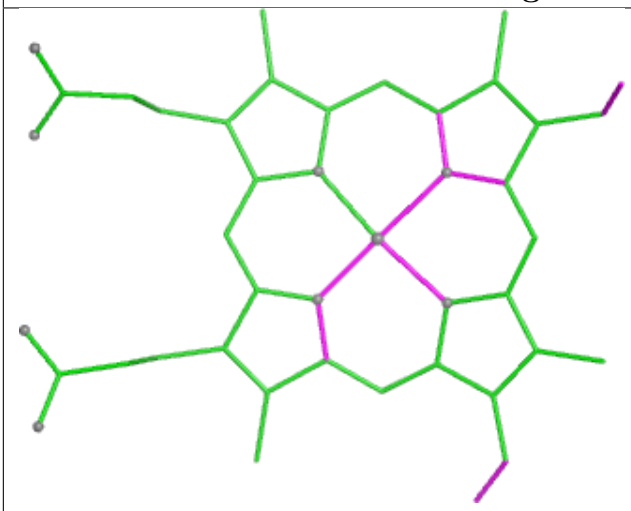


Rings

Ligand HEC V 600



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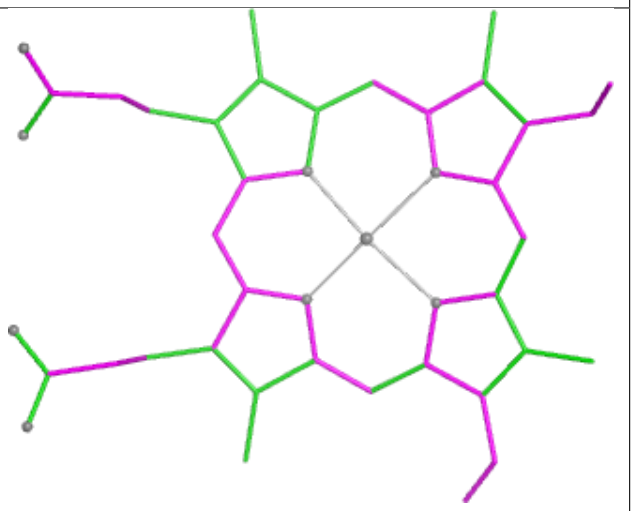
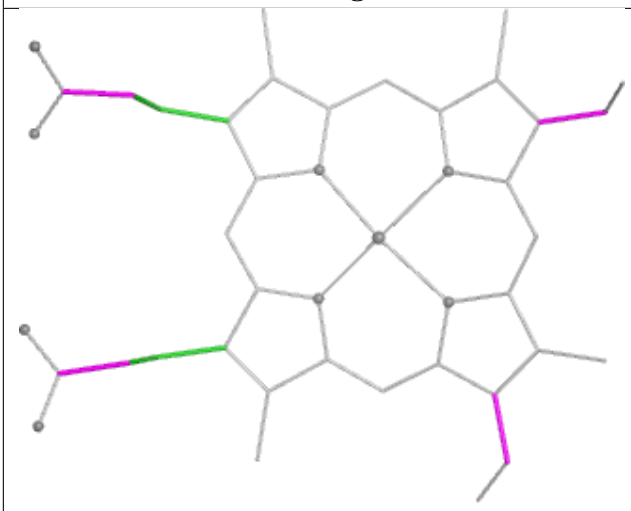


Bond angles



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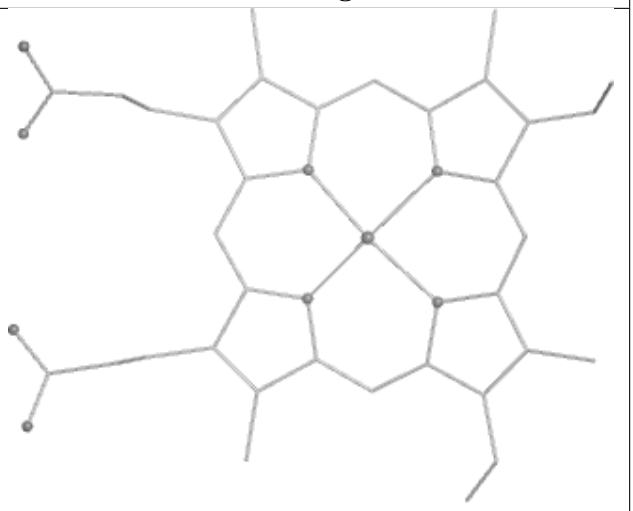
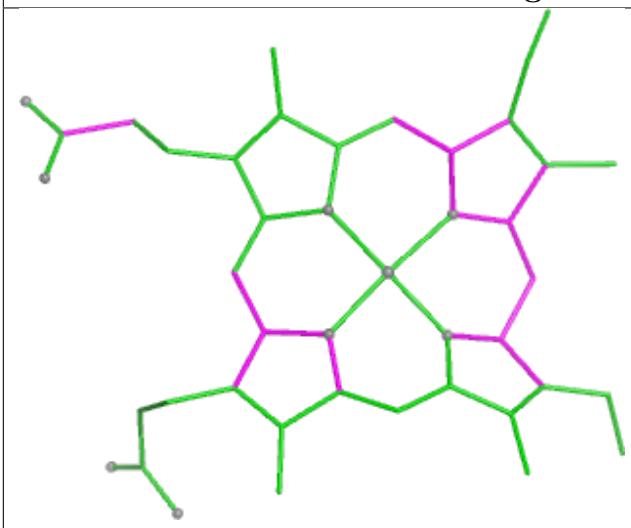
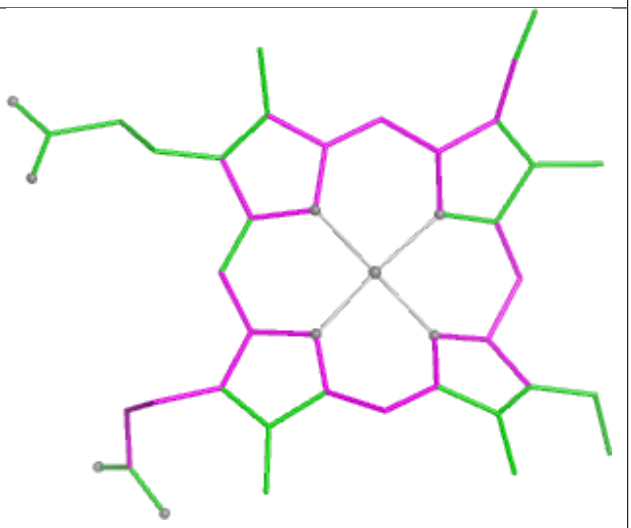


Rings

Ligand HEC F 603



Bond lengths



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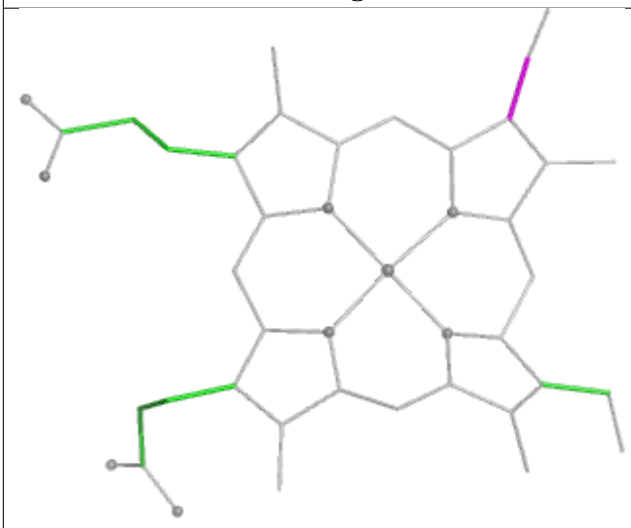

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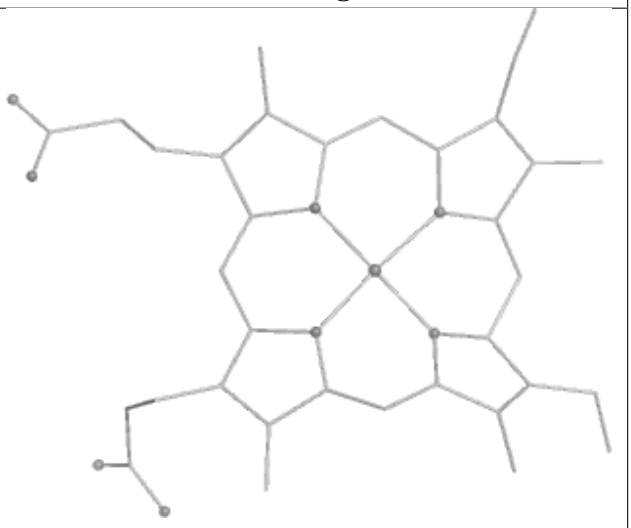
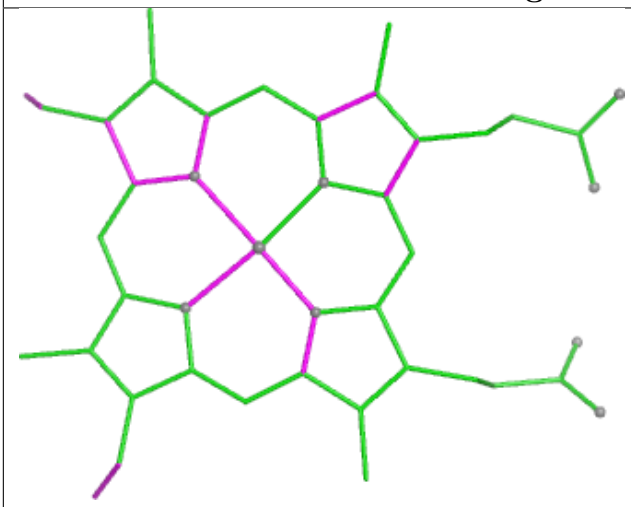


Rings

Ligand HEC S 604



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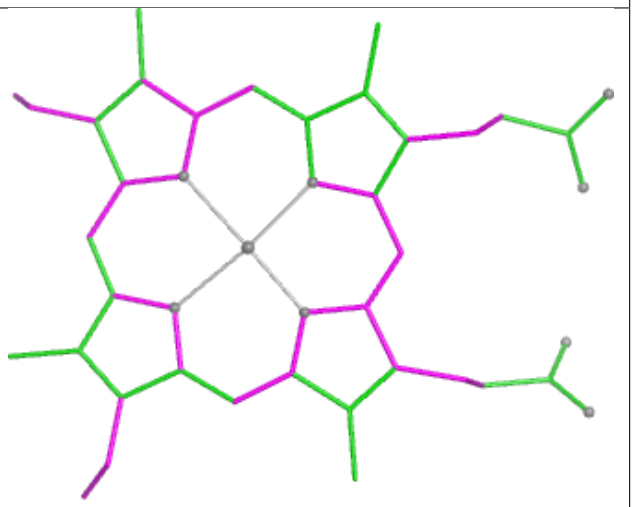

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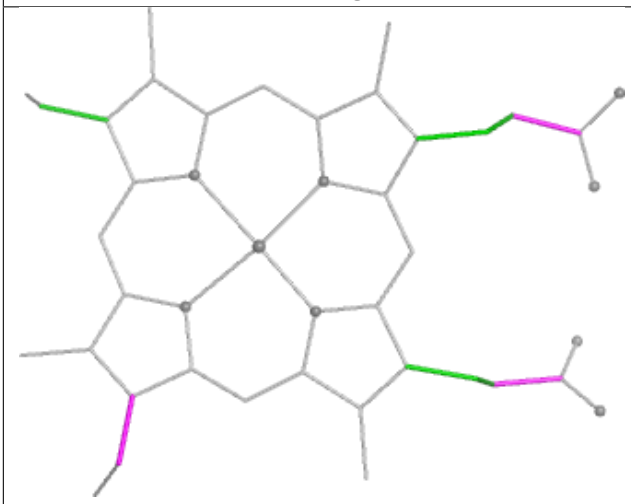

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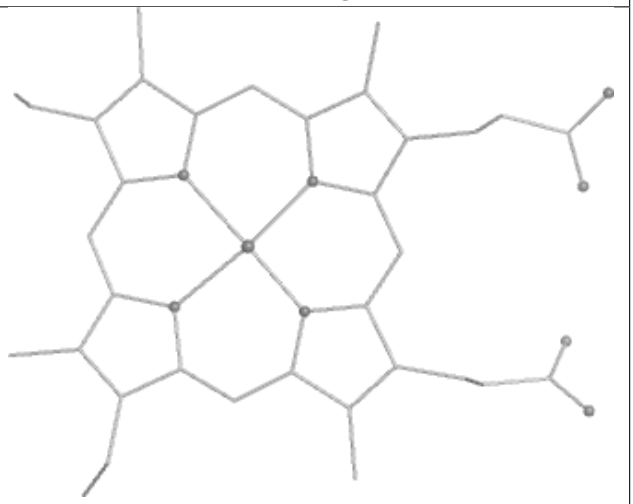
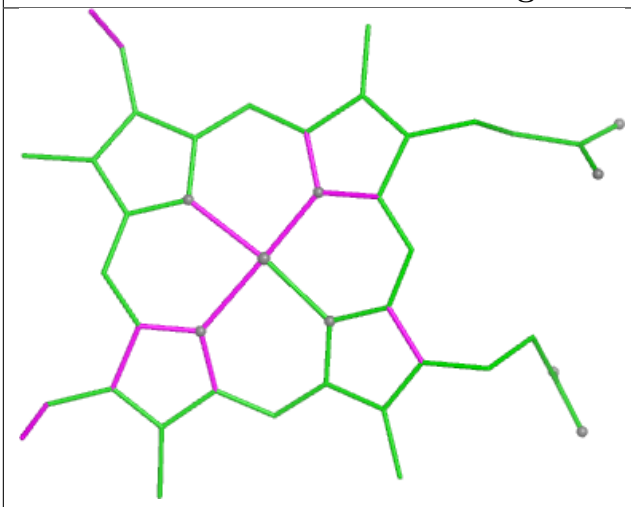


Rings

Ligand HEC W 607



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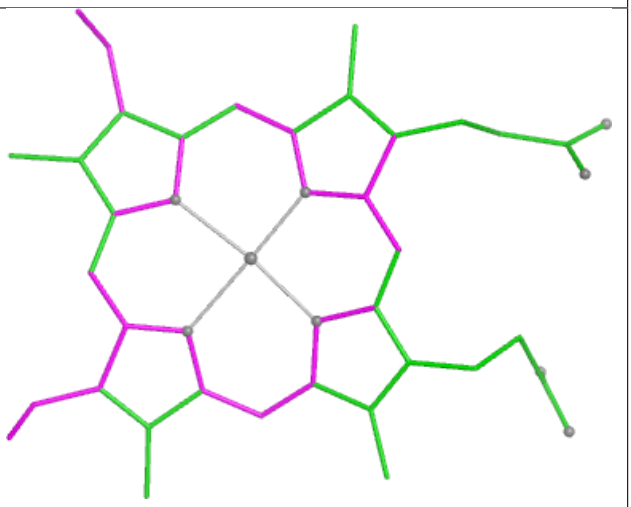

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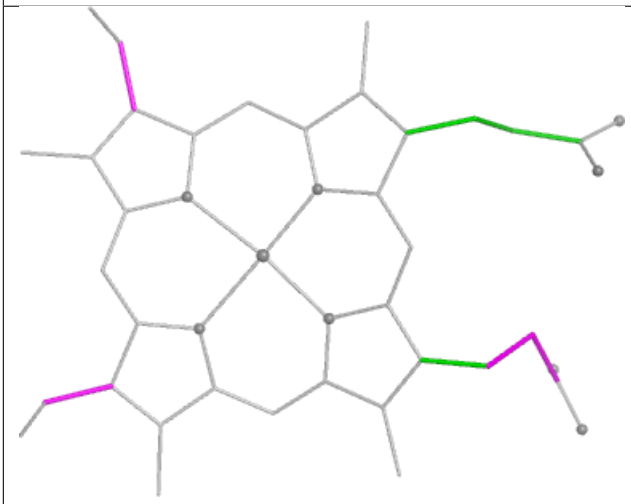

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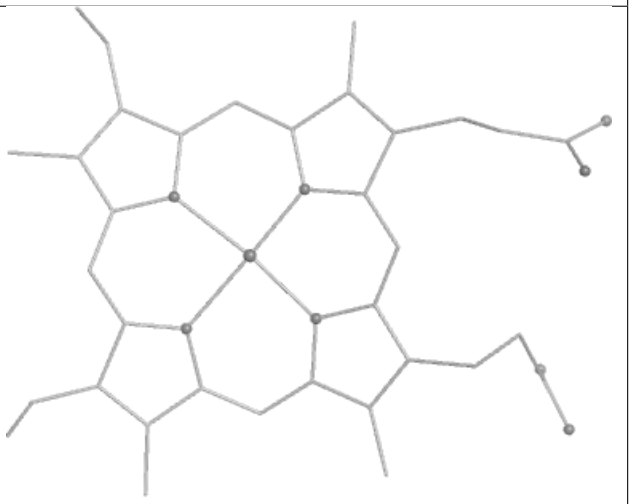

Rings

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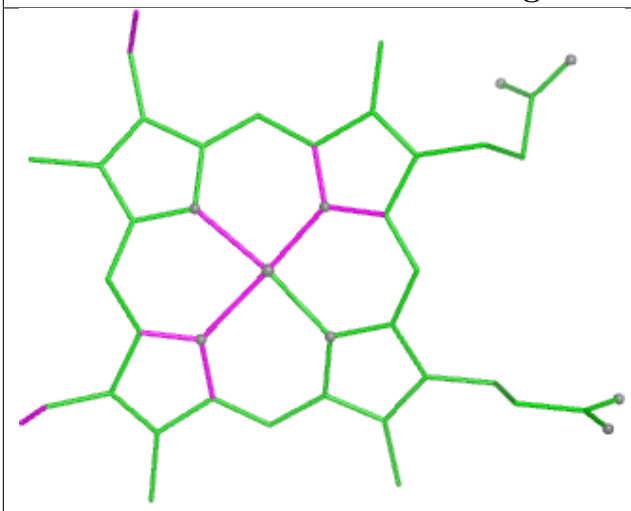

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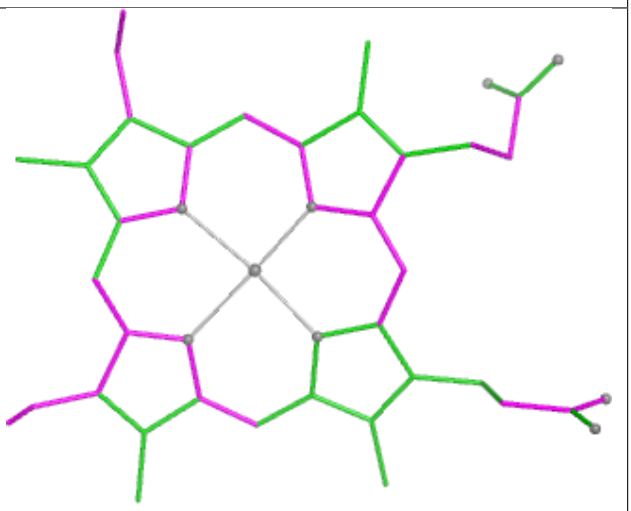

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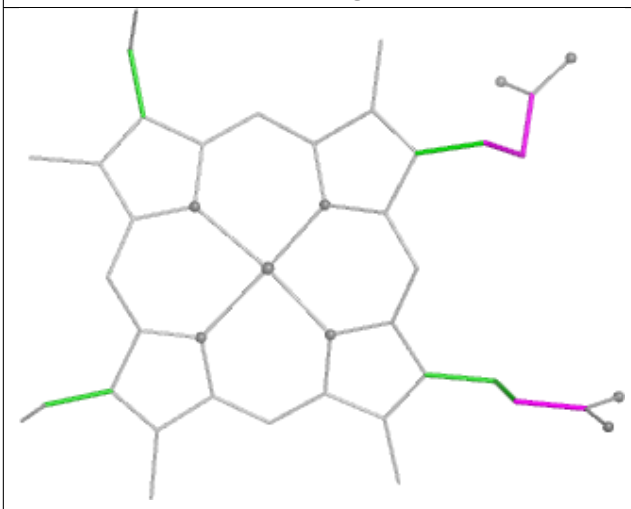

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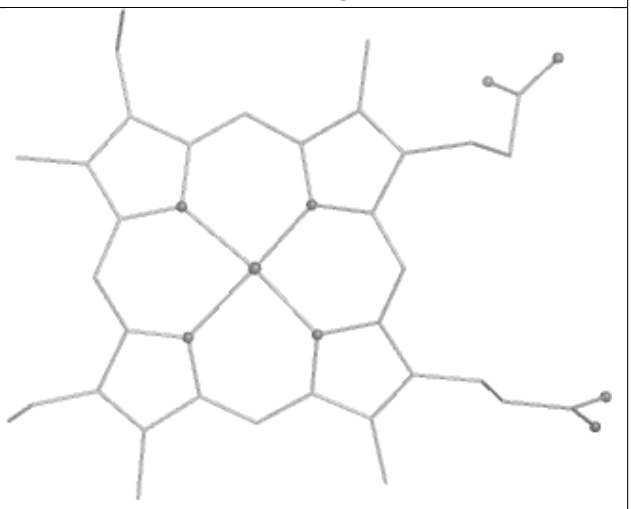

Rings

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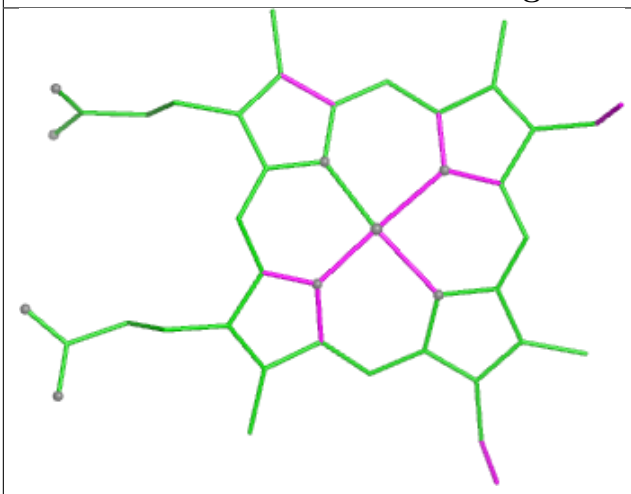

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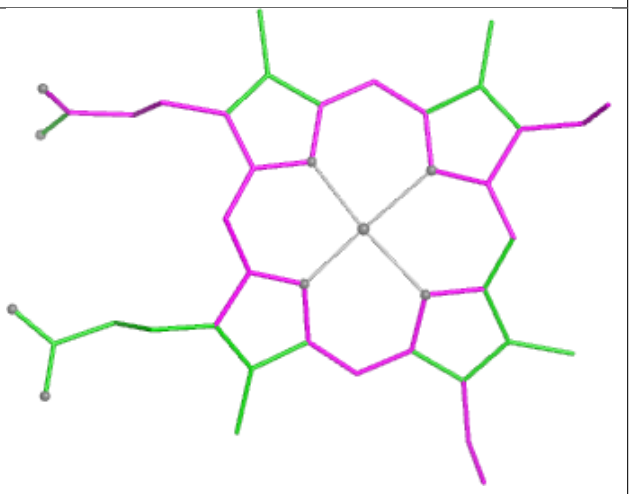

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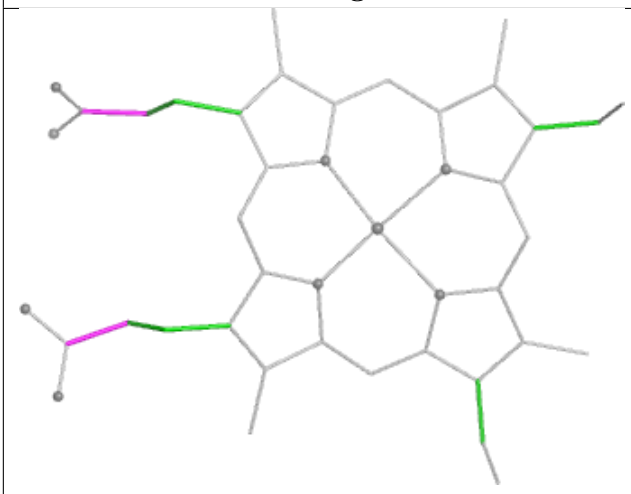

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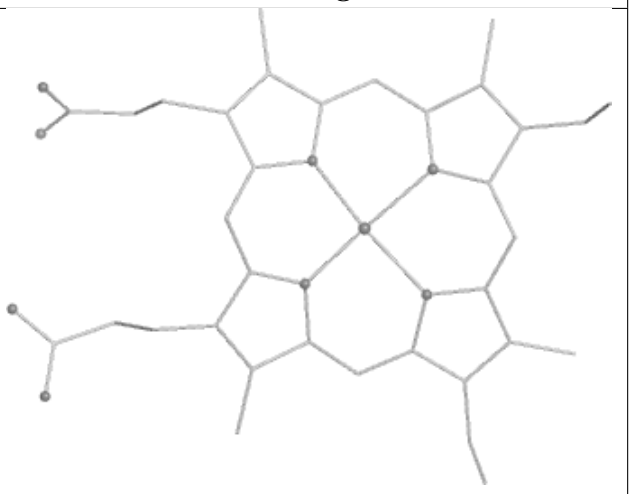

Rings

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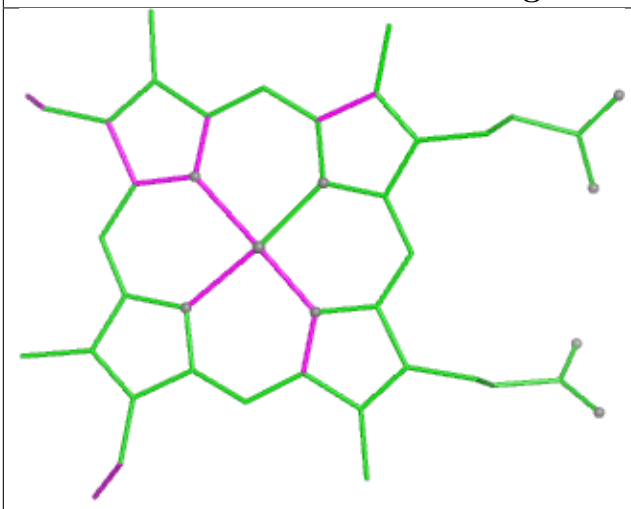

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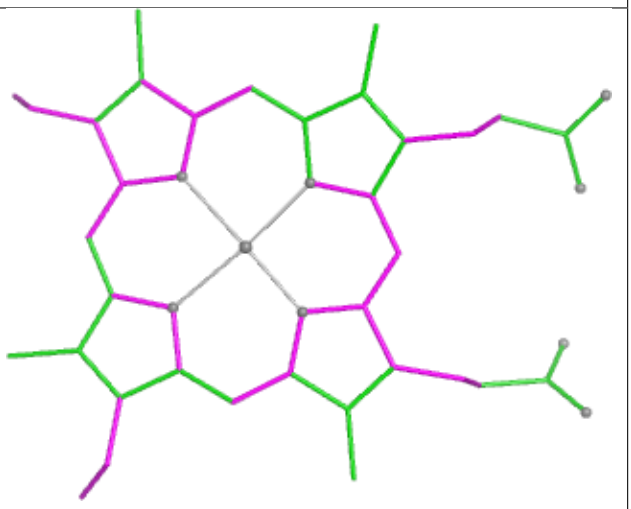

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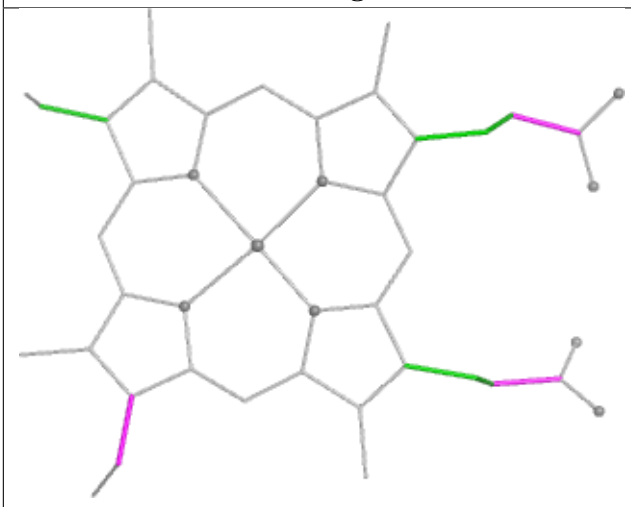

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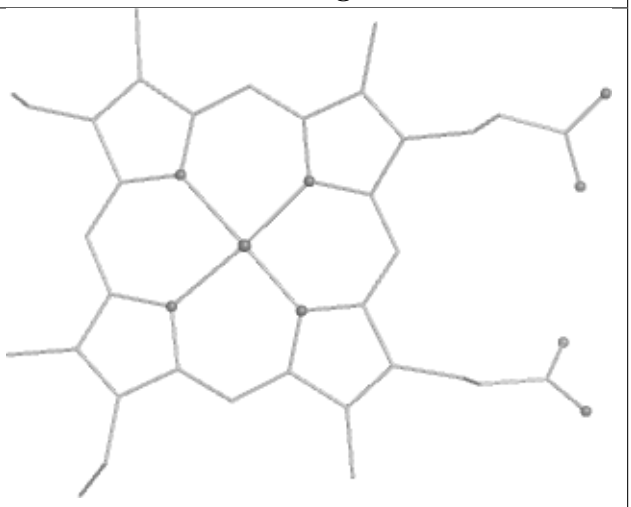
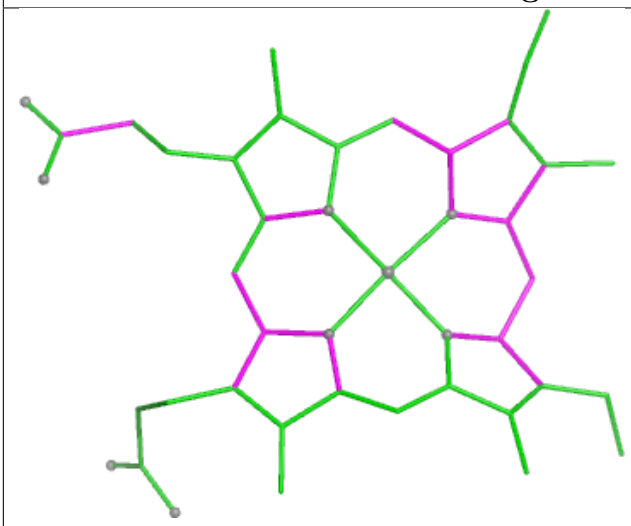


Rings

Ligand HEC G 603



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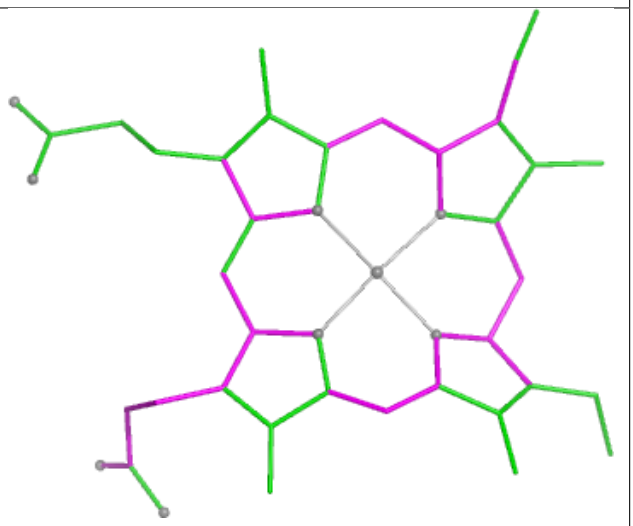
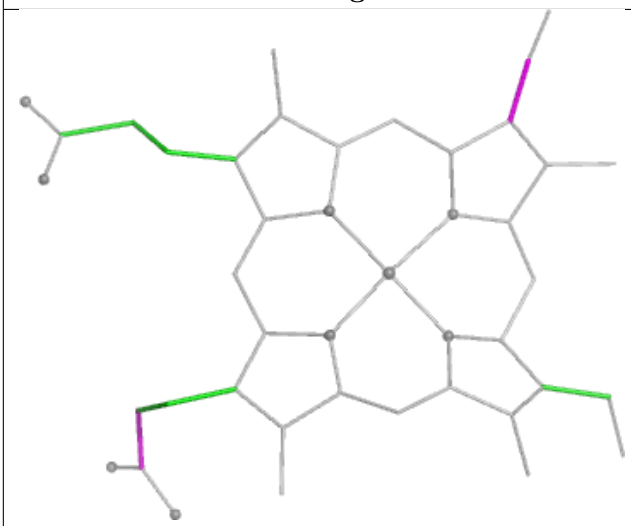


Bond angles



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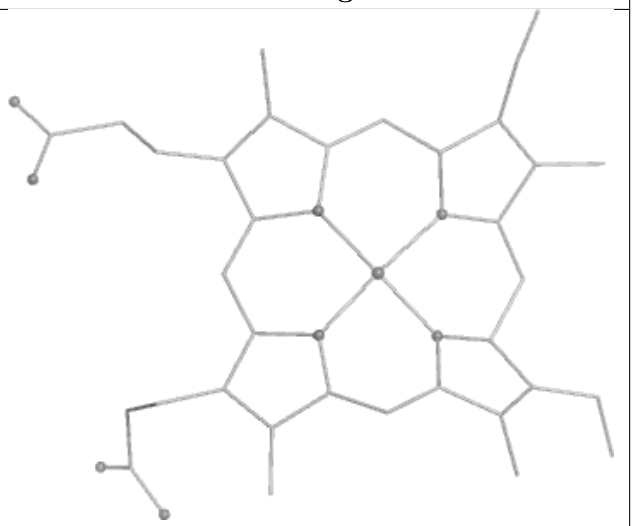
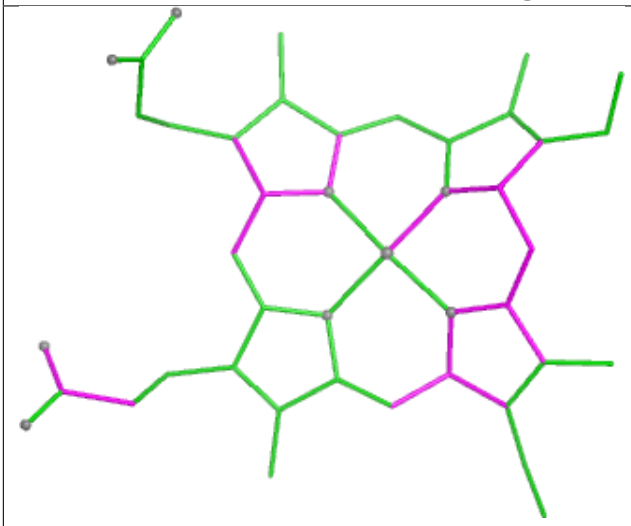


Rings

Ligand HEC M 603



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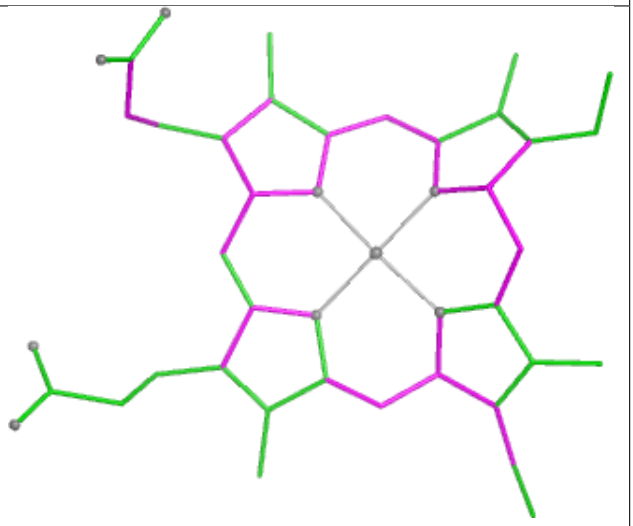

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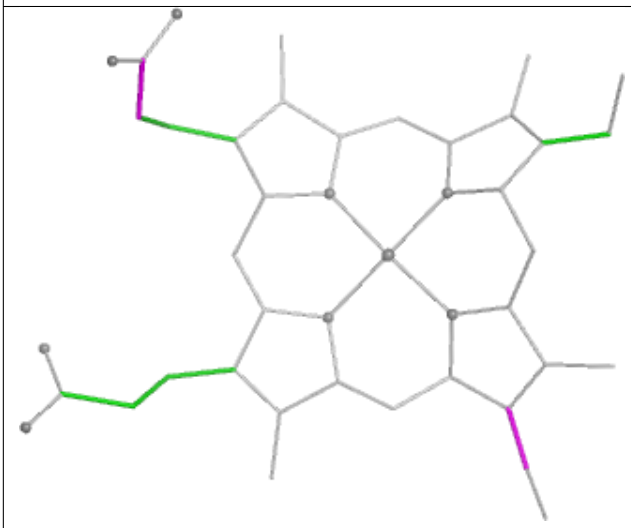

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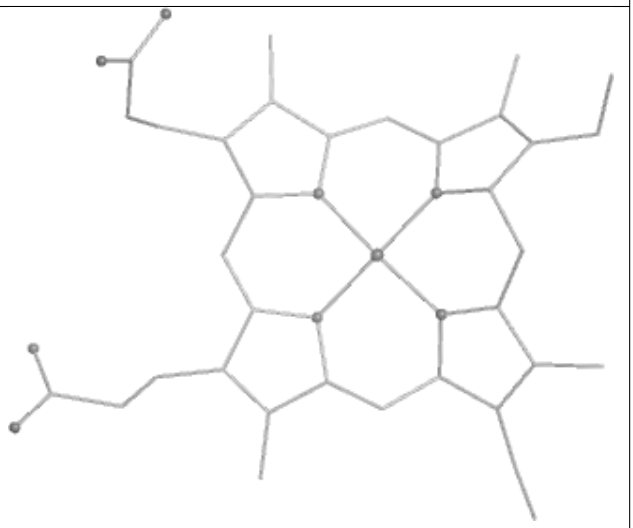
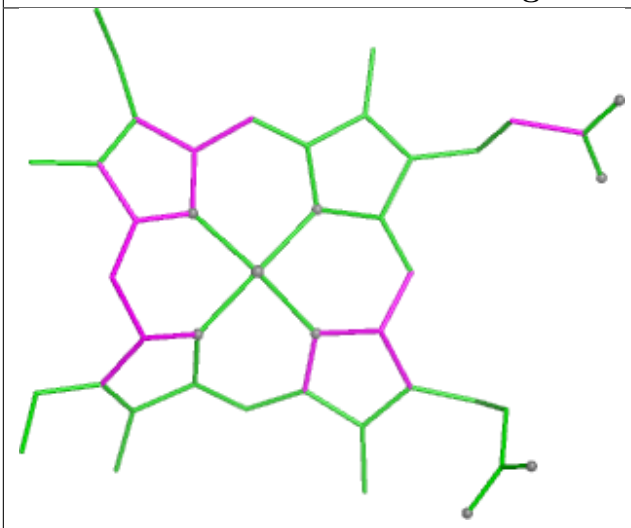


Rings

Ligand HEC X 603



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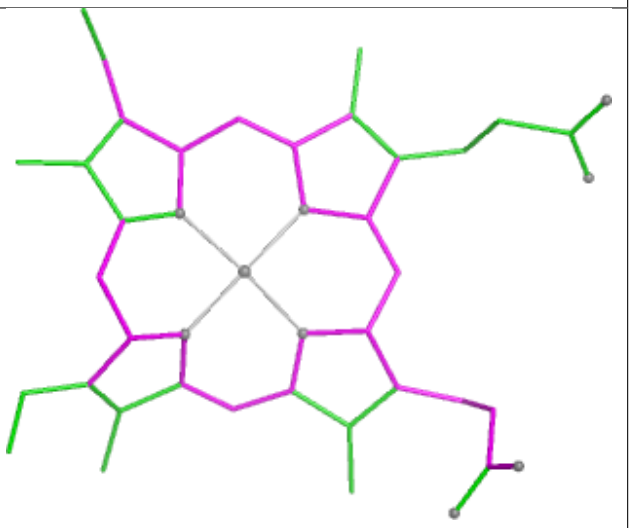

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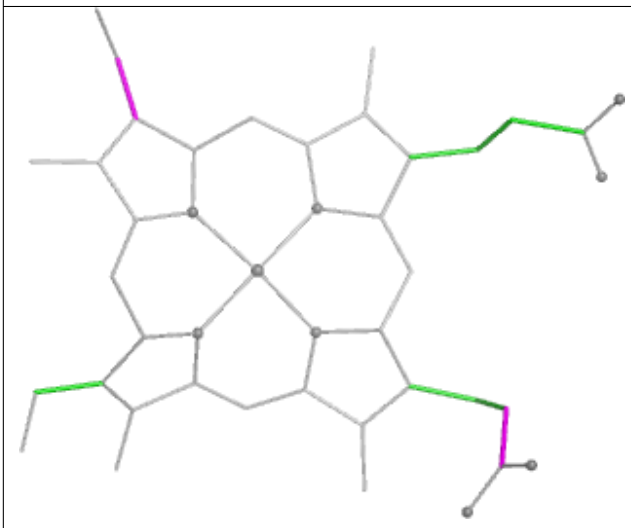

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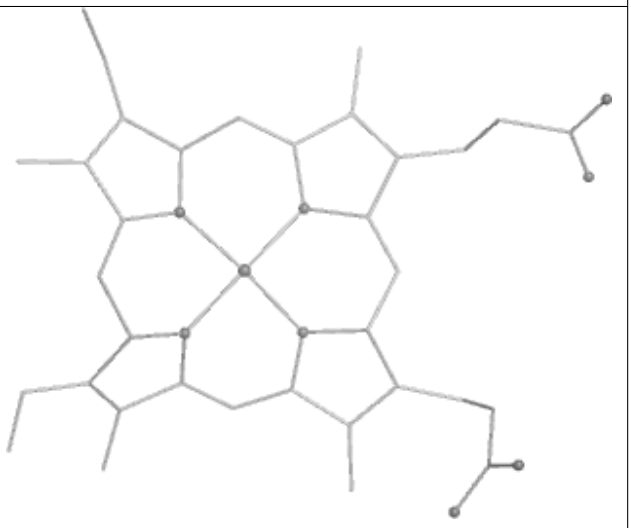
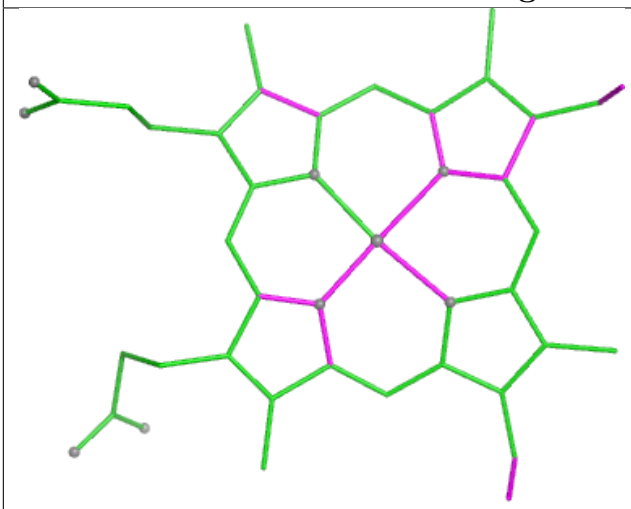


Rings

Ligand HEC M 602



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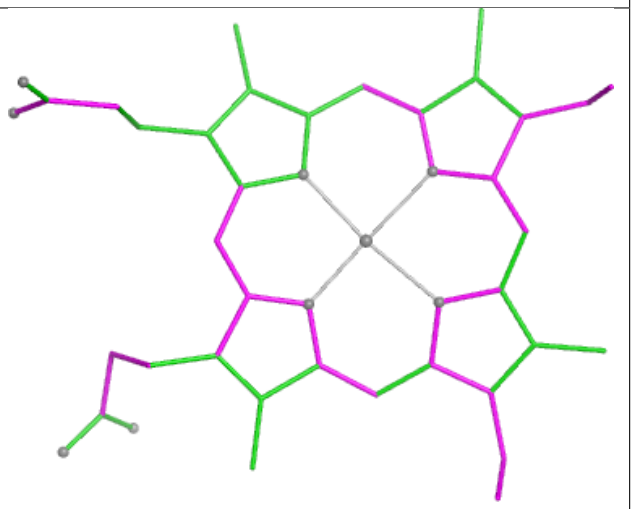
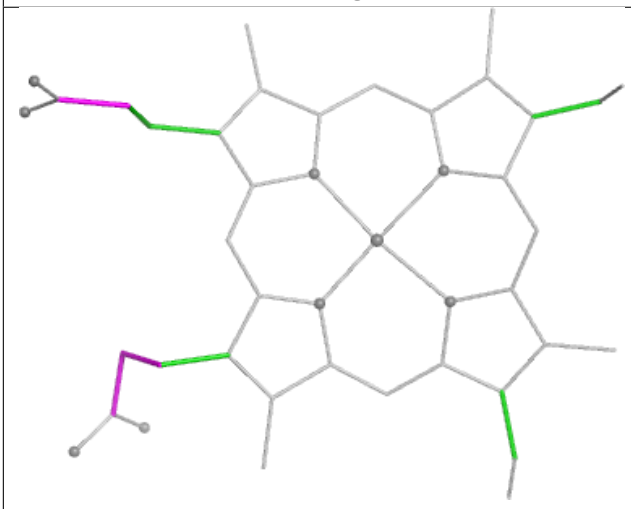


Bond angles



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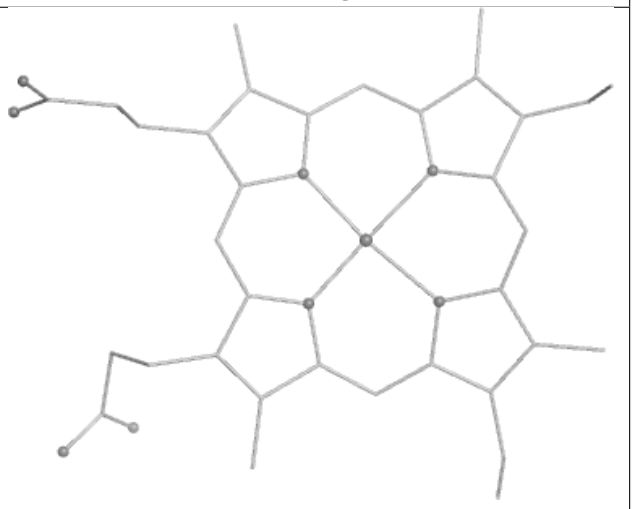

Rings

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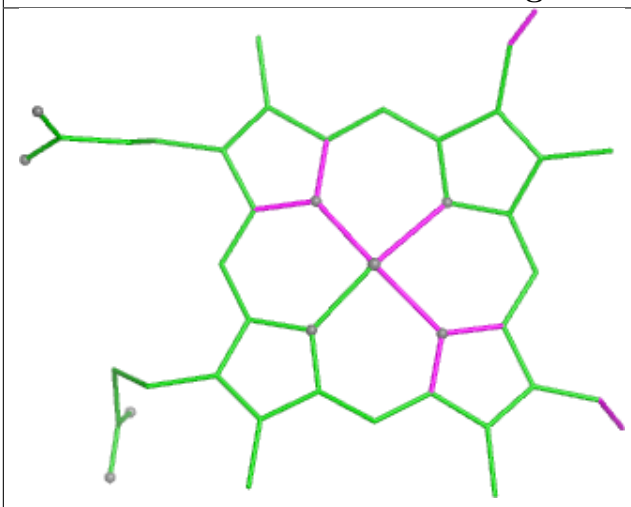

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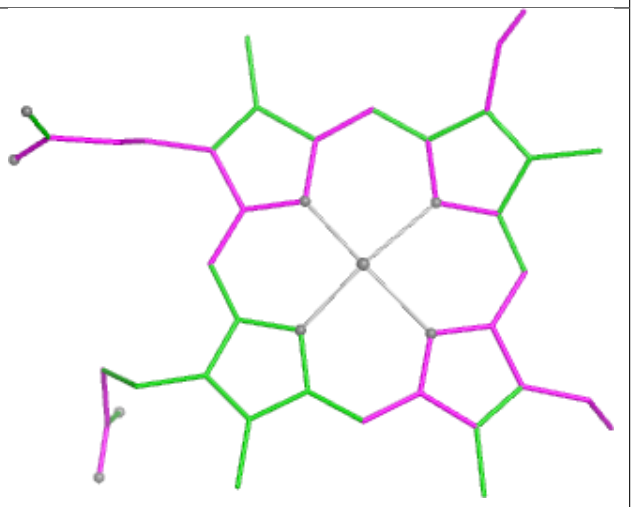

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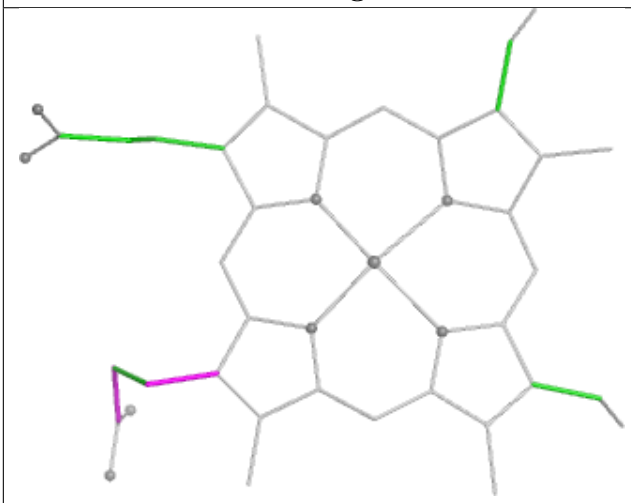

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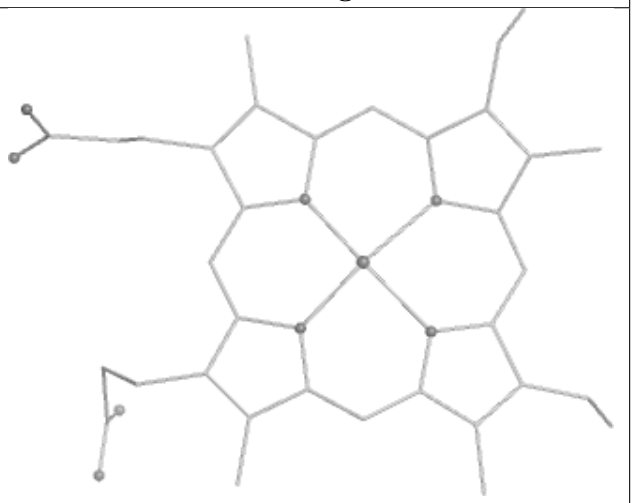
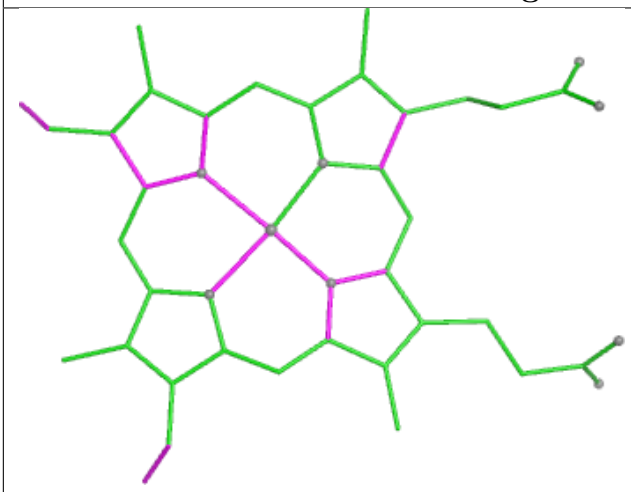


Rings

Ligand HEC N 605



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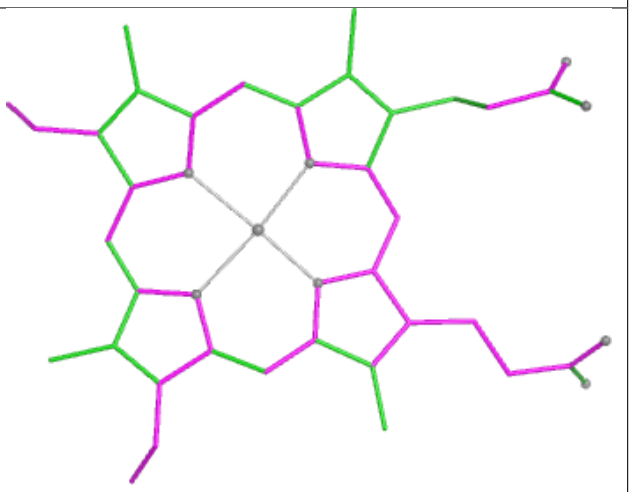

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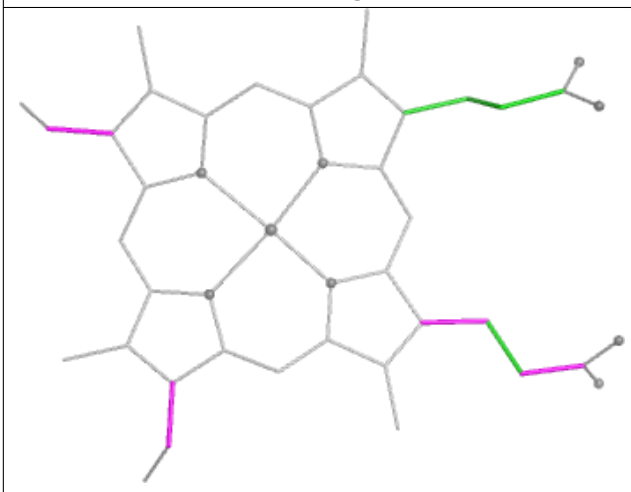

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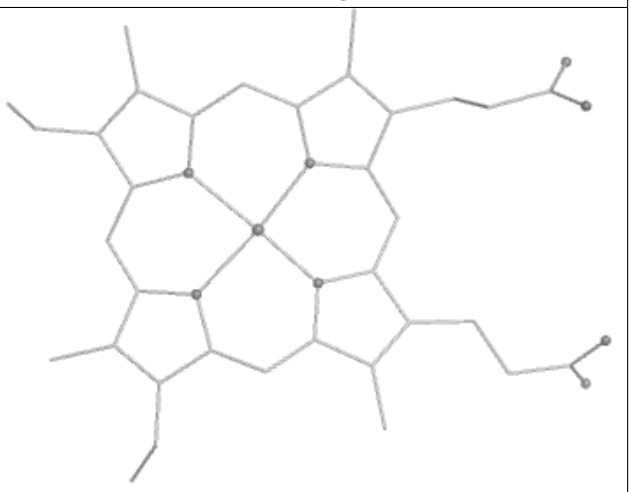
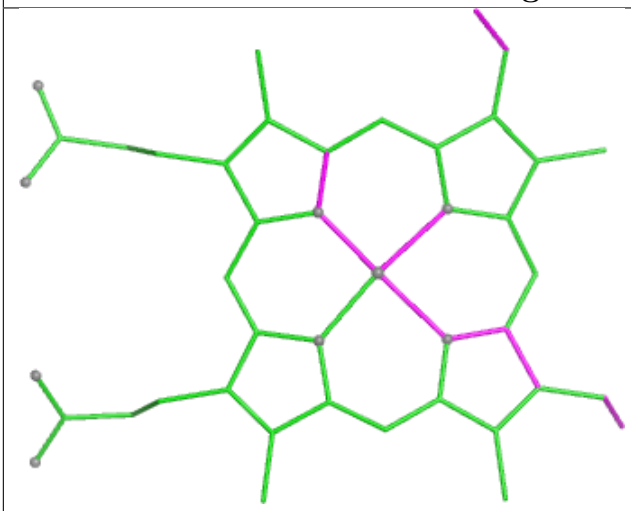


Rings

Ligand HEC U 600



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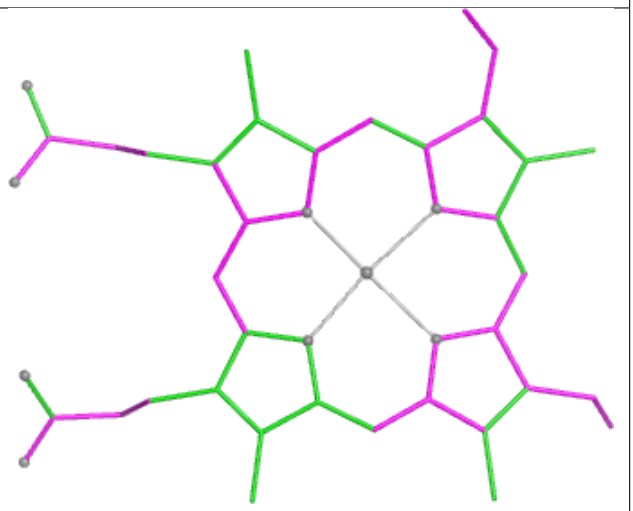
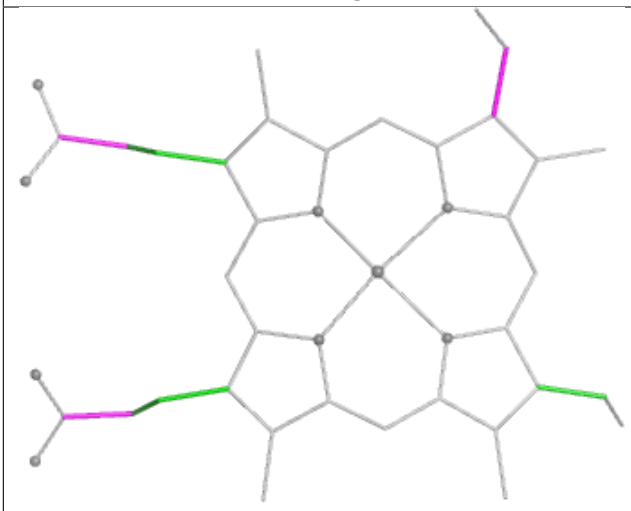


Bond angles



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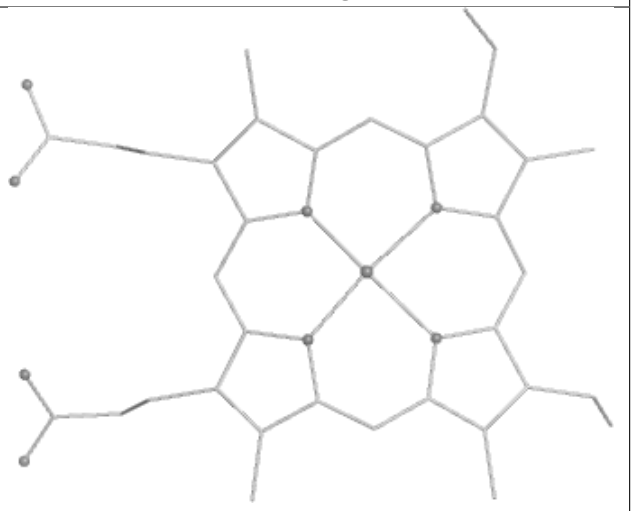
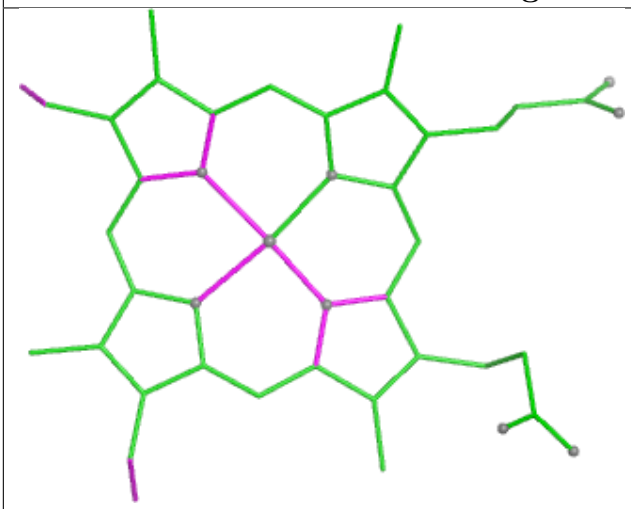


Rings

Ligand HEC N 602



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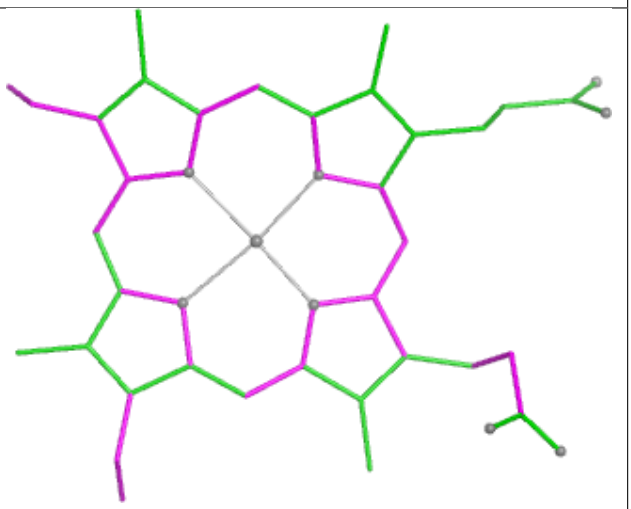

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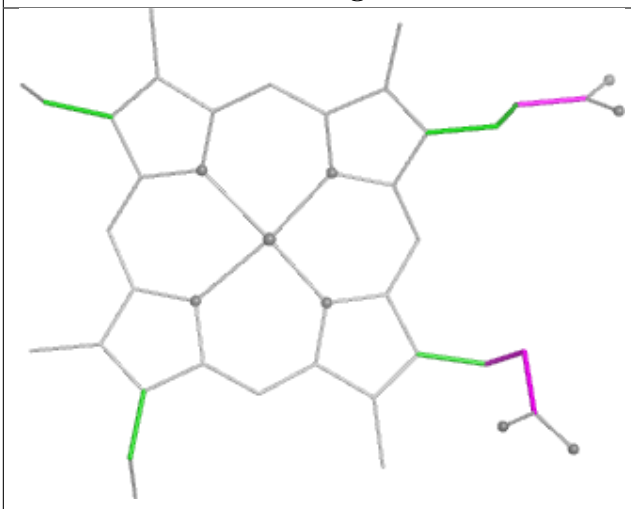

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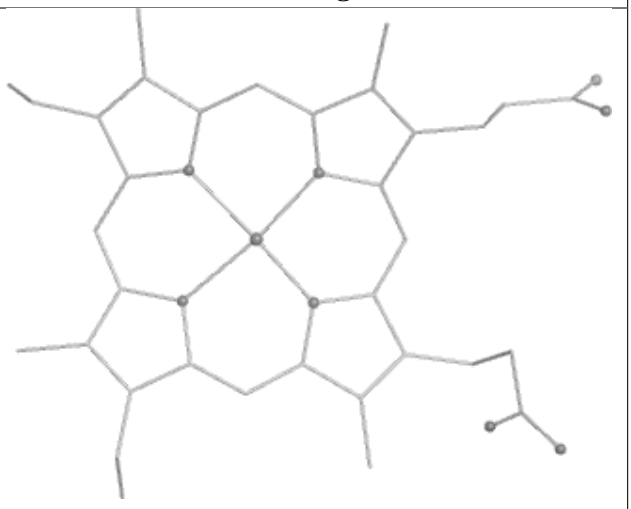
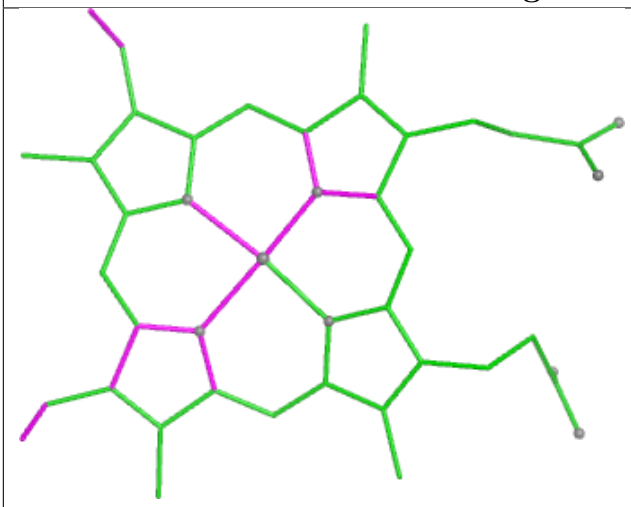


Rings

Ligand HEC B 607



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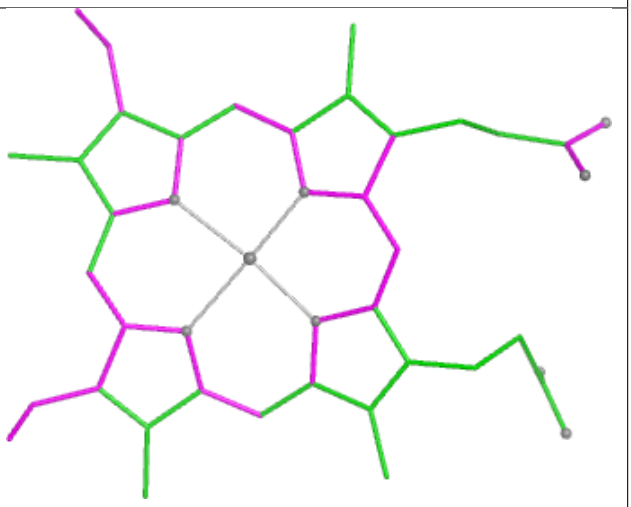
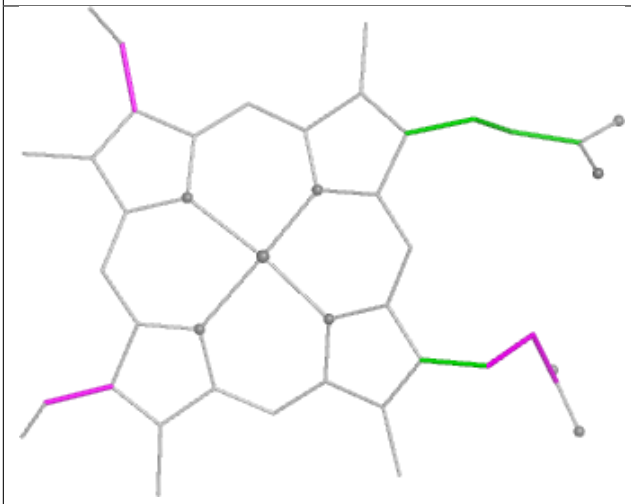


Bond angles



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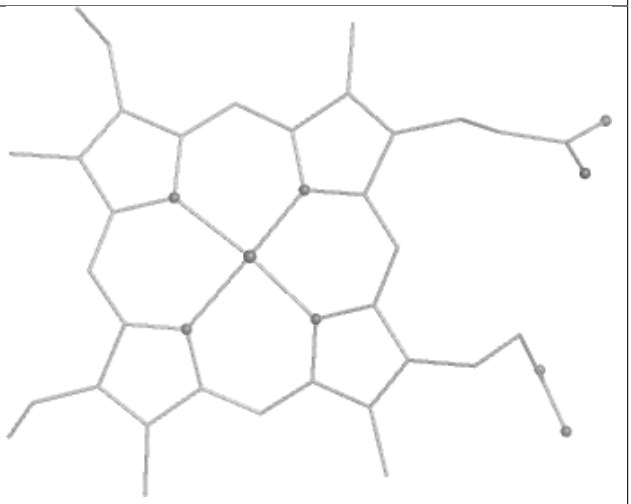
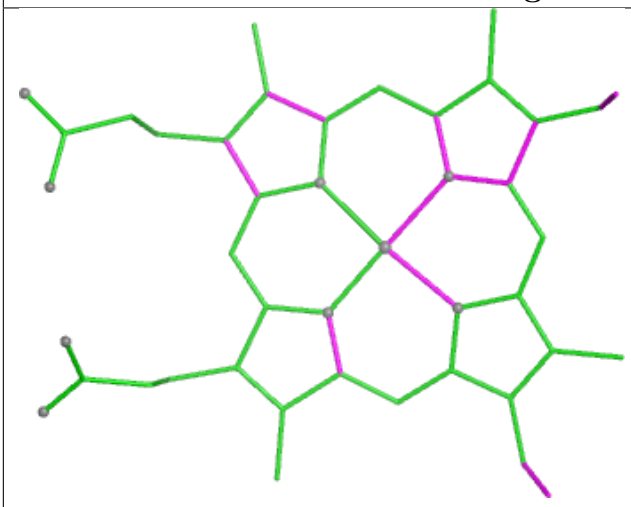


Rings

Ligand HEC E 604



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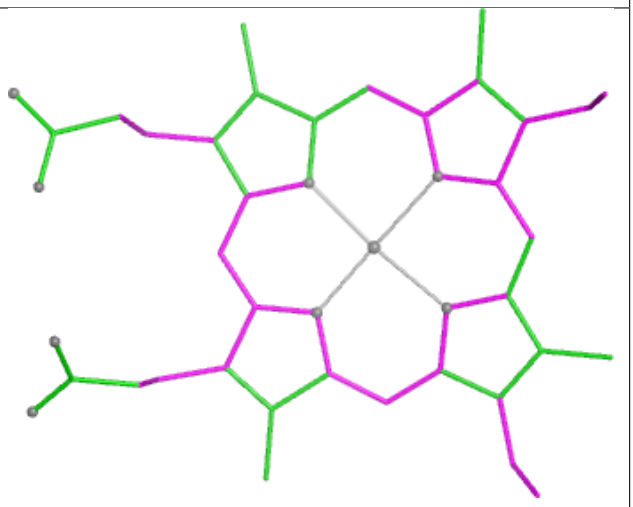

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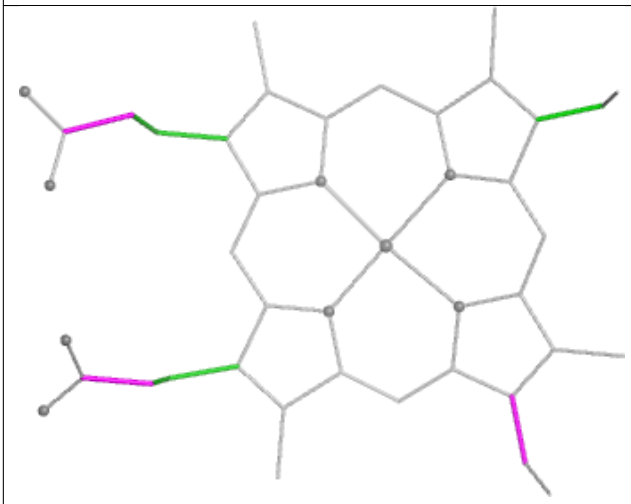

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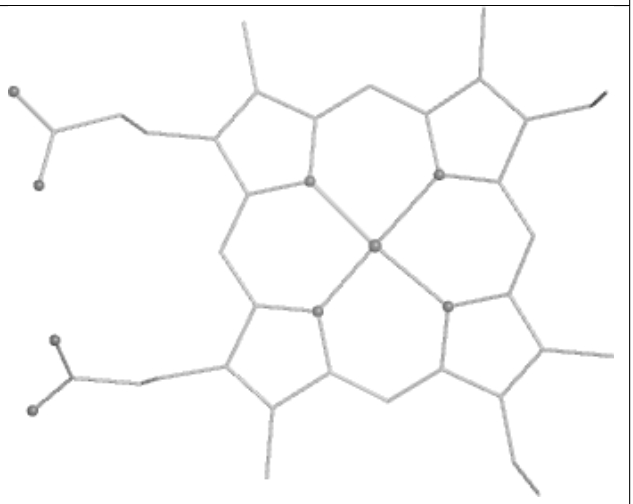
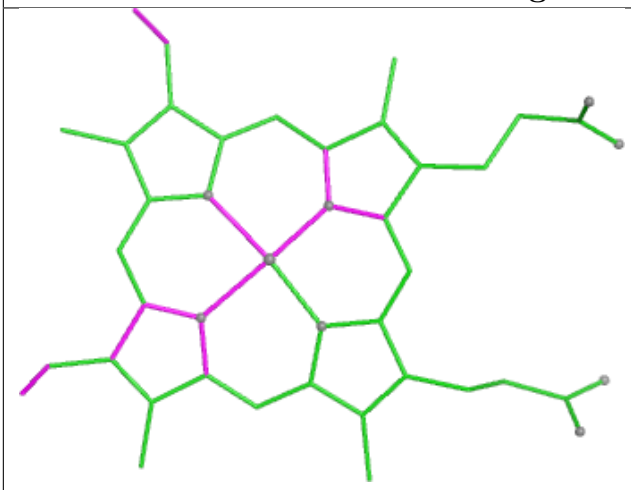


Rings

Ligand HEC I 605



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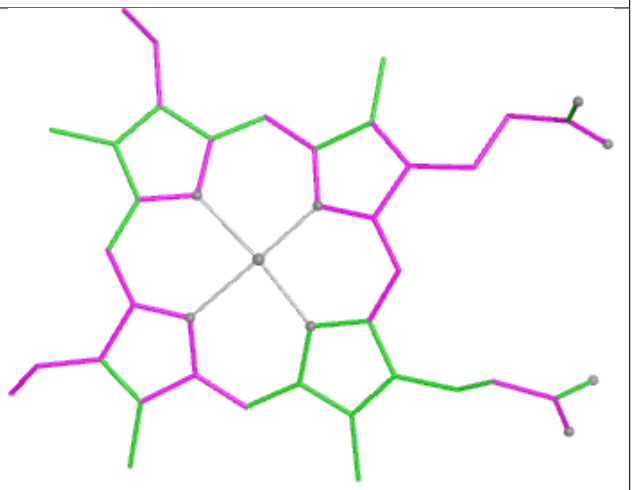

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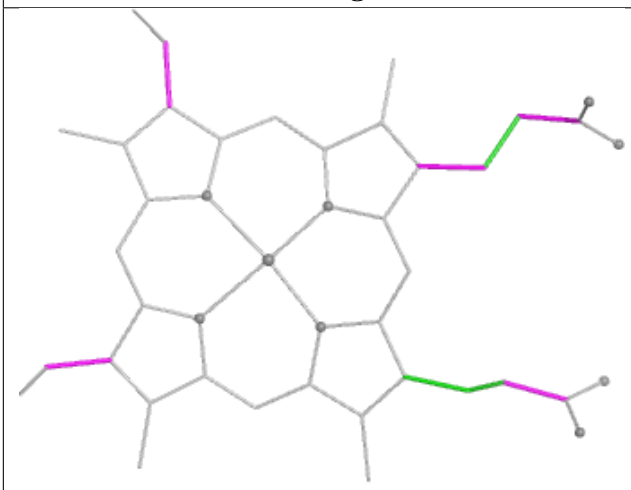

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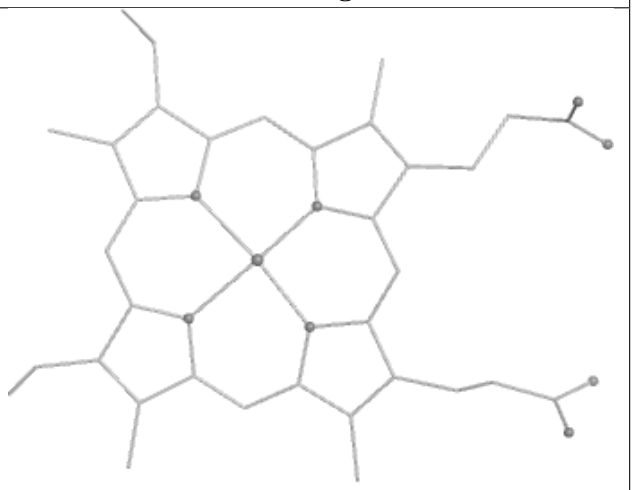

Rings

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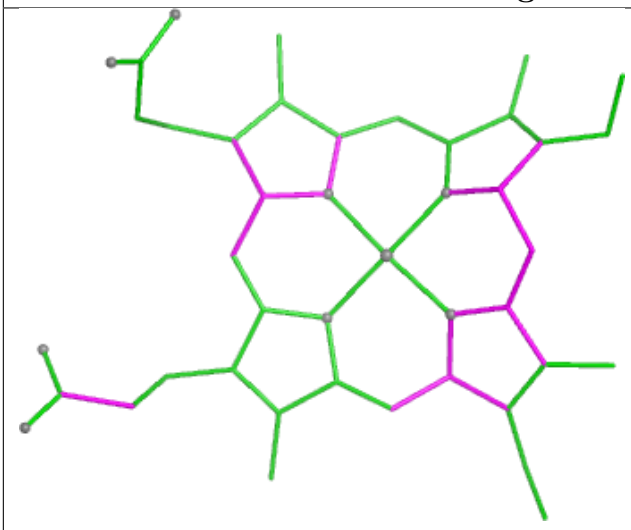

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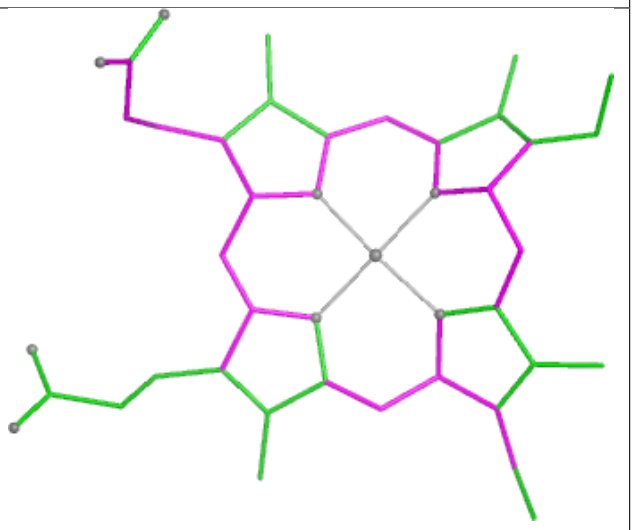

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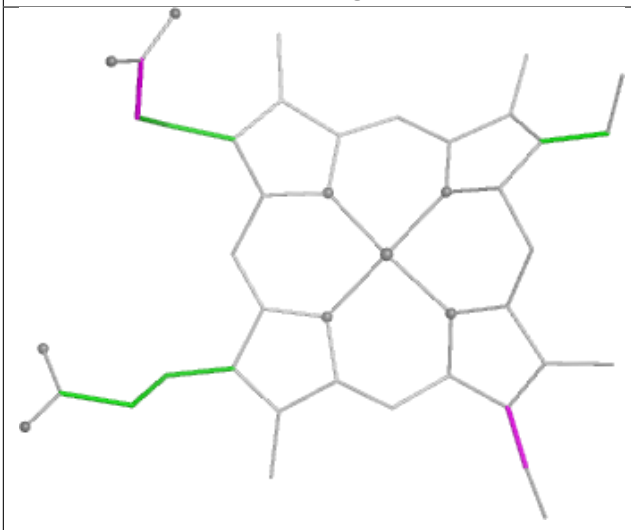

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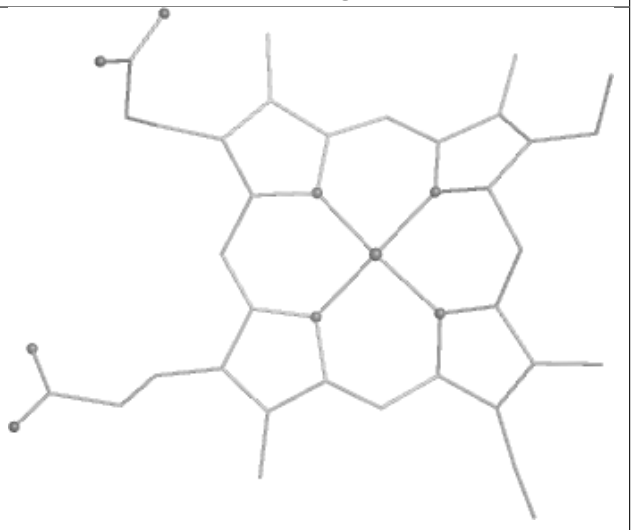

Rings

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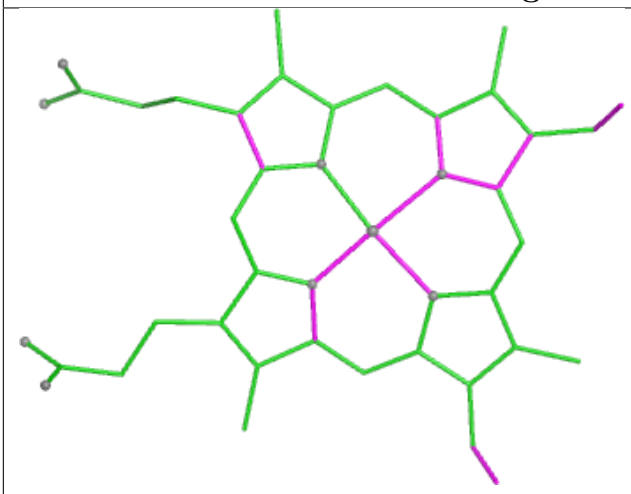

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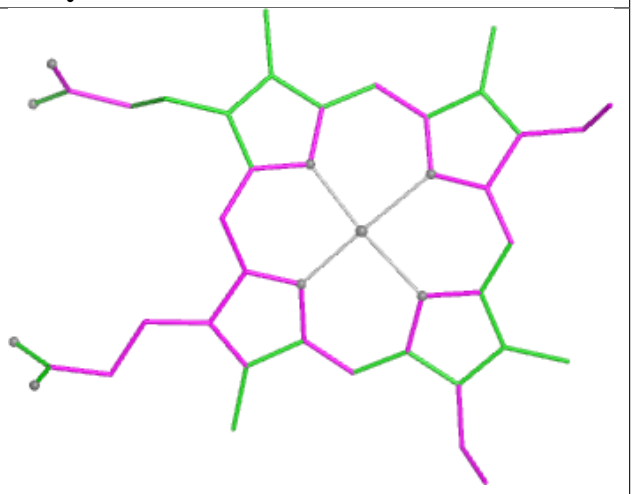

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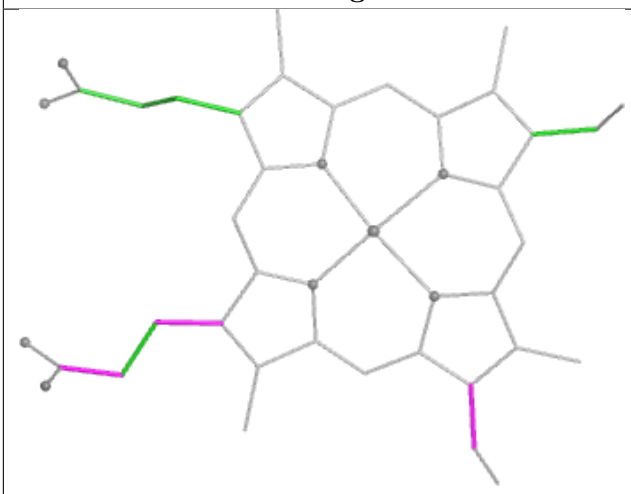

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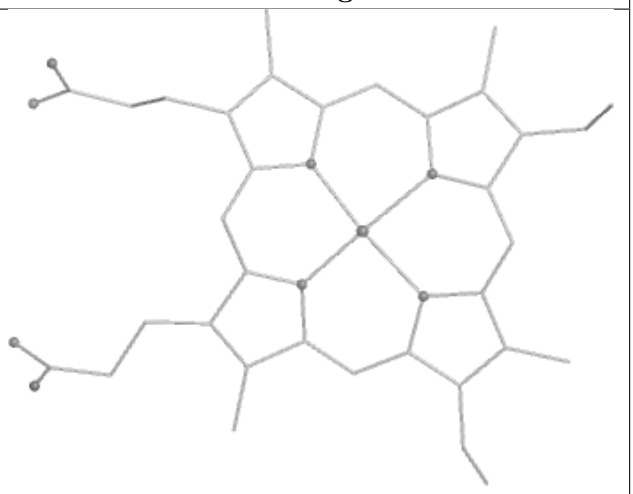
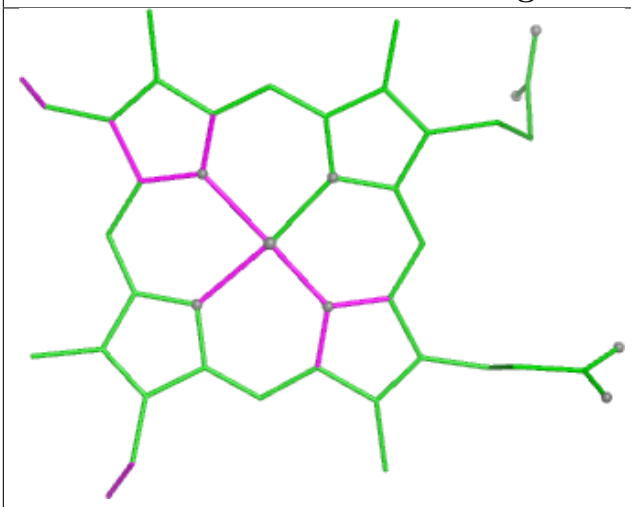


Rings

Ligand HEC W 601



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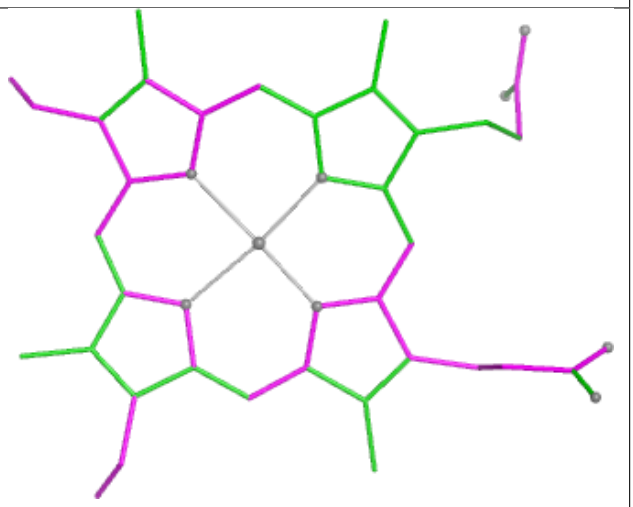

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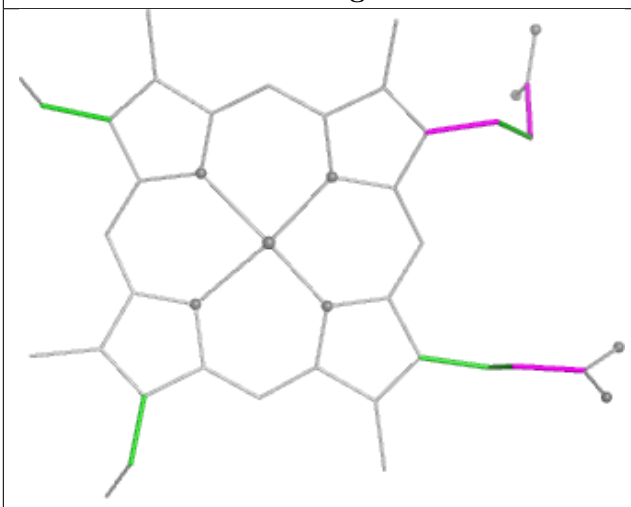

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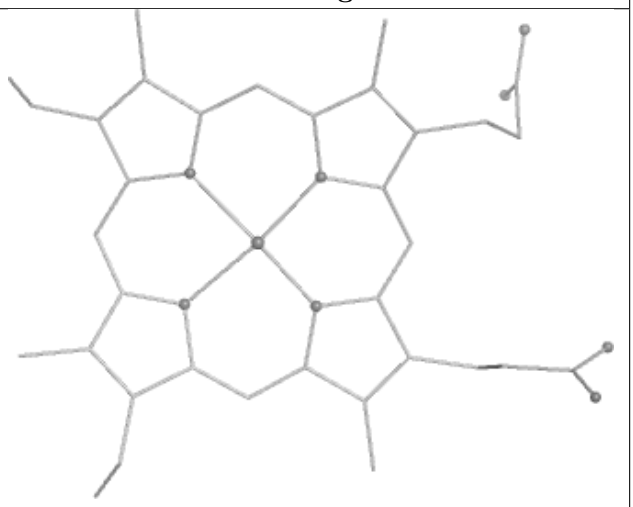

Rings

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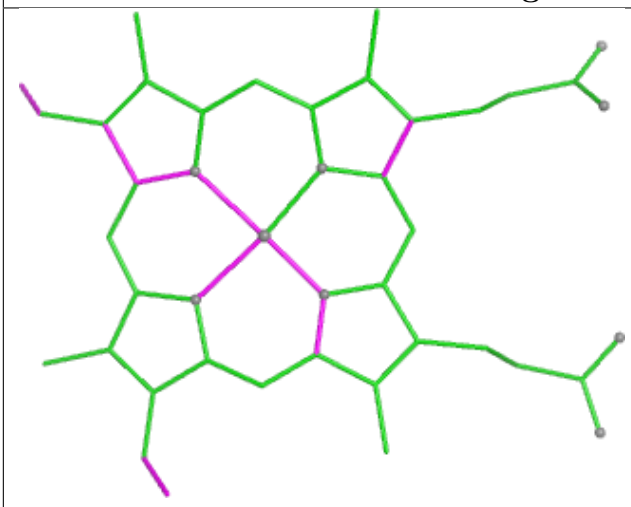

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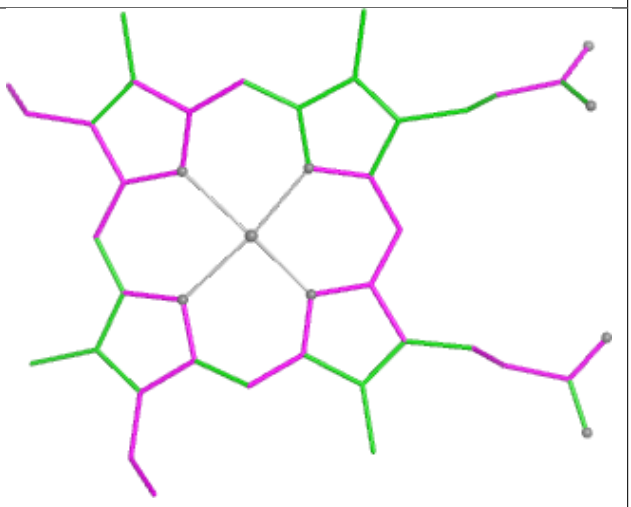

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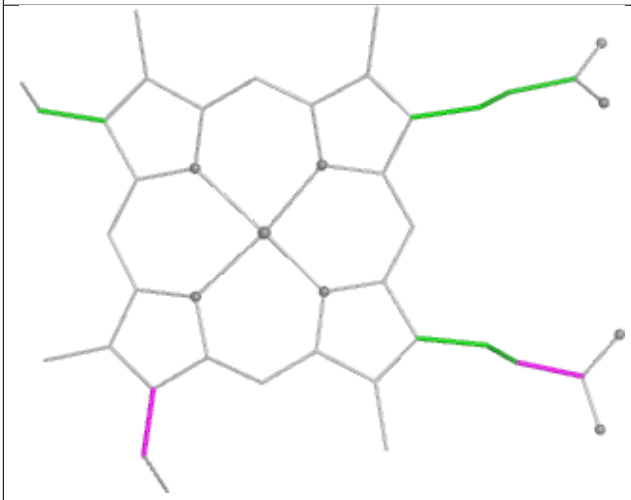

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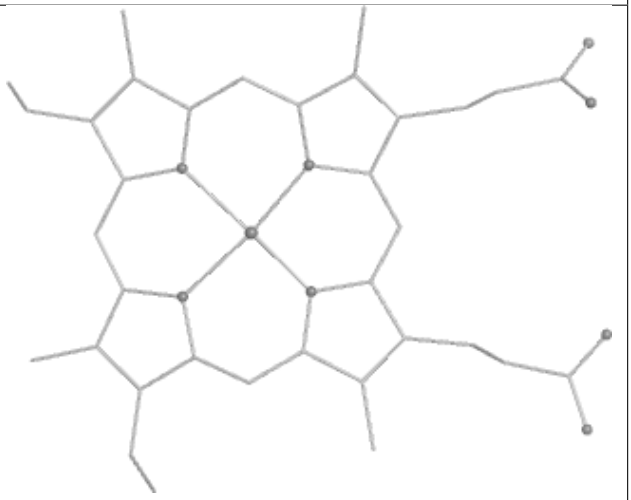

Rings

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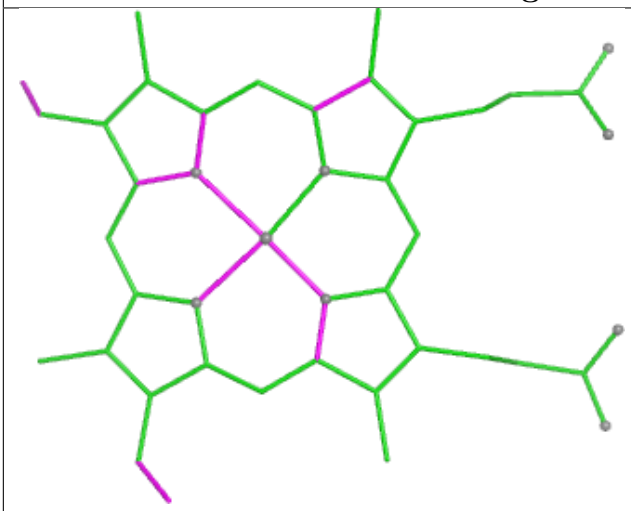

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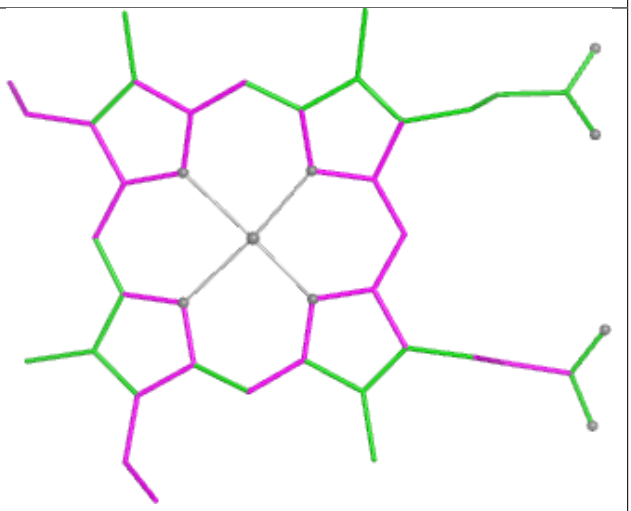

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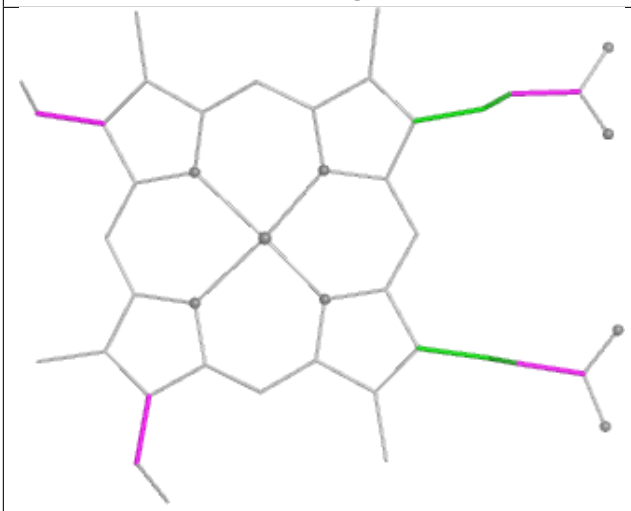

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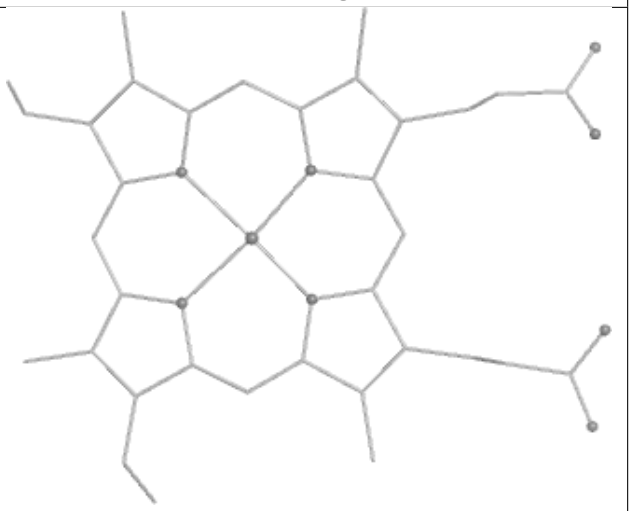

Rings

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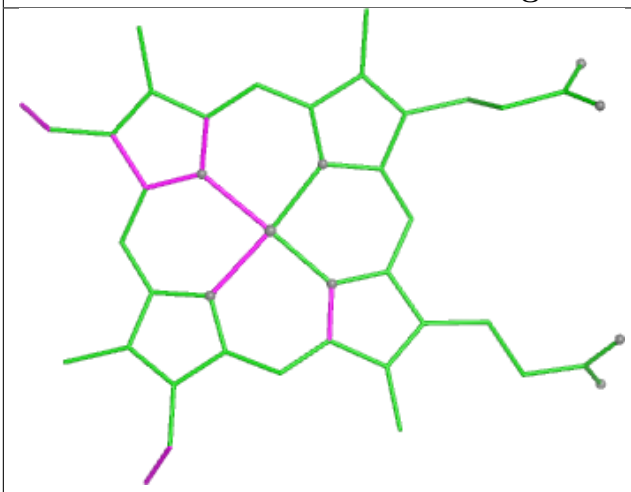

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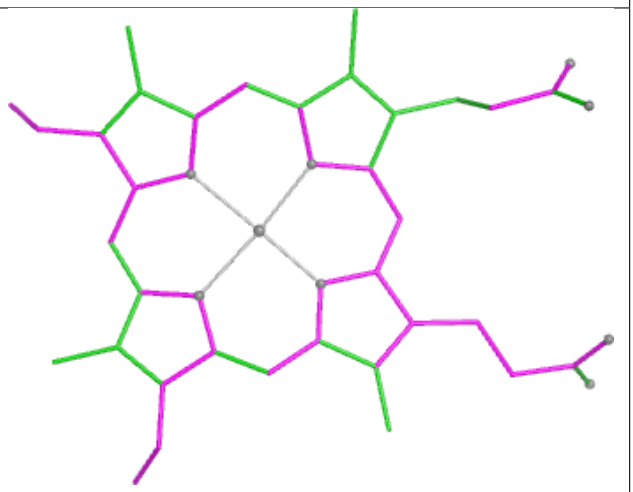

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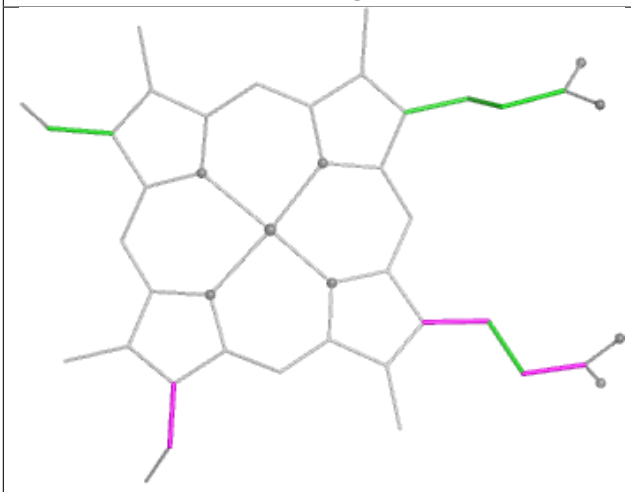

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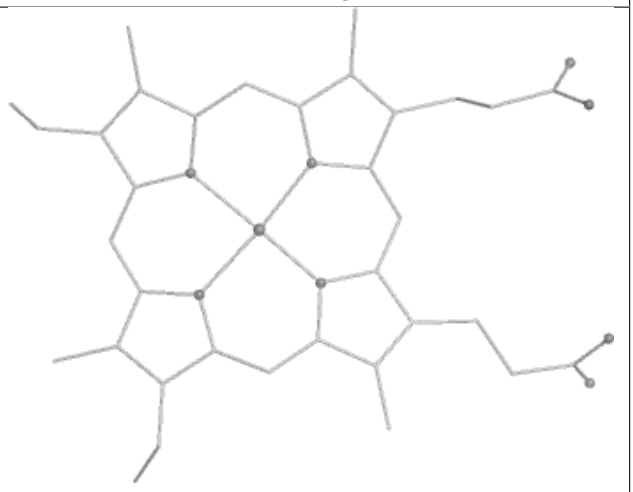

Rings

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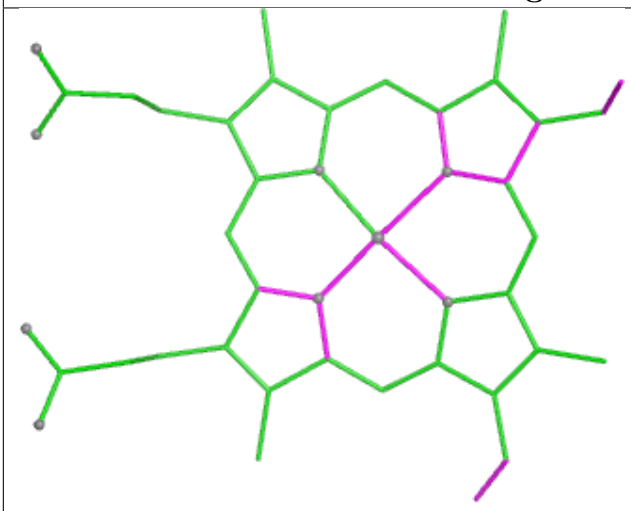

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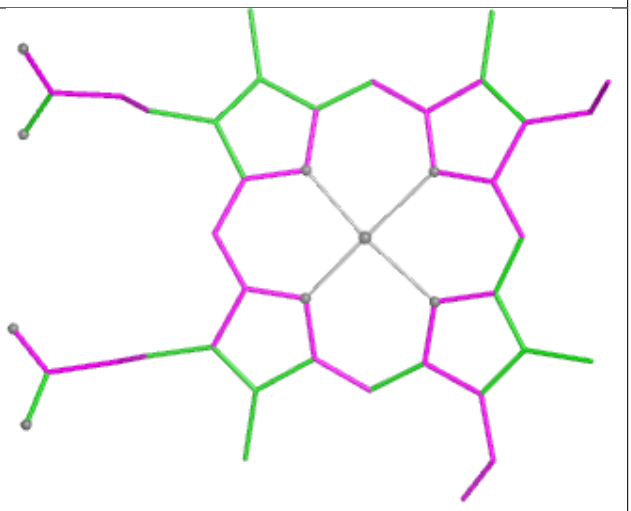

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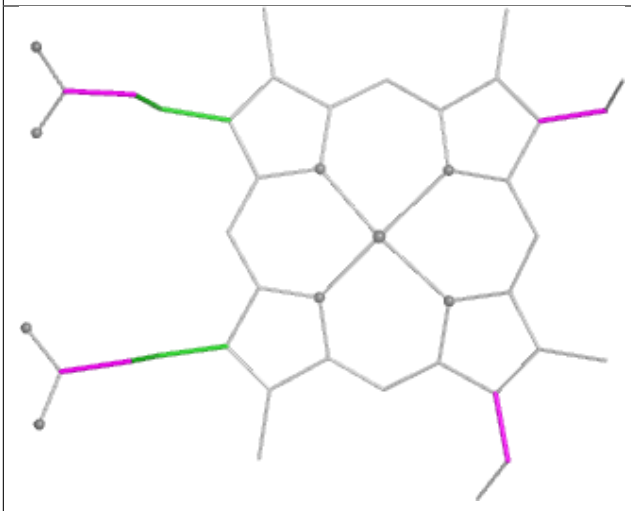

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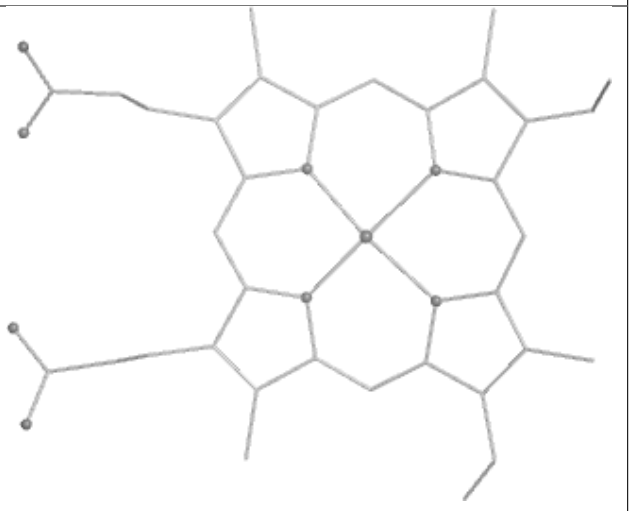

Rings

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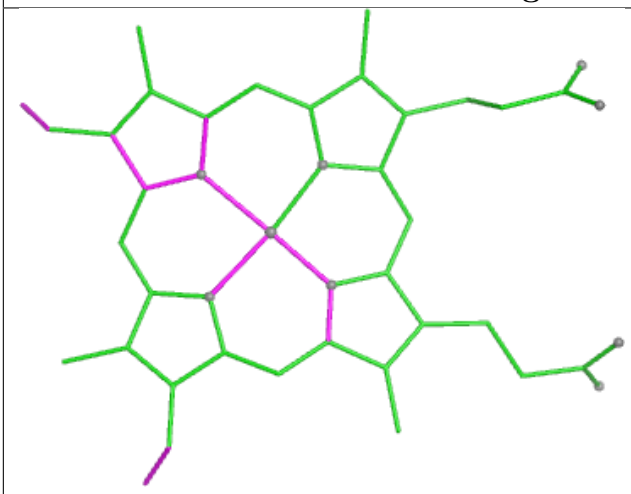

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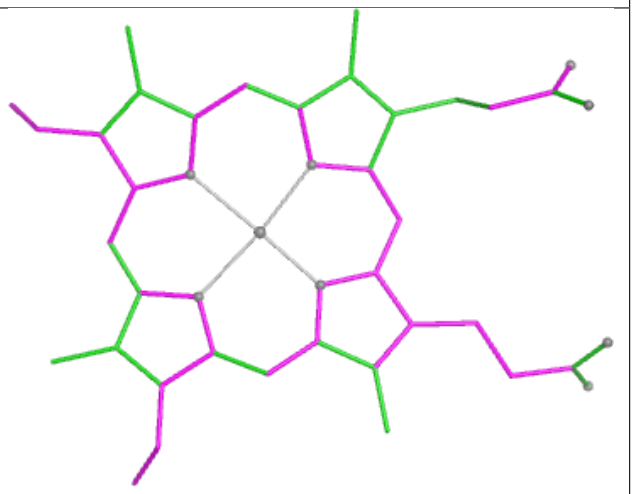

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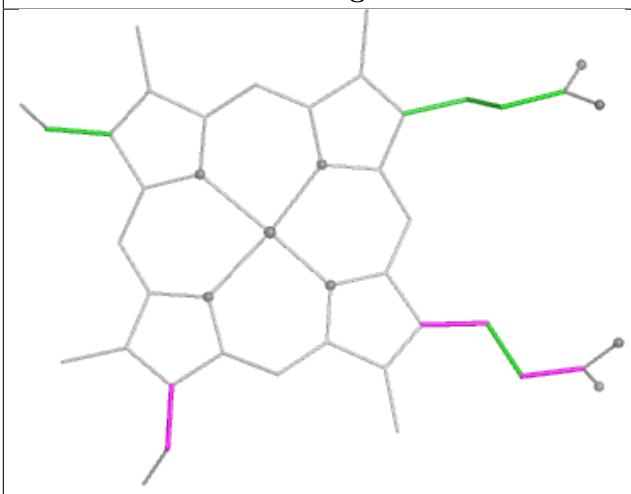

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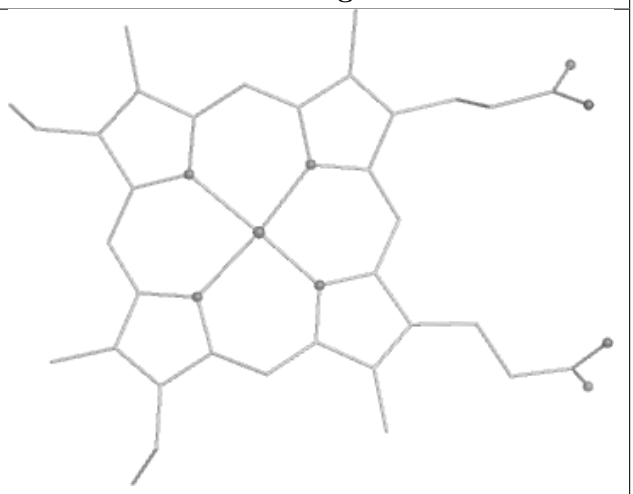
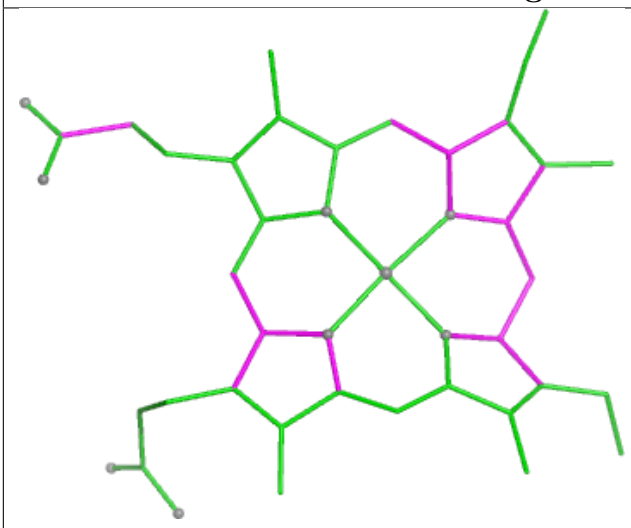


Rings

Ligand HEC L 603



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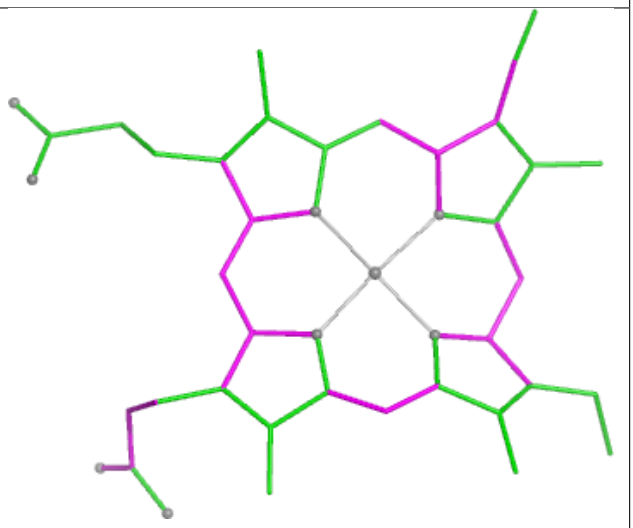

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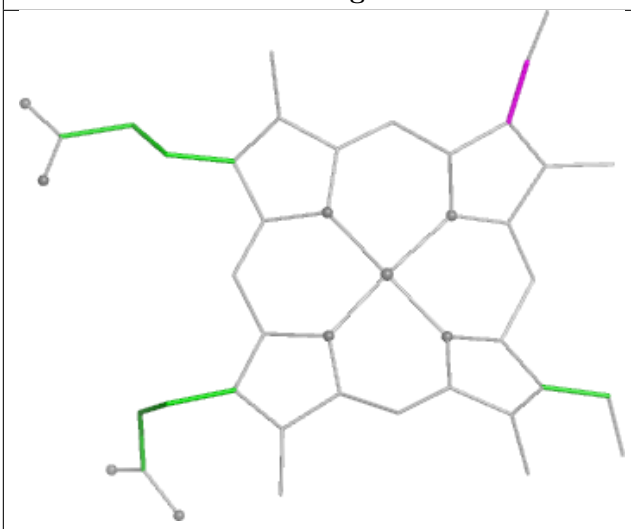

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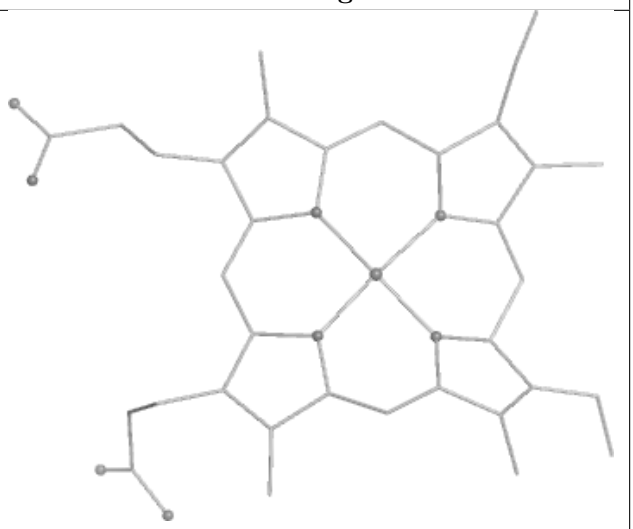
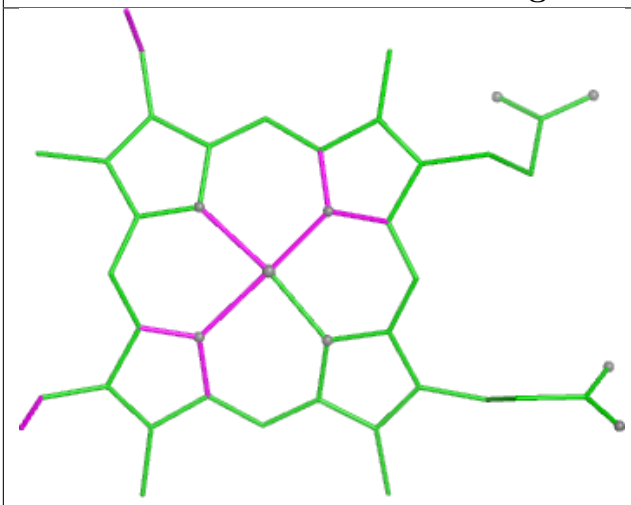


Rings

Ligand HEC I 602



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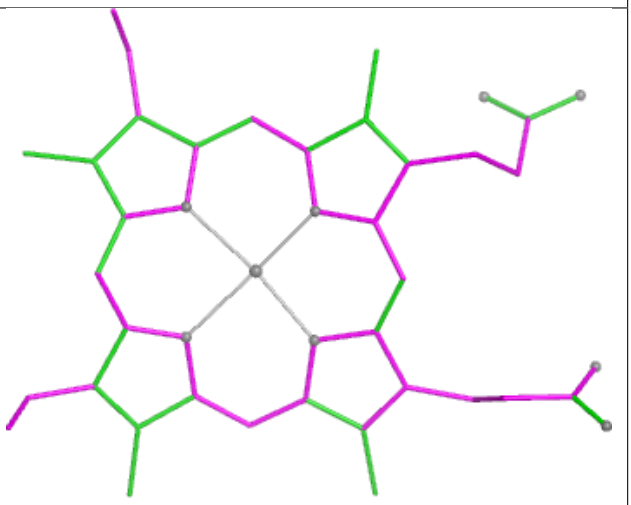

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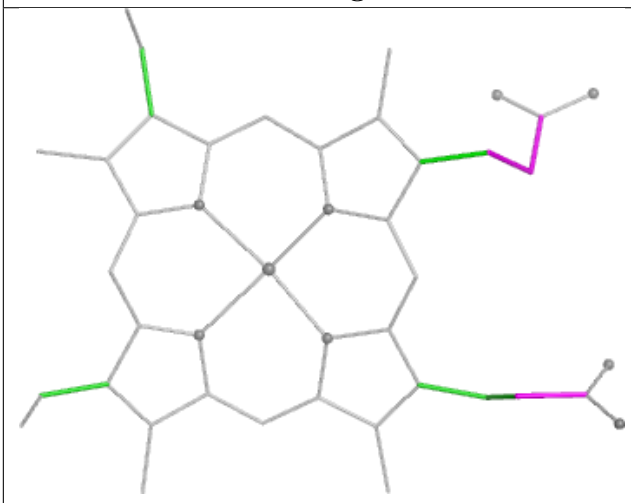

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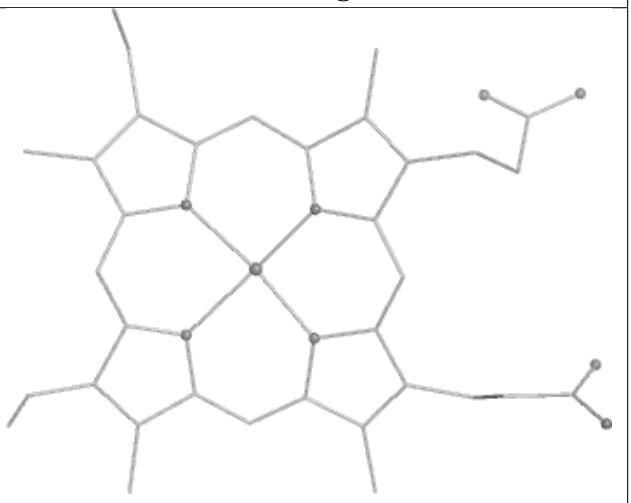
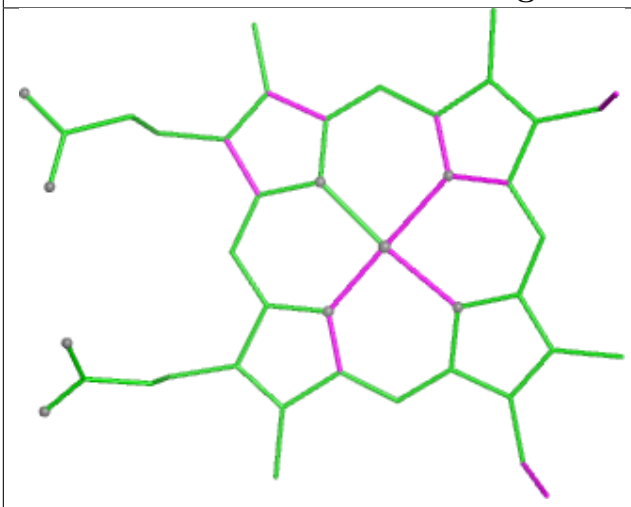


Rings

Ligand HEC W 604



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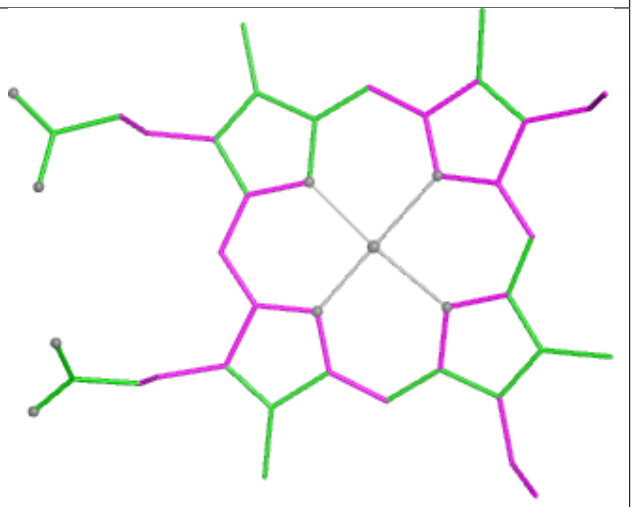

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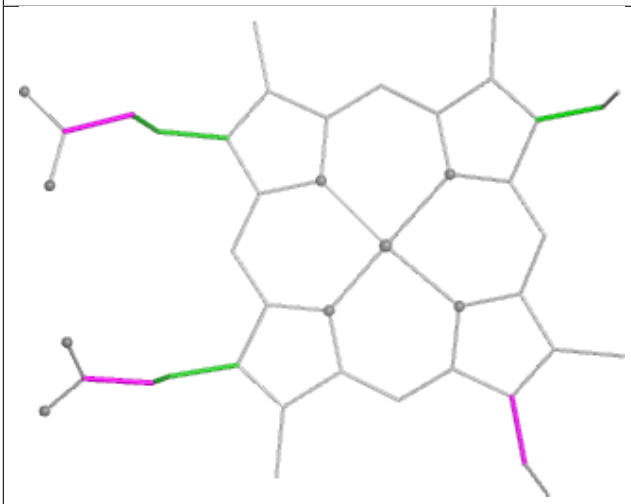

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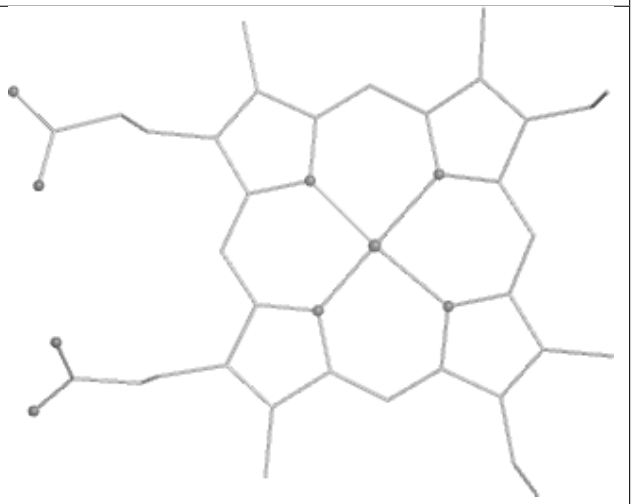
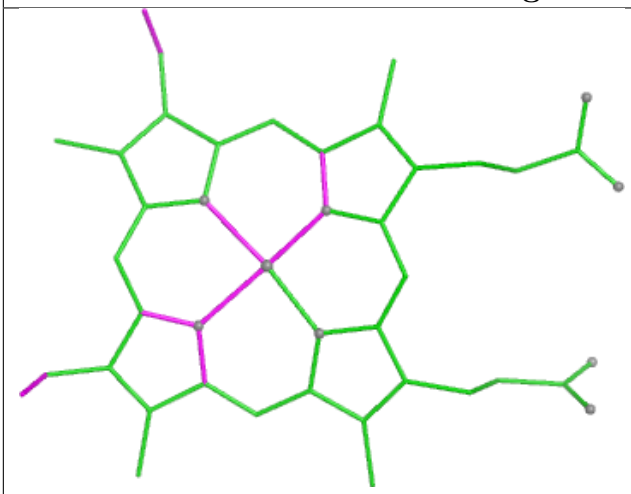


Rings

Ligand HEC C 606



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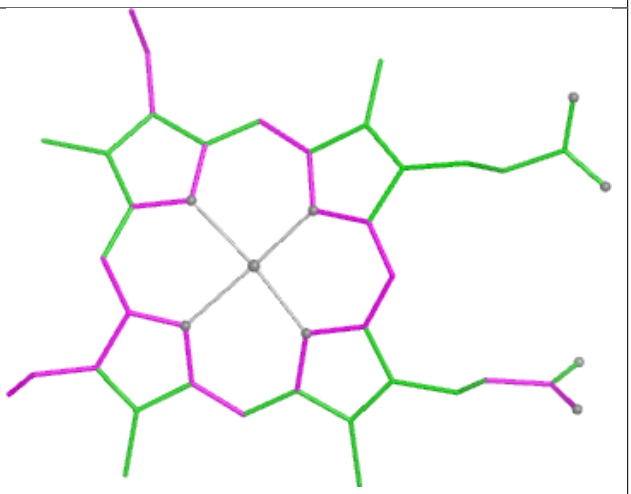
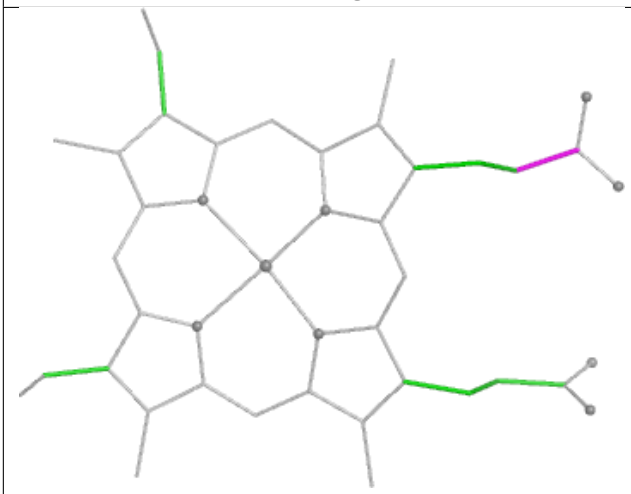


Bond angles



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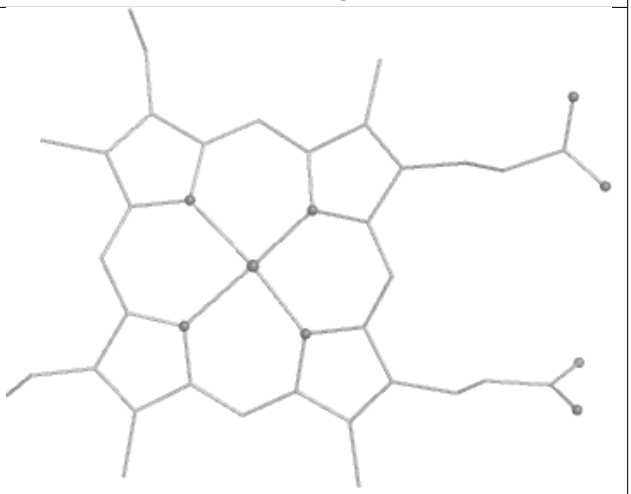
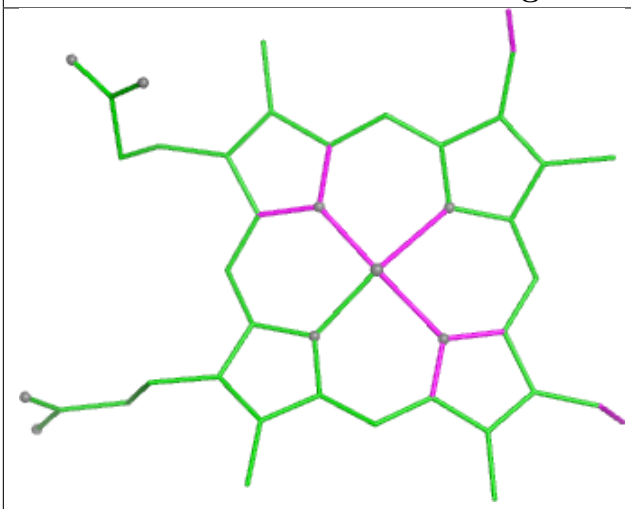


Rings

Ligand HEC H 602



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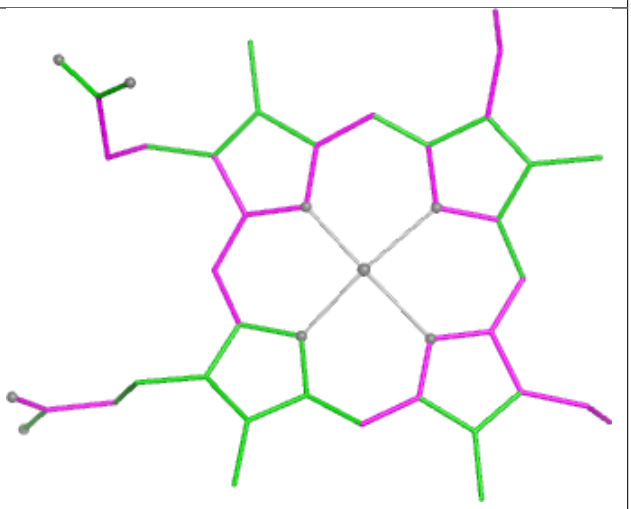
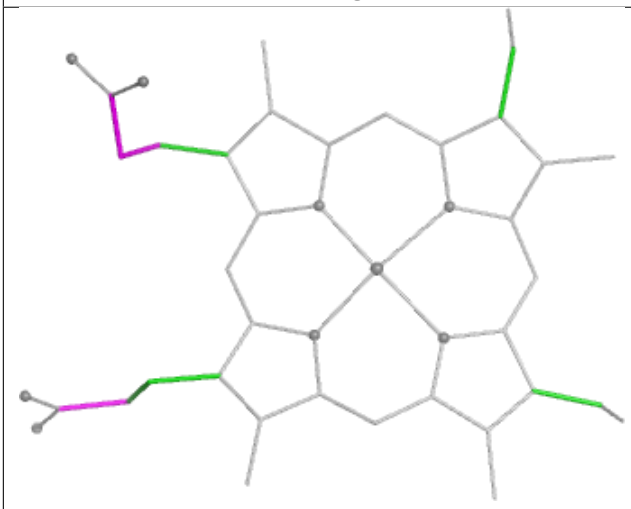


Bond angles



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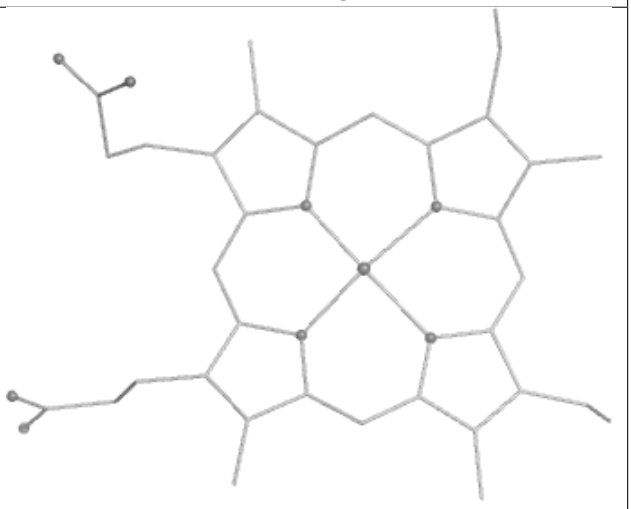
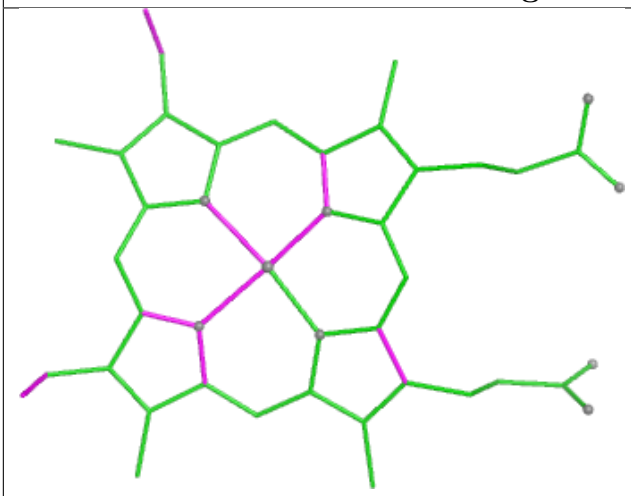


Rings

Ligand HEC H 606



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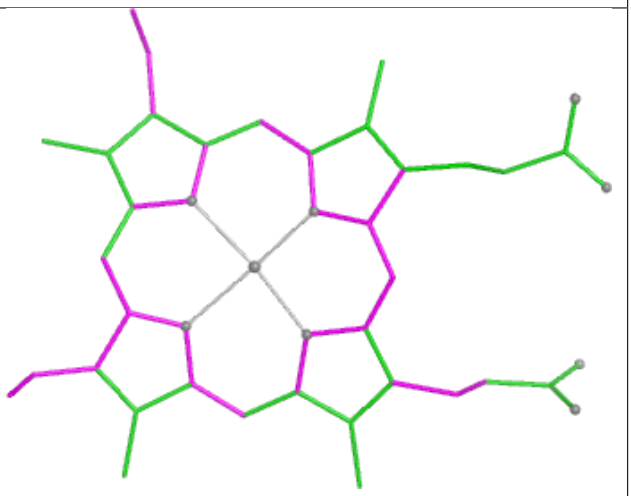

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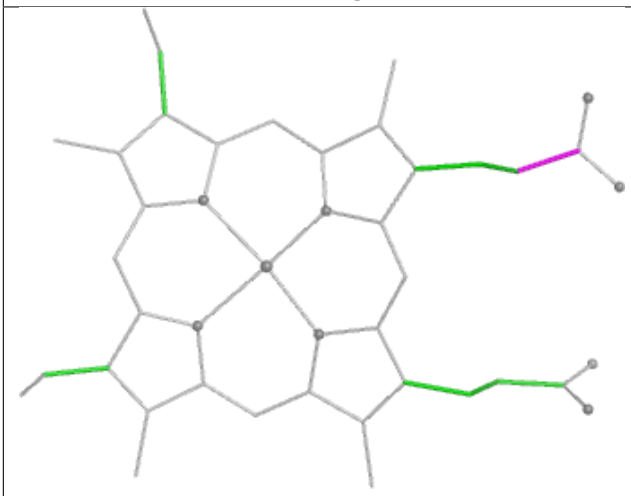

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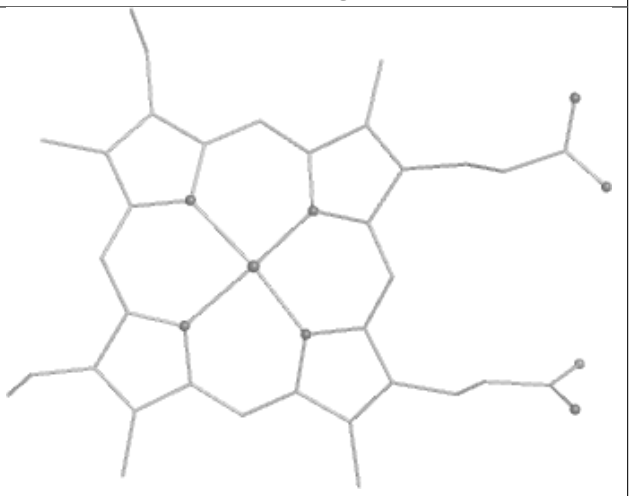

Rings

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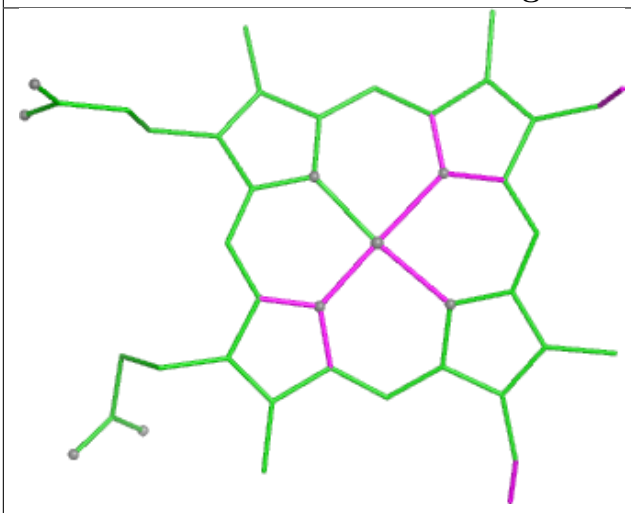

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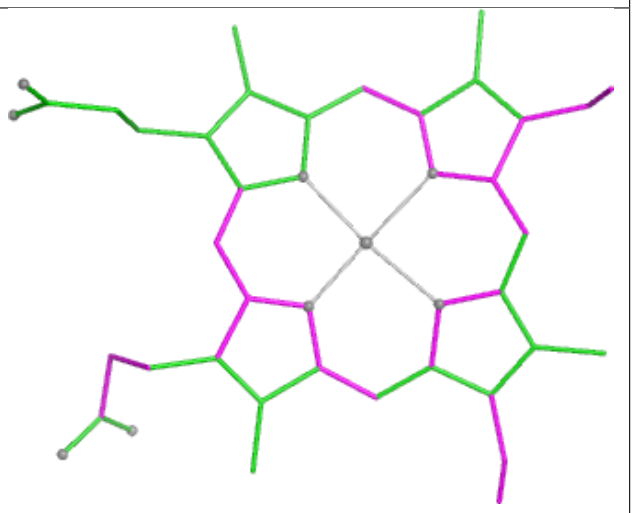

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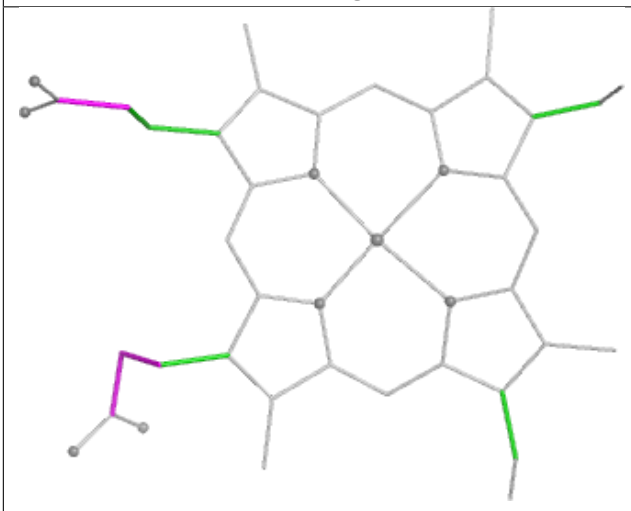

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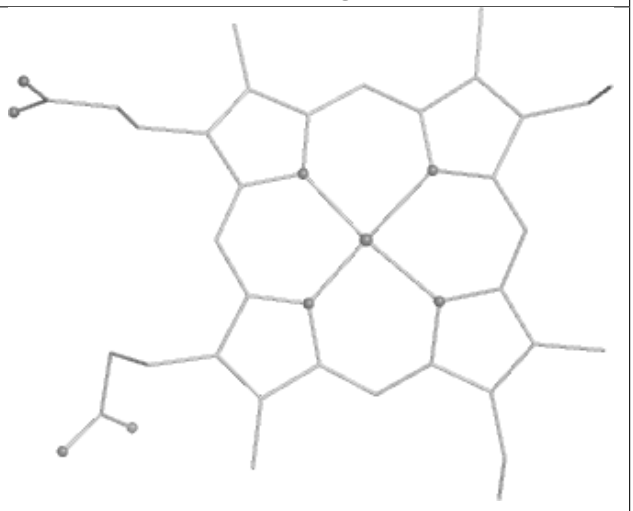

Rings

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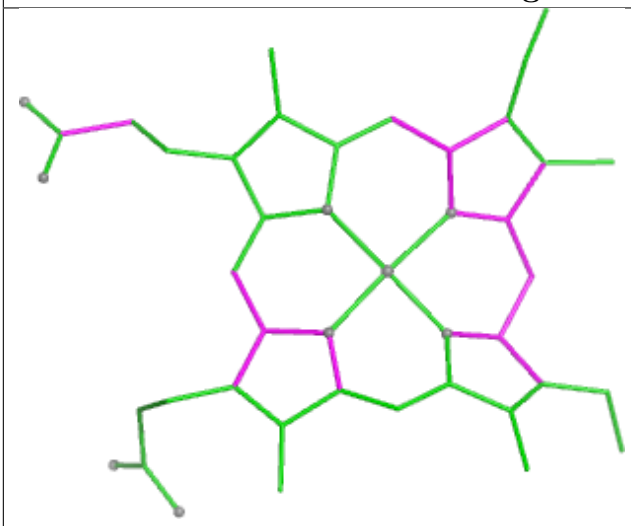

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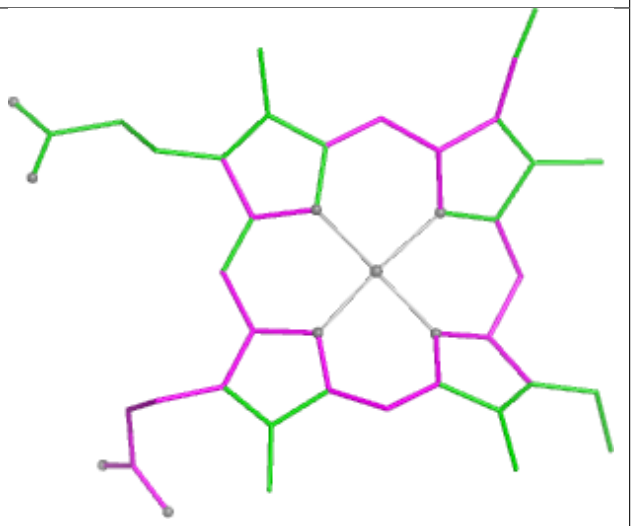

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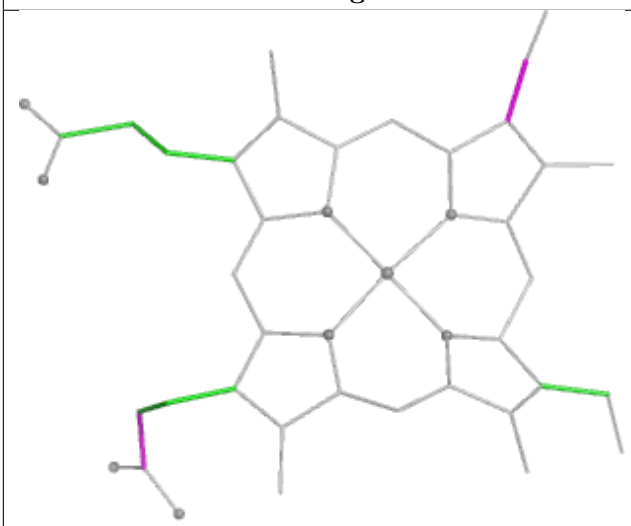

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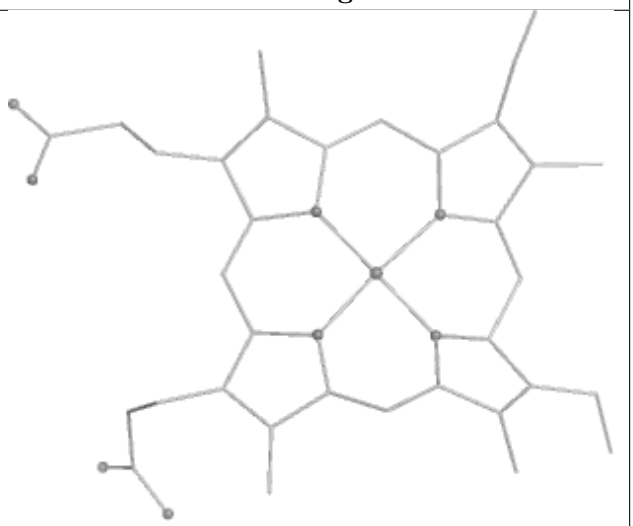

Rings

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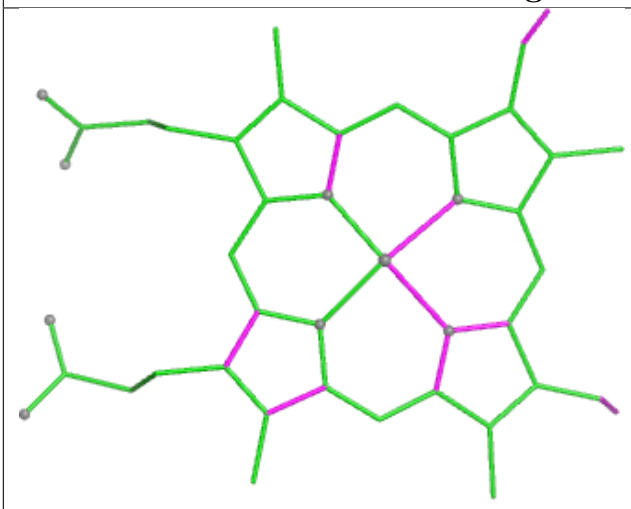

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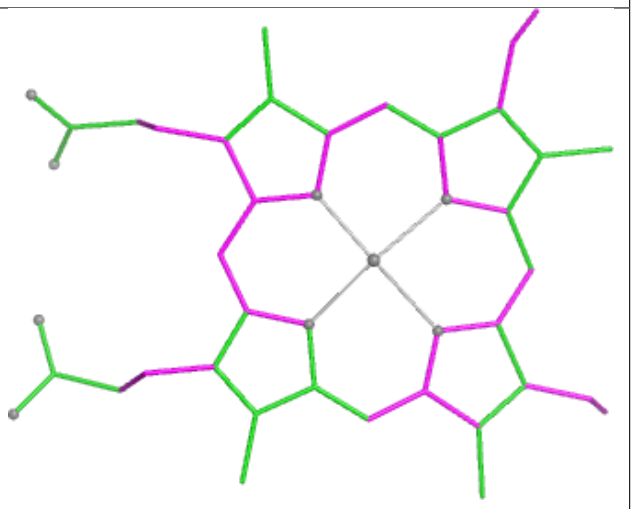

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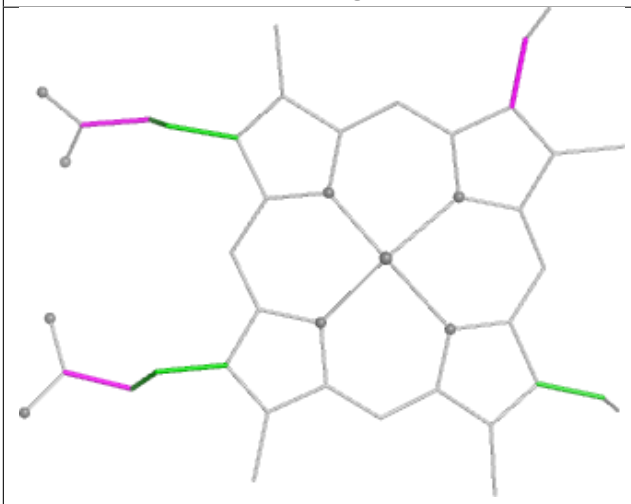

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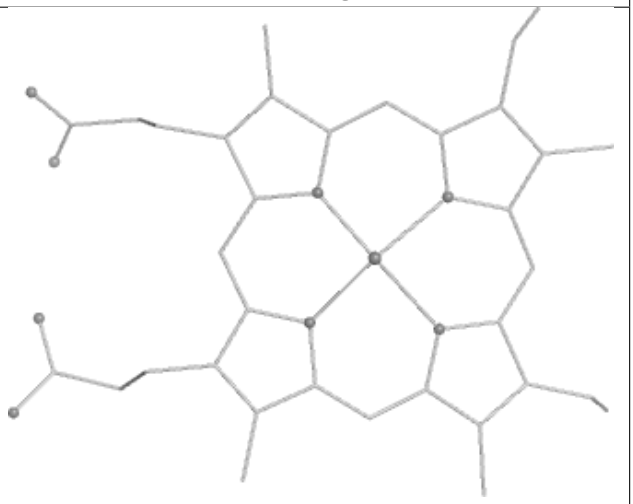

Rings

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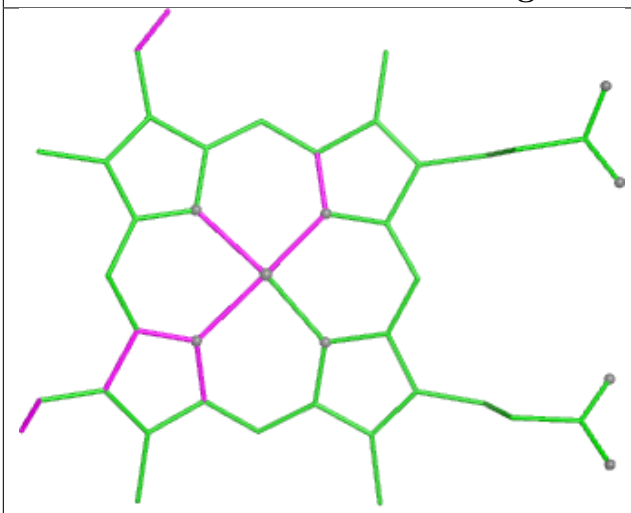

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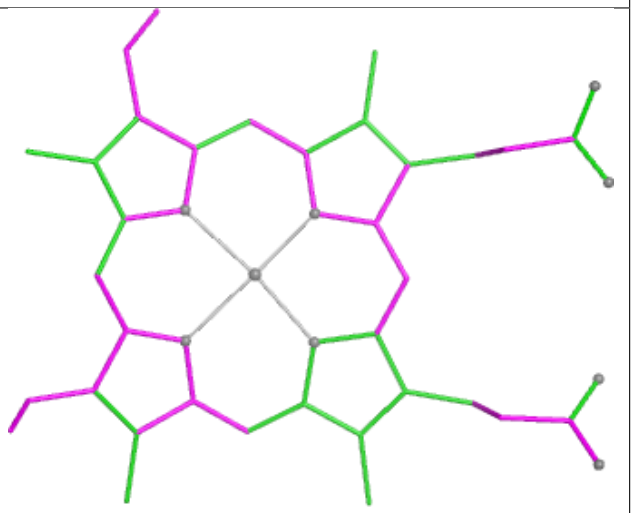

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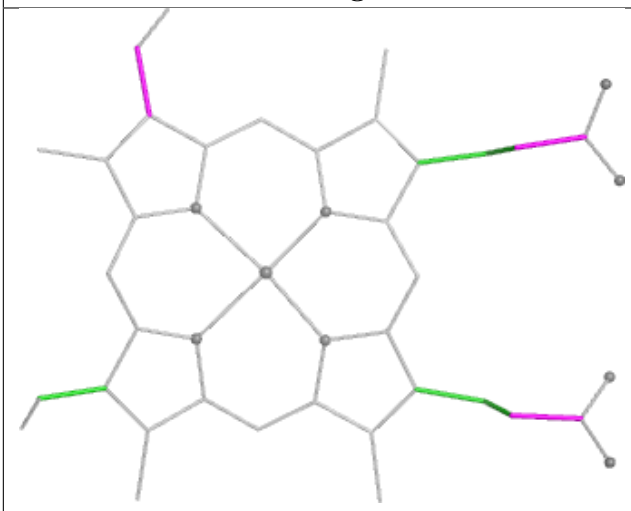

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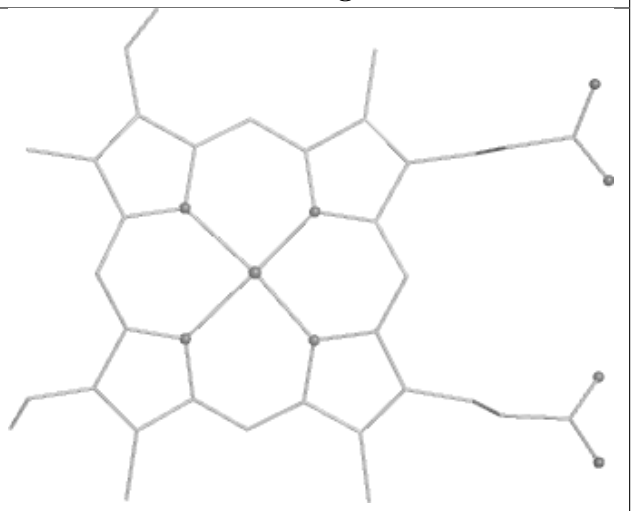

Rings

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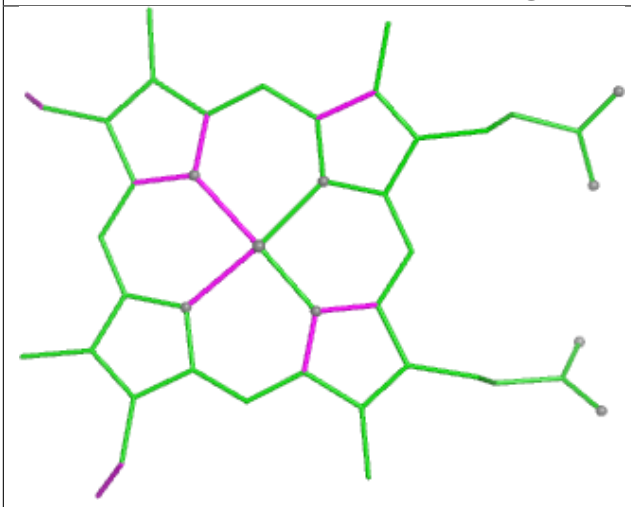

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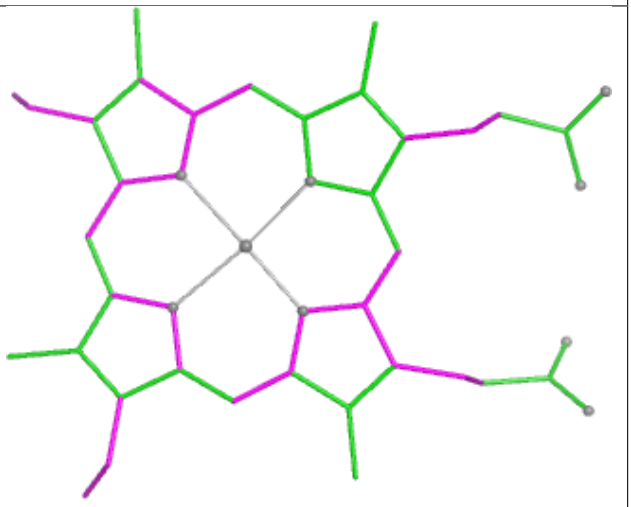

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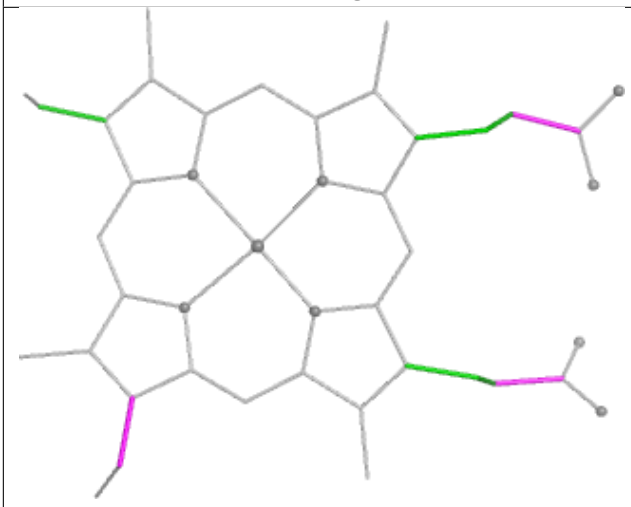

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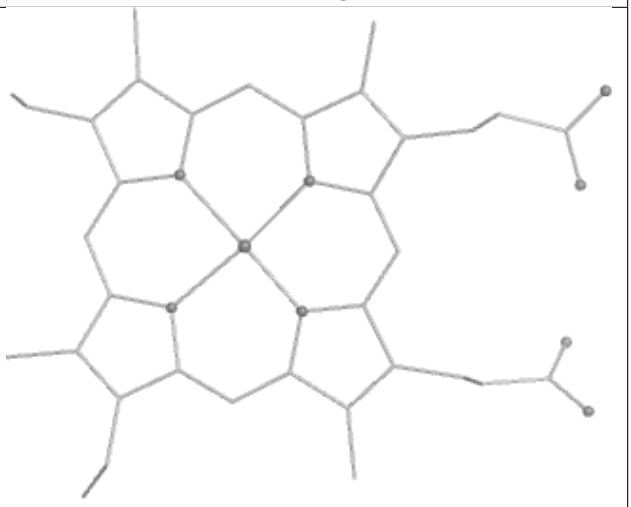

Rings

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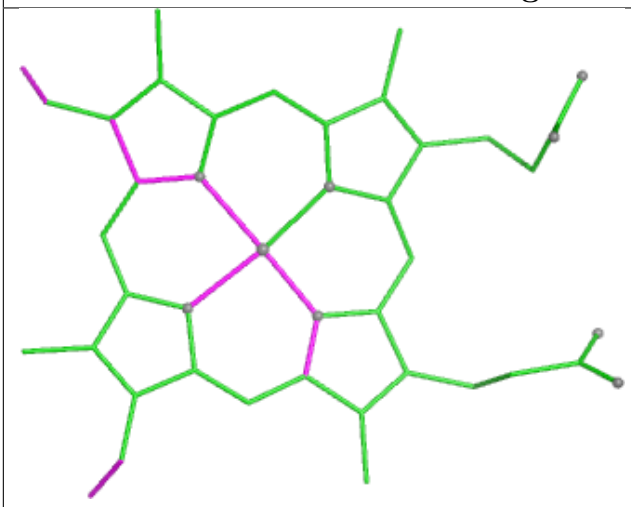

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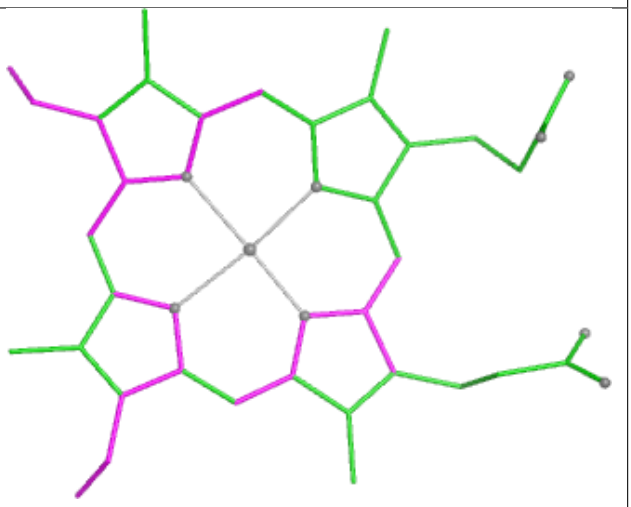

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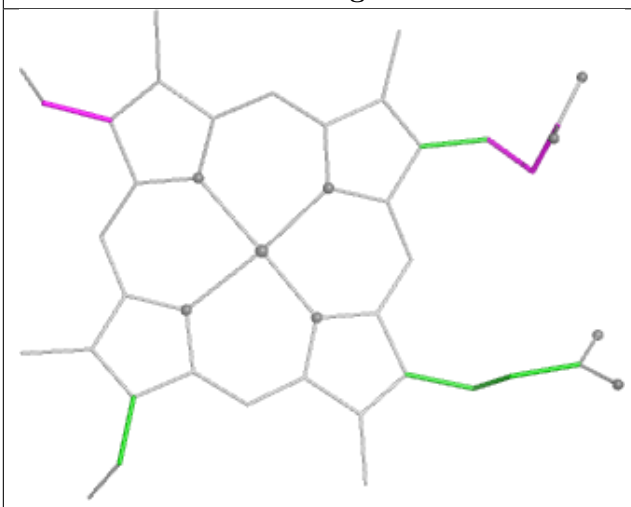

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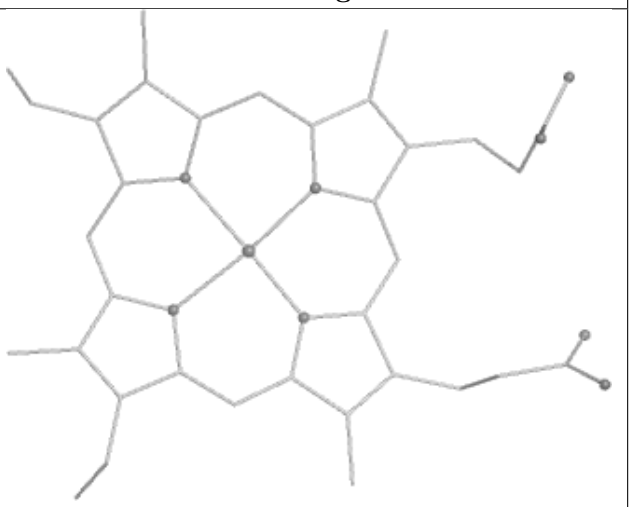

Rings

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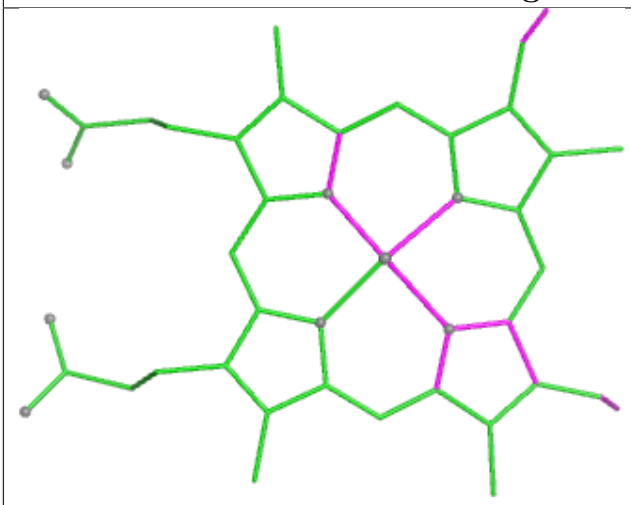

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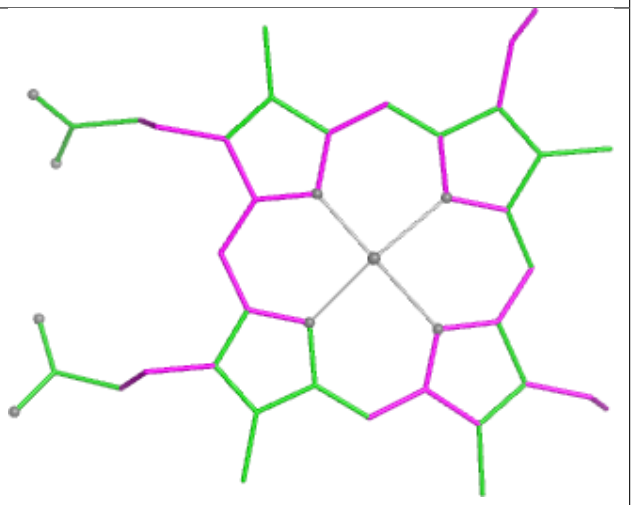

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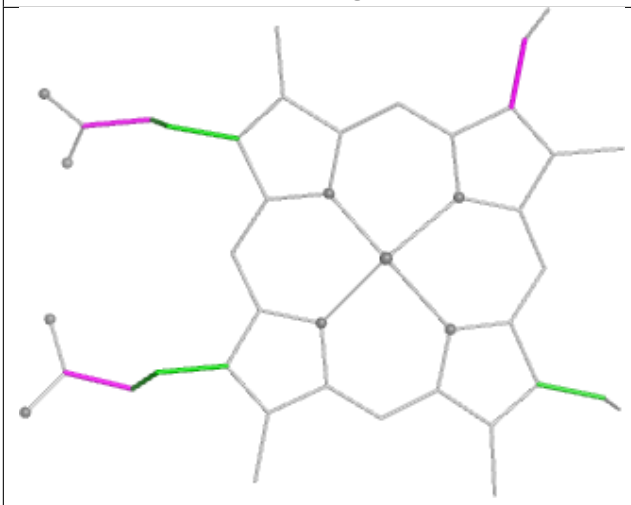

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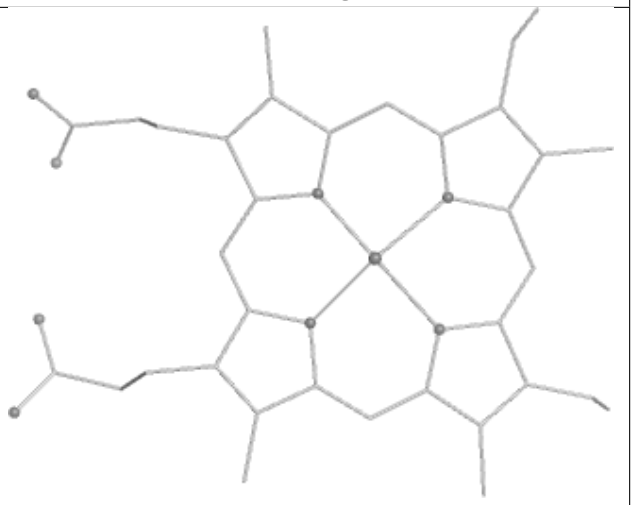

Rings

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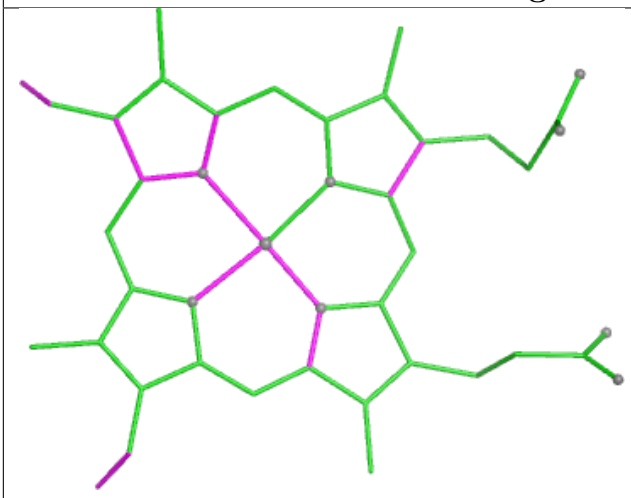

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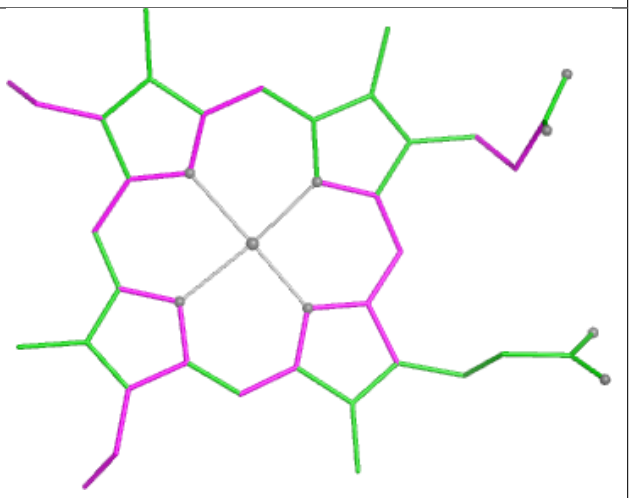

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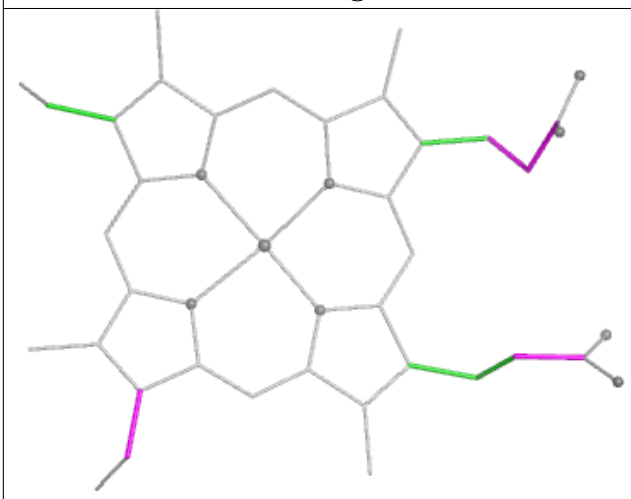

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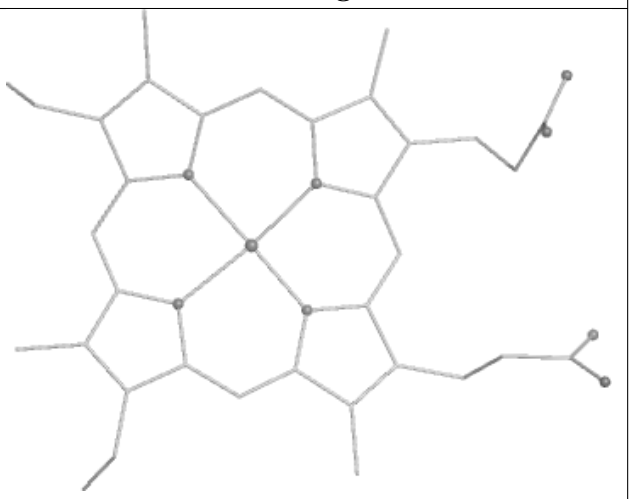

Rings

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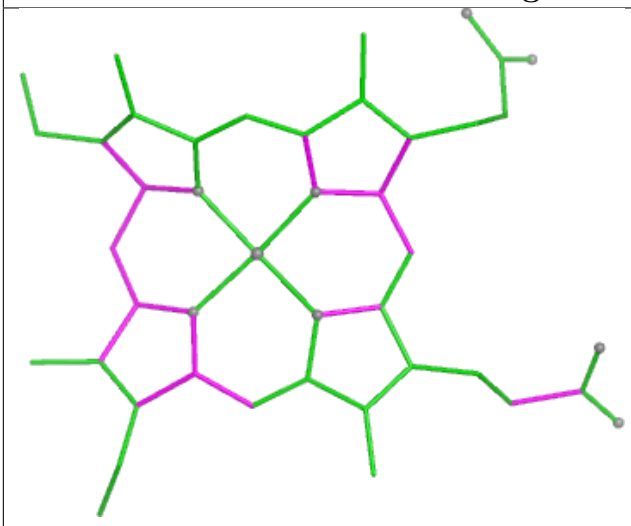

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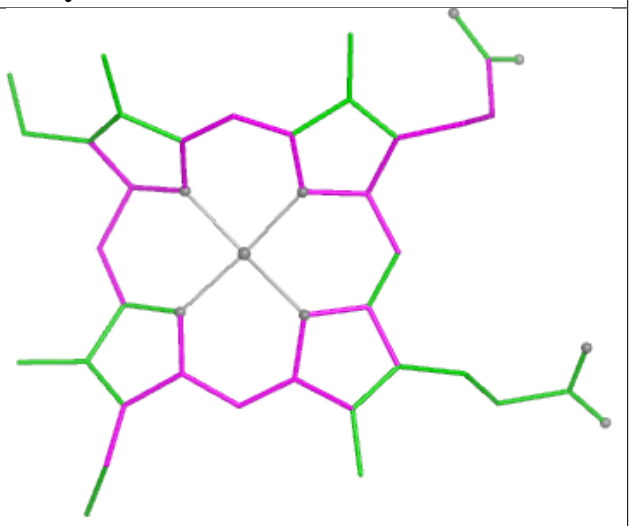

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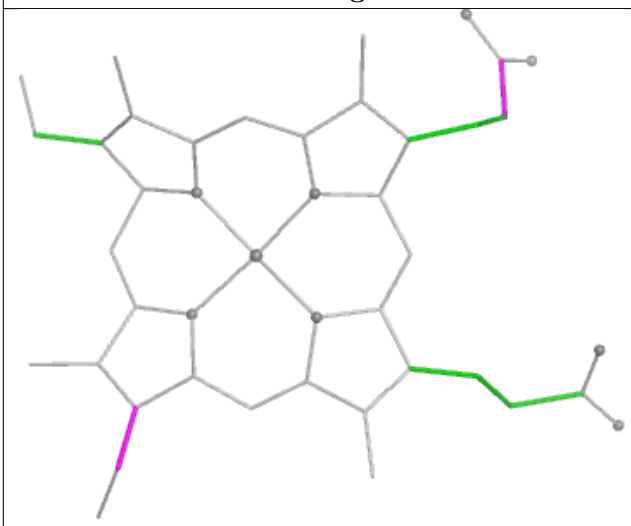

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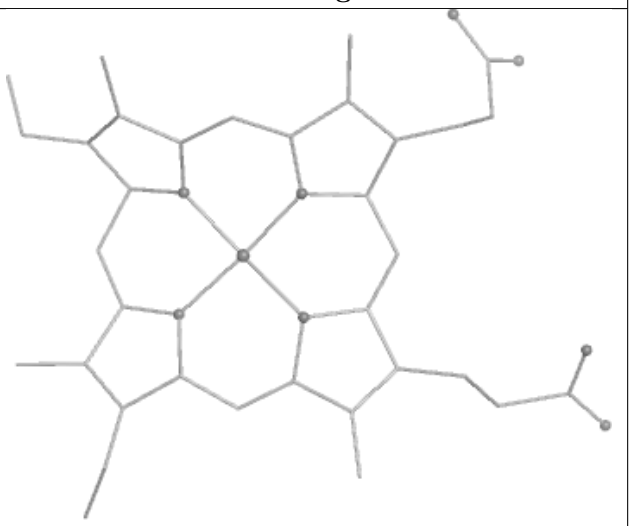
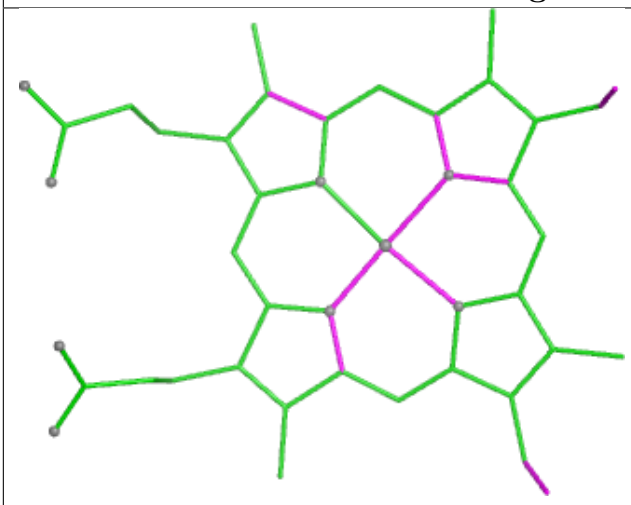


Rings

Ligand HEC I 604



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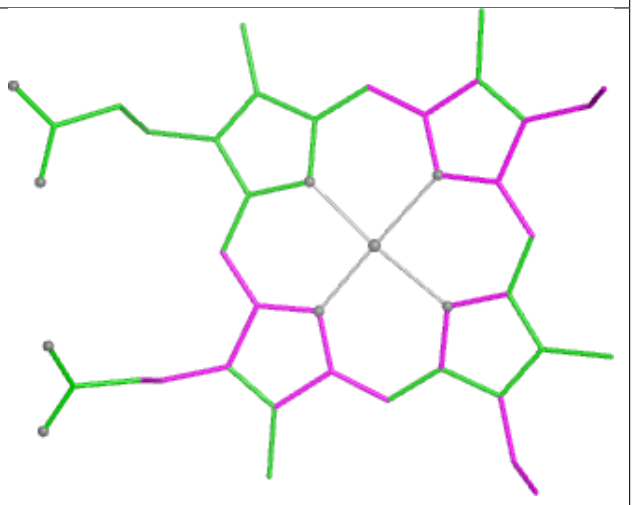

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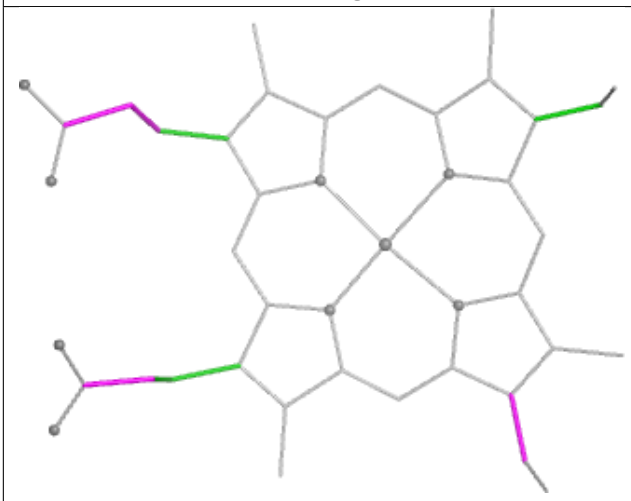

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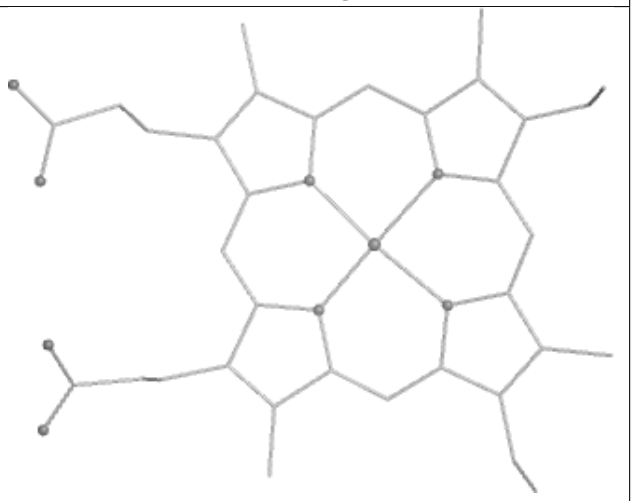
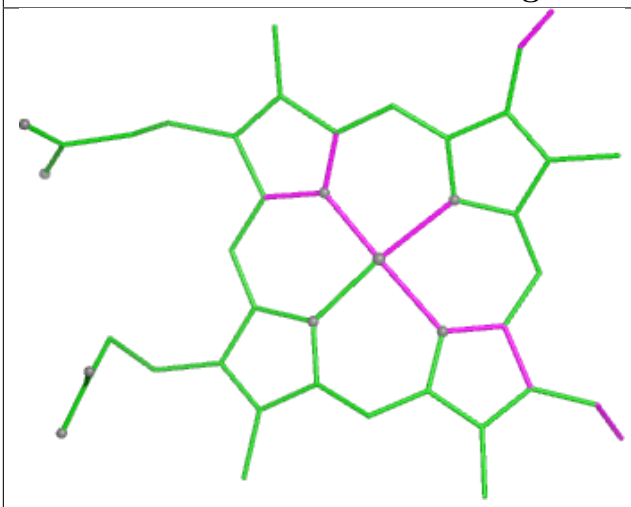


Rings

Ligand HEC U 607



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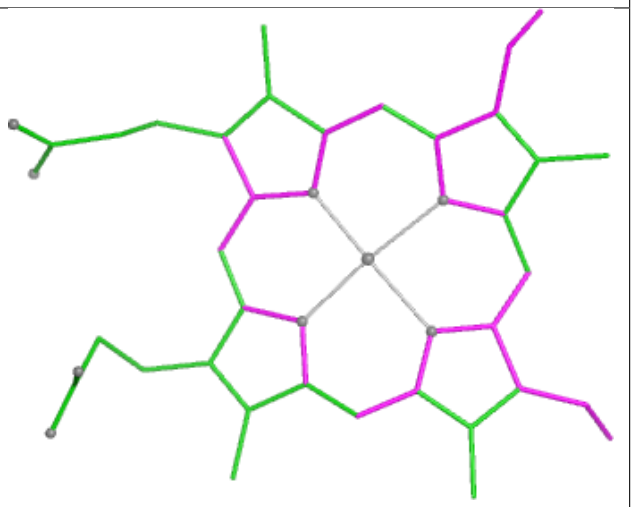

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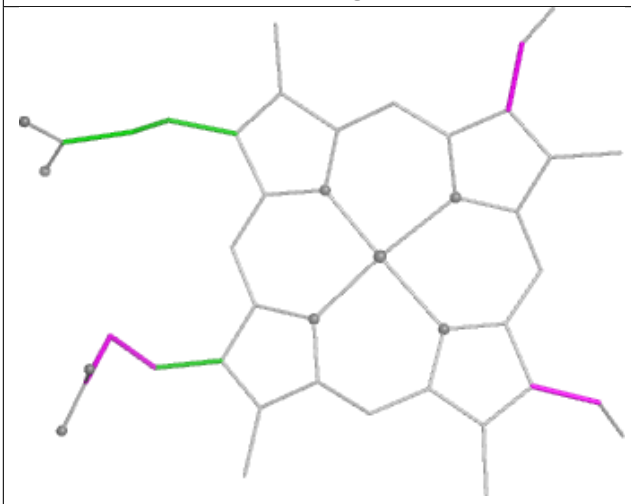

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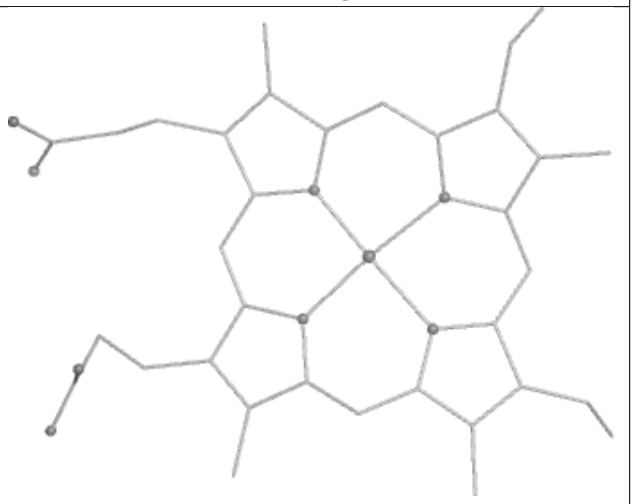

Rings

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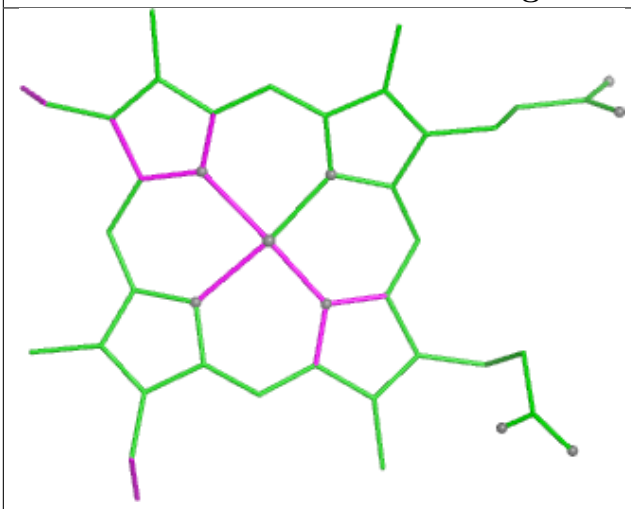

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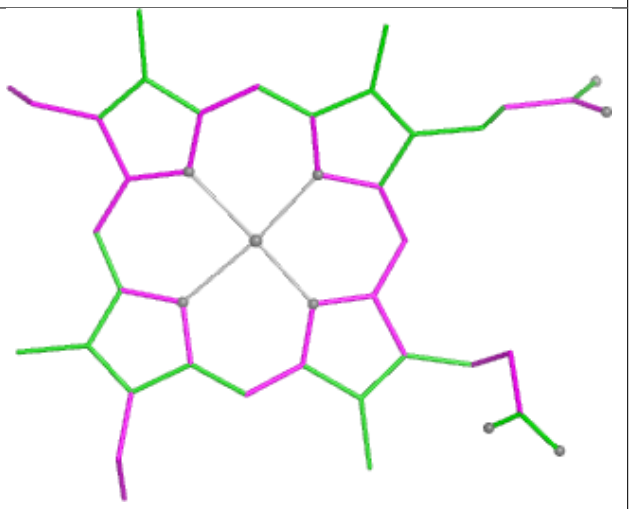

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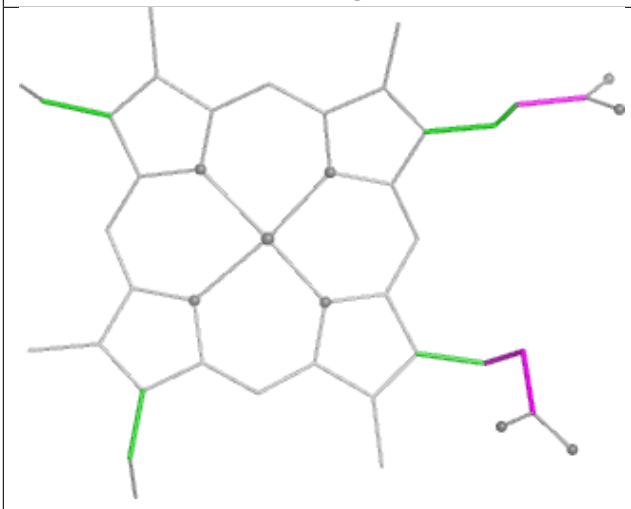

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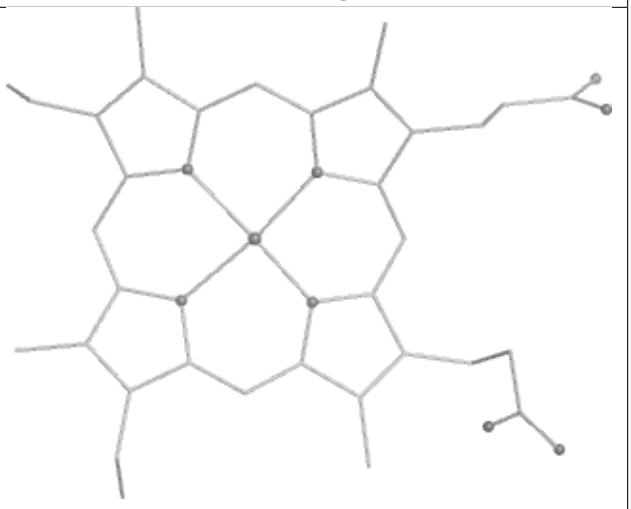
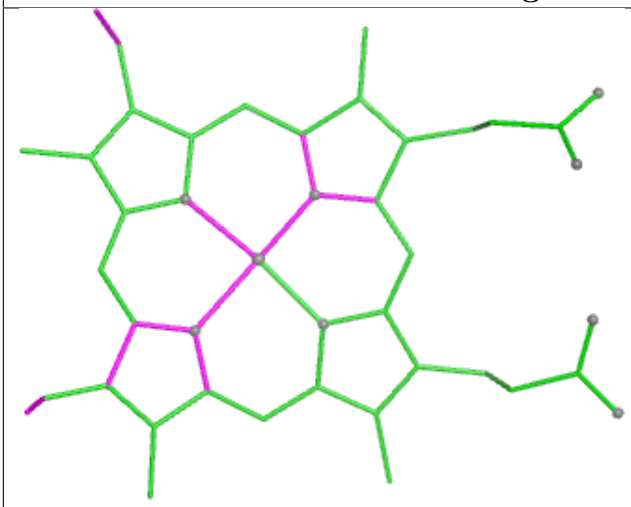


Rings

Ligand HEC U 604



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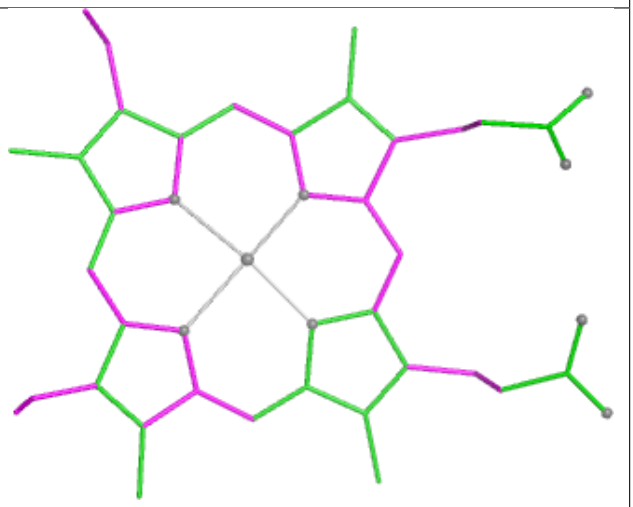
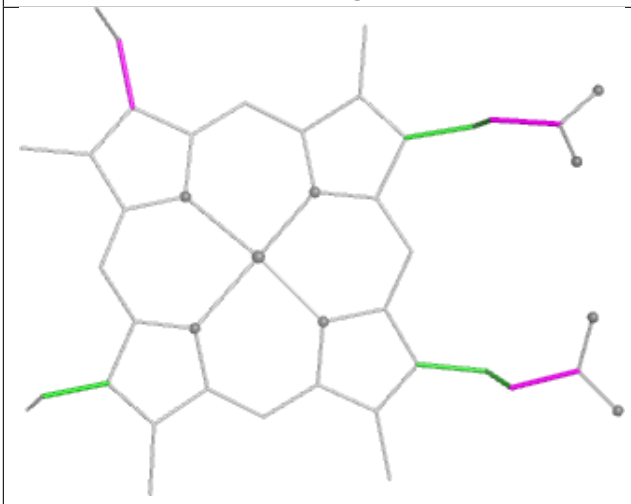


Bond angles



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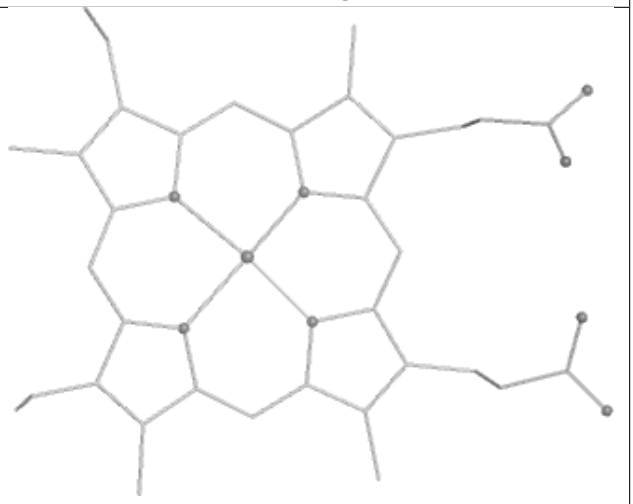
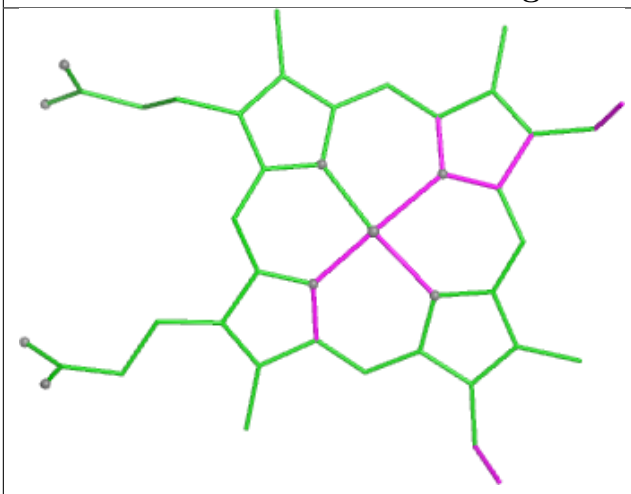


Rings

Ligand HEC A 605



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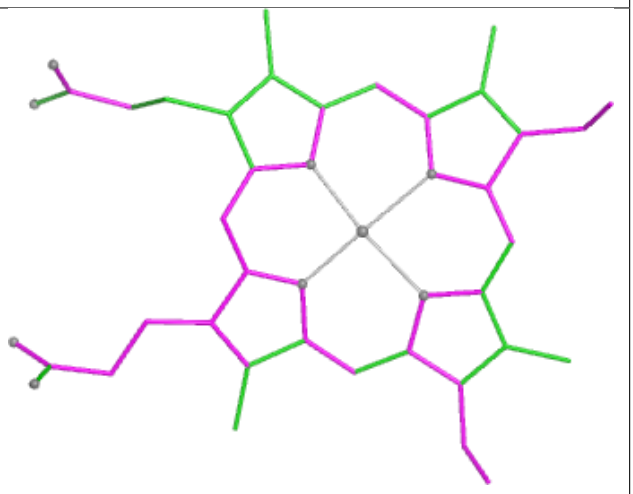

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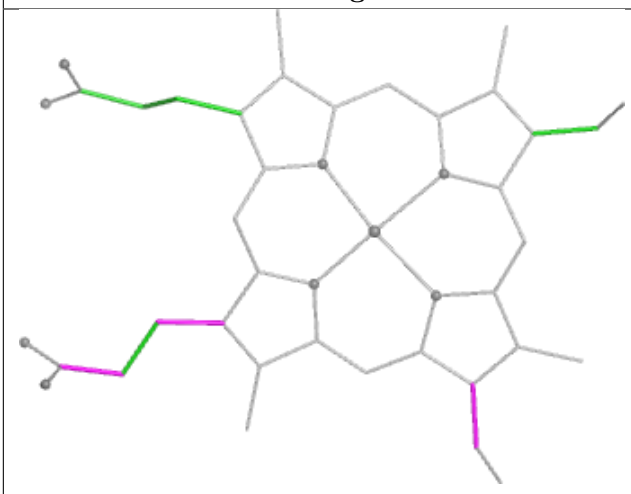

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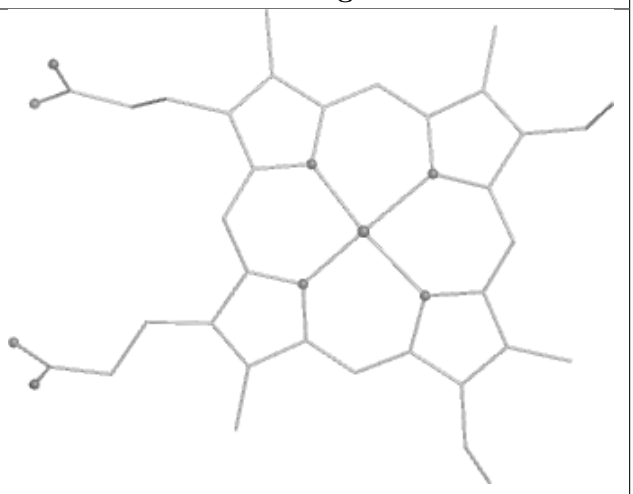
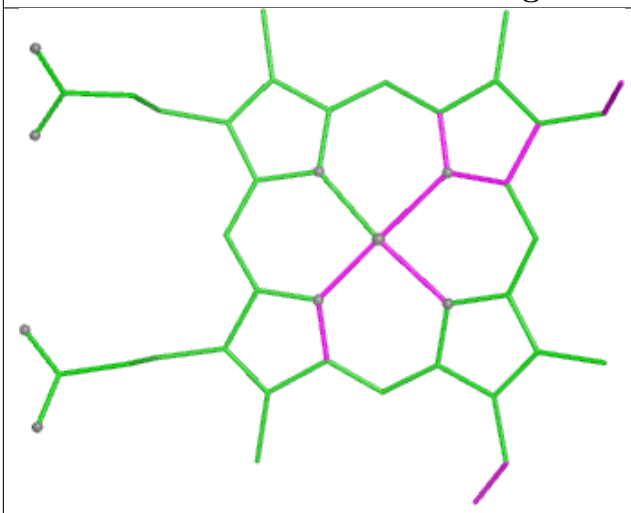


Rings

Ligand HEC Q 600



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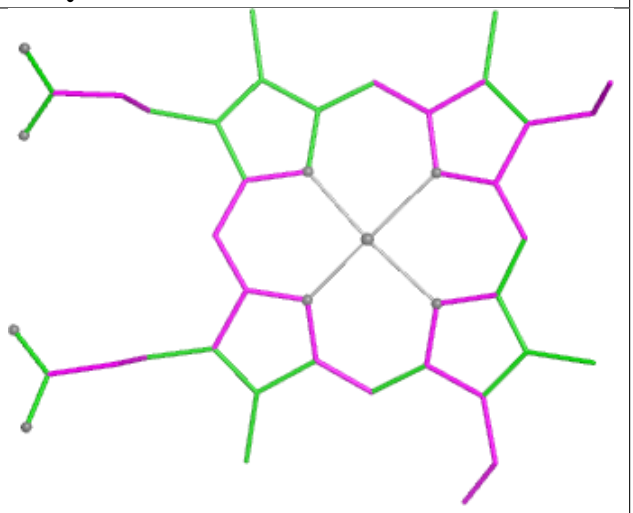

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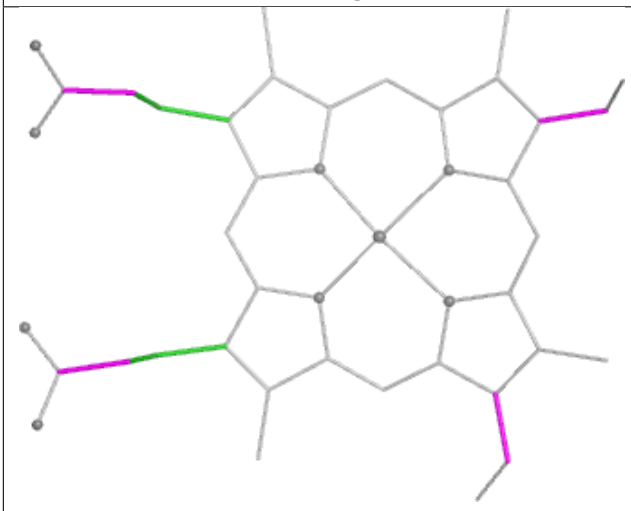

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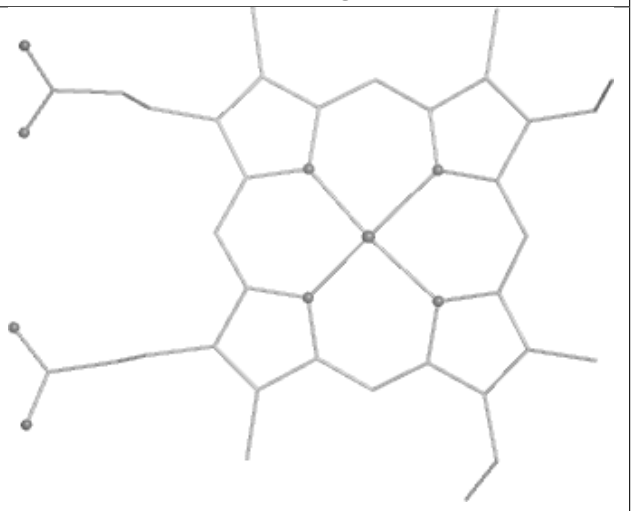
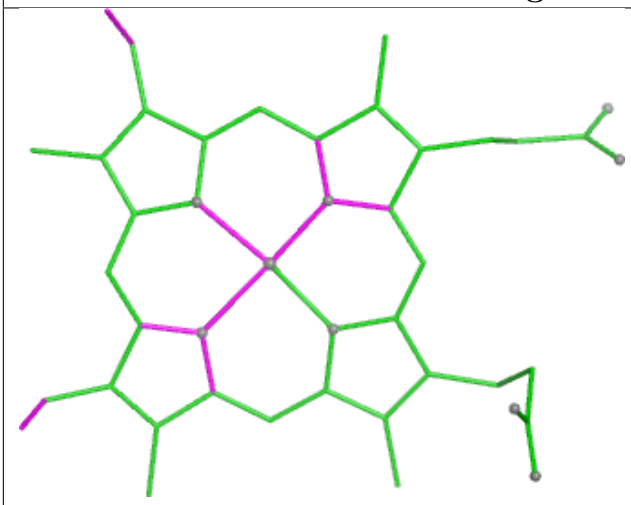


Rings

Ligand HEC J 601



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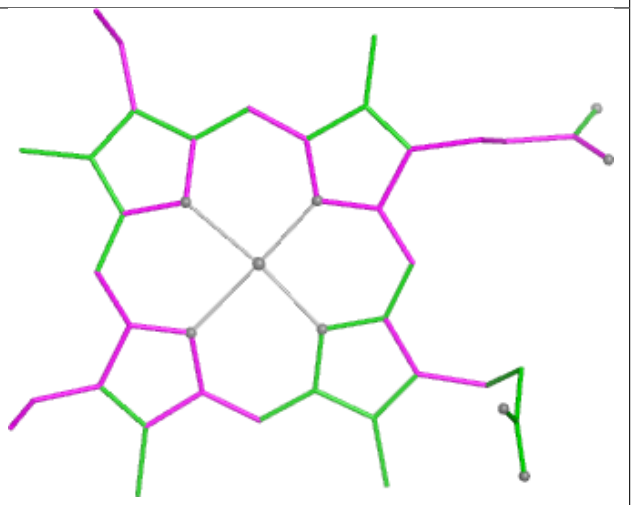

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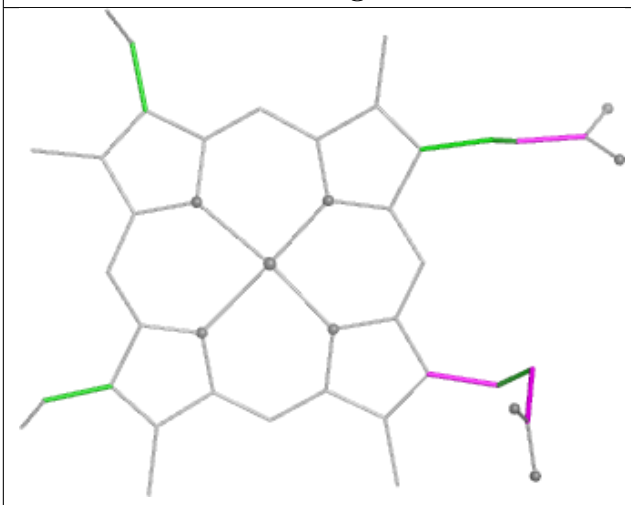

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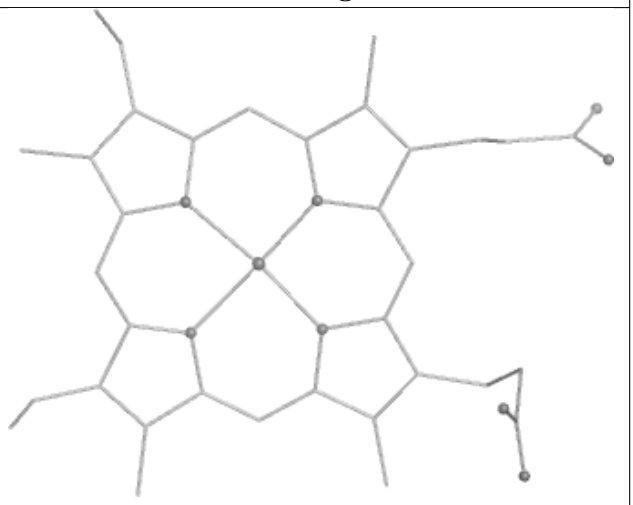
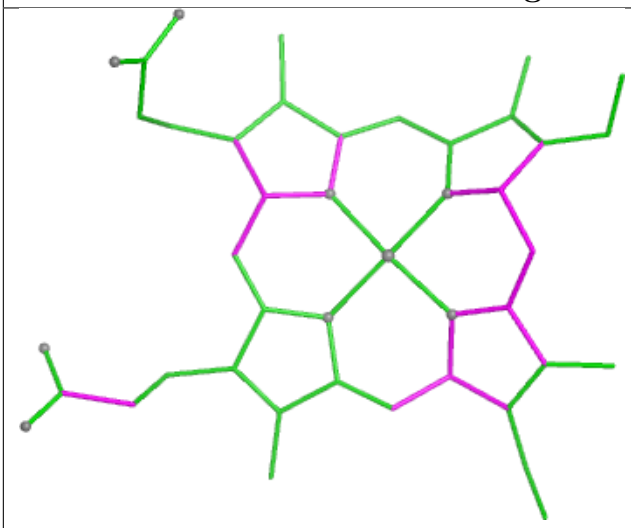


Rings

Ligand HEC E 603



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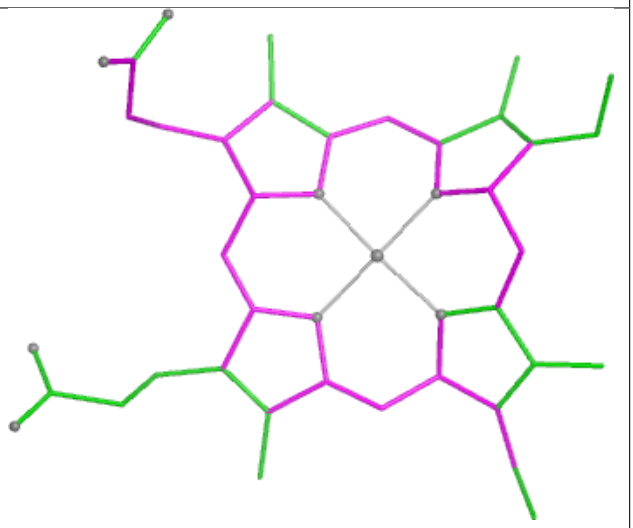

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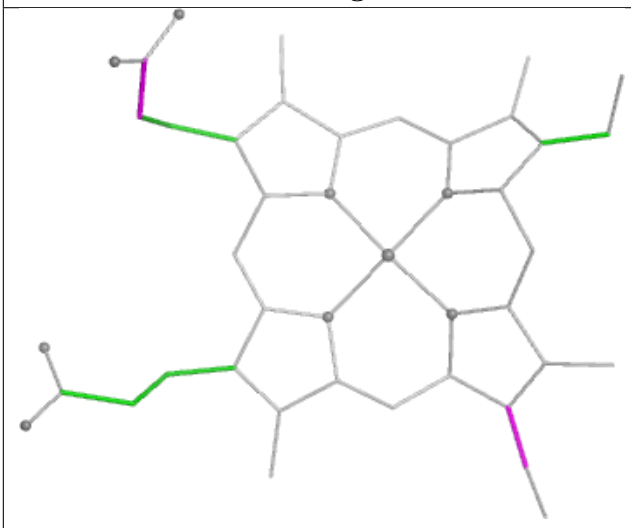

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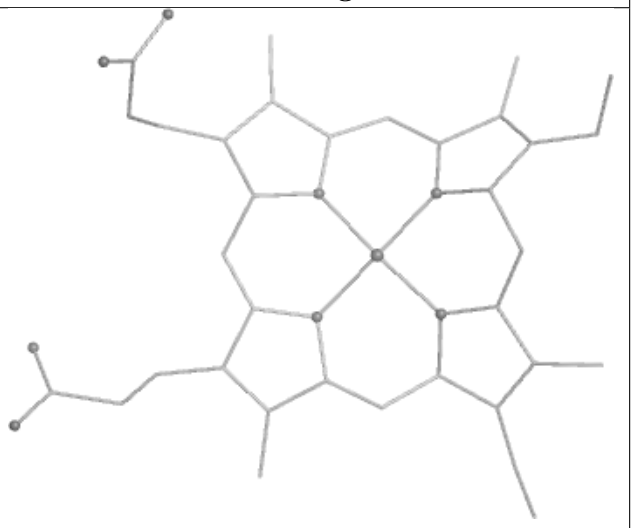
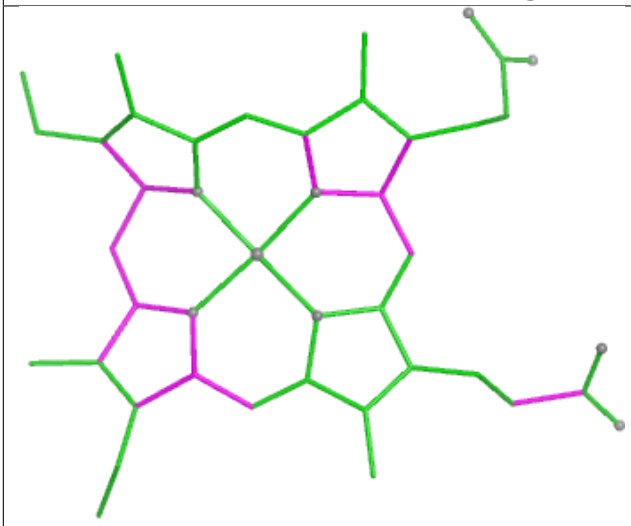


Rings

Ligand HEC N 603



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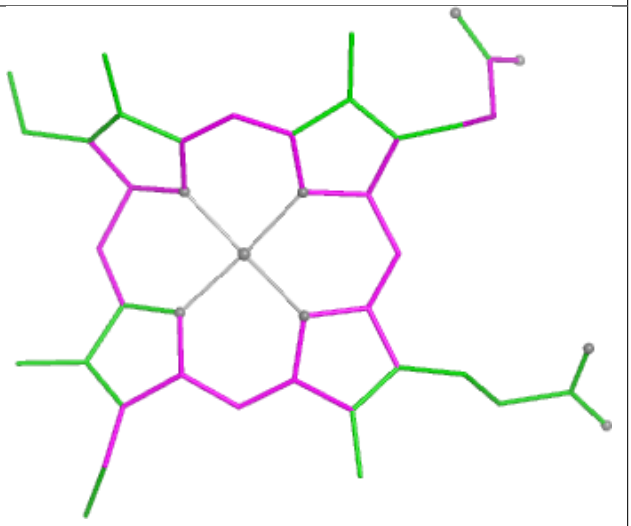

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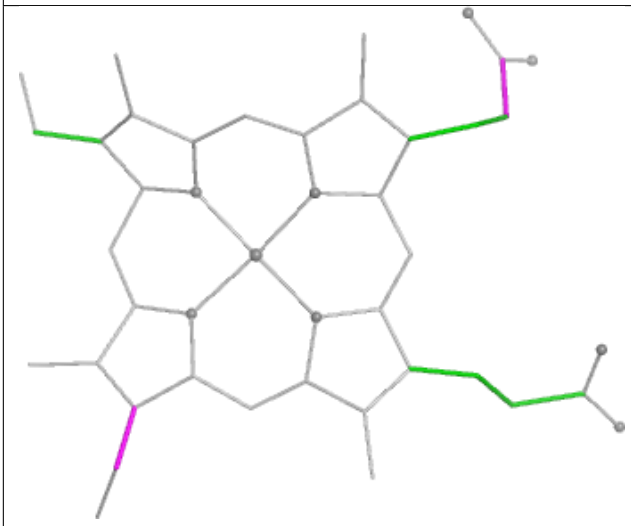

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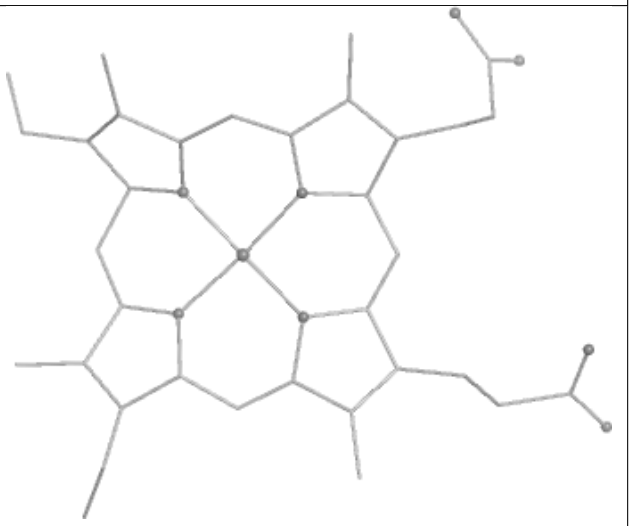
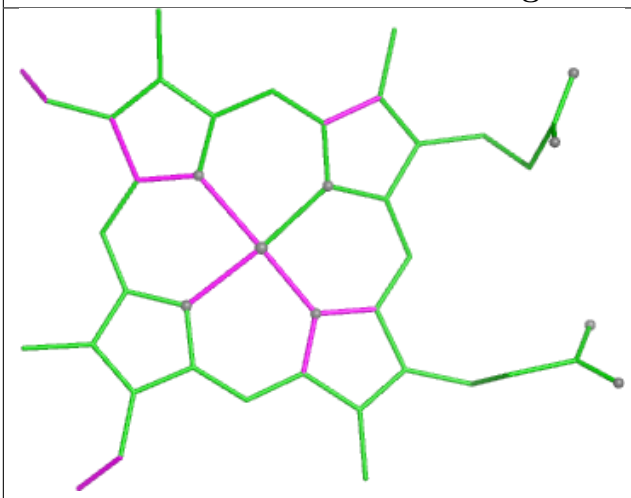


Rings

Ligand HEC D 607



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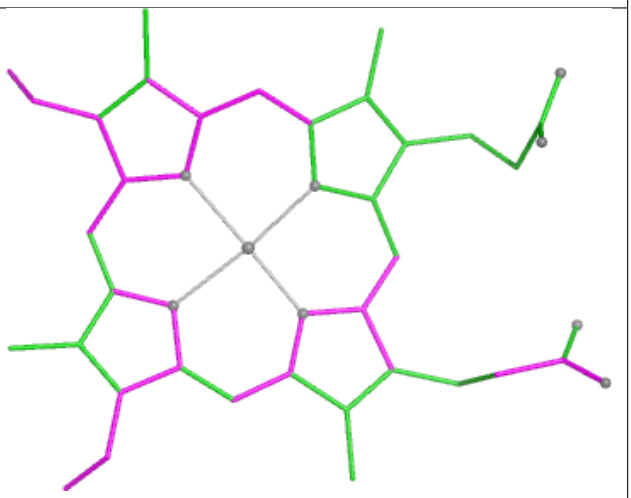

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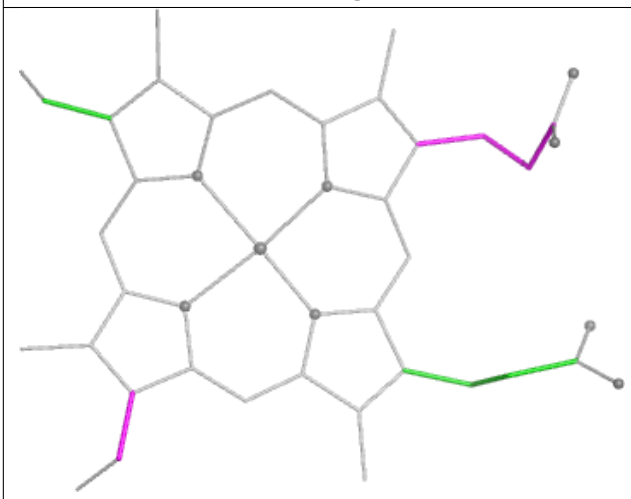

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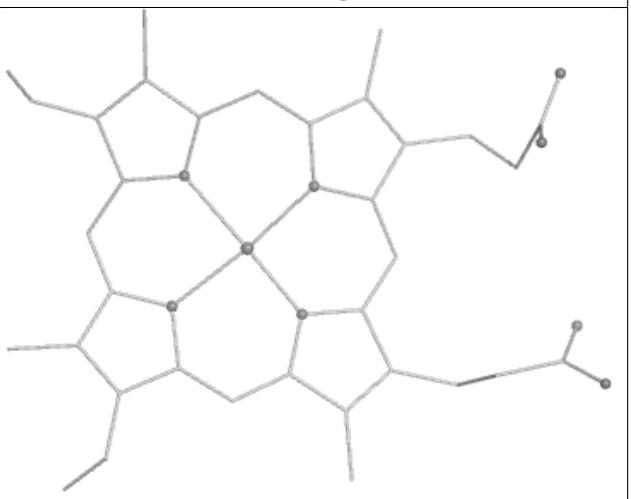
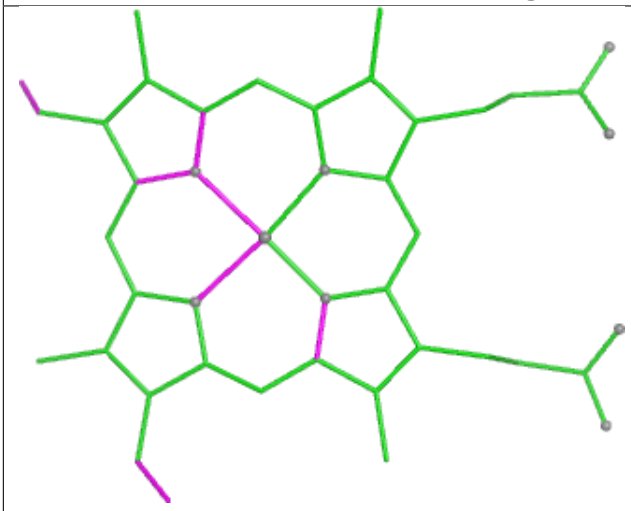


Rings

Ligand HEC X 600



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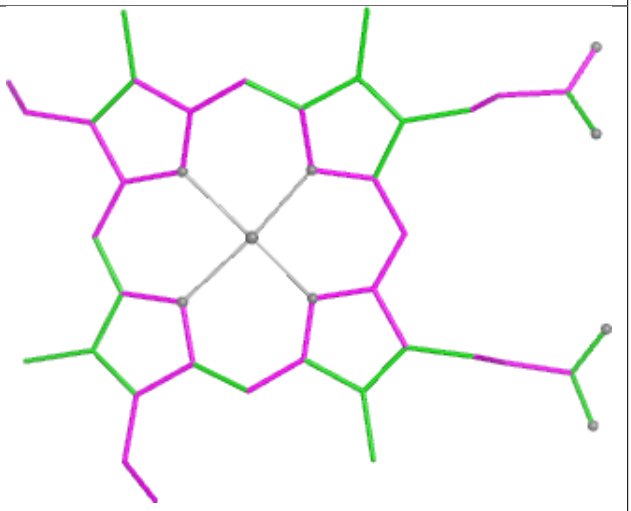

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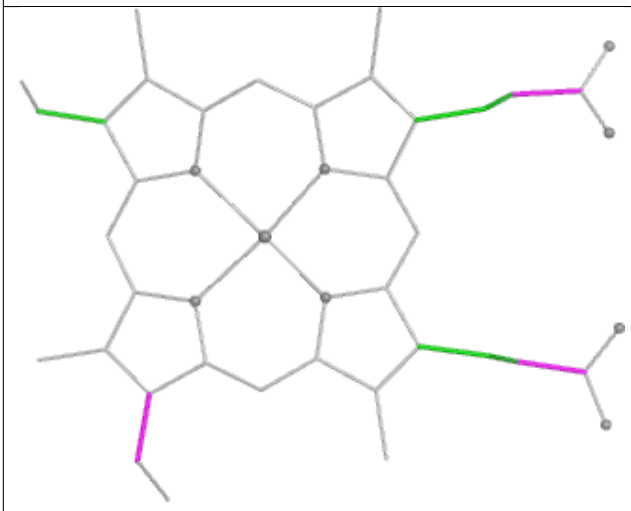

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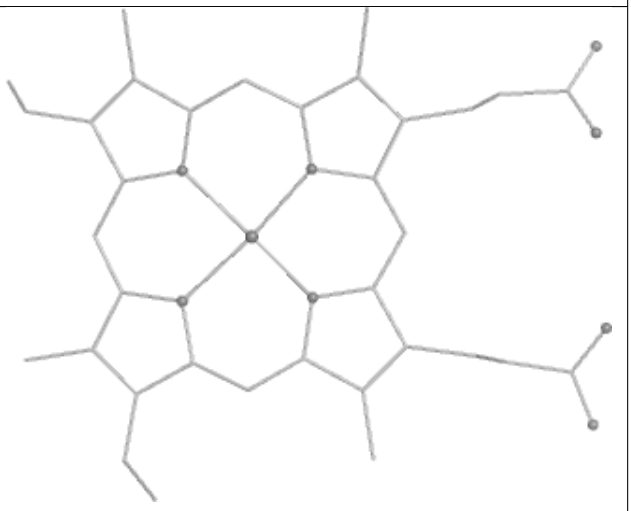

Rings

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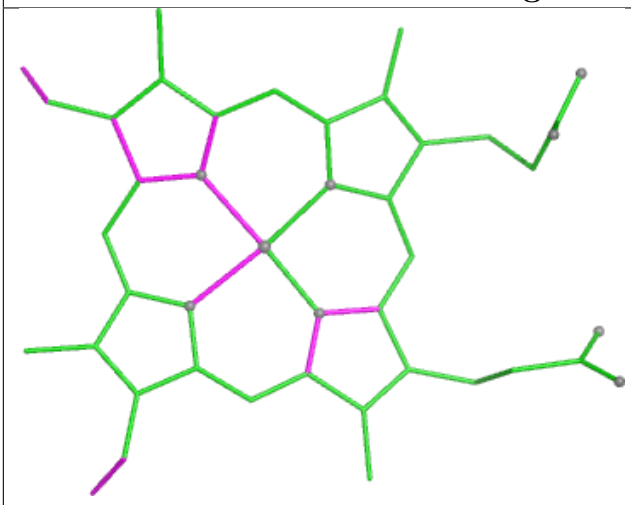

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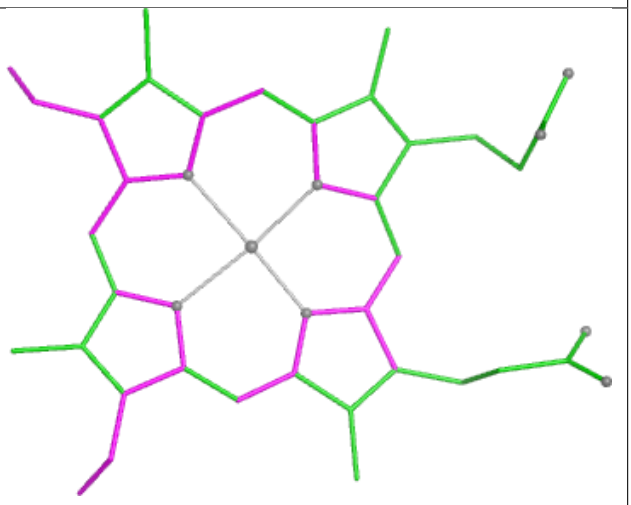

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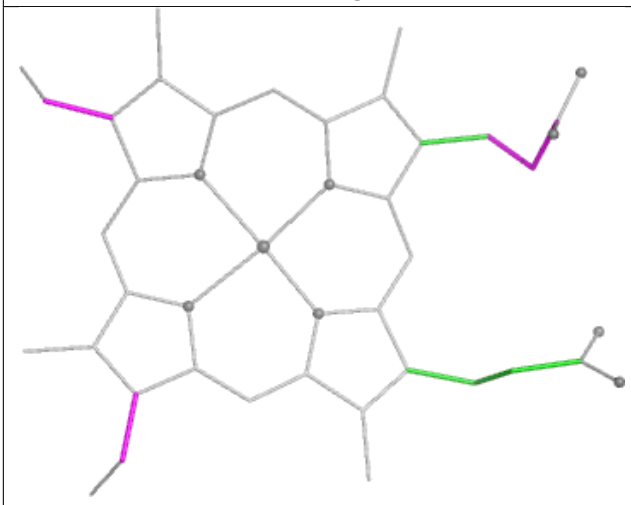

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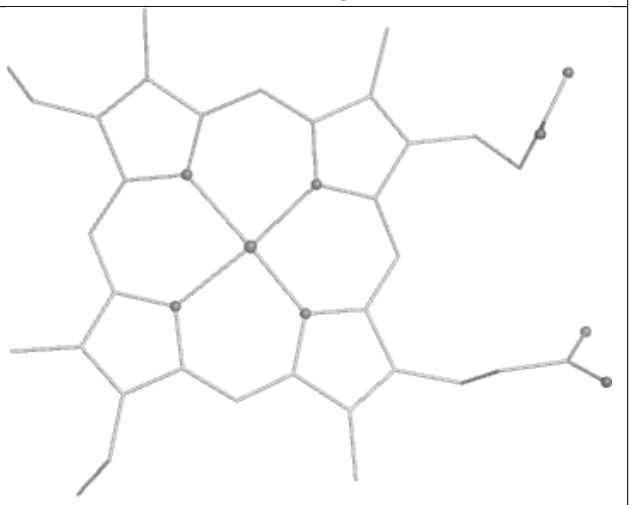

Rings

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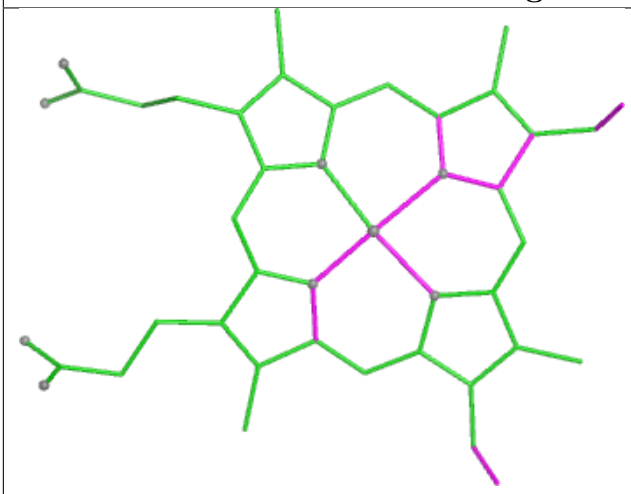

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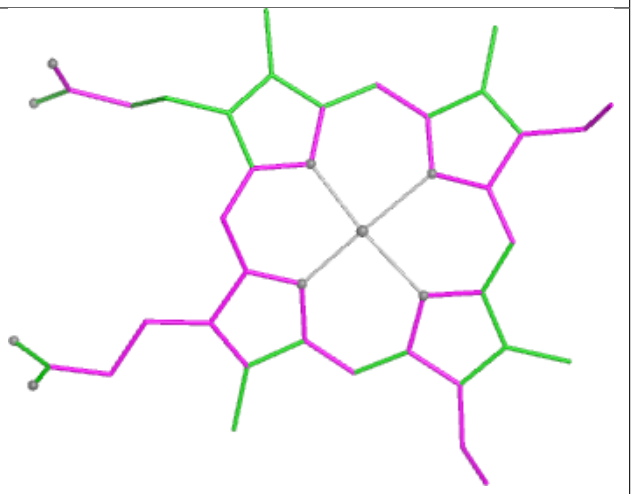

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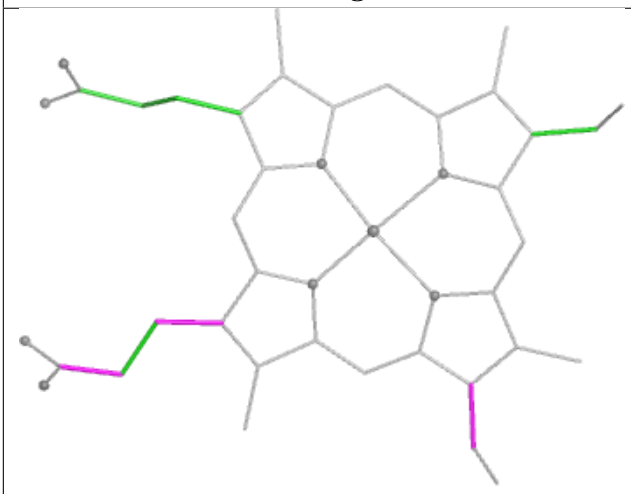

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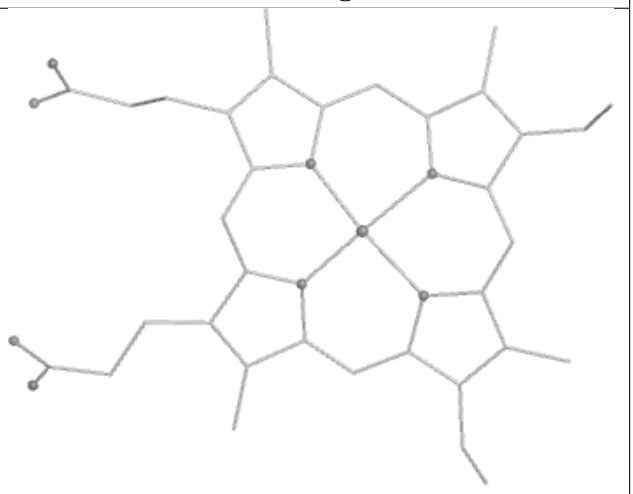

Rings

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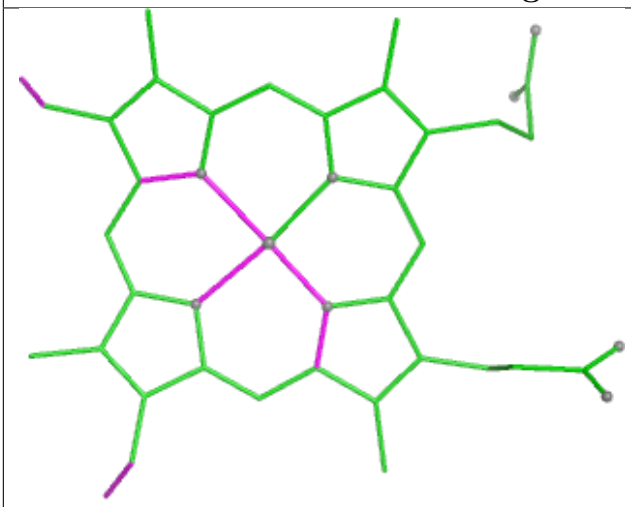

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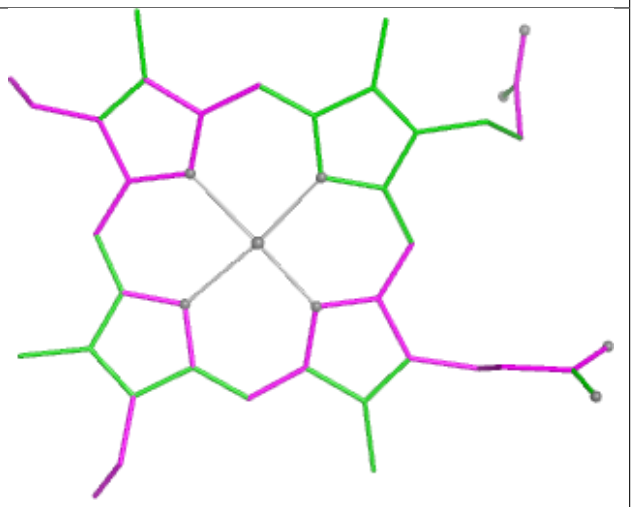

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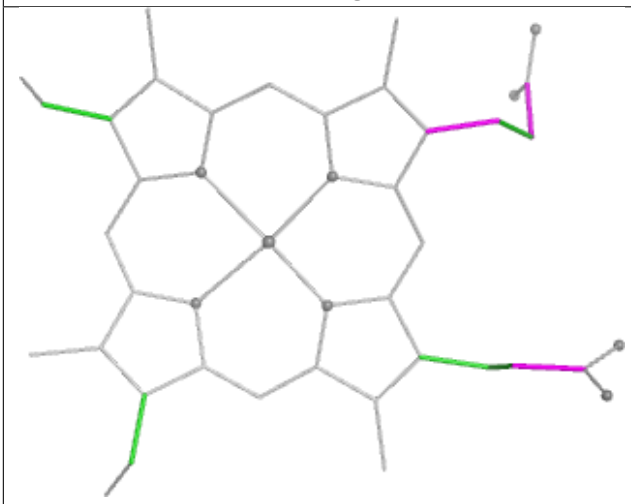

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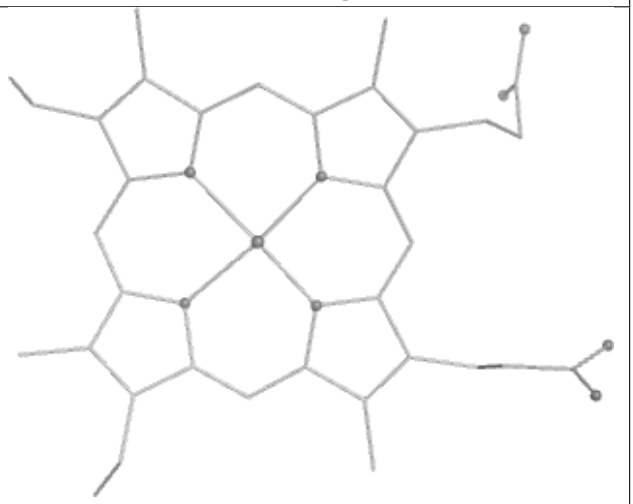
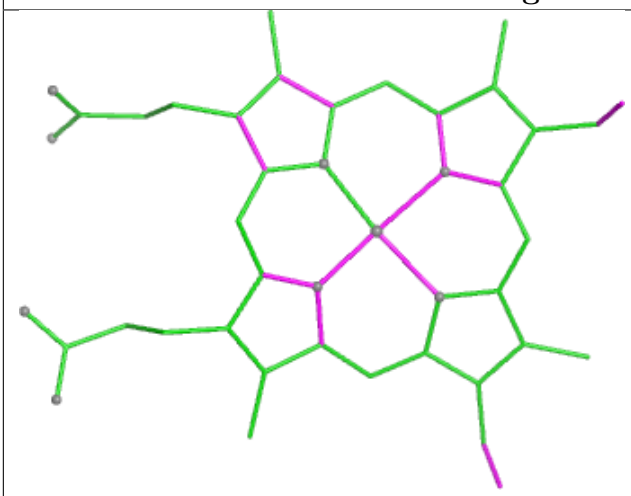


Rings

Ligand HEC R 606



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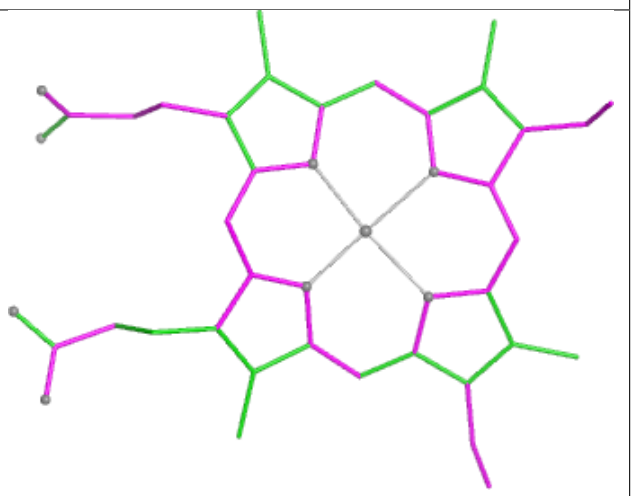

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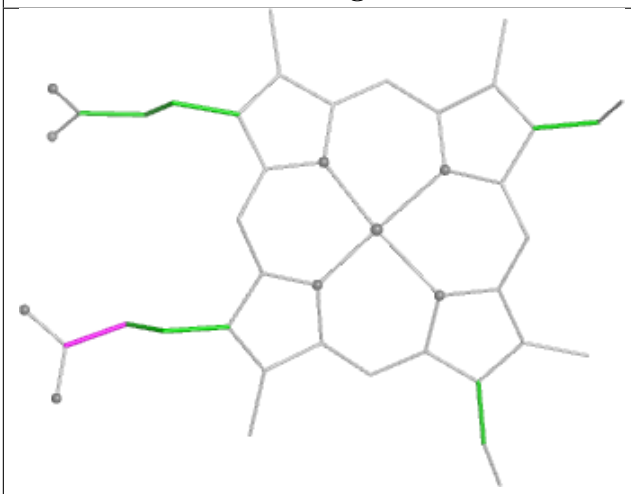

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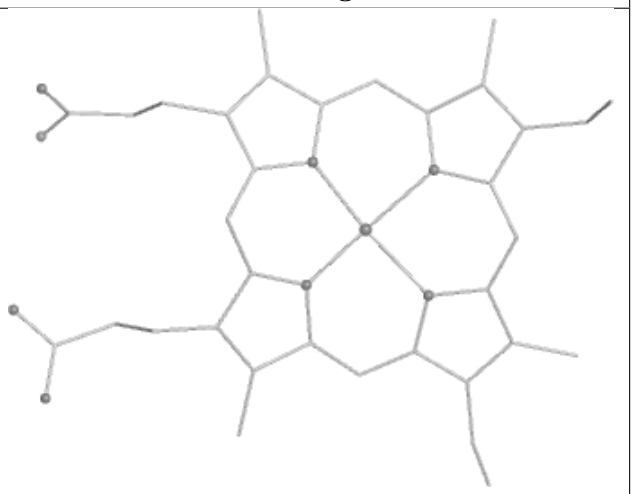

Rings

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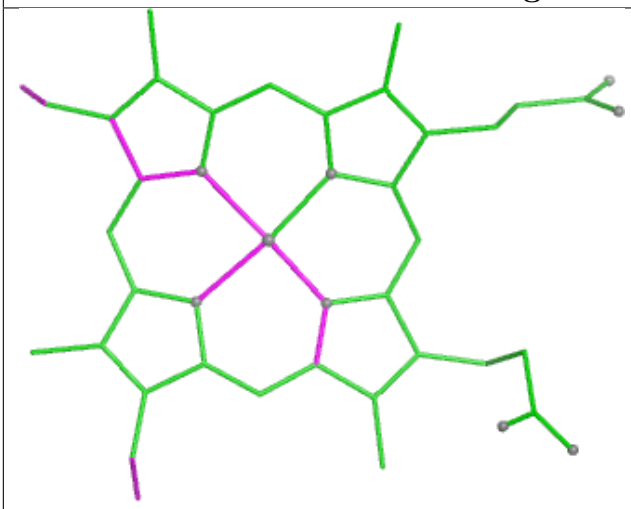

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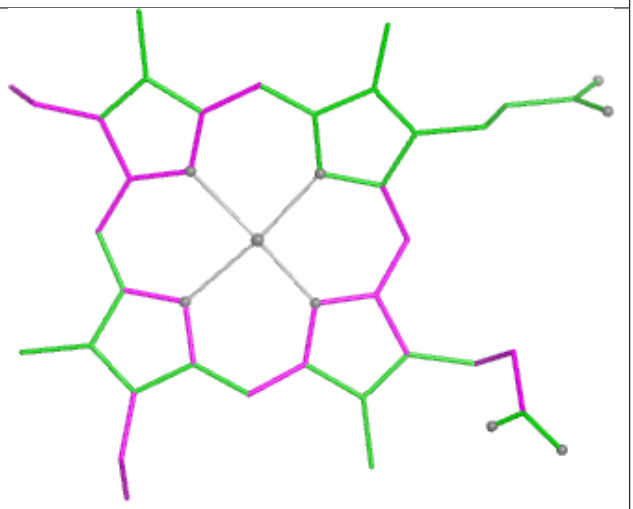

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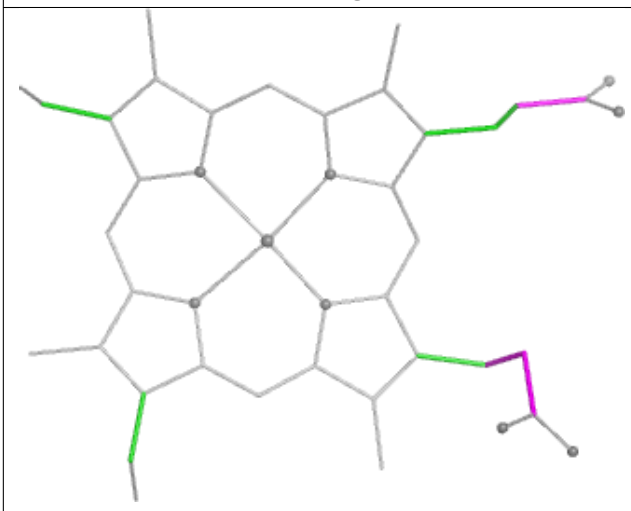

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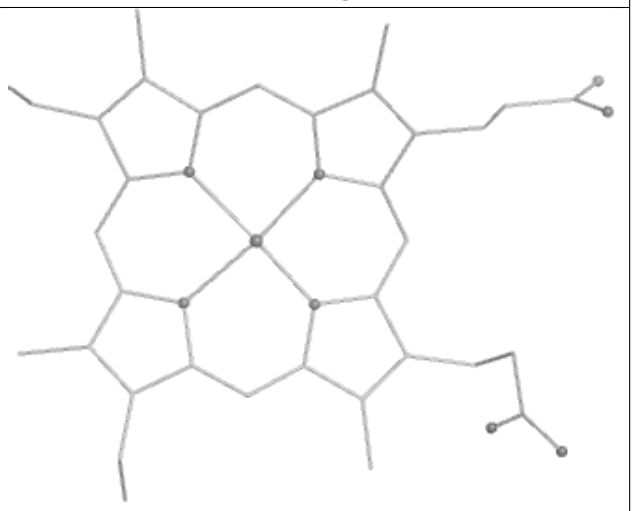
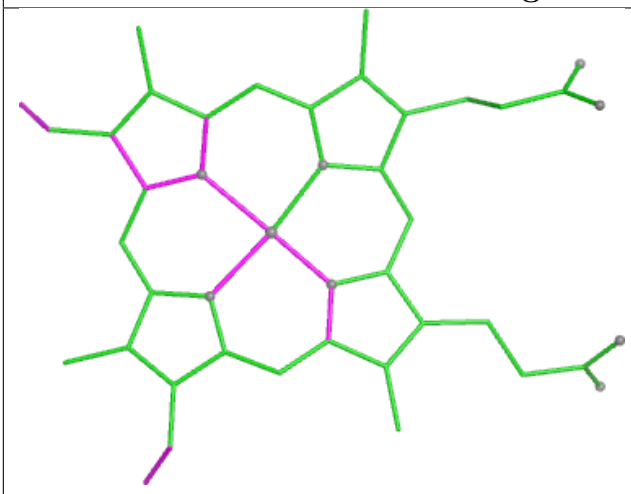


Rings

Ligand HEC O 605



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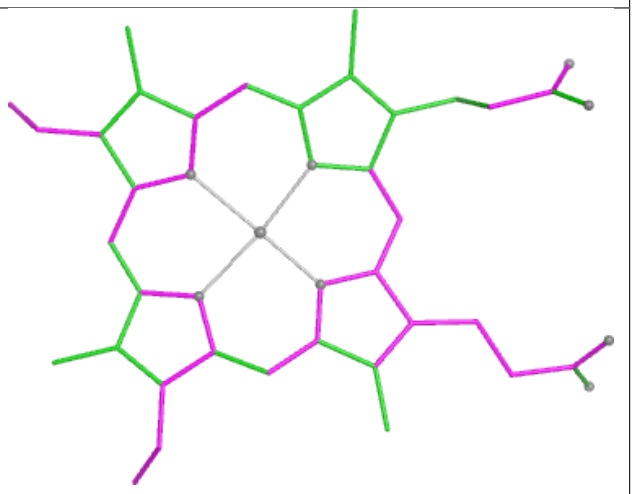

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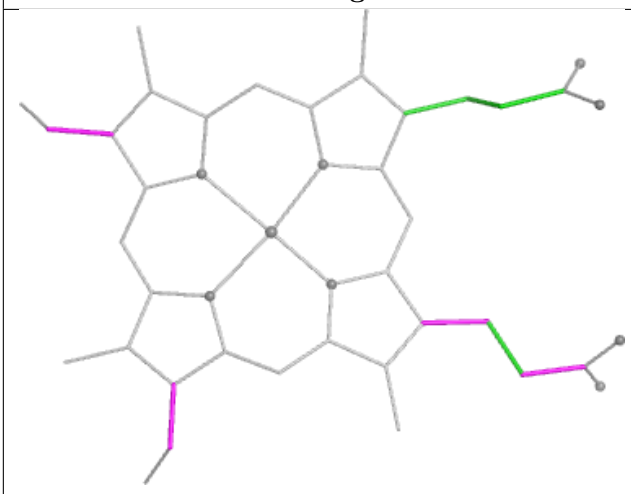

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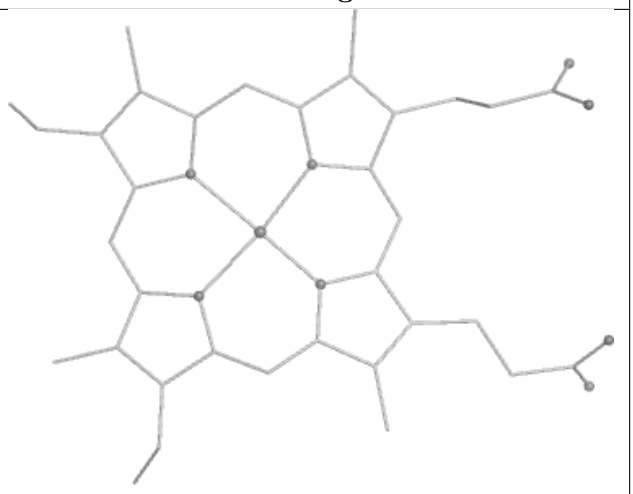
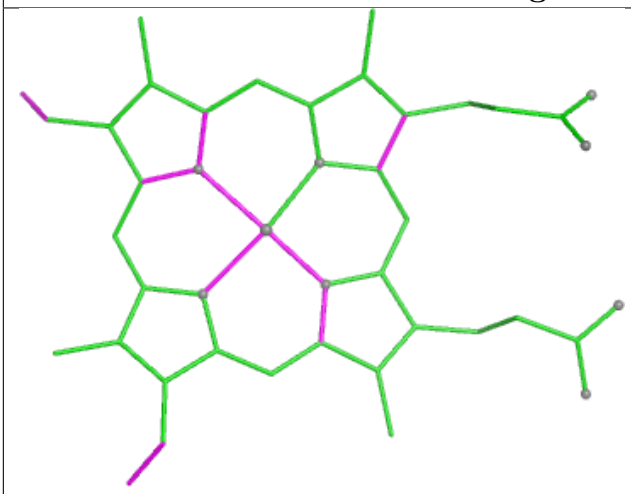


Rings

Ligand HEC I 606



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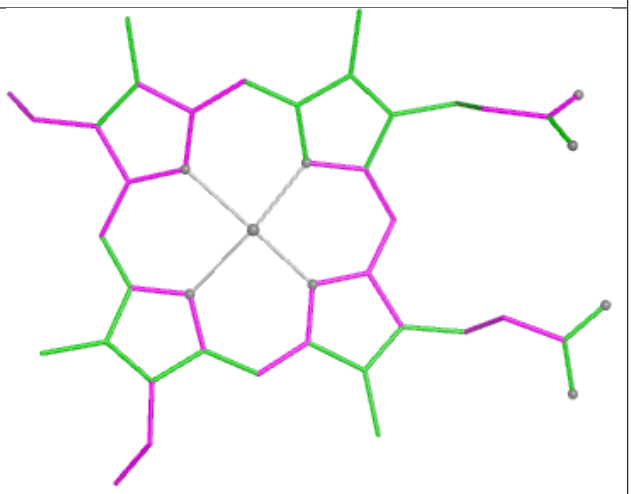

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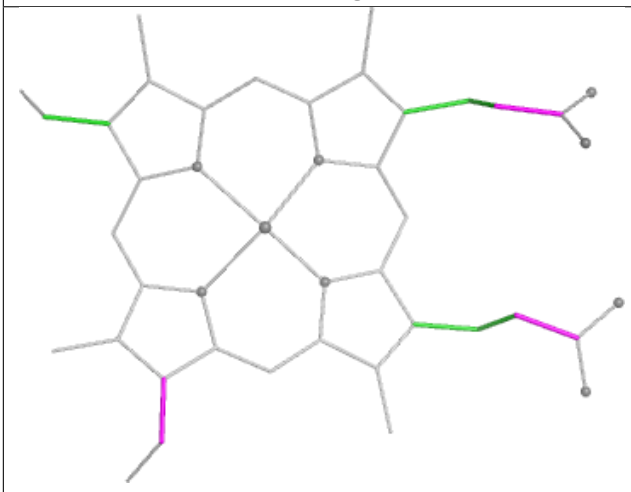

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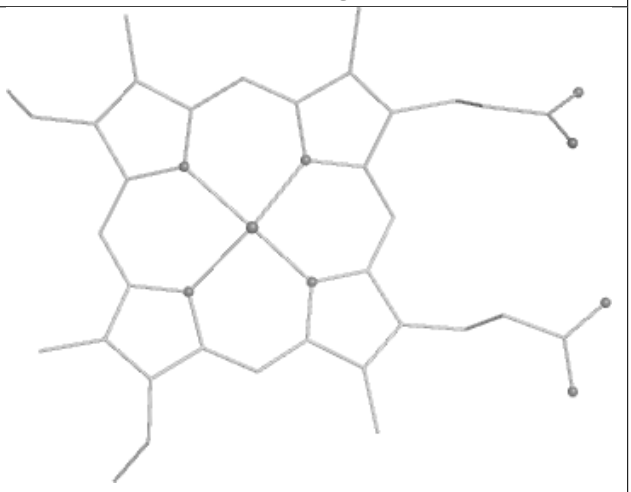
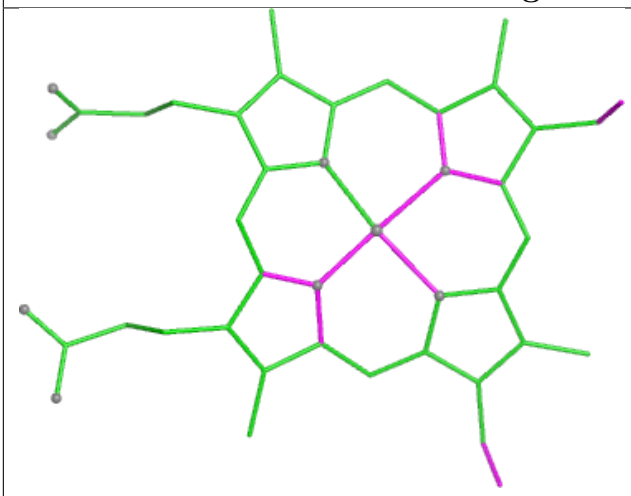


Rings

Ligand HEC O 606



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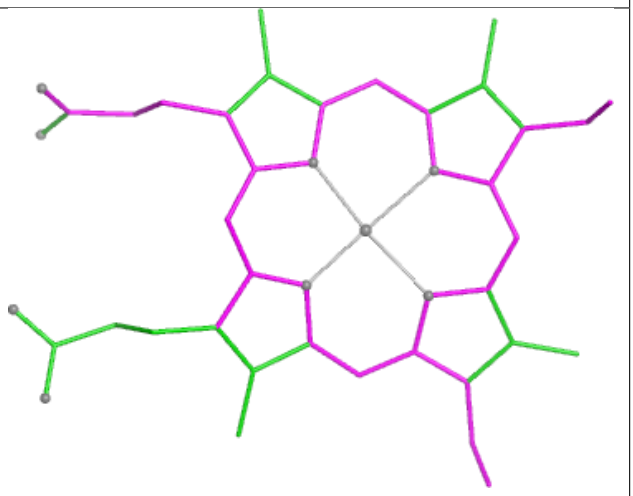
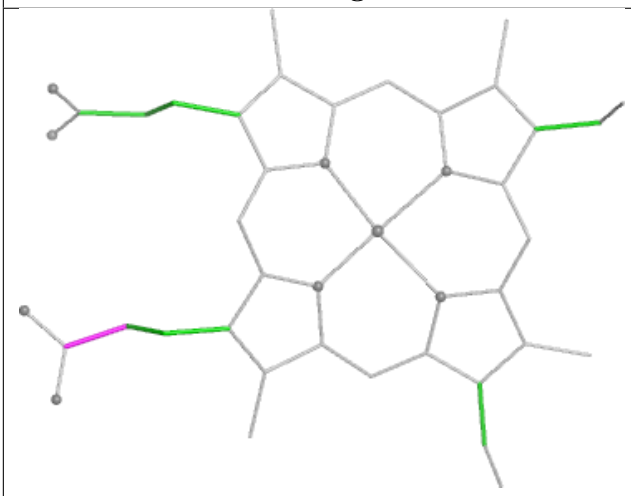
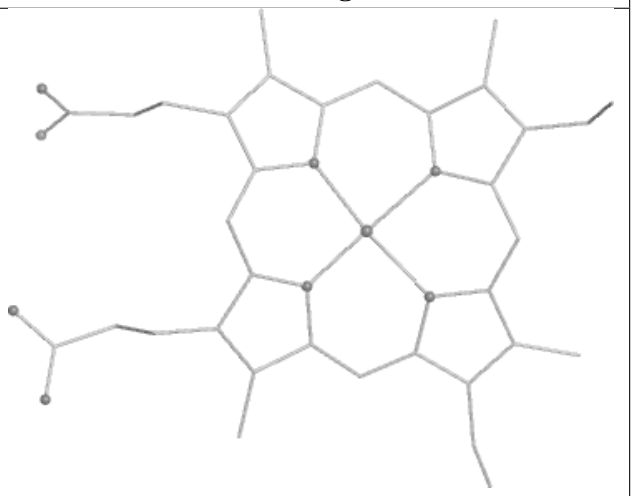


Bond angles

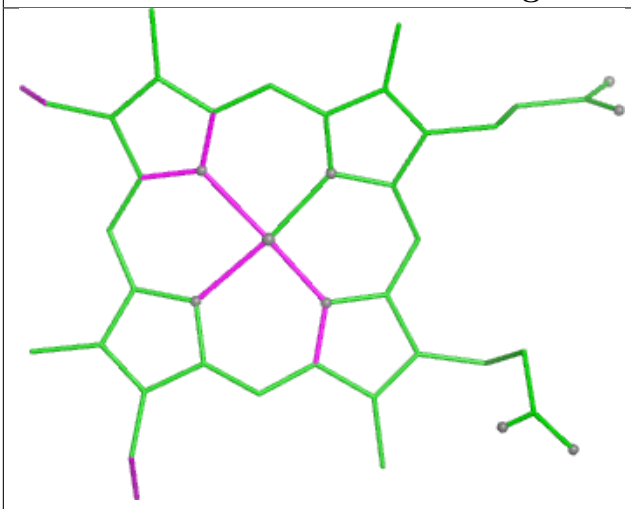


Torsions

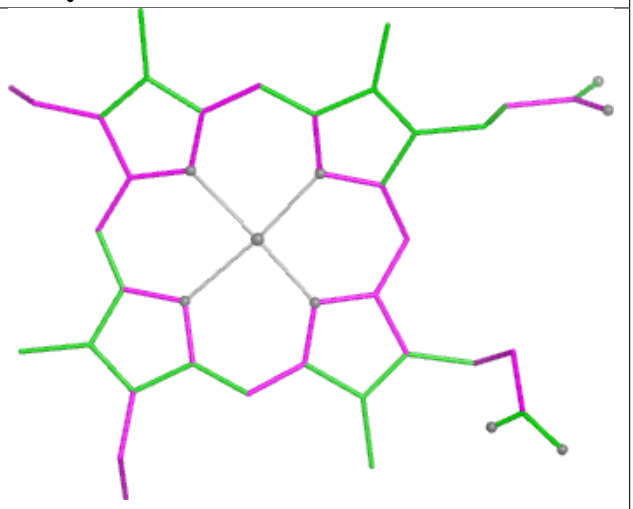


Rings

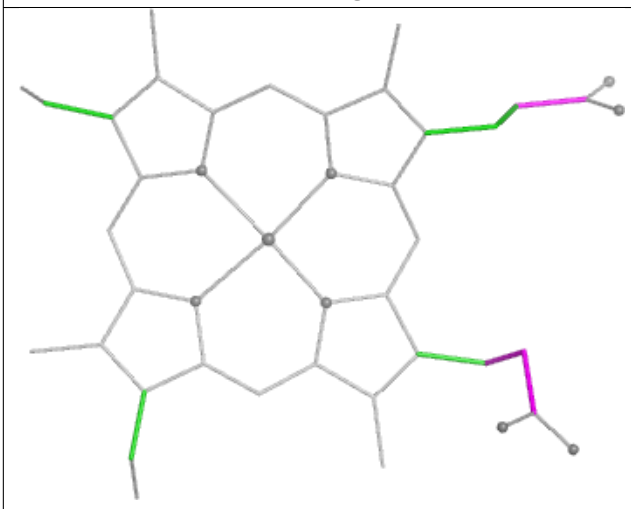
Ligand HEC Q 602



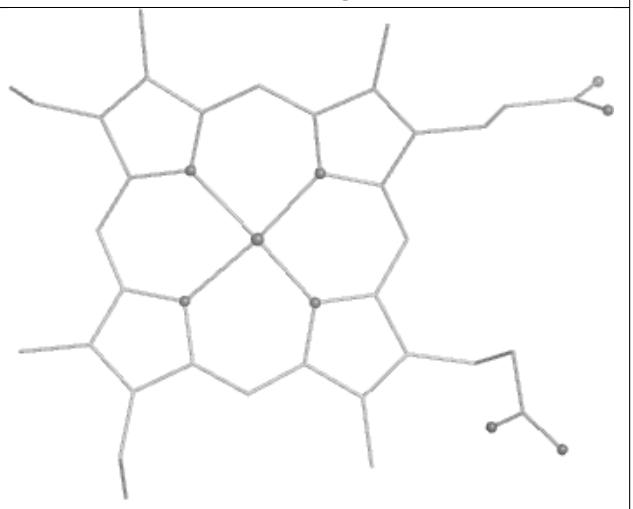
Bond lengths



Bond angles

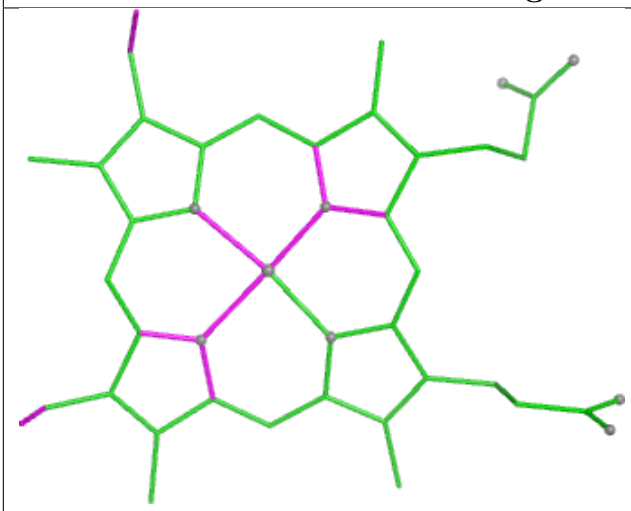


Torsions

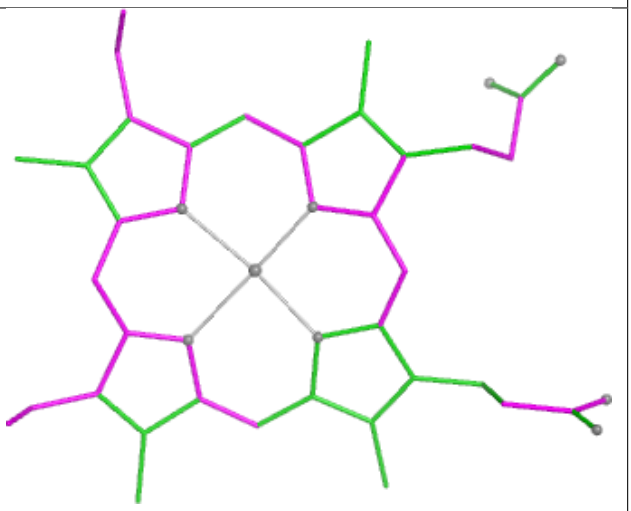


Rings

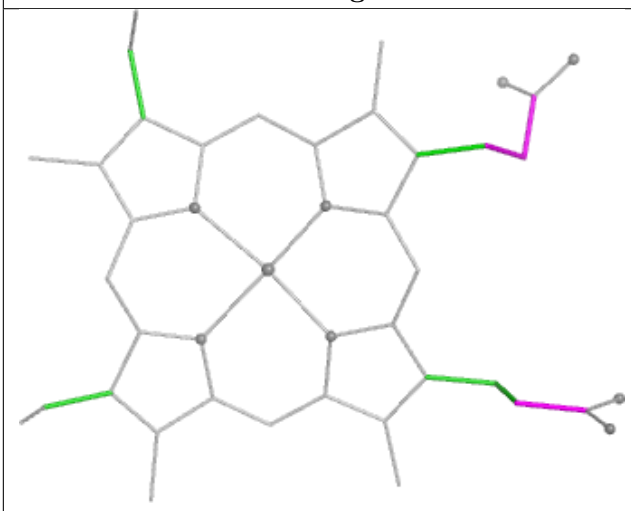
Ligand HEC S 602



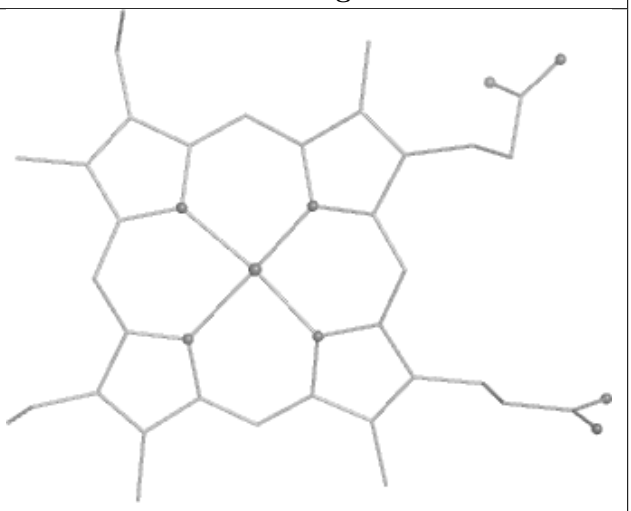
Bond lengths



Bond angles

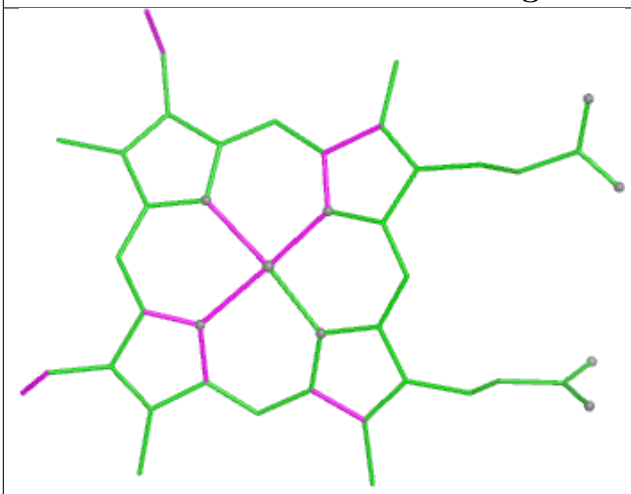


Torsions

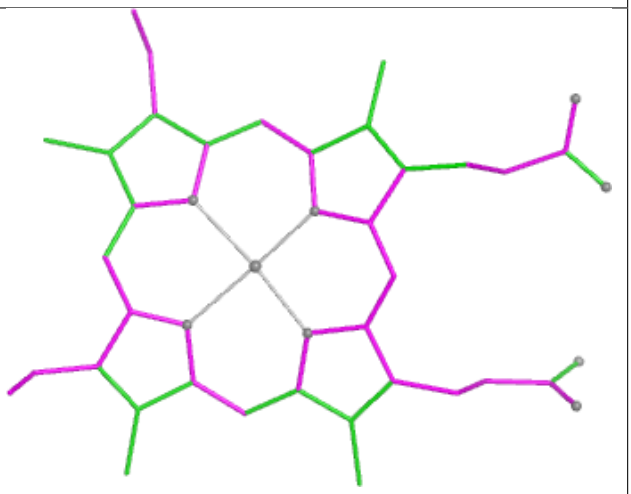


Rings

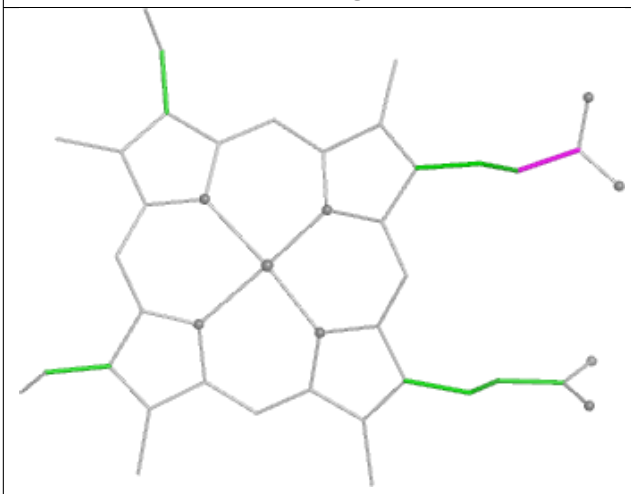
Ligand HEC G 606



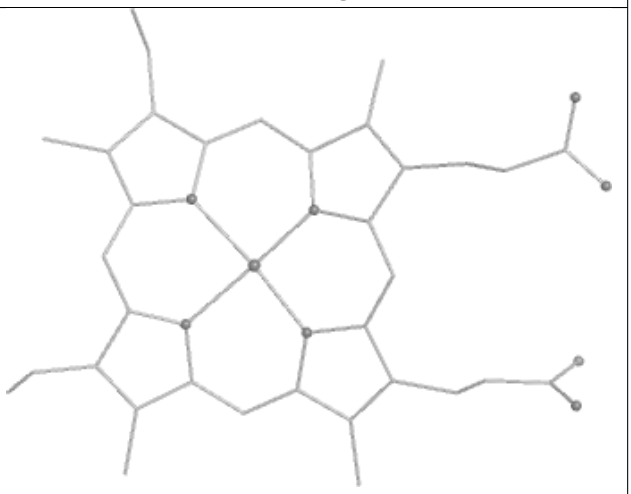
Bond lengths



Bond angles

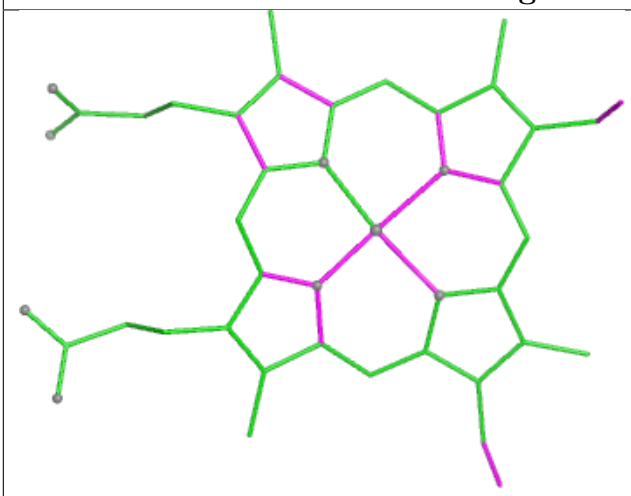


Torsions

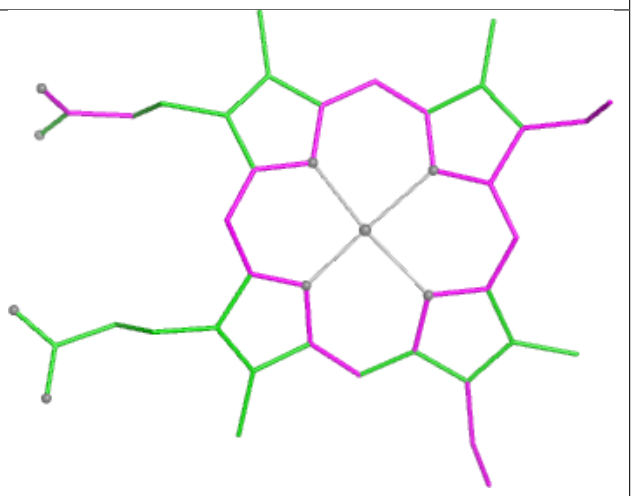


Rings

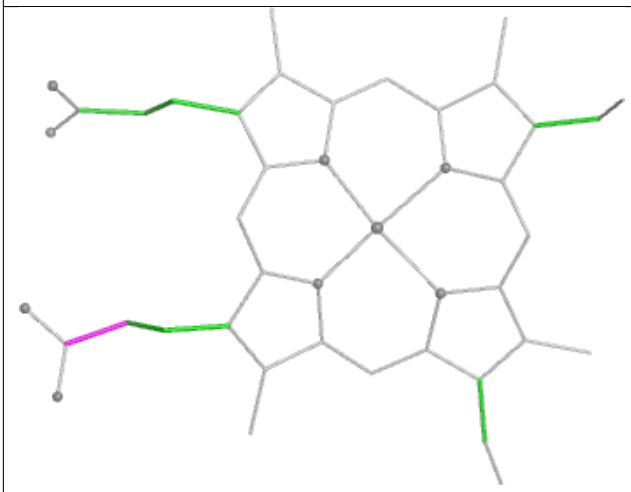
Ligand HEC M 606



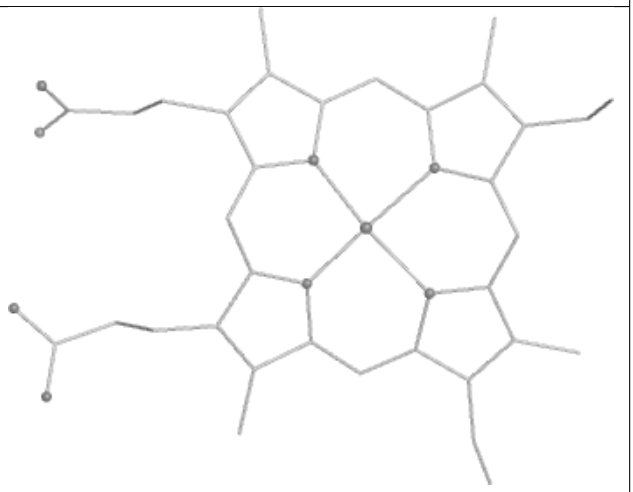
Bond lengths



Bond angles

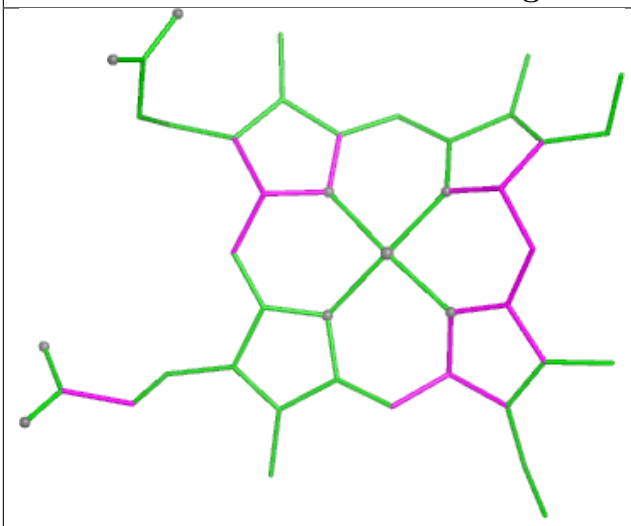


Torsions

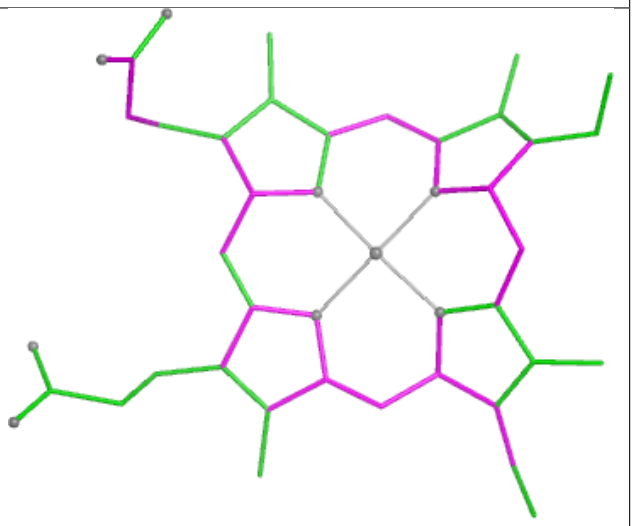


Rings

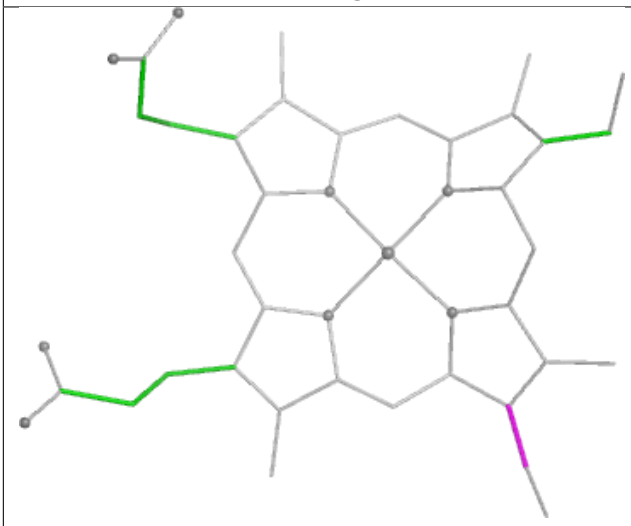
Ligand HEC V 603



Bond lengths



Bond angles



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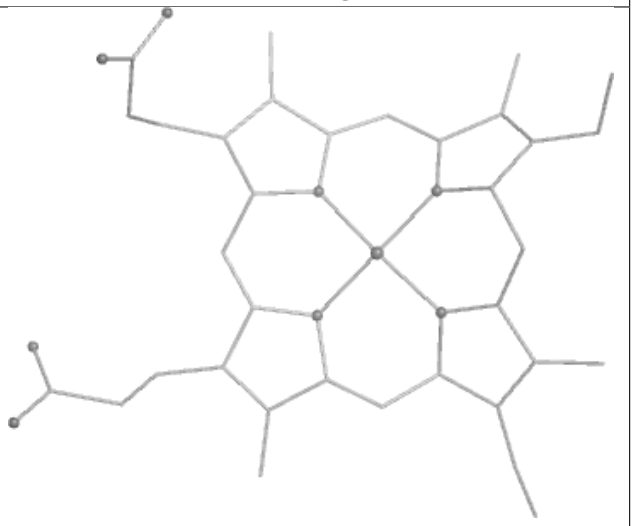
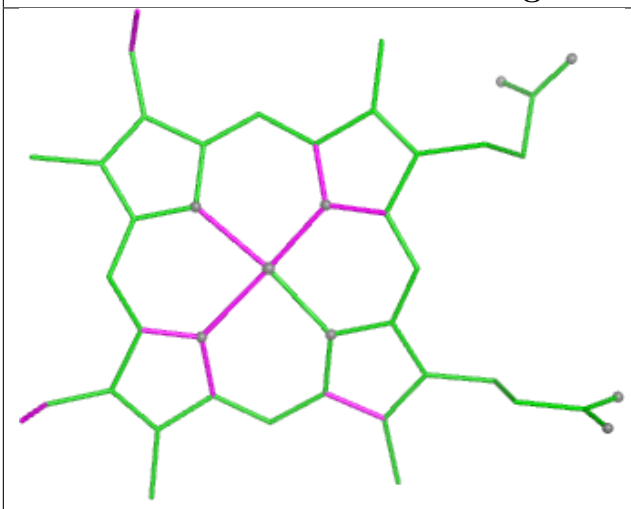
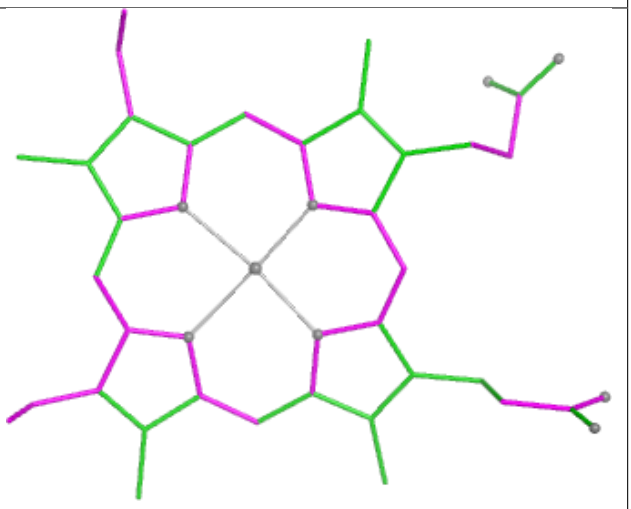


Rings

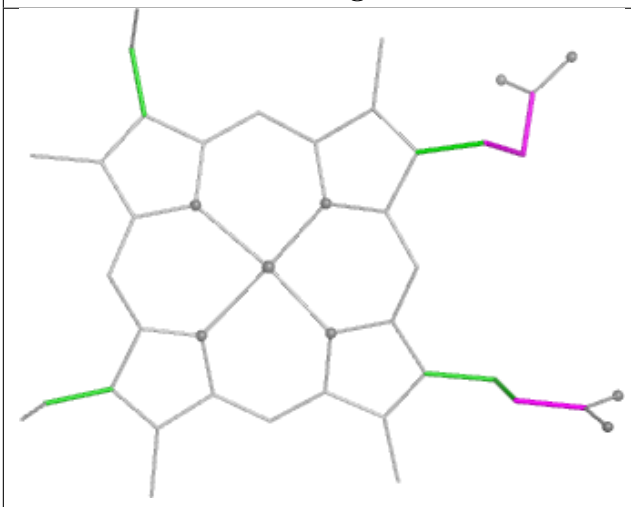
Ligand HEC T 602



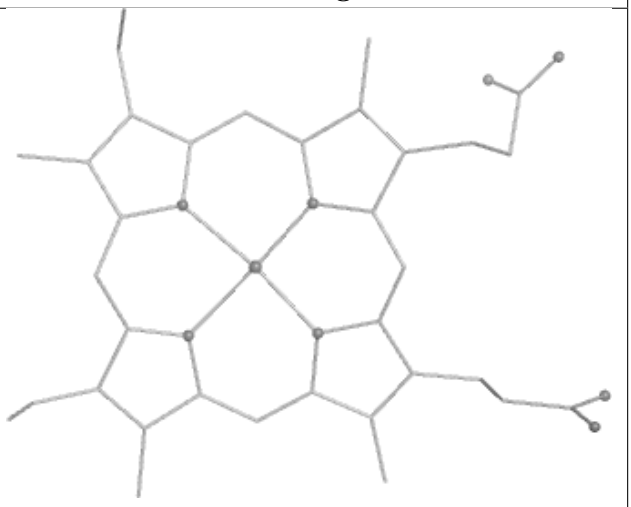
Bond lengths



Bond angles

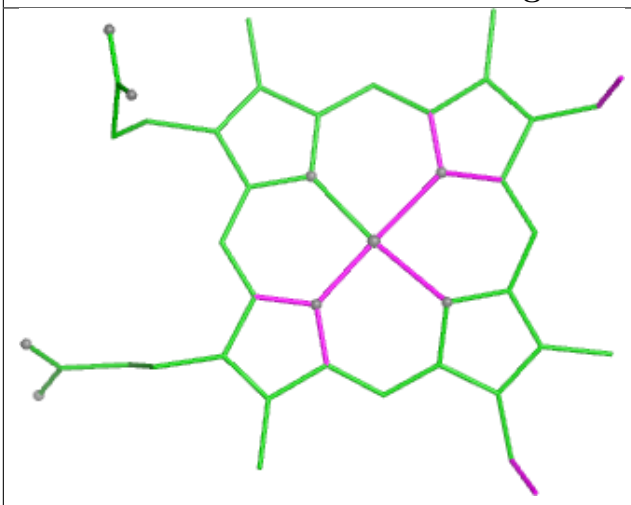


Torsions

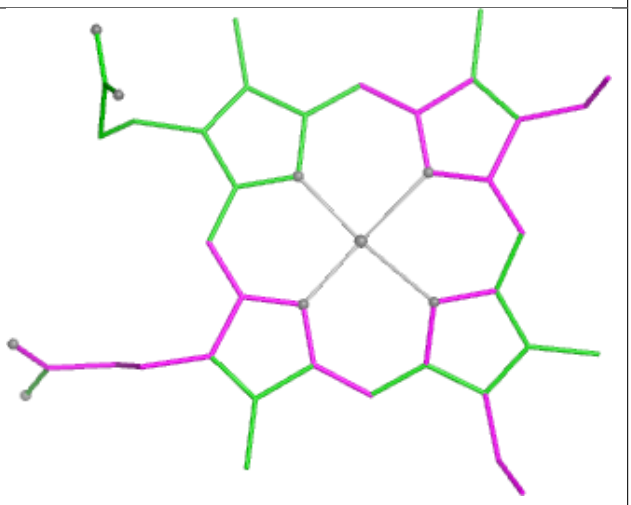


Rings

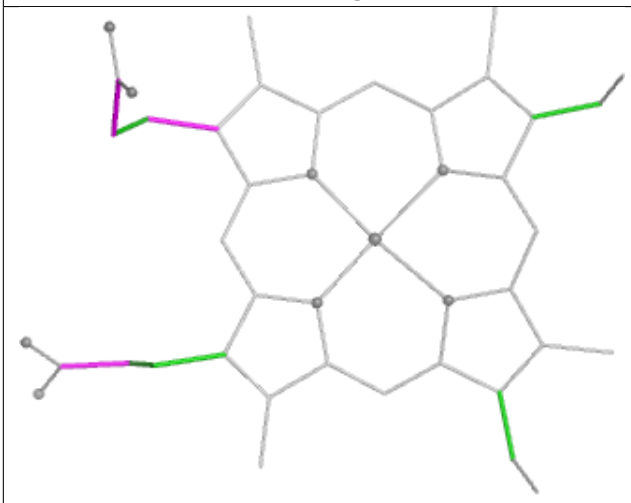
Ligand HEC P 601



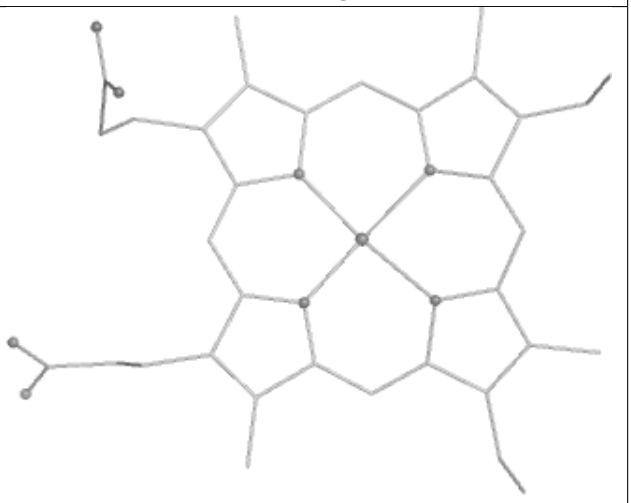
Bond lengths



Bond angles

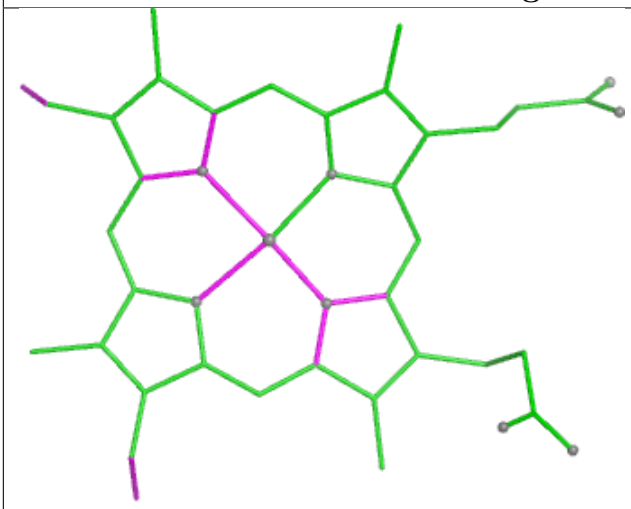


Torsions

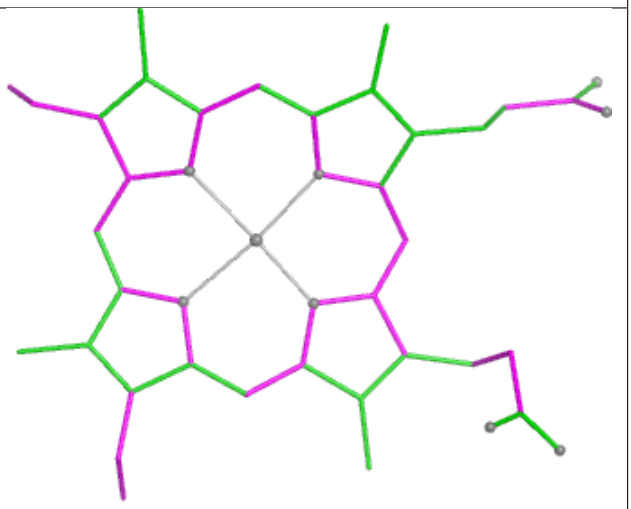


Rings

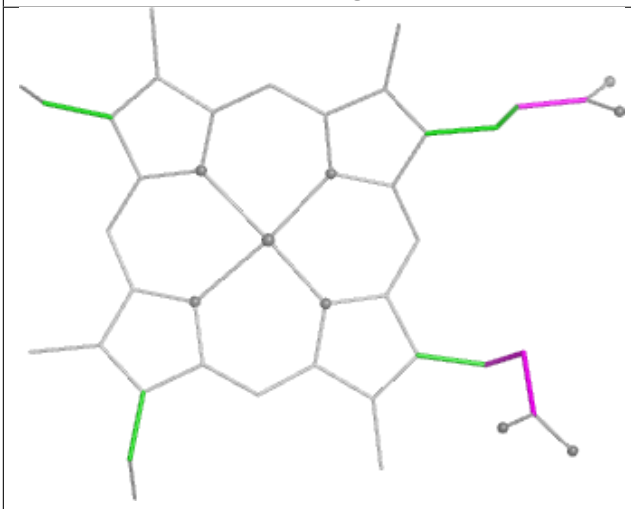
Ligand HEC X 602



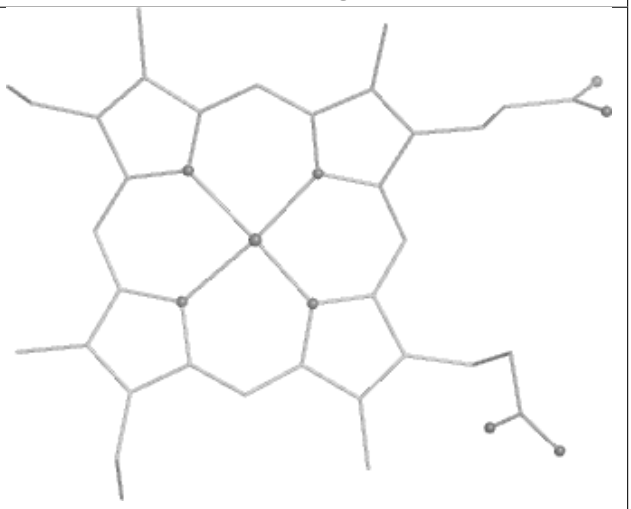
Bond lengths



Bond angles

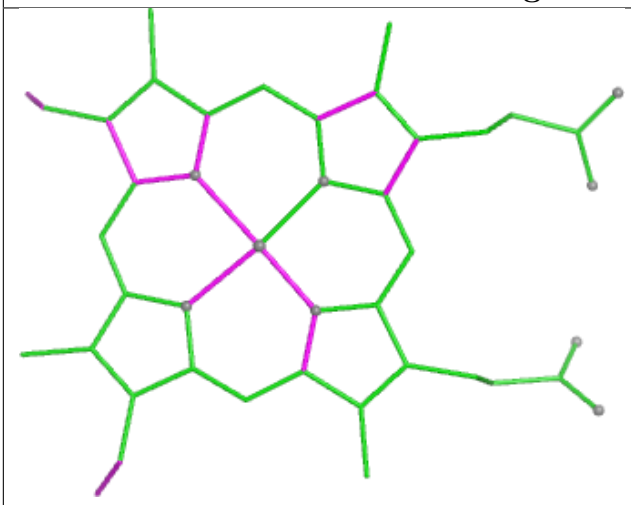


Torsions

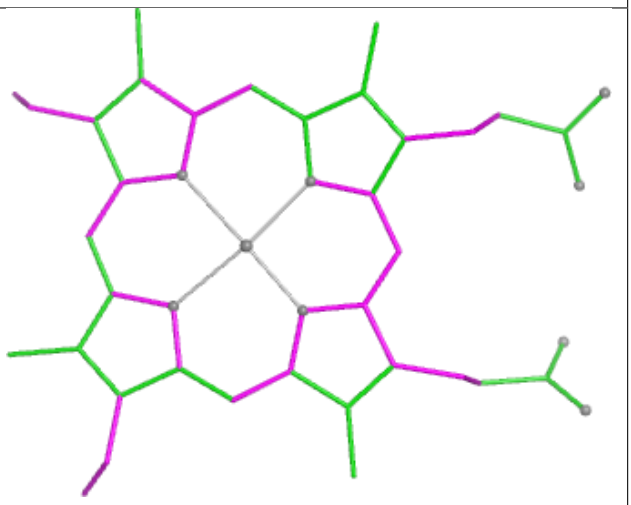


Rings

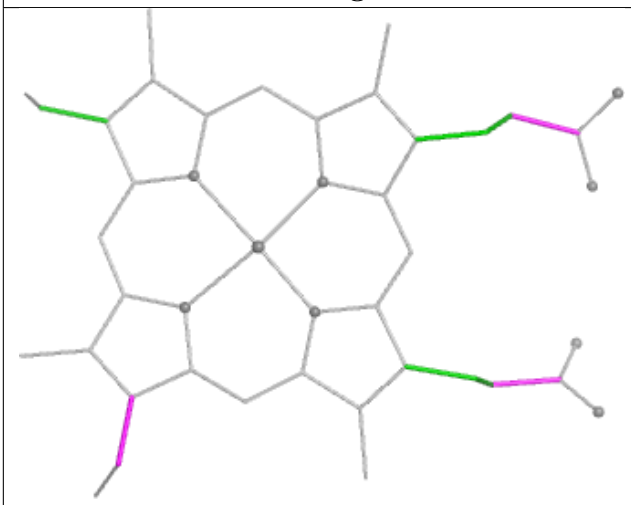
Ligand HEC T 604



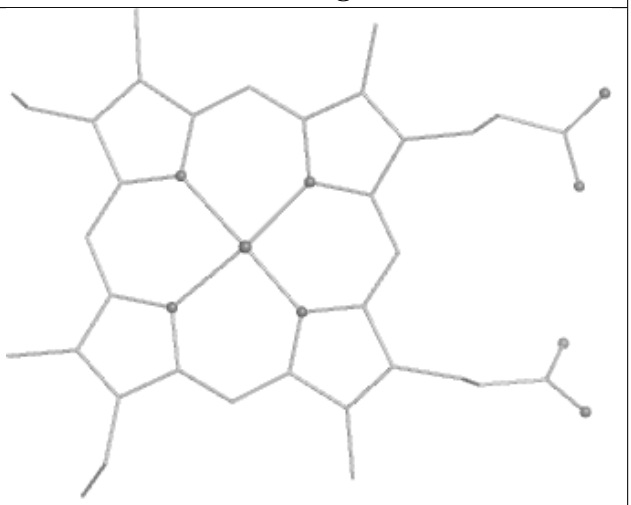
Bond lengths



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	531/582 (91%)	0.59	20 (3%) 44 35	39, 59, 87, 153	0
1	B	531/582 (91%)	0.43	11 (2%) 63 54	39, 57, 81, 173	0
1	C	531/582 (91%)	0.32	7 (1%) 75 66	40, 54, 84, 123	0
1	D	531/582 (91%)	0.52	25 (4%) 36 29	42, 68, 100, 140	0
1	E	531/582 (91%)	0.81	32 (6%) 27 21	39, 69, 104, 165	0
1	F	531/582 (91%)	1.18	84 (15%) 5 4	43, 76, 108, 158	0
1	G	531/582 (91%)	-0.08	6 (1%) 78 70	29, 41, 64, 139	0
1	H	531/582 (91%)	-0.08	8 (1%) 72 63	29, 39, 63, 156	0
1	I	527/582 (90%)	-0.34	0 100 100	27, 38, 57, 104	0
1	J	531/582 (91%)	-0.02	8 (1%) 72 63	29, 42, 66, 166	0
1	K	531/582 (91%)	0.04	8 (1%) 72 63	32, 44, 70, 159	0
1	L	531/582 (91%)	0.09	5 (0%) 81 74	32, 45, 73, 157	0
1	M	531/582 (91%)	0.31	11 (2%) 63 54	37, 54, 84, 150	0
1	N	531/582 (91%)	0.47	10 (1%) 66 57	37, 58, 85, 157	0
1	O	531/582 (91%)	0.21	6 (1%) 78 70	37, 51, 77, 133	0
1	P	531/582 (91%)	0.18	10 (1%) 66 57	37, 51, 72, 124	0
1	Q	531/582 (91%)	0.44	13 (2%) 59 49	34, 57, 82, 124	0
1	R	531/582 (91%)	0.28	11 (2%) 63 54	20, 52, 78, 142	1 (0%)
1	S	531/582 (91%)	1.07	71 (13%) 7 5	51, 80, 111, 158	0
1	T	531/582 (91%)	0.88	44 (8%) 17 12	50, 74, 107, 184	0
1	U	531/582 (91%)	1.06	70 (13%) 7 6	50, 80, 111, 150	0
1	V	531/582 (91%)	1.17	84 (15%) 5 4	52, 79, 108, 161	0
1	W	531/582 (91%)	1.18	97 (18%) 3 2	50, 80, 105, 163	0
1	X	531/582 (91%)	1.34	110 (20%) 2 2	56, 83, 111, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	Y	86/114 (75%)	0.66	6 (6%) 22 16	38, 54, 76, 105	0
2	Z	86/114 (75%)	1.43	18 (20%) 2 2	76, 96, 128, 192	0
2	a	86/114 (75%)	1.10	10 (11%) 9 7	64, 87, 116, 166	0
2	b	86/114 (75%)	1.08	11 (12%) 7 6	61, 83, 118, 167	0
2	c	86/114 (75%)	0.94	8 (9%) 14 10	58, 76, 101, 166	0
2	d	86/114 (75%)	0.93	9 (10%) 11 8	54, 68, 107, 152	0
2	e	86/114 (75%)	0.91	7 (8%) 18 13	57, 76, 109, 155	0
2	f	86/114 (75%)	1.34	16 (18%) 3 2	71, 96, 131, 168	0
2	g	86/114 (75%)	1.11	8 (9%) 14 10	68, 82, 114, 179	0
2	h	86/114 (75%)	1.43	20 (23%) 2 1	82, 96, 130, 166	0
2	i	86/114 (75%)	1.78	35 (40%) 0 0	85, 107, 137, 185	0
2	j	86/114 (75%)	1.39	15 (17%) 4 3	96, 109, 147, 178	0
All	All	13772/15336 (89%)	0.55	914 (6%) 24 18	20, 60, 104, 192	1 (0%)

The worst 5 of 914 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	h	110	PRO	7.0
2	Y	111	SER	6.5
2	c	110	PRO	6.2
2	d	110	PRO	6.1
2	a	110	PRO	5.4

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
4	SO4	X	610	5/5	0.31	0.13	158,161,161,162	0
6	K	X	612	1/1	0.44	0.20	93,93,93,93	0
6	K	K	616	1/1	0.46	0.17	85,85,85,85	0
4	SO4	c	201	5/5	0.54	0.12	132,133,135,135	0
6	K	H	616	1/1	0.54	0.17	82,82,82,82	0
4	SO4	X	611	5/5	0.55	0.12	139,139,141,144	0
4	SO4	a	201	5/5	0.63	0.11	139,139,140,140	0
4	SO4	X	609	5/5	0.64	0.11	107,108,110,112	0
4	SO4	O	610	5/5	0.66	0.12	109,111,112,112	0
4	SO4	S	609	5/5	0.66	0.11	129,133,135,135	0
4	SO4	Q	611	5/5	0.67	0.12	112,118,119,119	0
4	SO4	A	611	5/5	0.68	0.14	117,118,119,120	0
4	SO4	H	610	5/5	0.69	0.14	106,111,113,114	0
4	SO4	H	613	5/5	0.70	0.17	116,120,125,127	0
4	SO4	U	611	5/5	0.70	0.12	127,130,131,133	0
4	SO4	L	612	5/5	0.71	0.14	110,112,115,115	0
4	SO4	V	611	5/5	0.71	0.11	131,133,134,135	0
4	SO4	C	609	5/5	0.72	0.14	96,102,106,108	0
5	GOL	A	614	6/6	0.73	0.21	82,89,90,91	0
6	K	Q	612	1/1	0.73	0.10	96,96,96,96	0
4	SO4	I	612	5/5	0.73	0.13	120,121,124,125	0
4	SO4	C	610	5/5	0.74	0.27	143,145,147,149	0
4	SO4	C	611	5/5	0.74	0.13	111,111,114,116	0
4	SO4	M	610	5/5	0.74	0.23	134,135,138,139	0
4	SO4	Y	202	5/5	0.75	0.09	130,130,132,136	0
4	SO4	M	612	5/5	0.75	0.14	121,122,123,125	0
4	SO4	G	611	5/5	0.77	0.12	139,139,143,149	0
4	SO4	N	610	5/5	0.77	0.16	101,105,107,109	0
4	SO4	H	612	5/5	0.78	0.14	110,113,116,118	0
5	GOL	J	612	6/6	0.78	0.18	58,64,67,67	0
4	SO4	K	611	5/5	0.79	0.15	102,104,105,105	0
4	SO4	I	611	5/5	0.79	0.11	115,115,116,117	0
4	SO4	J	611	5/5	0.79	0.21	118,118,120,123	0
4	SO4	Q	609	5/5	0.79	0.11	84,87,88,89	0
5	GOL	I	615	6/6	0.80	0.15	51,55,56,57	0
4	SO4	W	609	5/5	0.80	0.09	114,118,119,124	0
4	SO4	M	611	5/5	0.80	0.20	129,131,136,137	0
4	SO4	F	610	5/5	0.80	0.10	135,136,139,139	0
5	GOL	G	615	6/6	0.80	0.20	61,67,68,68	0
4	SO4	E	610	5/5	0.80	0.09	103,105,106,109	0
4	SO4	L	610	5/5	0.81	0.13	142,143,145,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	H	615	6/6	0.81	0.37	78,86,90,100	0
4	SO4	U	610	5/5	0.81	0.11	99,101,103,104	0
4	SO4	Y	201	5/5	0.81	0.11	136,136,137,141	0
4	SO4	L	611	5/5	0.81	0.10	116,119,121,122	0
4	SO4	G	612	5/5	0.81	0.16	120,124,126,126	0
4	SO4	H	609	5/5	0.81	0.17	78,81,82,83	0
4	SO4	B	609	5/5	0.81	0.18	116,117,119,124	0
5	GOL	A	612	6/6	0.82	0.17	76,78,79,81	0
4	SO4	O	611	5/5	0.82	0.10	114,114,119,120	0
5	GOL	D	610	6/6	0.82	0.15	86,88,88,89	0
5	GOL	K	612	6/6	0.82	0.24	76,80,86,90	0
4	SO4	Q	610	5/5	0.83	0.20	133,136,137,137	0
4	SO4	T	609	5/5	0.84	0.10	98,100,102,102	0
4	SO4	B	610	5/5	0.84	0.14	88,89,91,91	0
4	SO4	P	609	5/5	0.84	0.19	95,95,96,98	0
4	SO4	F	609	5/5	0.85	0.08	95,99,102,104	0
4	SO4	N	611	5/5	0.85	0.10	123,126,127,129	0
4	SO4	A	610	5/5	0.85	0.13	73,77,79,80	0
5	GOL	A	613	6/6	0.85	0.14	74,77,78,79	0
4	SO4	H	611	5/5	0.85	0.13	97,100,101,105	0
4	SO4	R	610	5/5	0.85	0.15	75,77,79,79	0
4	SO4	R	611	5/5	0.85	0.21	142,143,145,147	0
4	SO4	K	610	5/5	0.86	0.15	84,84,86,88	0
4	SO4	L	609	5/5	0.87	0.10	91,94,94,97	0
4	SO4	J	610	5/5	0.87	0.13	99,100,101,103	0
5	GOL	I	613	6/6	0.87	0.13	59,64,66,73	0
4	SO4	G	610	5/5	0.87	0.24	104,106,107,108	0
4	SO4	S	610	5/5	0.87	0.13	92,93,94,95	0
4	SO4	V	610	5/5	0.88	0.12	94,97,98,99	0
4	SO4	D	609	5/5	0.89	0.10	82,82,84,87	0
4	SO4	G	614	5/5	0.89	0.14	91,94,95,95	0
4	SO4	O	609	5/5	0.89	0.11	77,78,80,82	0
5	GOL	L	613	6/6	0.89	0.17	56,59,60,61	0
5	GOL	J	613	6/6	0.90	0.16	58,61,62,63	0
4	SO4	J	609	5/5	0.90	0.11	77,79,80,80	0
5	GOL	K	615	6/6	0.90	0.33	53,55,58,59	0
5	GOL	H	614	6/6	0.90	0.30	56,63,64,68	0
4	SO4	M	609	5/5	0.91	0.12	89,90,91,92	0
4	SO4	V	609	5/5	0.91	0.10	56,59,60,62	0
5	GOL	K	613	6/6	0.91	0.09	45,51,52,53	0
5	GOL	I	614	6/6	0.92	0.33	67,78,80,83	0
4	SO4	E	609	5/5	0.92	0.10	50,51,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	G	613	5/5	0.93	0.10	63,63,64,66	0
3	HEC	V	602	43/43	0.93	0.14	68,73,87,100	0
3	HEC	W	606	43/43	0.93	0.14	64,76,88,96	0
3	HEC	X	606	43/43	0.93	0.15	69,83,87,90	0
5	GOL	G	616	6/6	0.93	0.10	37,40,41,41	0
4	SO4	U	609	5/5	0.93	0.10	57,58,60,64	0
3	HEC	V	603	43/43	0.94	0.12	51,65,82,86	0
3	HEC	W	603	43/43	0.94	0.13	67,77,85,89	0
5	GOL	K	614	6/6	0.94	0.20	49,56,57,59	0
3	HEC	W	605	43/43	0.94	0.13	74,81,87,89	0
3	HEC	S	603	43/43	0.94	0.13	72,77,88,94	0
3	HEC	U	606	43/43	0.94	0.13	65,72,88,96	0
4	SO4	G	609	5/5	0.94	0.10	72,72,74,74	0
3	HEC	S	605	43/43	0.94	0.13	63,72,82,83	0
4	SO4	I	610	5/5	0.94	0.10	67,67,69,69	0
3	HEC	V	606	43/43	0.95	0.11	57,60,76,81	0
3	HEC	V	607	43/43	0.95	0.11	54,66,69,70	0
3	HEC	E	605	43/43	0.95	0.12	53,63,75,82	0
3	HEC	E	606	43/43	0.95	0.13	55,60,68,75	0
3	HEC	F	603	43/43	0.95	0.12	62,70,74,79	0
3	HEC	F	605	43/43	0.95	0.11	54,60,69,78	0
3	HEC	X	603	43/43	0.95	0.12	70,80,103,109	0
3	HEC	X	601	43/43	0.95	0.11	62,69,78,82	0
3	HEC	X	602	43/43	0.95	0.12	69,75,91,106	0
3	HEC	X	605	43/43	0.95	0.15	79,86,97,100	0
3	HEC	N	601	43/43	0.95	0.11	41,44,55,65	0
3	HEC	Q	602	43/43	0.95	0.13	64,68,88,97	0
3	HEC	S	602	43/43	0.95	0.13	63,71,86,104	0
3	HEC	S	604	43/43	0.95	0.12	59,66,75,86	0
3	HEC	A	604	43/43	0.95	0.11	47,50,61,73	0
3	HEC	S	606	43/43	0.95	0.11	61,69,74,79	0
3	HEC	A	606	43/43	0.95	0.12	45,60,73,78	0
3	HEC	T	602	43/43	0.95	0.12	59,68,83,97	0
3	HEC	T	607	43/43	0.95	0.11	49,57,60,62	0
3	HEC	U	603	43/43	0.95	0.11	61,72,83,85	0
3	HEC	U	600	43/43	0.95	0.11	58,64,71,72	0
3	HEC	U	605	43/43	0.95	0.12	62,68,80,87	0
3	HEC	D	600	43/43	0.95	0.10	54,60,68,74	0
3	HEC	E	603	43/43	0.95	0.11	56,66,92,96	0
3	HEC	V	605	43/43	0.95	0.12	56,65,73,76	0
4	SO4	I	609	5/5	0.96	0.08	28,28,29,30	0
3	HEC	S	607	43/43	0.96	0.11	51,57,59,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	E	602	43/43	0.96	0.11	48,53,73,94	0
3	HEC	T	603	43/43	0.96	0.10	60,66,71,73	0
3	HEC	T	600	43/43	0.96	0.10	53,60,68,69	0
3	HEC	T	601	43/43	0.96	0.10	55,58,61,63	0
3	HEC	E	604	43/43	0.96	0.10	40,45,53,63	0
3	HEC	T	604	43/43	0.96	0.10	59,65,70,80	0
3	HEC	T	605	43/43	0.96	0.11	54,60,74,76	0
3	HEC	T	606	43/43	0.96	0.10	52,56,65,74	0
3	HEC	A	605	43/43	0.96	0.11	50,59,63,64	0
3	HEC	A	600	43/43	0.96	0.10	47,49,56,59	0
3	HEC	E	607	43/43	0.96	0.10	47,54,60,62	0
3	HEC	U	601	43/43	0.96	0.11	54,57,67,73	0
3	HEC	U	602	43/43	0.96	0.11	60,69,94,116	0
3	HEC	U	604	43/43	0.96	0.11	52,60,72,81	0
3	HEC	A	607	43/43	0.96	0.10	41,45,50,53	0
3	HEC	F	600	43/43	0.96	0.10	46,52,62,68	0
3	HEC	U	607	43/43	0.96	0.11	53,70,73,74	0
3	HEC	V	600	43/43	0.96	0.11	67,70,84,91	0
3	HEC	V	601	43/43	0.96	0.10	52,63,65,67	0
3	HEC	F	601	43/43	0.96	0.12	51,55,68,70	0
3	HEC	V	604	43/43	0.96	0.11	59,71,81,85	0
3	HEC	F	602	43/43	0.96	0.12	64,75,85,96	0
3	HEC	F	604	43/43	0.96	0.10	58,65,74,84	0
3	HEC	A	603	43/43	0.96	0.11	54,66,71,73	0
4	SO4	R	609	5/5	0.96	0.08	36,39,40,40	0
3	HEC	F	606	43/43	0.96	0.11	50,56,67,76	0
3	HEC	F	607	43/43	0.96	0.11	49,56,57,60	0
3	HEC	W	600	43/43	0.96	0.10	61,68,74,77	0
3	HEC	W	601	43/43	0.96	0.11	61,70,77,80	0
3	HEC	W	602	43/43	0.96	0.11	54,58,83,99	0
3	HEC	W	604	43/43	0.96	0.10	50,57,67,74	0
3	HEC	H	602	43/43	0.96	0.10	35,44,64,77	0
3	HEC	I	602	43/43	0.96	0.10	37,42,59,70	0
3	HEC	W	607	43/43	0.96	0.11	63,68,71,71	0
3	HEC	J	600	43/43	0.96	0.10	37,41,52,60	0
3	HEC	X	600	43/43	0.96	0.10	57,63,75,81	0
3	HEC	J	602	43/43	0.96	0.11	38,41,67,86	0
3	HEC	K	600	43/43	0.96	0.10	38,40,46,55	0
3	HEC	X	604	43/43	0.96	0.10	63,73,78,80	0
3	HEC	L	600	43/43	0.96	0.10	41,44,50,51	0
3	HEC	M	600	43/43	0.96	0.10	44,48,56,62	0
3	HEC	X	607	43/43	0.96	0.11	57,61,65,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	N	600	43/43	0.96	0.10	46,49,57,63	0
3	HEC	B	602	43/43	0.96	0.10	49,56,80,99	0
3	HEC	N	602	43/43	0.96	0.11	48,52,75,92	0
3	HEC	N	605	43/43	0.96	0.10	48,52,66,73	0
3	HEC	N	606	43/43	0.96	0.11	47,51,60,64	0
3	HEC	O	600	43/43	0.96	0.09	44,48,58,60	0
4	SO4	A	609	5/5	0.96	0.07	47,49,49,52	0
3	HEC	O	602	43/43	0.96	0.10	47,51,72,91	0
3	HEC	P	601	43/43	0.96	0.10	39,44,46,47	0
3	HEC	P	602	43/43	0.96	0.09	41,45,63,76	0
3	HEC	Q	603	43/43	0.96	0.09	52,55,58,59	0
3	HEC	Q	600	43/43	0.96	0.10	47,52,59,65	0
3	HEC	Q	601	43/43	0.96	0.11	46,50,54,56	0
3	HEC	B	604	43/43	0.96	0.10	44,51,62,67	0
3	HEC	Q	604	43/43	0.96	0.11	54,60,68,76	0
3	HEC	Q	606	43/43	0.96	0.11	44,55,65,69	0
3	HEC	R	603	43/43	0.96	0.09	37,43,48,52	0
3	HEC	R	600	43/43	0.96	0.10	49,54,62,64	0
3	HEC	S	600	43/43	0.96	0.10	60,65,73,75	0
3	HEC	S	601	43/43	0.96	0.12	67,70,81,85	0
3	HEC	C	606	43/43	0.96	0.10	41,43,59,65	0
3	HEC	C	607	43/43	0.96	0.10	44,48,49,52	0
3	HEC	A	602	43/43	0.96	0.10	51,56,79,99	0
3	HEC	G	602	43/43	0.96	0.10	34,38,59,77	0
3	HEC	B	603	43/43	0.97	0.08	45,49,53,54	0
3	HEC	H	604	43/43	0.97	0.08	38,43,53,64	0
3	HEC	H	606	43/43	0.97	0.08	32,34,39,44	0
3	HEC	I	600	43/43	0.97	0.08	39,43,50,52	0
3	HEC	I	601	43/43	0.97	0.08	35,37,41,44	0
3	HEC	D	601	43/43	0.97	0.10	51,59,61,62	0
3	HEC	D	602	43/43	0.97	0.10	45,48,65,79	0
3	HEC	D	605	43/43	0.97	0.10	48,53,61,66	0
3	HEC	J	604	43/43	0.97	0.09	32,35,44,55	0
3	HEC	J	605	43/43	0.97	0.09	32,38,43,47	0
3	HEC	J	606	43/43	0.97	0.09	33,39,41,46	0
3	HEC	D	606	43/43	0.97	0.09	46,51,62,66	0
3	HEC	K	601	43/43	0.97	0.08	33,34,38,43	0
3	HEC	K	602	43/43	0.97	0.10	44,47,65,81	0
3	HEC	K	604	43/43	0.97	0.09	36,41,49,57	0
3	HEC	K	605	43/43	0.97	0.09	35,38,43,48	0
3	HEC	K	606	43/43	0.97	0.09	33,39,42,46	0
3	HEC	L	603	43/43	0.97	0.08	35,41,50,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	D	603	43/43	0.97	0.09	54,66,69,72	0
4	SO4	N	609	5/5	0.97	0.07	40,40,41,42	0
3	HEC	L	601	43/43	0.97	0.09	36,40,45,46	0
3	HEC	L	602	43/43	0.97	0.10	42,45,57,72	0
3	HEC	L	604	43/43	0.97	0.09	35,41,48,58	0
3	HEC	L	605	43/43	0.97	0.09	35,37,41,45	0
3	HEC	L	606	43/43	0.97	0.08	35,37,43,47	0
3	HEC	B	600	43/43	0.97	0.10	48,52,59,61	0
3	HEC	M	601	43/43	0.97	0.09	41,44,47,51	0
3	HEC	M	602	43/43	0.97	0.10	44,48,72,89	0
3	HEC	M	604	43/43	0.97	0.09	40,43,51,62	0
3	HEC	M	605	43/43	0.97	0.10	36,38,46,51	0
3	HEC	M	606	43/43	0.97	0.10	37,40,50,55	0
3	HEC	M	607	43/43	0.97	0.09	36,39,52,62	0
3	HEC	M	603	43/43	0.97	0.09	42,46,49,50	0
3	HEC	N	603	43/43	0.97	0.08	47,56,60,62	0
3	HEC	E	600	43/43	0.97	0.09	39,41,53,55	0
3	HEC	E	601	43/43	0.97	0.09	39,43,47,55	0
3	HEC	B	601	43/43	0.97	0.09	43,47,56,68	0
3	HEC	N	604	43/43	0.97	0.08	42,47,56,59	0
3	HEC	G	601	43/43	0.97	0.09	37,41,43,48	0
3	HEC	A	601	43/43	0.97	0.09	44,47,53,54	0
3	HEC	N	607	43/43	0.97	0.09	37,41,44,46	0
3	HEC	O	603	43/43	0.97	0.09	40,44,49,51	0
3	HEC	B	605	43/43	0.97	0.09	42,45,53,59	0
3	HEC	B	607	43/43	0.97	0.07	37,40,45,47	0
3	HEC	O	604	43/43	0.97	0.10	34,41,50,60	0
3	HEC	O	605	43/43	0.97	0.09	36,41,49,52	0
3	HEC	O	606	43/43	0.97	0.09	37,41,49,52	0
3	HEC	O	607	43/43	0.97	0.08	34,37,38,39	0
3	HEC	P	600	43/43	0.97	0.09	44,46,51,53	0
3	HEC	C	603	43/43	0.97	0.10	44,48,58,63	0
3	HEC	C	600	43/43	0.97	0.09	49,52,56,58	0
3	HEC	P	604	43/43	0.97	0.08	36,40,52,63	0
3	HEC	P	605	43/43	0.97	0.08	43,46,49,50	0
3	HEC	P	606	43/43	0.97	0.09	43,47,48,49	0
3	HEC	P	607	43/43	0.97	0.09	38,48,52,54	0
3	HEC	P	603	43/43	0.97	0.10	40,49,56,62	0
3	HEC	C	601	43/43	0.97	0.09	41,45,50,51	0
3	HEC	C	602	43/43	0.97	0.09	45,48,66,80	0
3	HEC	C	604	43/43	0.97	0.09	42,47,53,60	0
3	HEC	C	605	43/43	0.97	0.09	38,43,53,57	0

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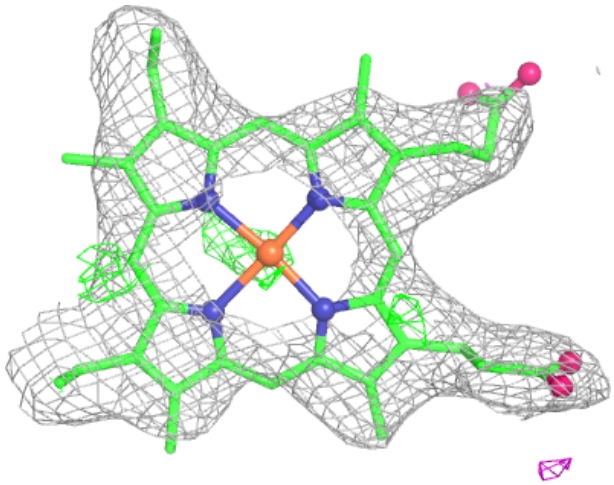
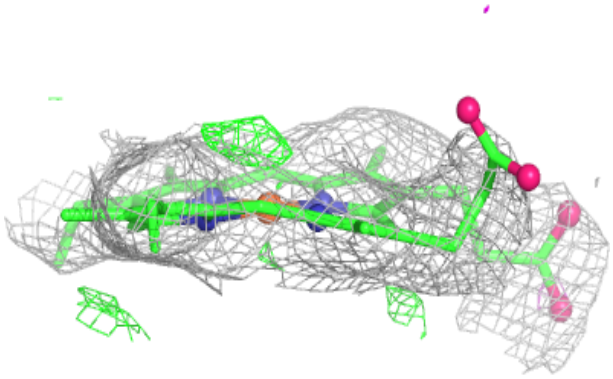
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEC	G	600	43/43	0.97	0.09	40,42,45,49	0
3	HEC	Q	605	43/43	0.97	0.09	45,51,57,60	0
3	HEC	G	604	43/43	0.97	0.08	31,34,49,57	0
3	HEC	Q	607	43/43	0.97	0.08	36,40,44,46	0
3	HEC	H	600	43/43	0.97	0.07	32,37,42,44	0
3	HEC	H	601	43/43	0.97	0.09	34,36,41,47	0
3	HEC	R	601	43/43	0.97	0.09	43,48,50,50	0
3	HEC	R	602	43/43	0.97	0.10	45,48,74,89	0
3	HEC	R	604	43/43	0.97	0.09	38,43,53,61	0
3	HEC	R	606	43/43	0.97	0.09	37,43,59,63	0
3	HEC	R	607	43/43	0.97	0.08	37,38,43,48	0
3	HEC	J	603	43/43	0.98	0.07	37,39,44,46	0
3	HEC	K	603	43/43	0.98	0.07	37,39,42,44	0
3	HEC	B	606	43/43	0.98	0.09	39,42,50,57	0
3	HEC	H	607	43/43	0.98	0.07	28,30,32,35	0
3	HEC	I	603	43/43	0.98	0.06	30,33,37,39	0
3	HEC	G	607	43/43	0.98	0.07	30,31,34,34	0
3	HEC	G	603	43/43	0.98	0.07	34,36,39,42	0
3	HEC	H	603	43/43	0.98	0.07	31,34,42,48	0
3	HEC	K	607	43/43	0.98	0.07	30,32,34,36	0
4	SO4	K	609	5/5	0.98	0.06	28,28,29,30	0
3	HEC	I	604	43/43	0.98	0.07	36,38,51,58	0
3	HEC	I	605	43/43	0.98	0.07	29,33,38,40	0
3	HEC	I	606	43/43	0.98	0.07	34,35,44,47	0
3	HEC	I	607	43/43	0.98	0.07	32,34,36,38	0
3	HEC	D	604	43/43	0.98	0.08	44,47,54,60	0
3	HEC	O	601	43/43	0.98	0.09	40,44,49,56	0
3	HEC	J	601	43/43	0.98	0.08	34,37,41,47	0
3	HEC	G	605	43/43	0.98	0.08	33,36,41,43	0
3	HEC	L	607	43/43	0.98	0.07	32,34,35,36	0
3	HEC	G	606	43/43	0.98	0.08	35,37,42,46	0
3	HEC	R	605	43/43	0.98	0.07	35,40,45,46	0
3	HEC	D	607	43/43	0.98	0.08	40,45,55,61	0
3	HEC	H	605	43/43	0.98	0.07	28,32,34,35	0
3	HEC	J	607	43/43	0.98	0.08	28,30,33,37	0

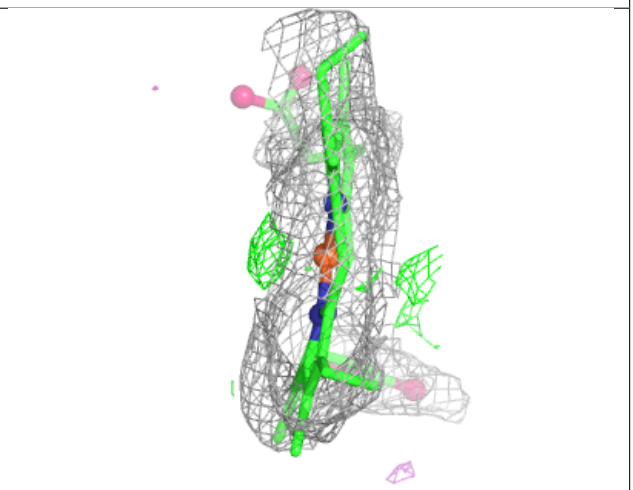
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC V 602:

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

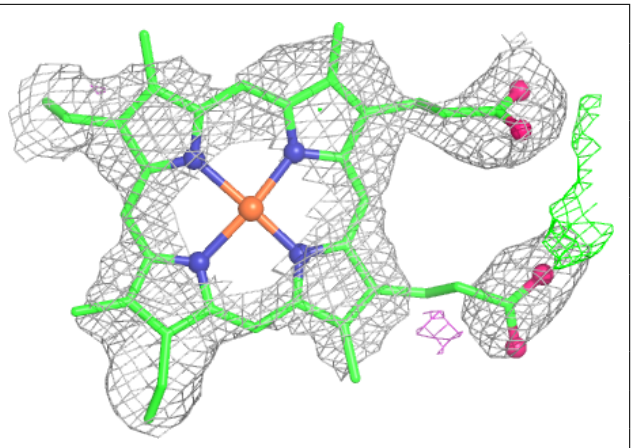


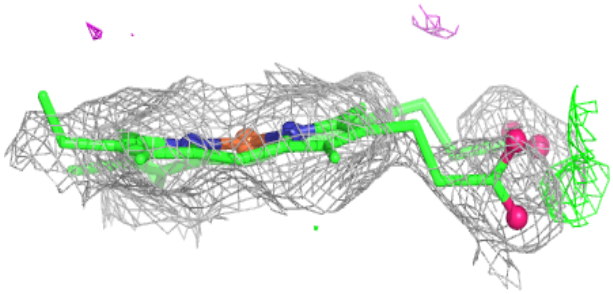


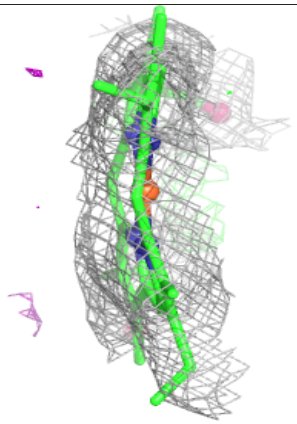


Electron density around HEC W 606:

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

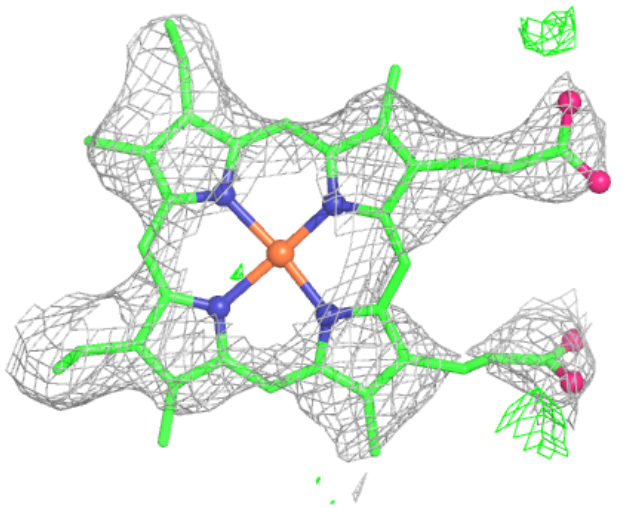


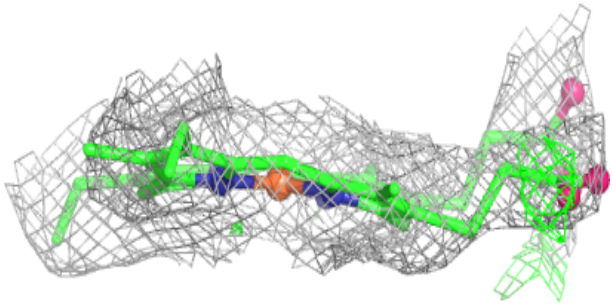


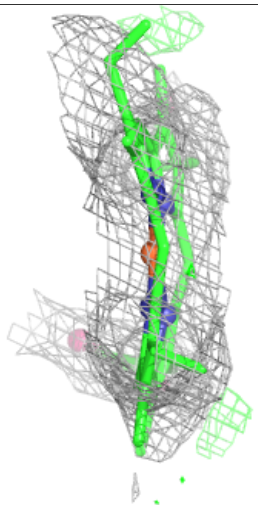


Electron density around HEC X 606:

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

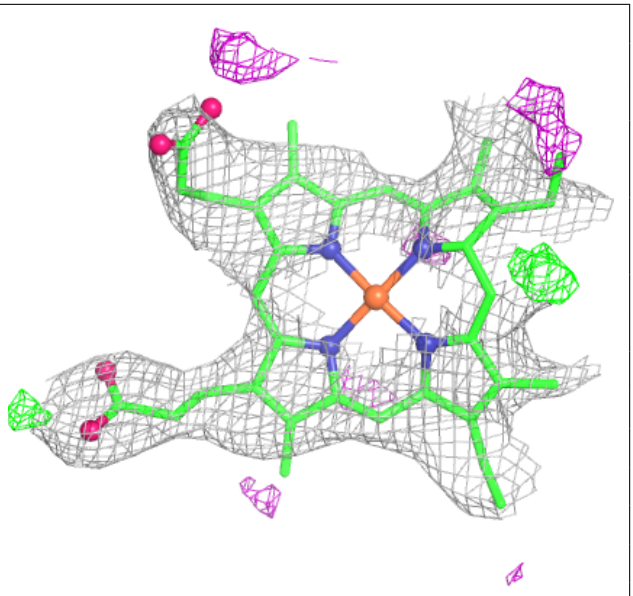


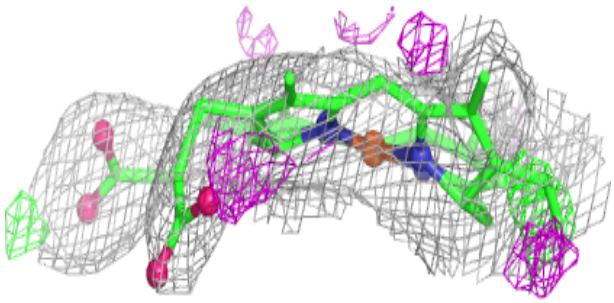


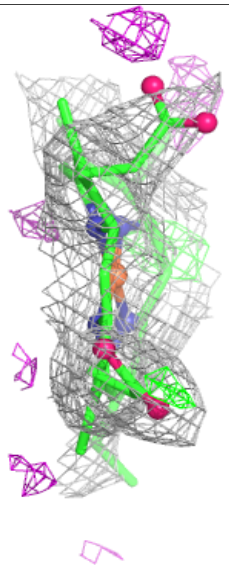


Electron density around HEC V 603:

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

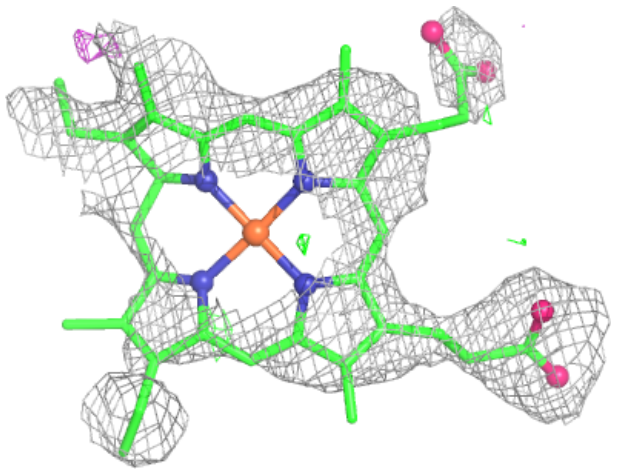


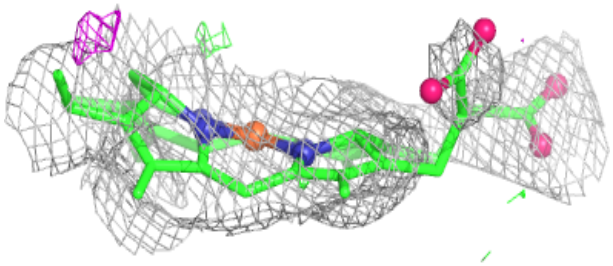


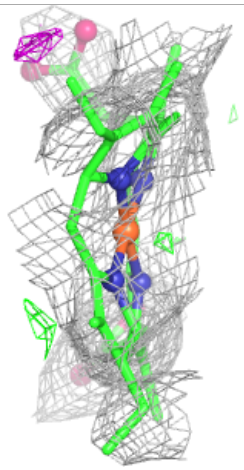


Electron density around HEC W 603:

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

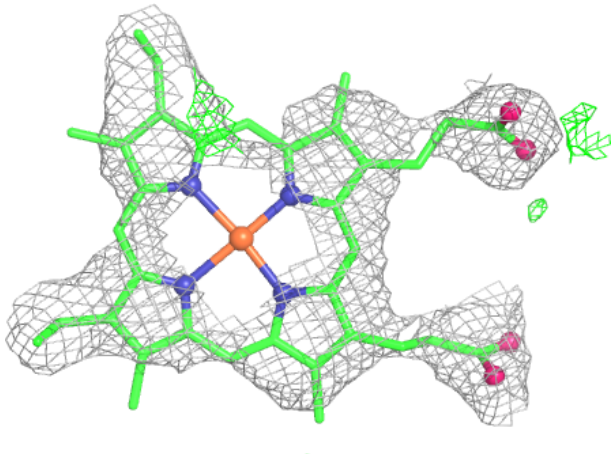


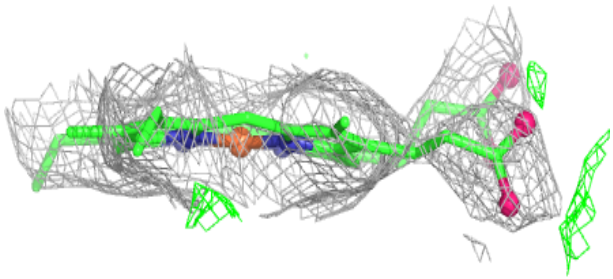


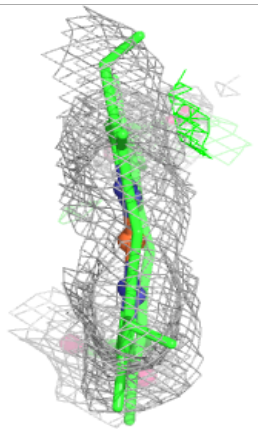


Electron density around HEC W 605:

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

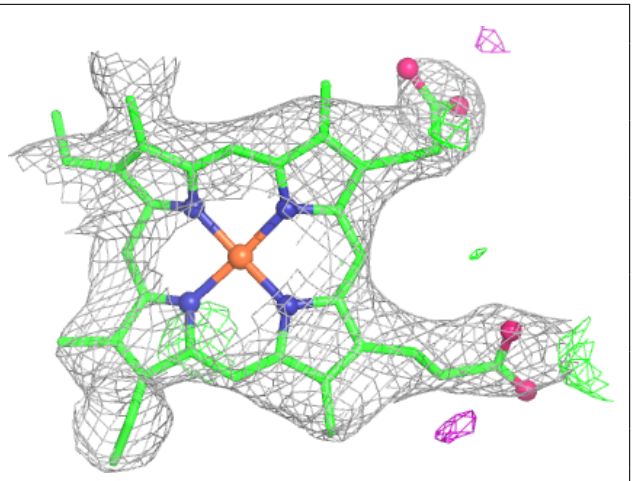


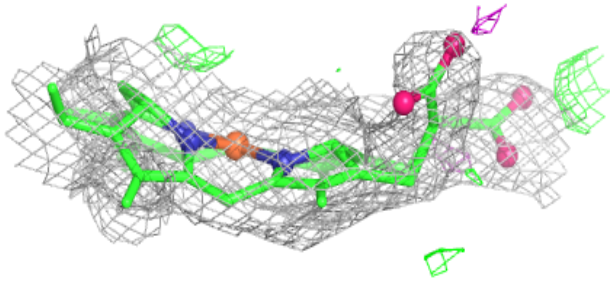


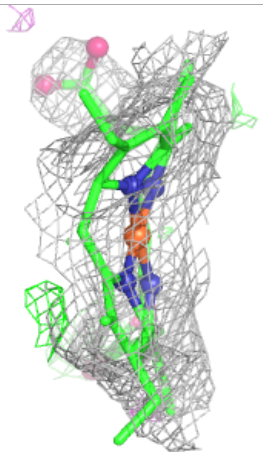


Electron density around HEC S 603:

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

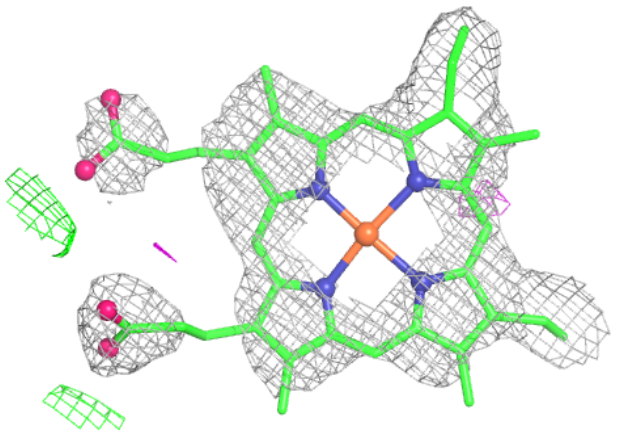


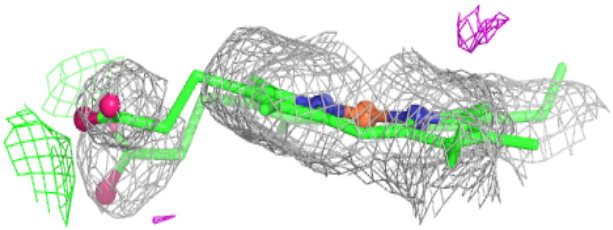


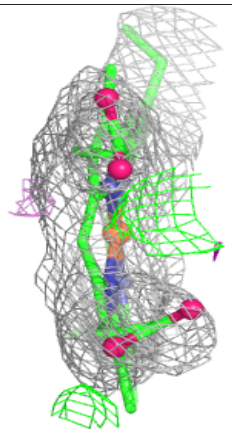


Electron density around HEC U 606:

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

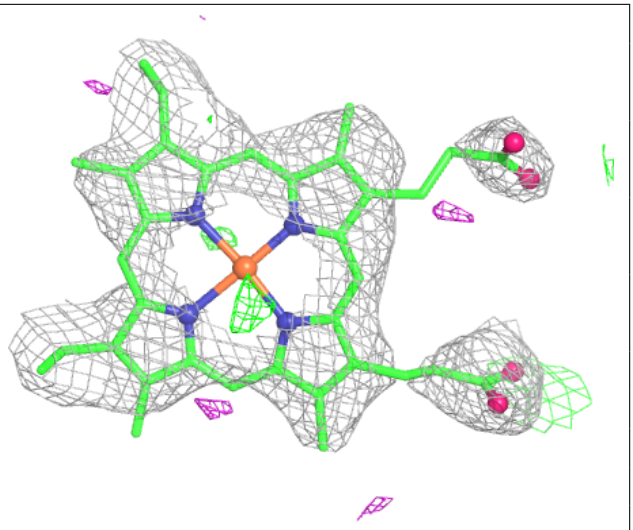


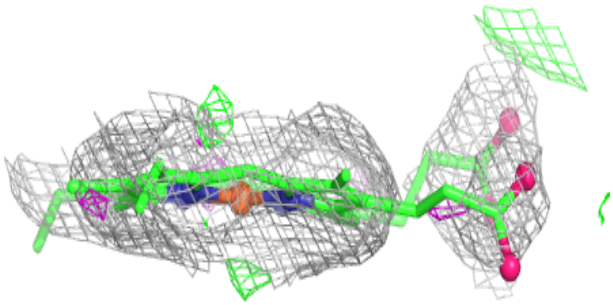


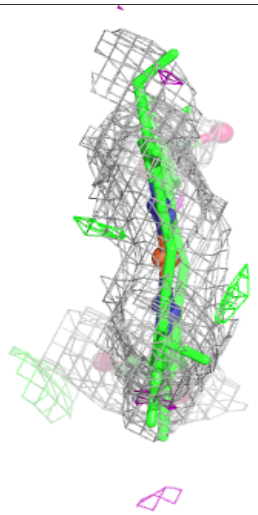


Electron density around HEC S 605:

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

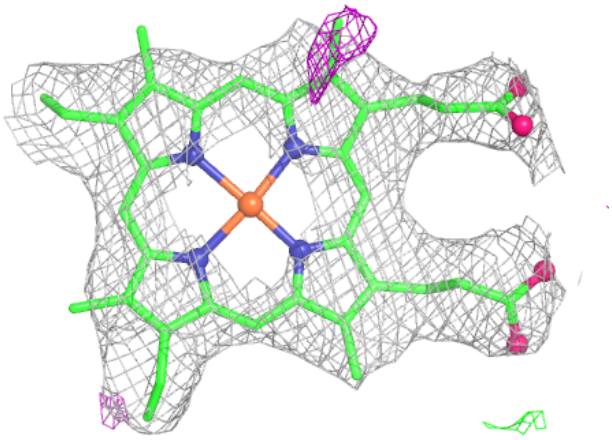


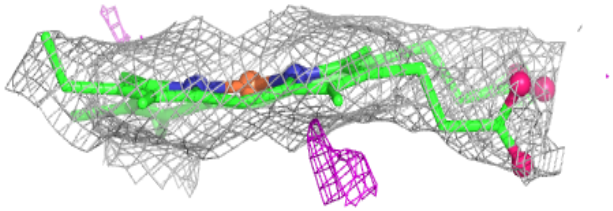


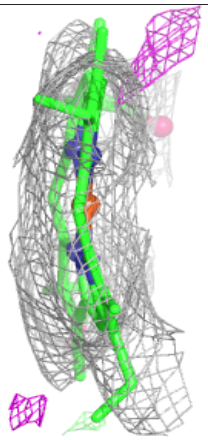


Electron density around HEC V 606:

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

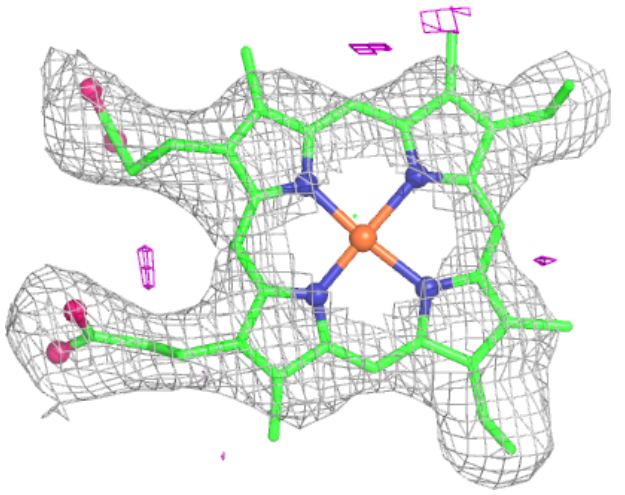


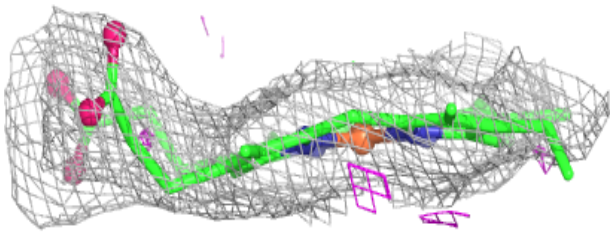


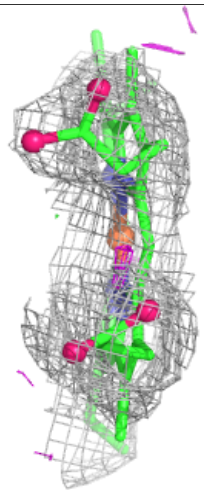


Electron density around HEC V 607:

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

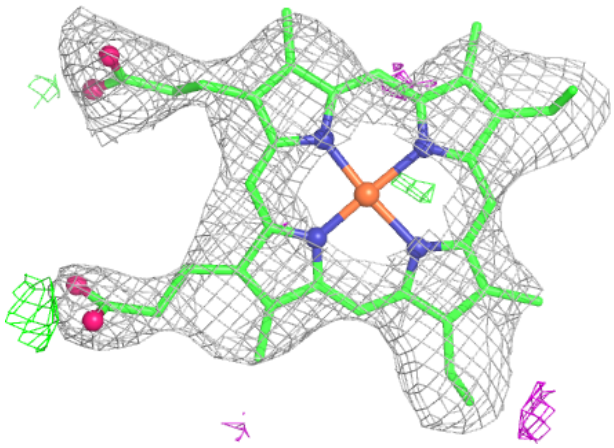


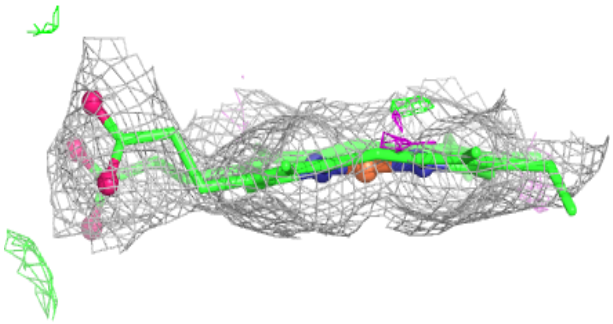


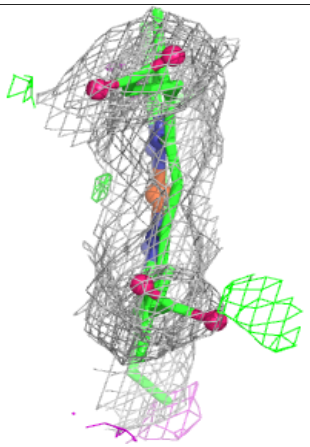


Electron density around HEC E 605:

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

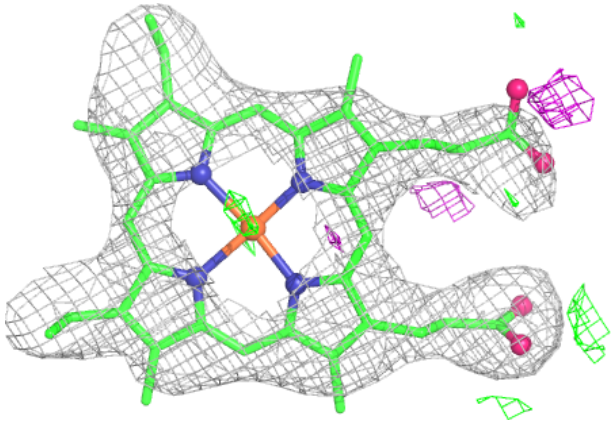


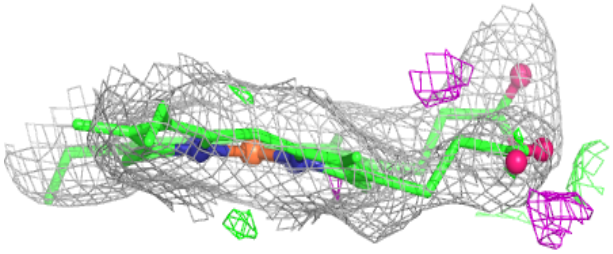


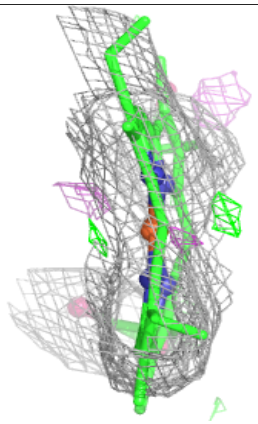


Electron density around HEC E 606:

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

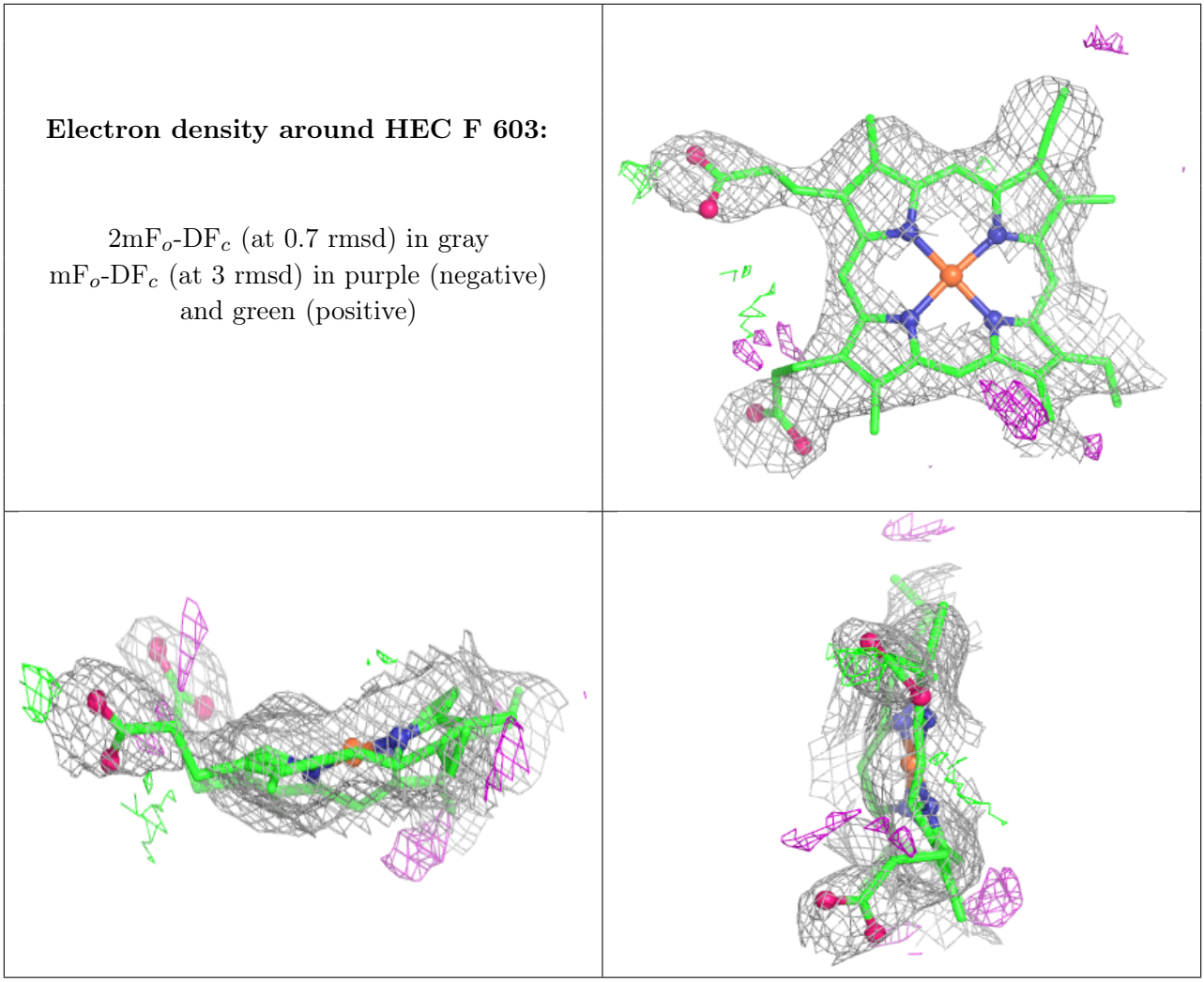






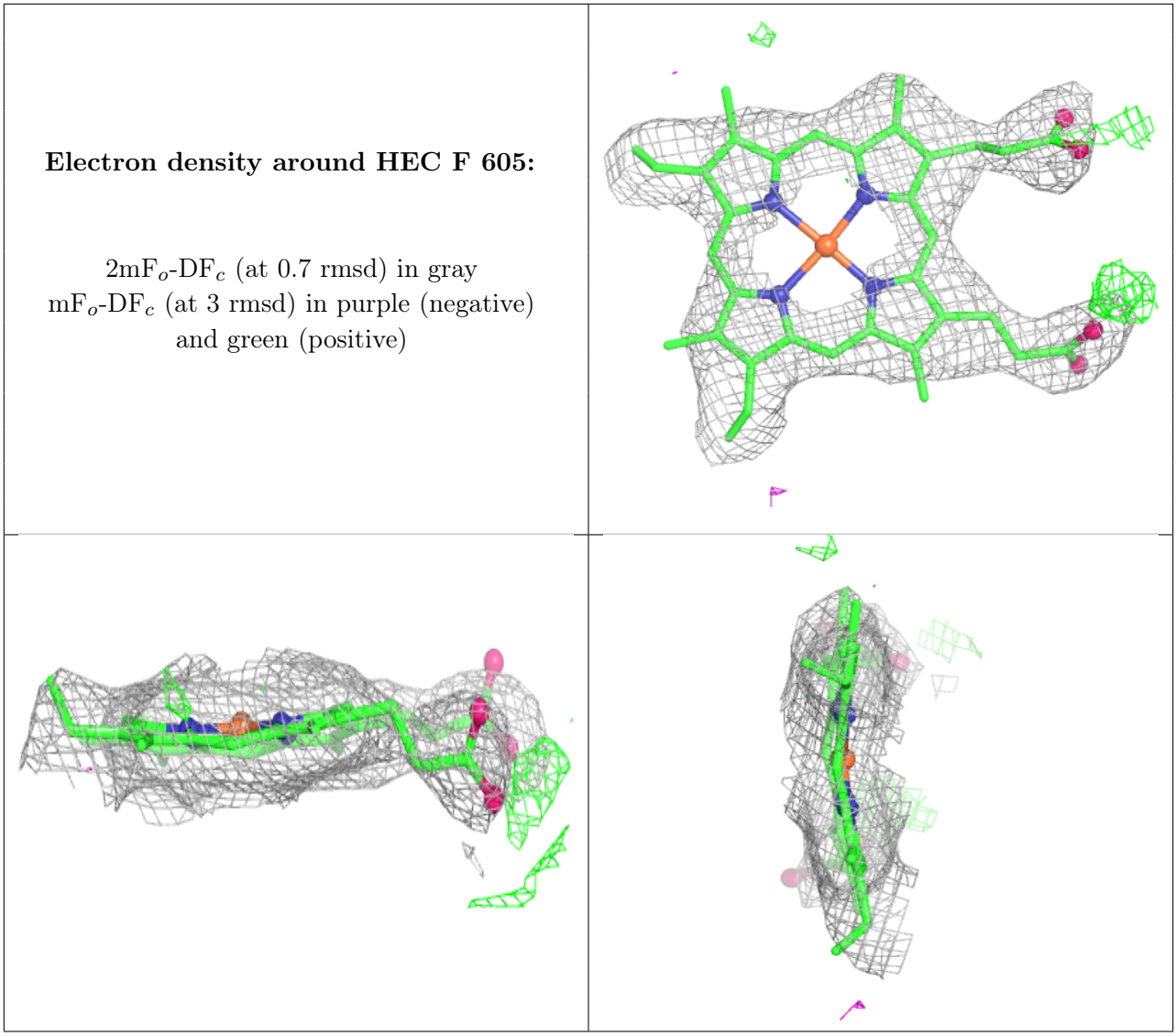
Electron density around HEC F 603:

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



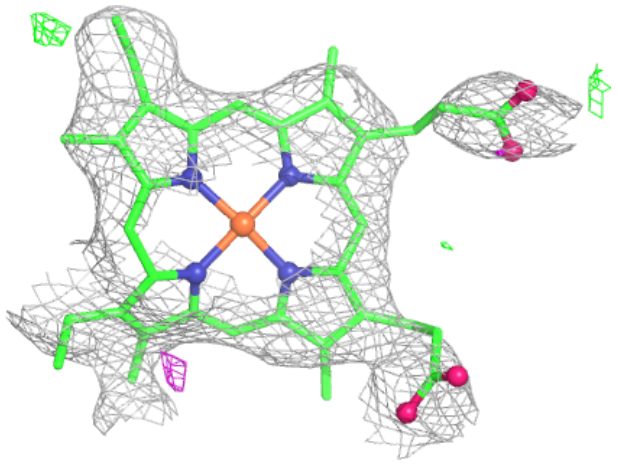
Electron density around HEC F 605:

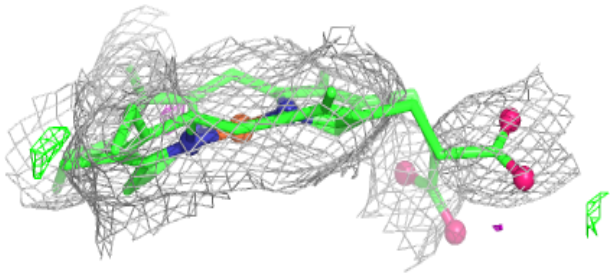
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

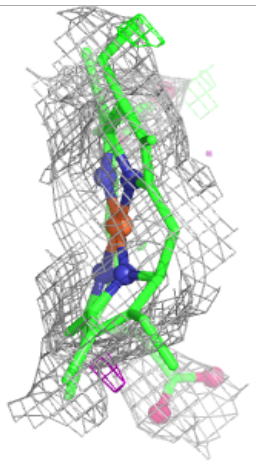


Electron density around HEC X 603:

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

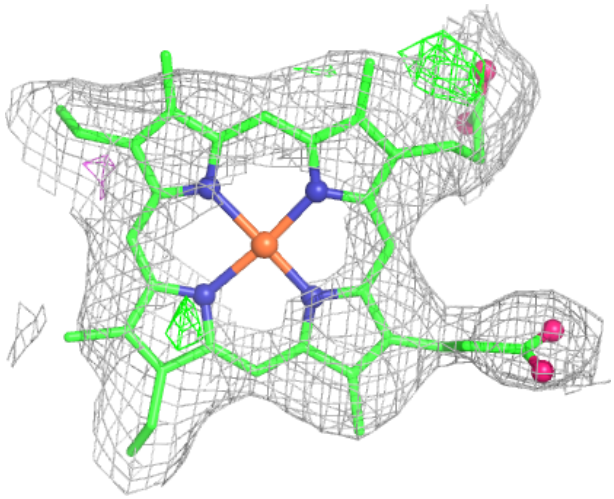


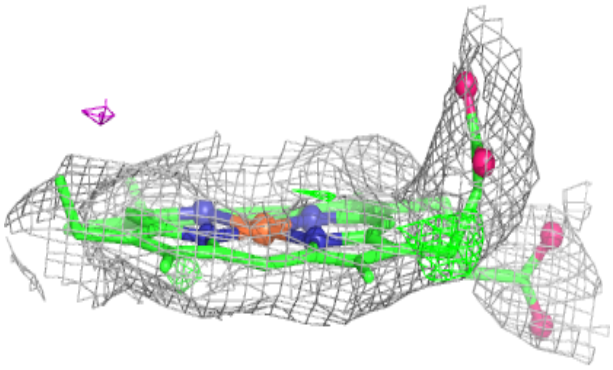


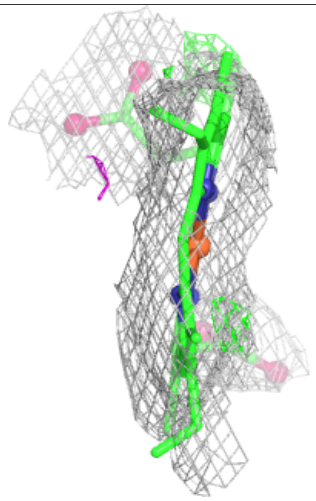


Electron density around HEC X 601:

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

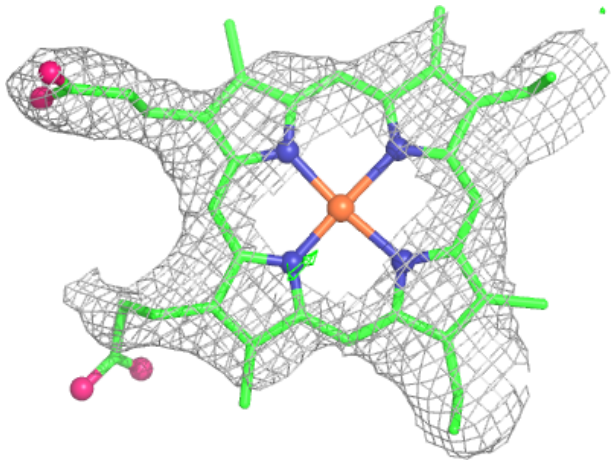


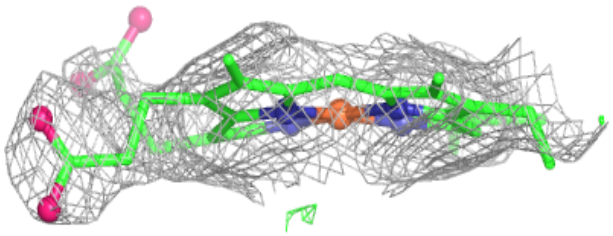


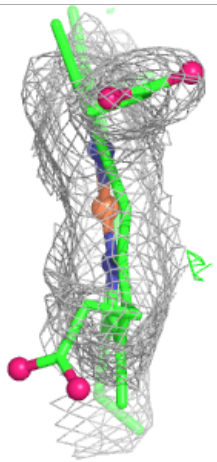


Electron density around HEC X 602:

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

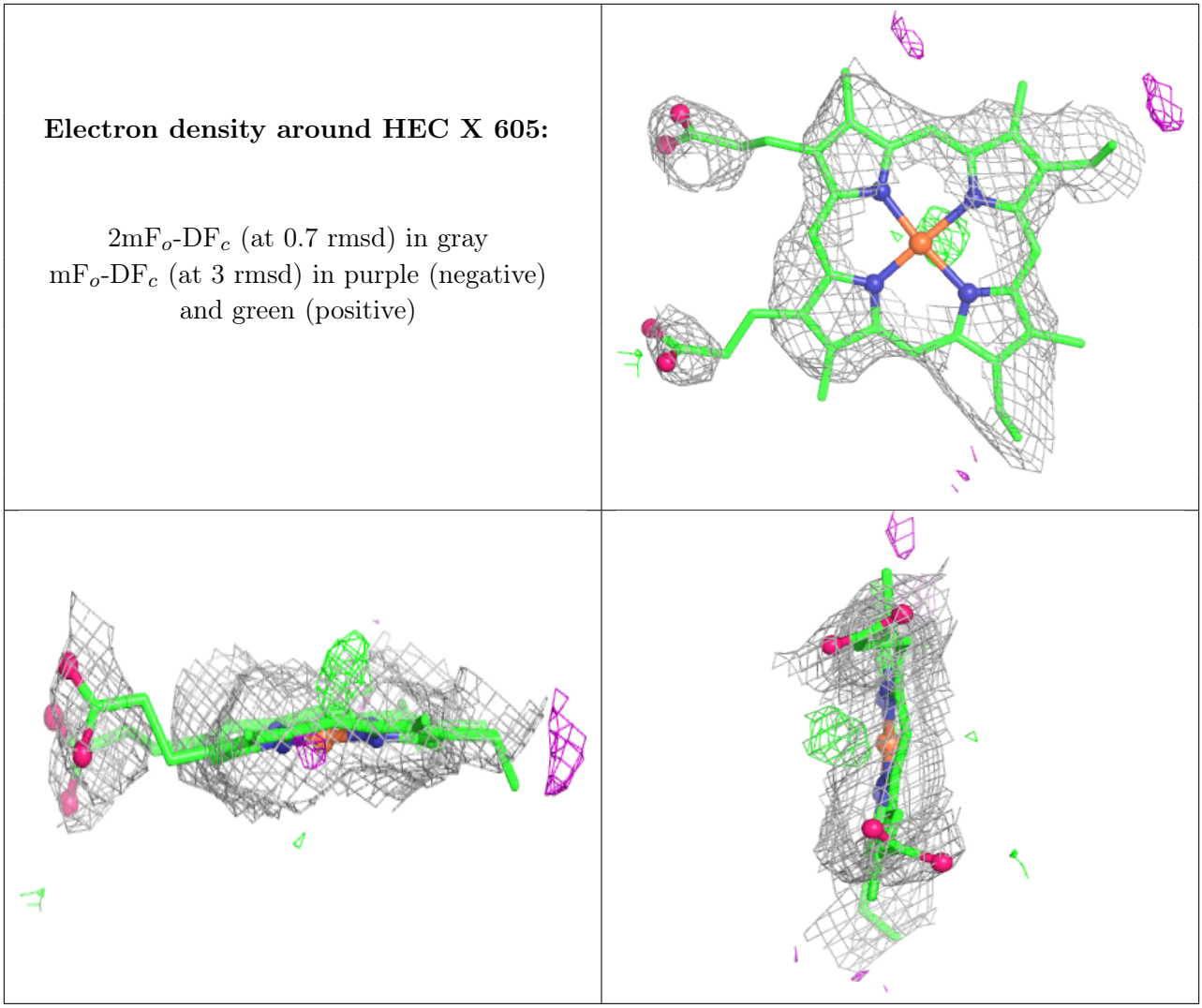






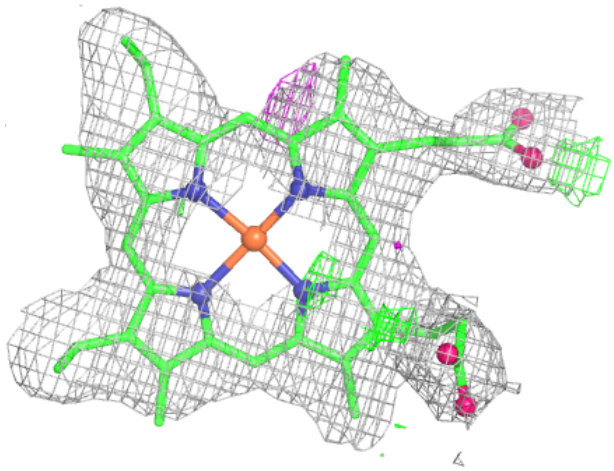
Electron density around HEC X 605:

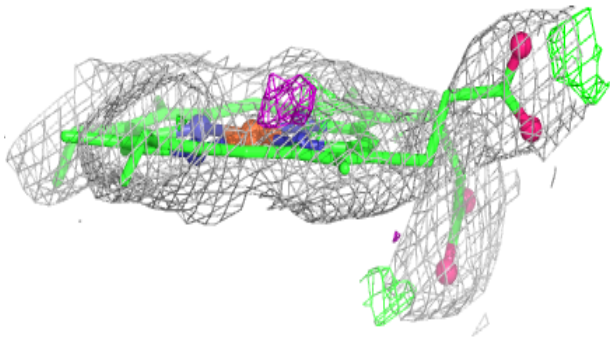
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

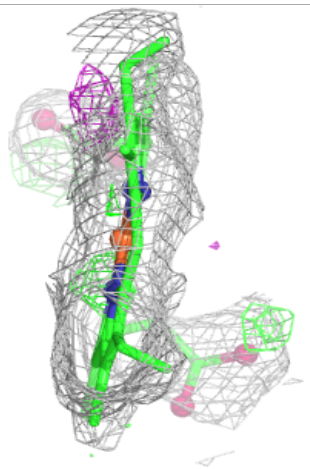


Electron density around HEC N 601:

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

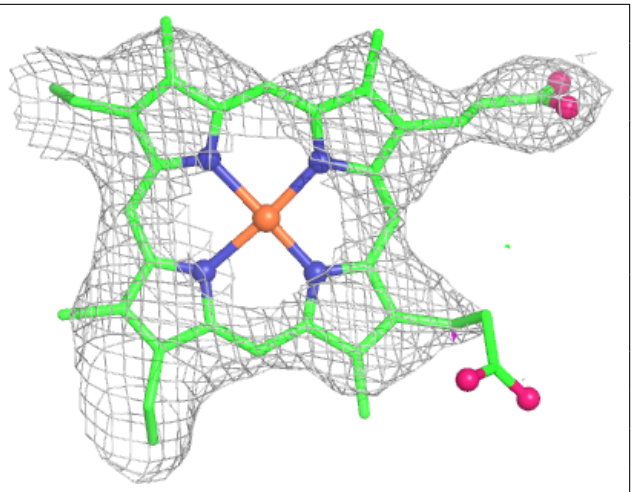


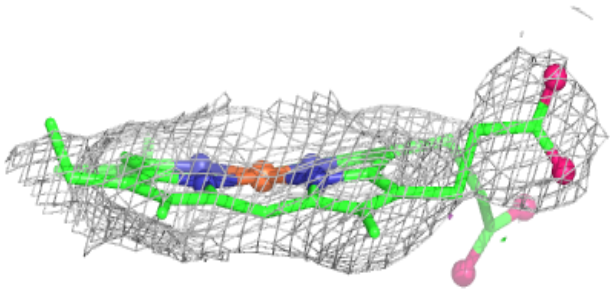


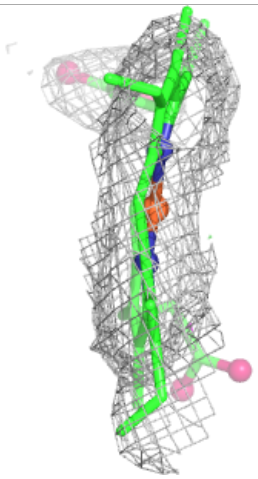


Electron density around HEC Q 602:

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

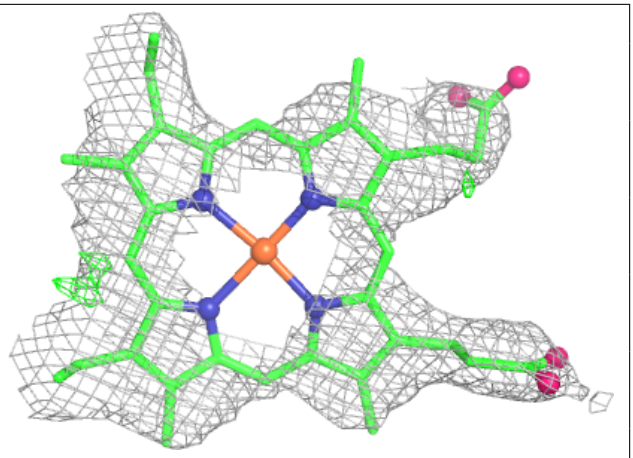


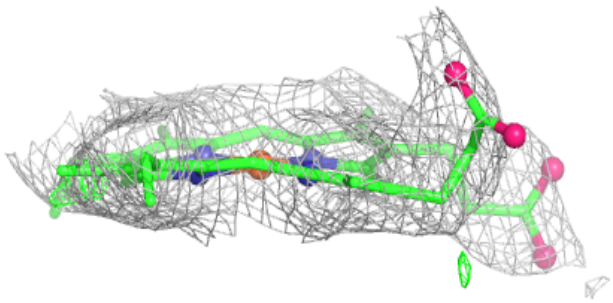


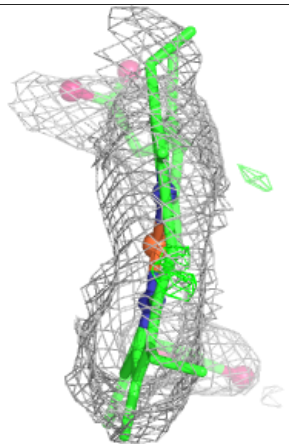


Electron density around HEC S 602:

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

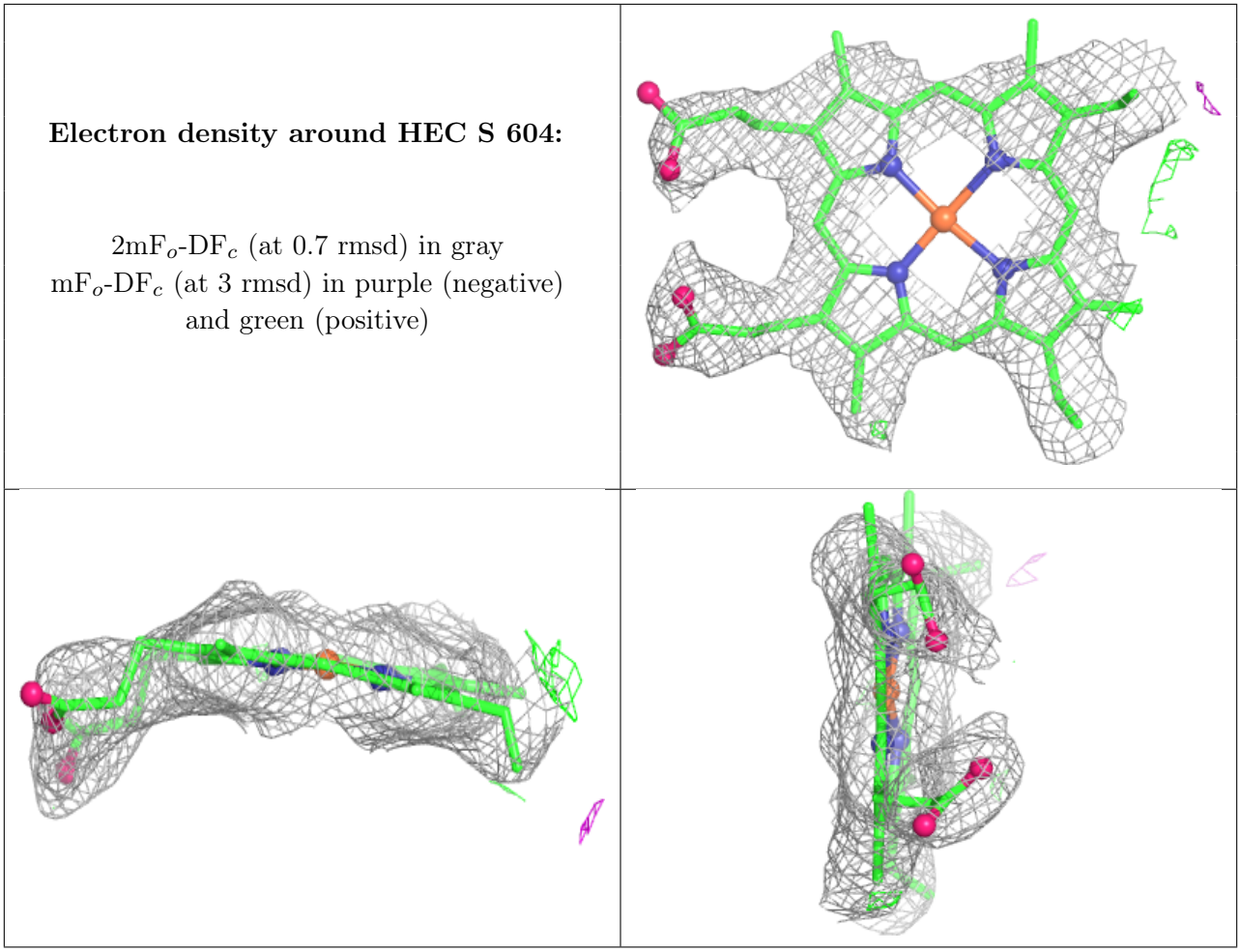






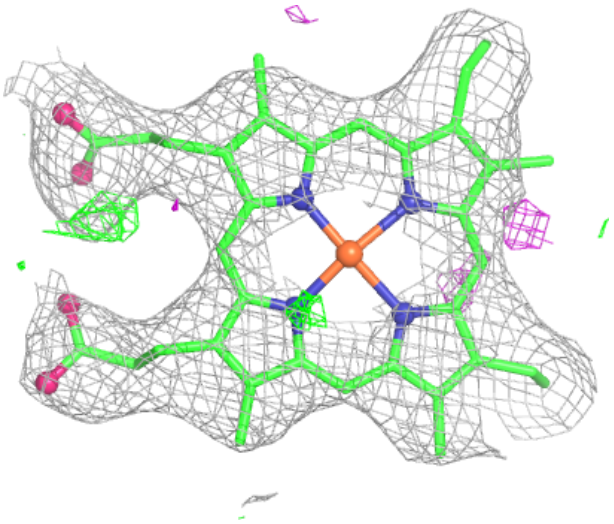
Electron density around HEC S 604:

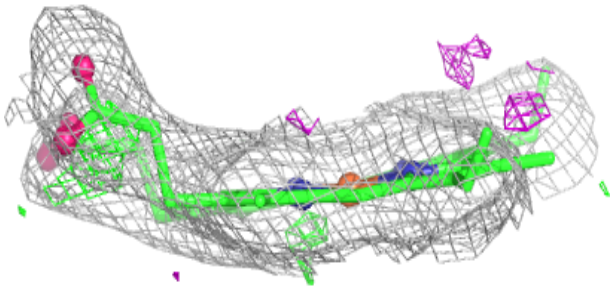
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

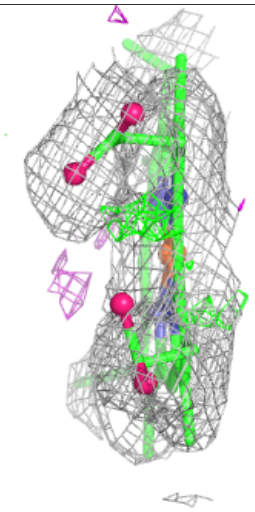


Electron density around HEC A 604:

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

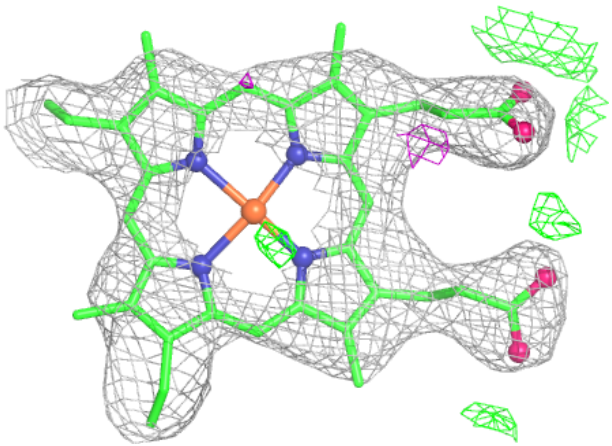


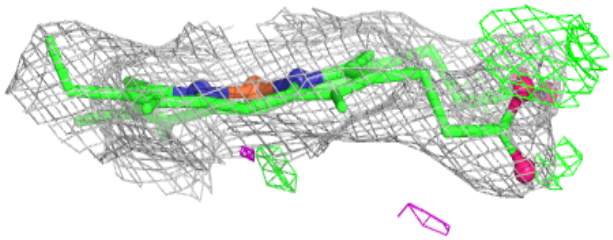


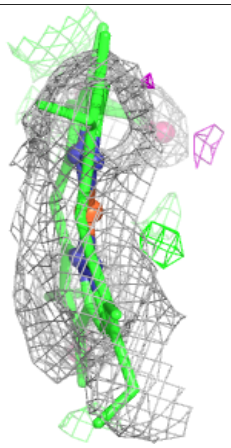


Electron density around HEC S 606:

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

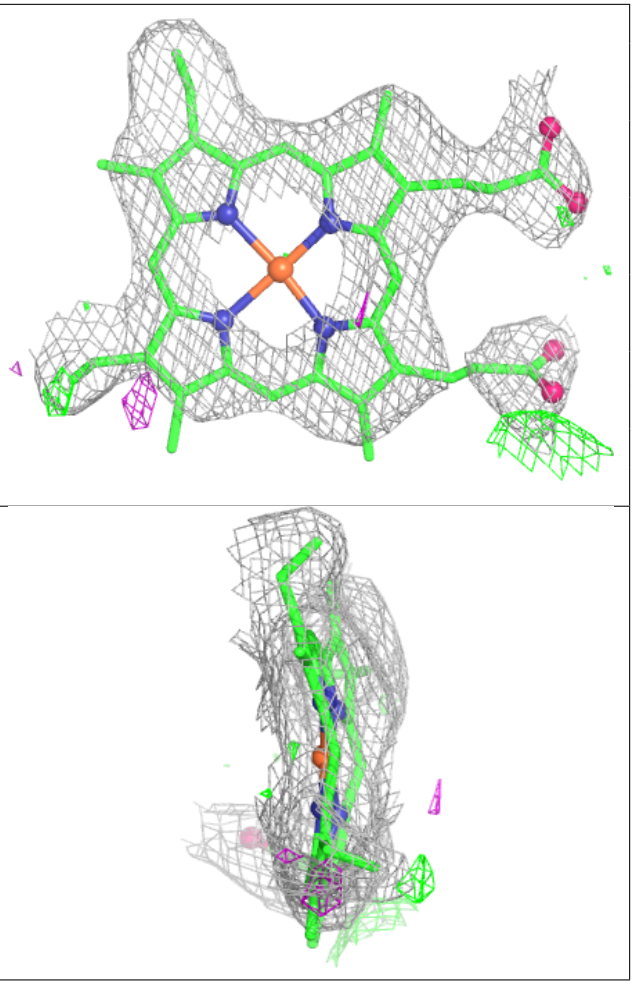






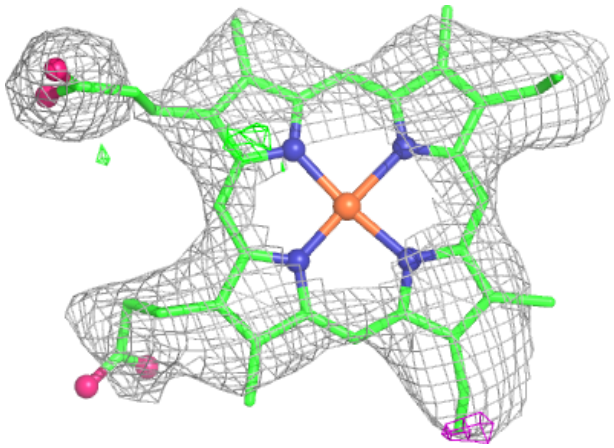
Electron density around HEC A 606:

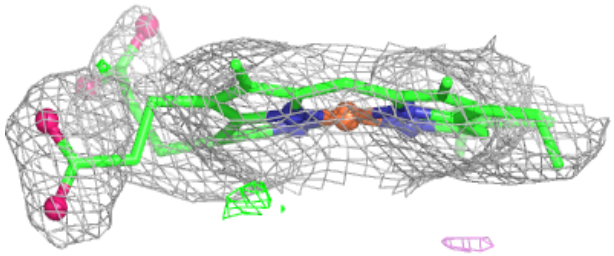
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

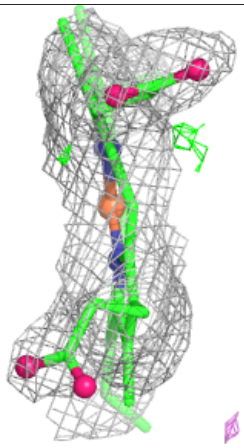


Electron density around HEC T 602:

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

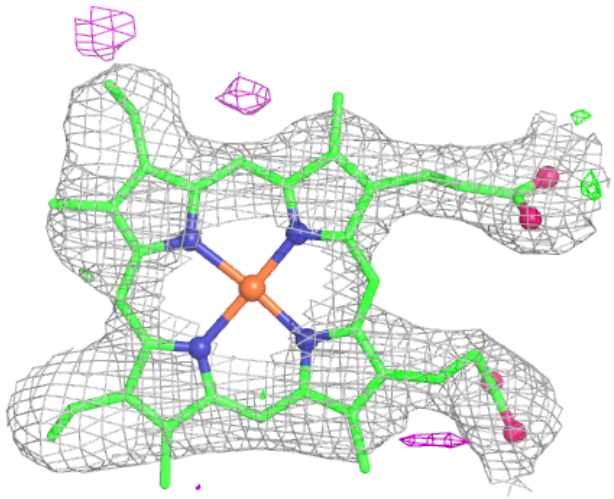


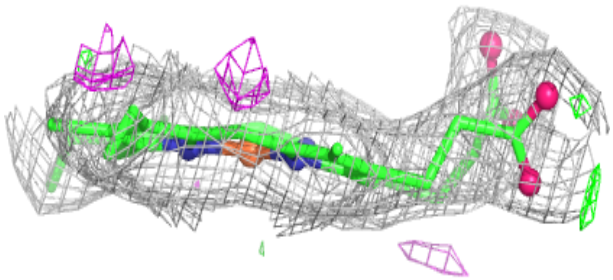


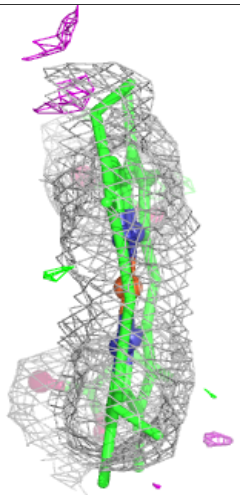


Electron density around HEC T 607:

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

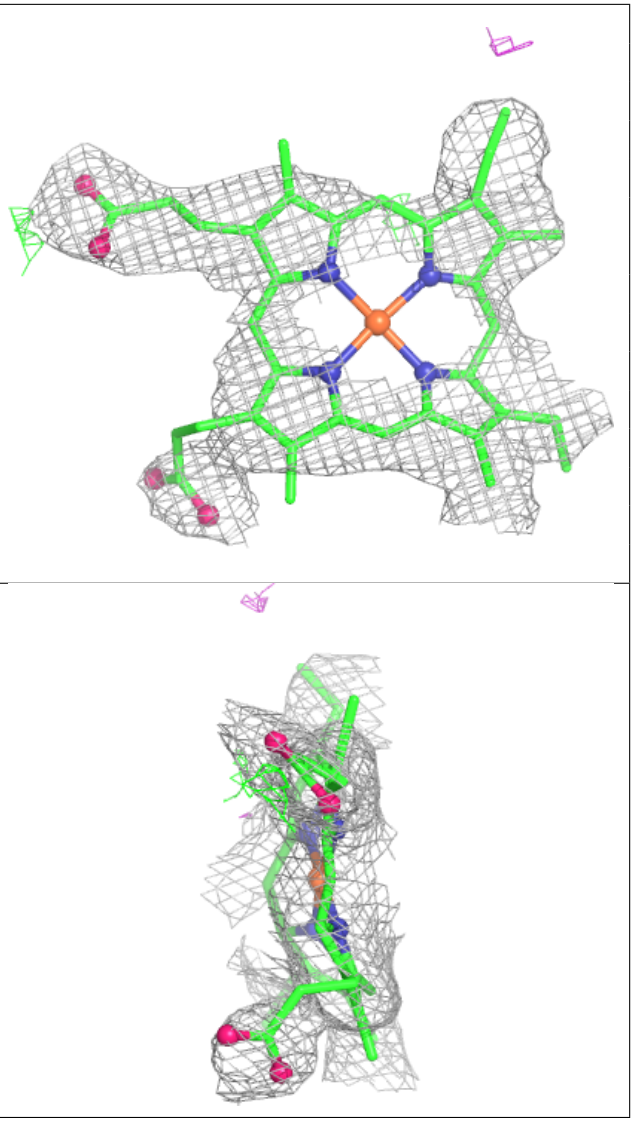


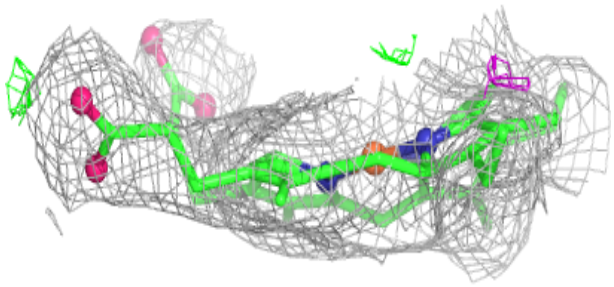




Electron density around HEC U 603:

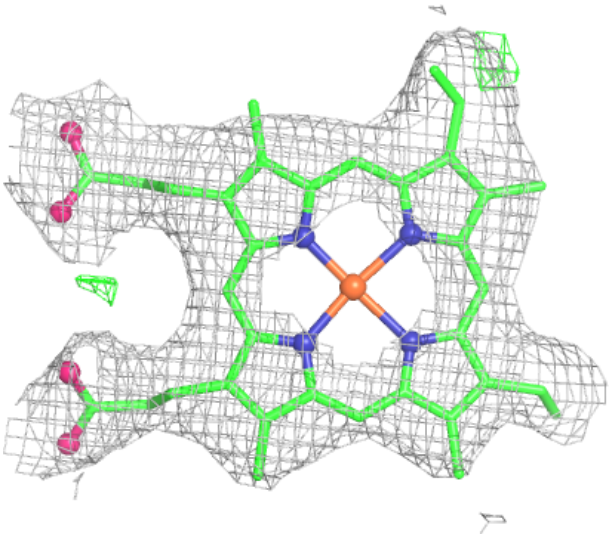
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

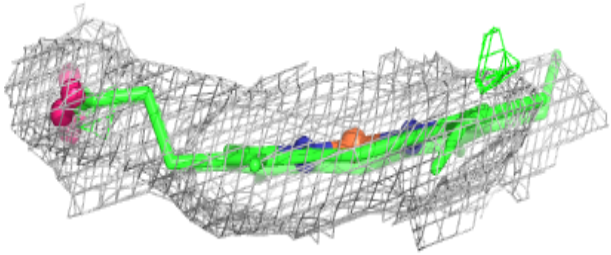


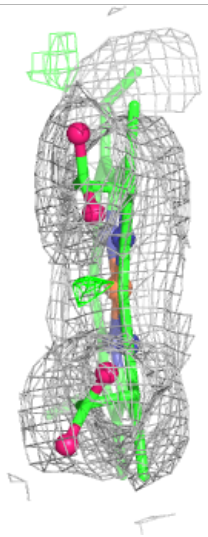


Electron density around HEC U 600:

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

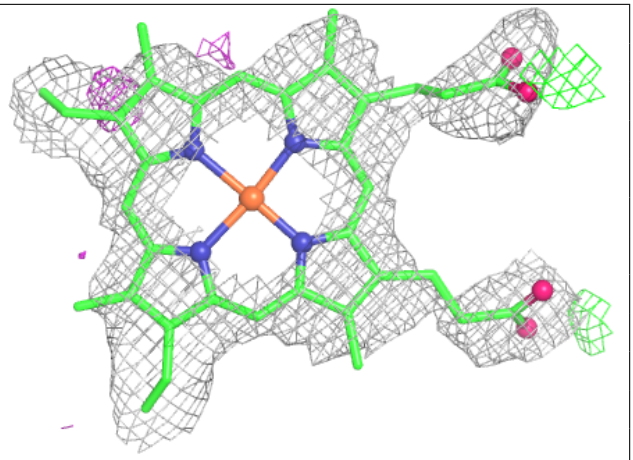


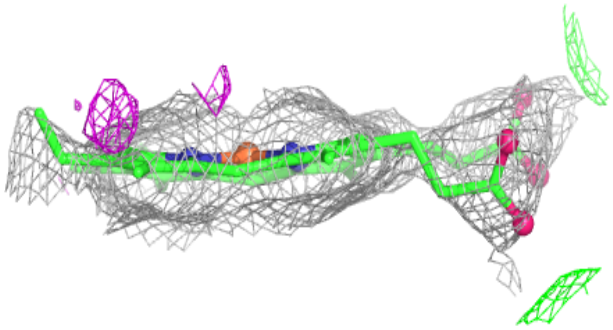


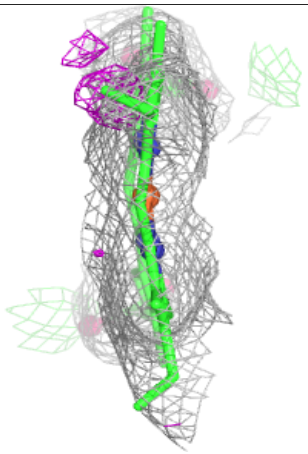


Electron density around HEC U 605:

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

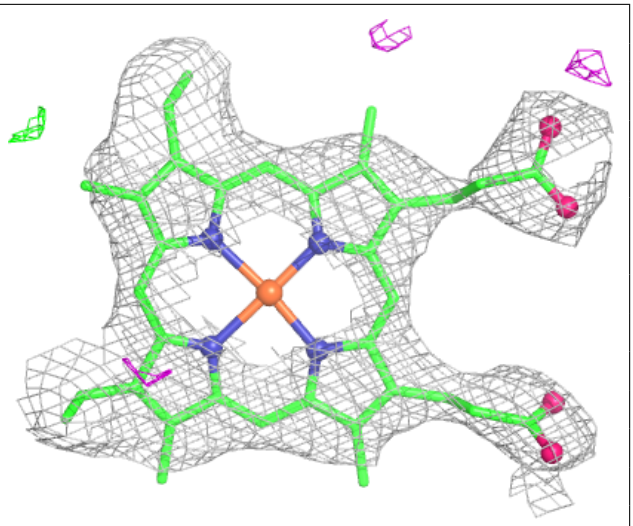


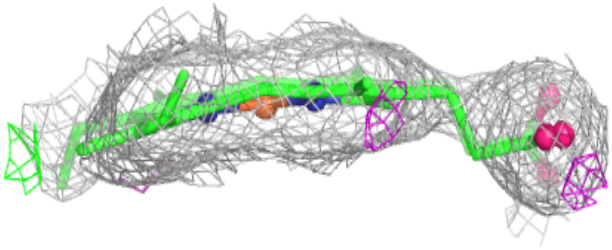


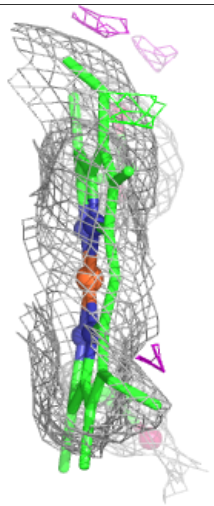


Electron density around HEC D 600:

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

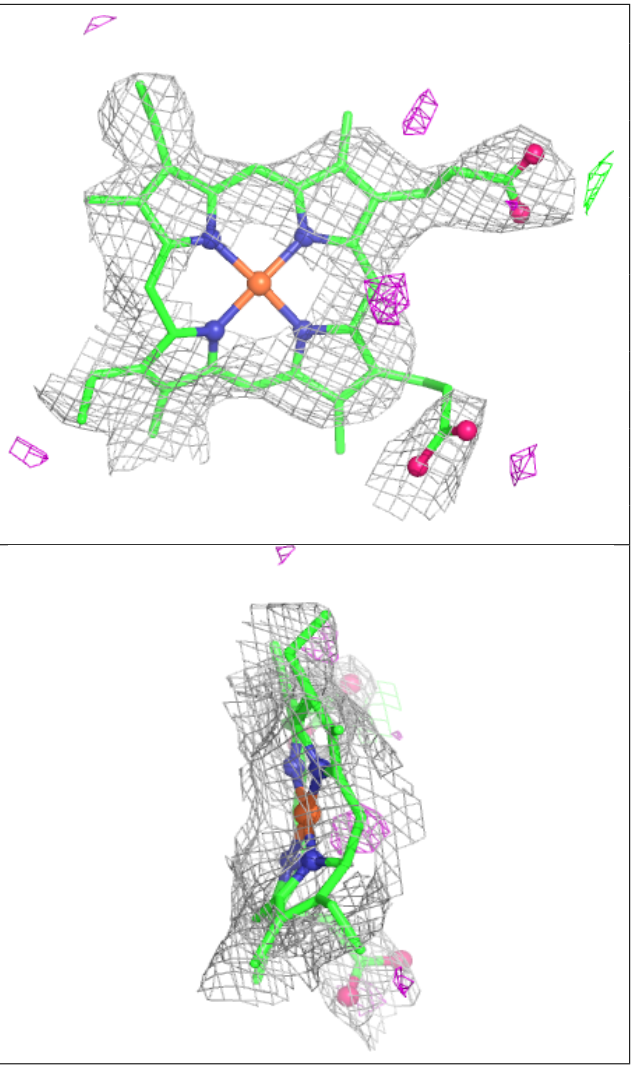






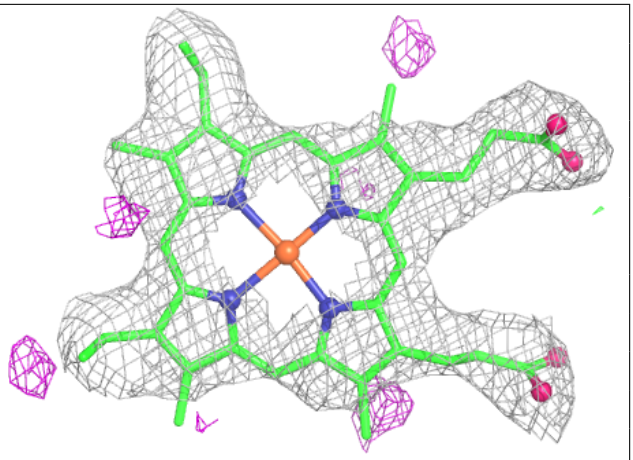
Electron density around HEC E 603:

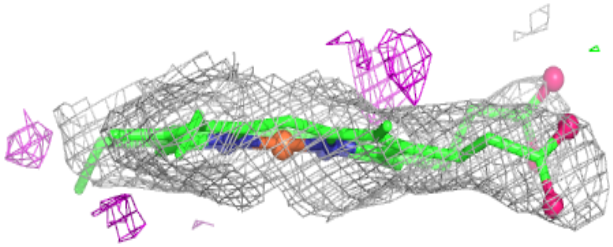
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

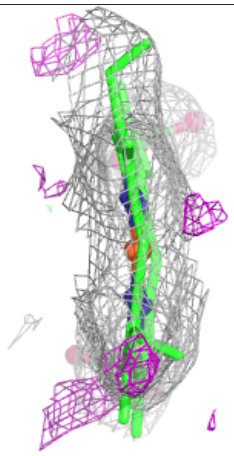


Electron density around HEC V 605:

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

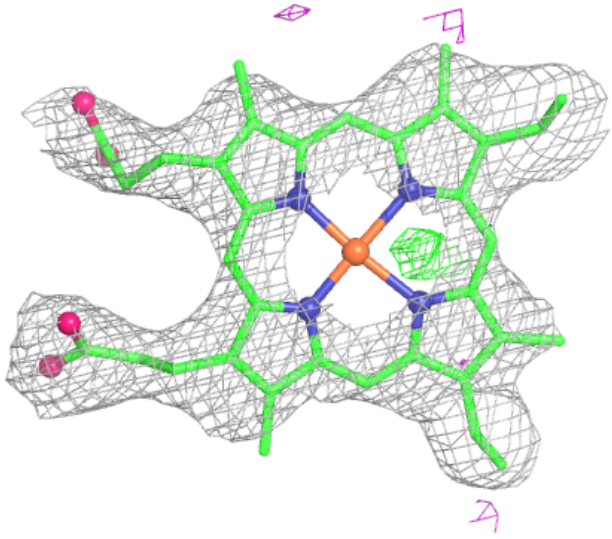


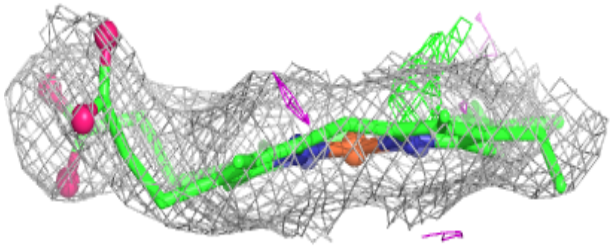


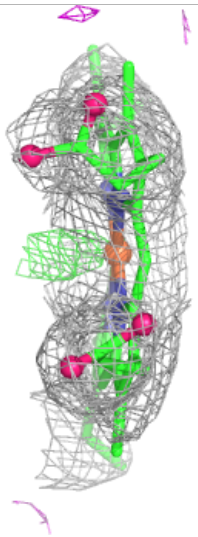


Electron density around HEC S 607:

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

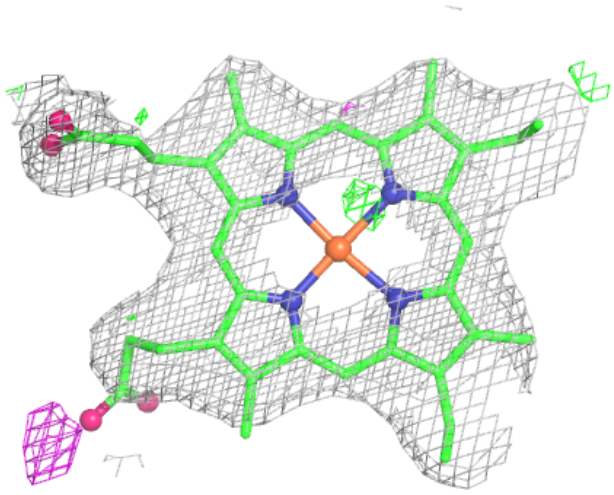


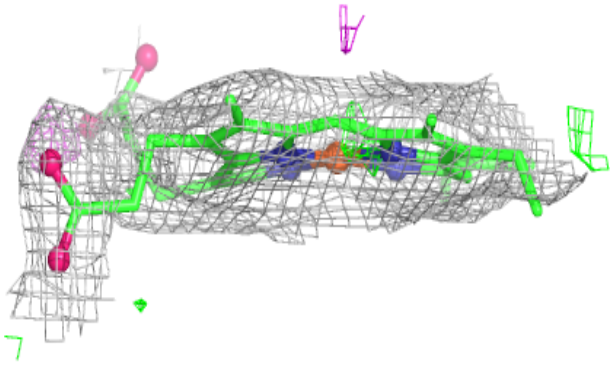


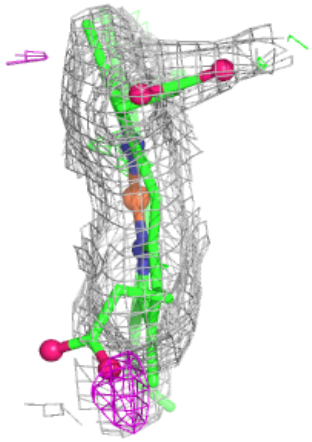


Electron density around HEC E 602:

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

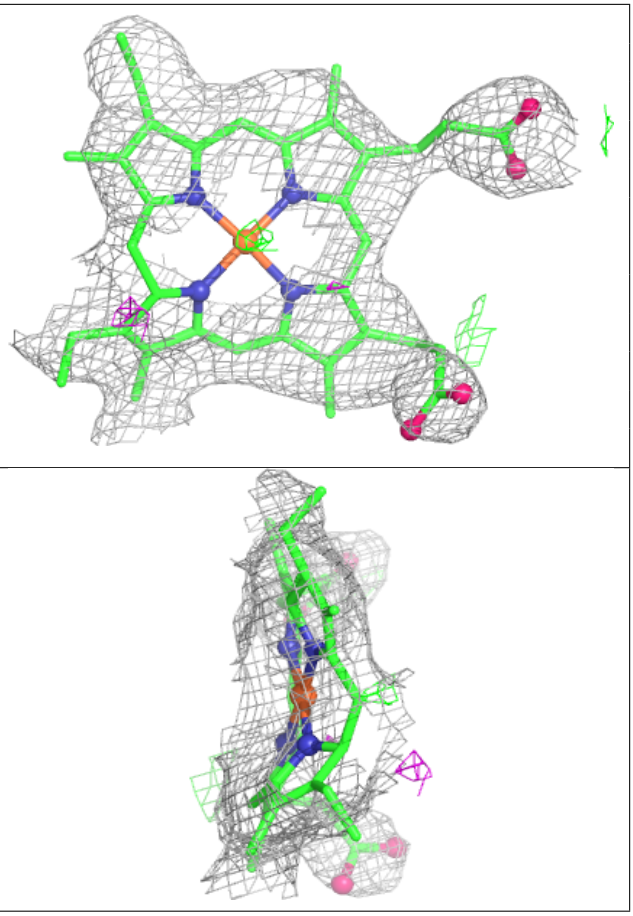






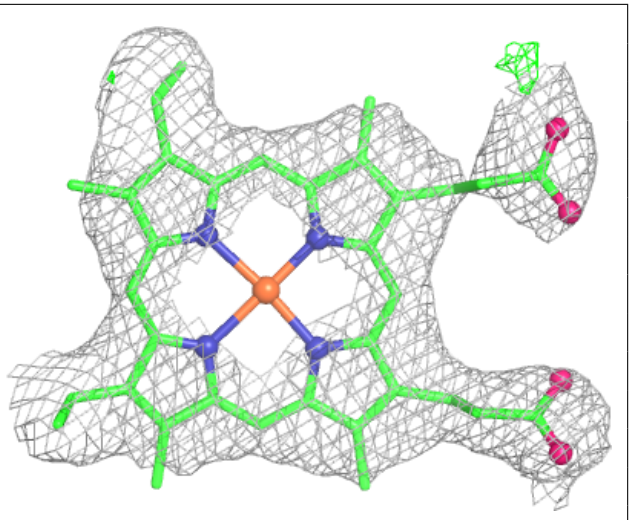
Electron density around HEC T 603:

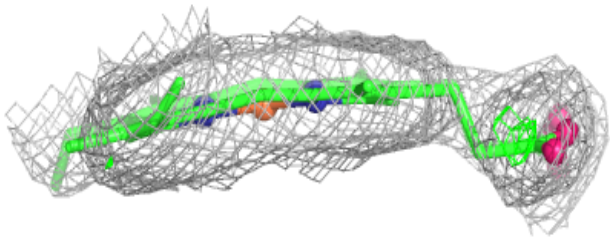
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

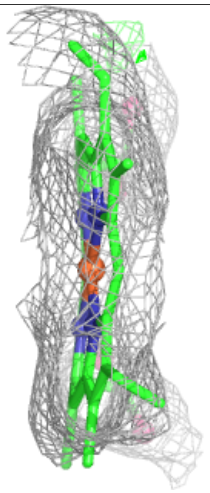


Electron density around HEC T 600:

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

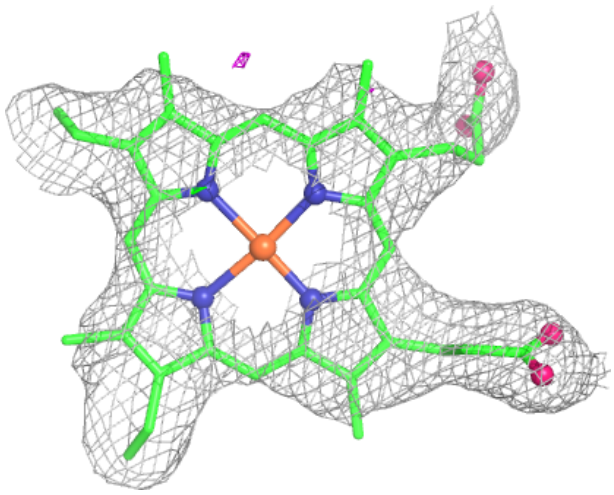


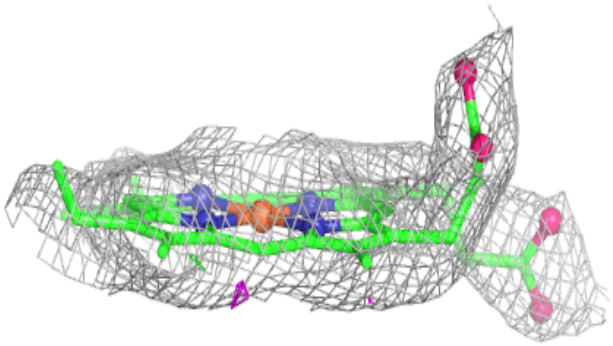


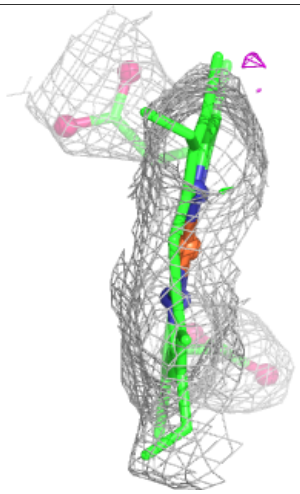


Electron density around HEC T 601:

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

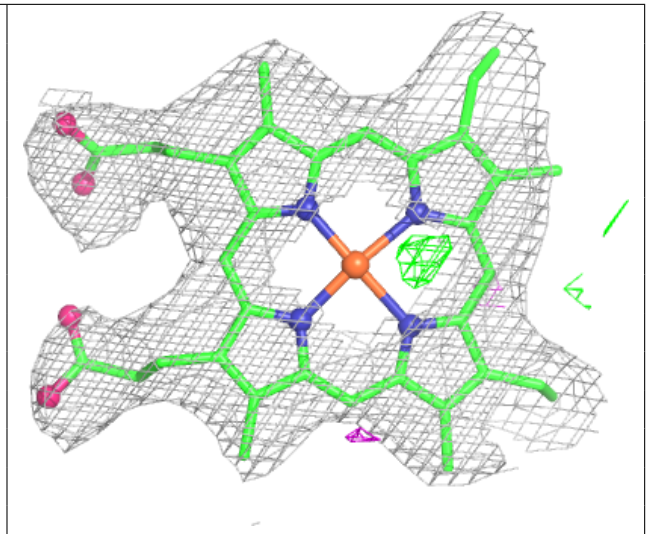


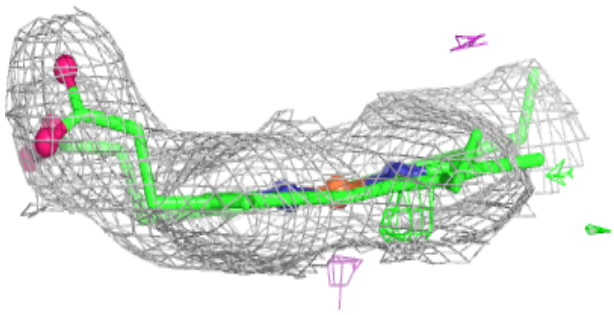


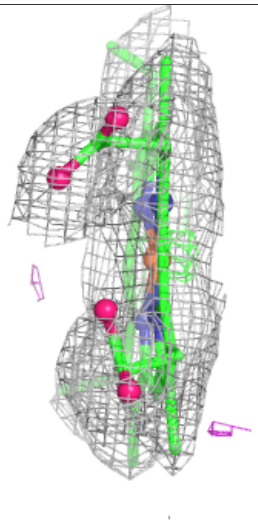


Electron density around HEC E 604:

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

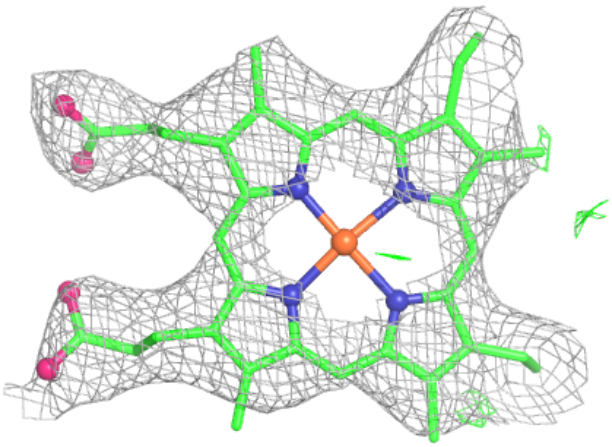


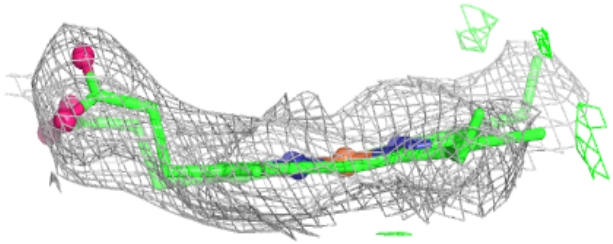


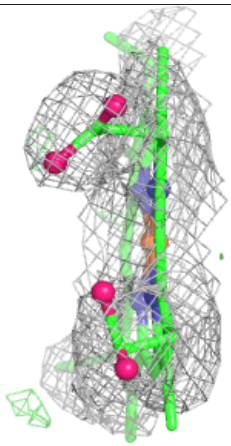


Electron density around HEC T 604:

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

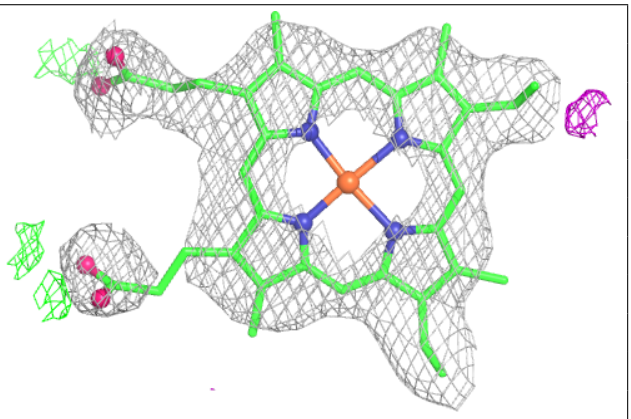


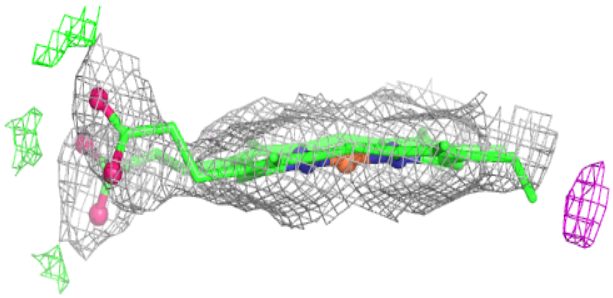




Electron density around HEC T 605:

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

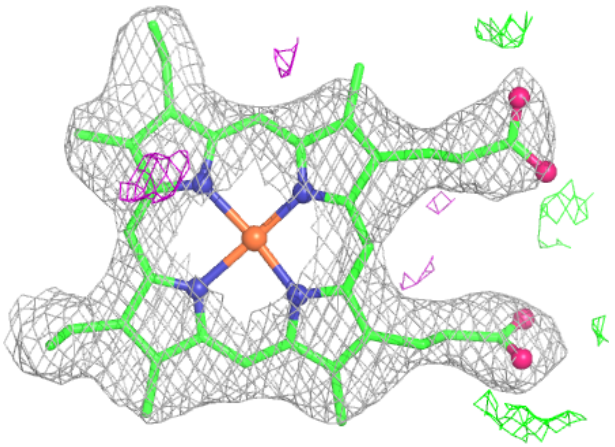


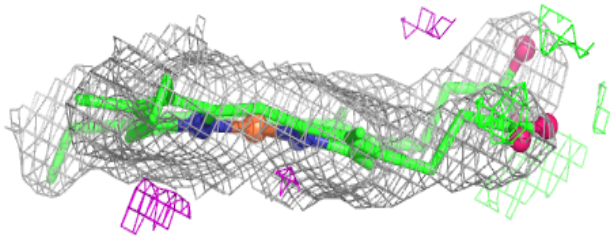


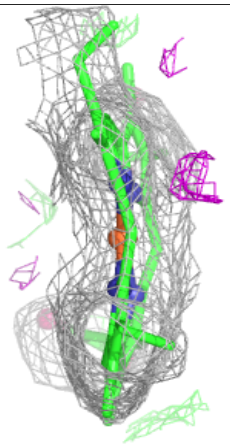


Electron density around HEC T 606:

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

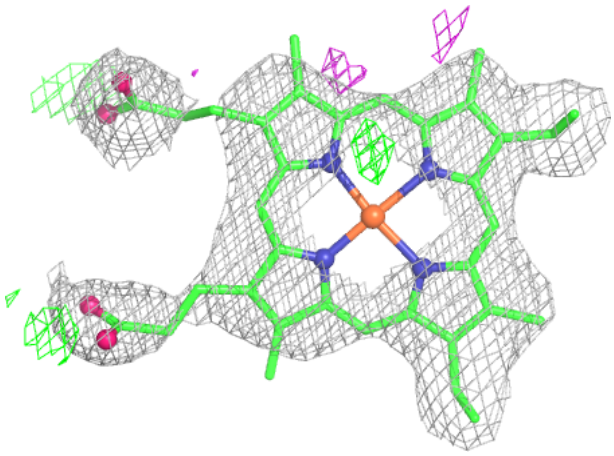


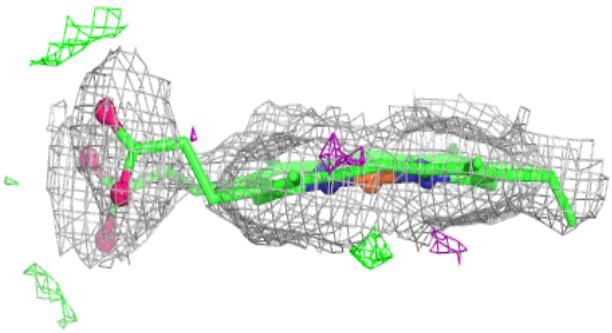


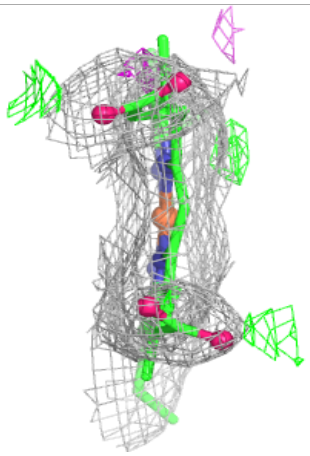


Electron density around HEC A 605:

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

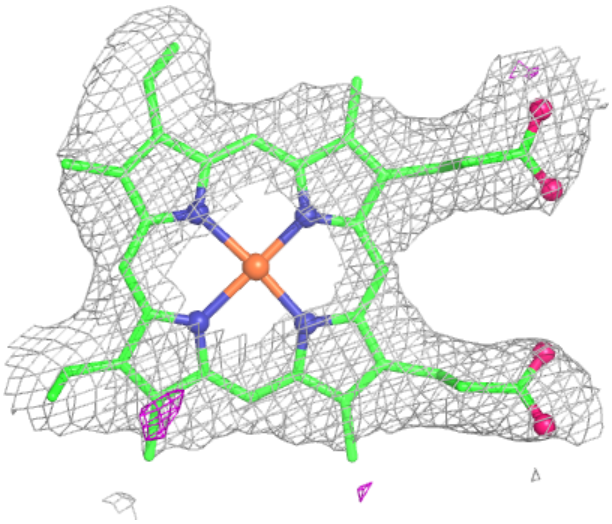


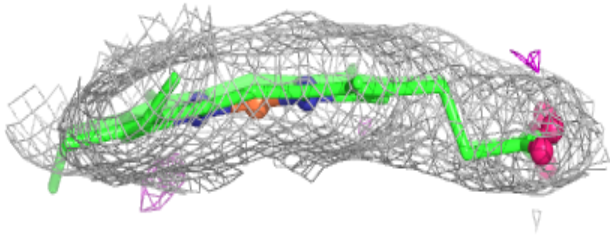


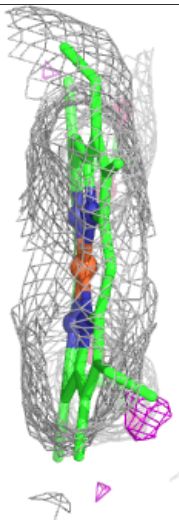


Electron density around HEC A 600:

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

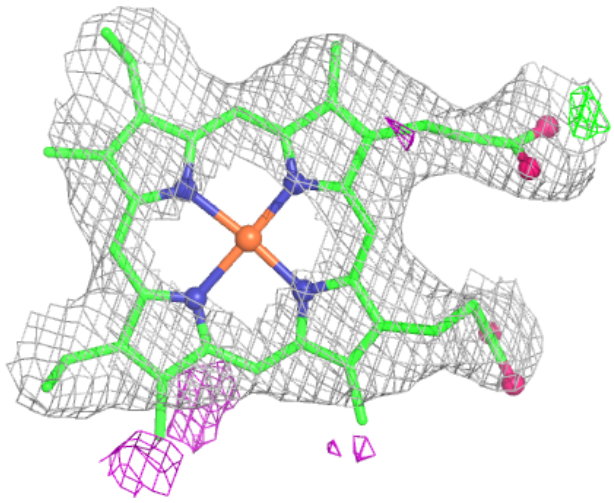


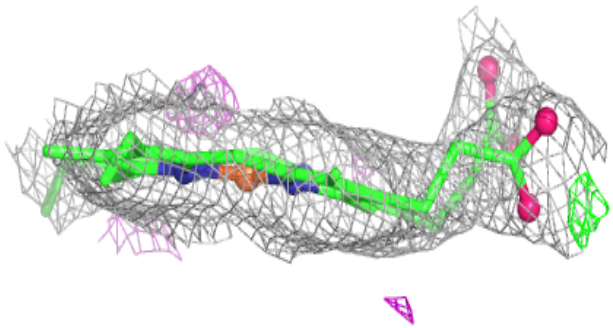


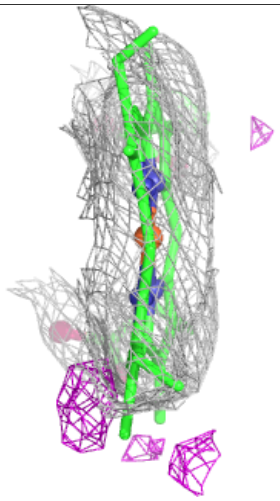


Electron density around HEC E 607:

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

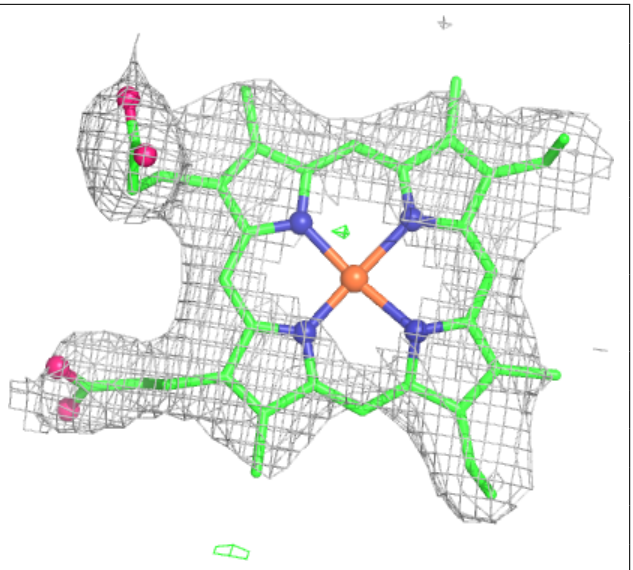


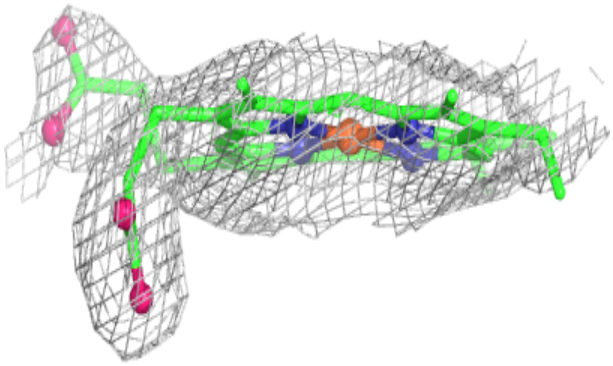


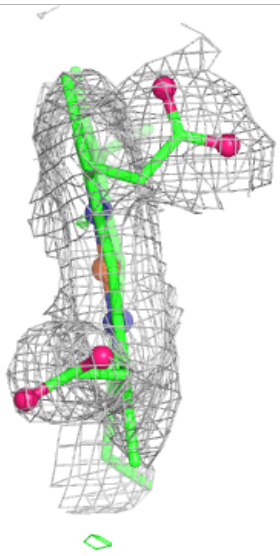


Electron density around HEC U 601:

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

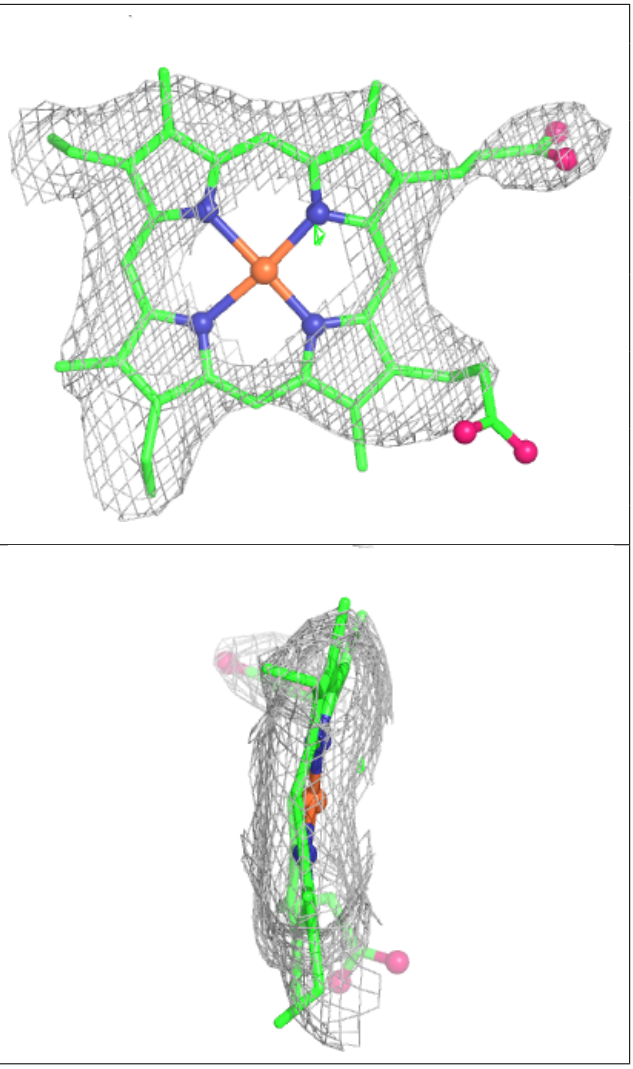


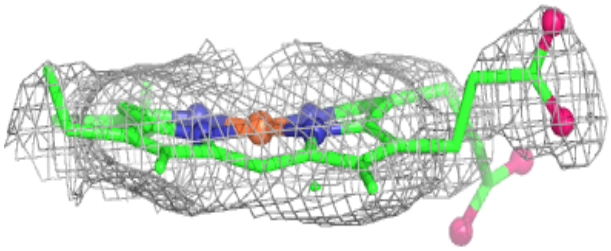




Electron density around HEC U 602:

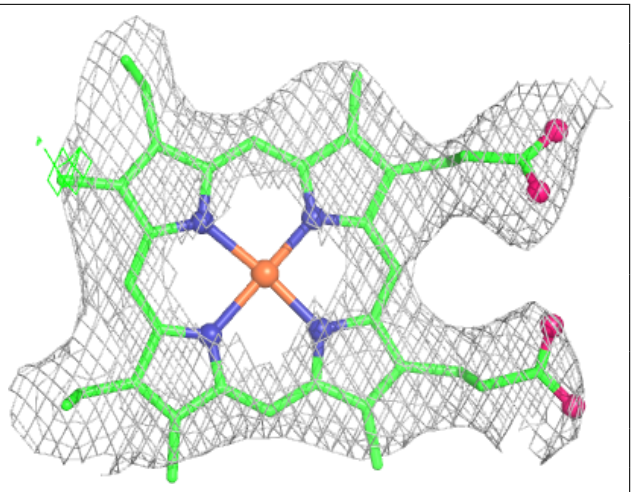
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

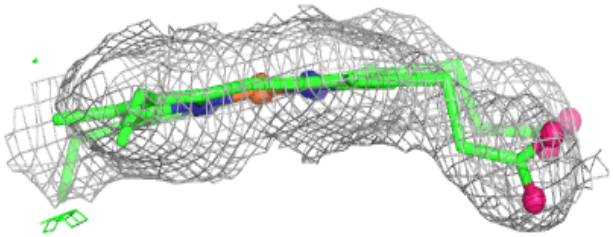


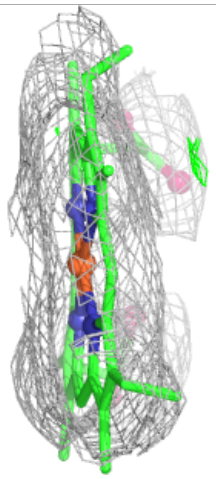


Electron density around HEC U 604:

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

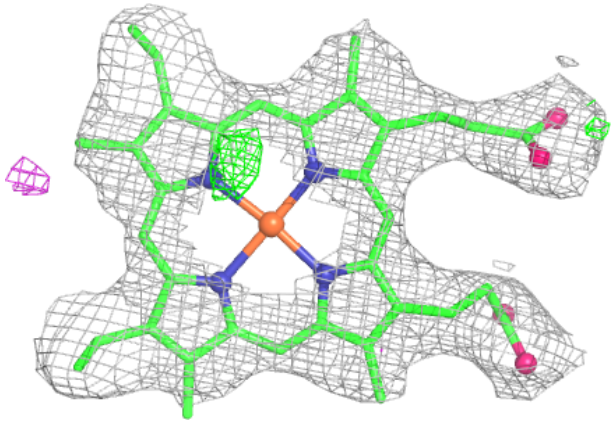


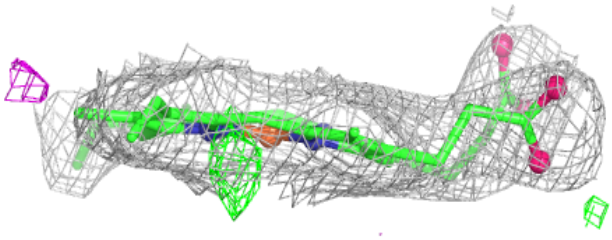


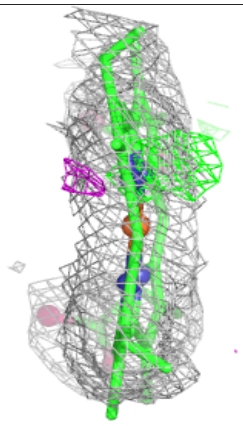


Electron density around HEC A 607:

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

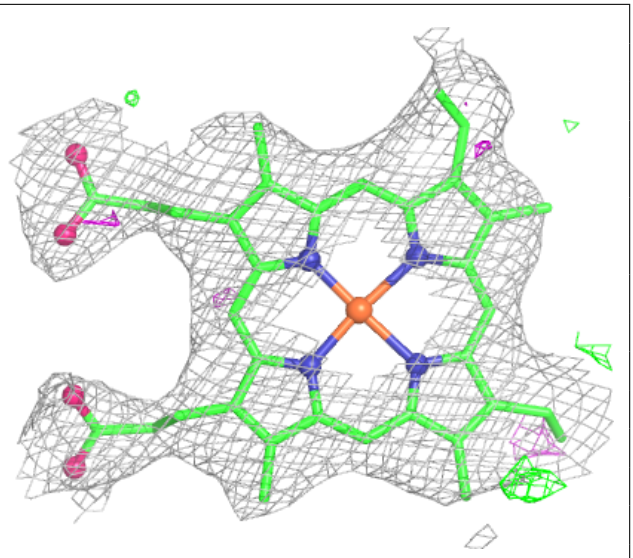


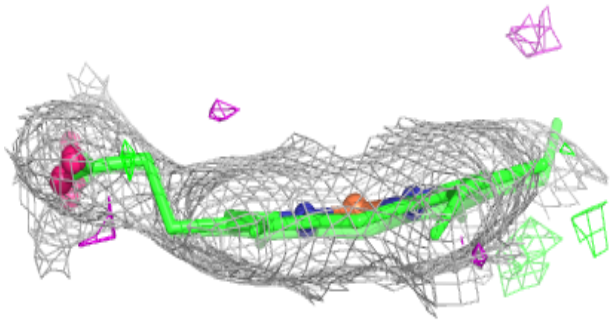


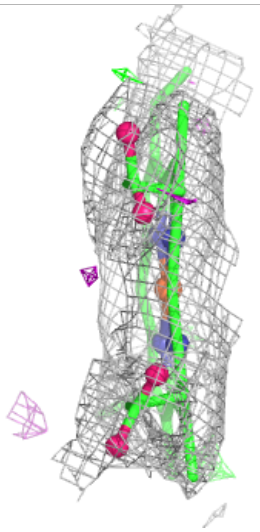


Electron density around HEC F 600:

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

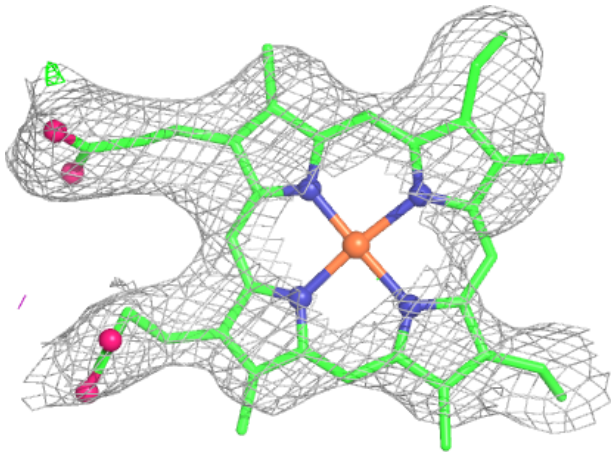


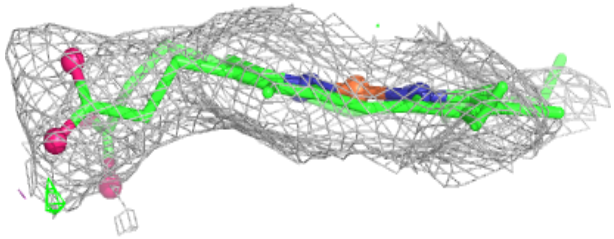


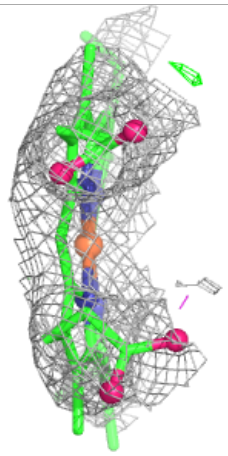


Electron density around HEC U 607:

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

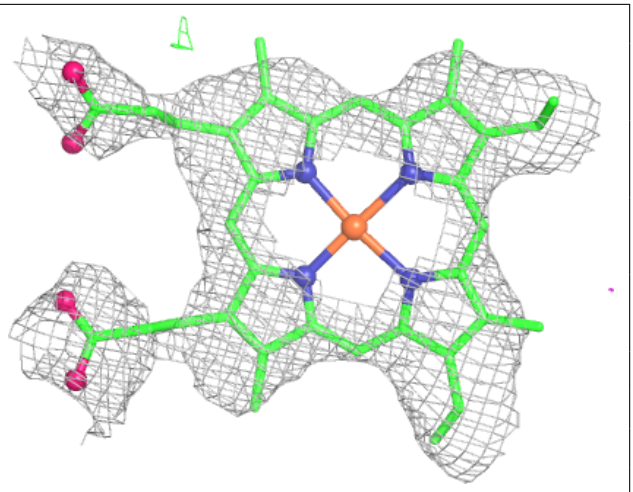


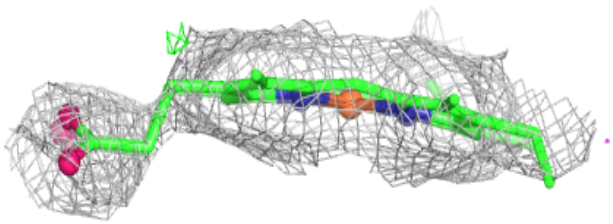


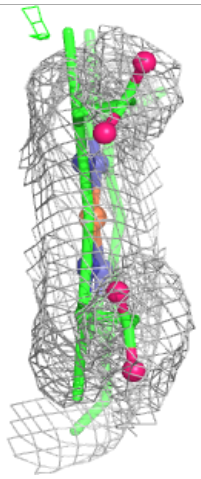


Electron density around HEC V 600:

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

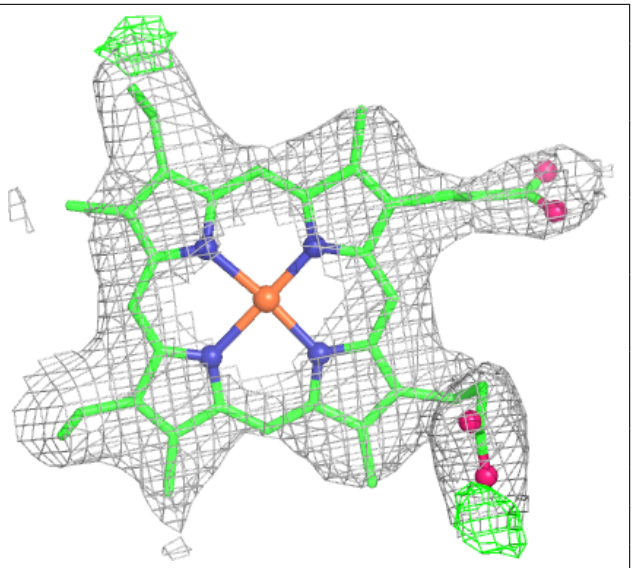


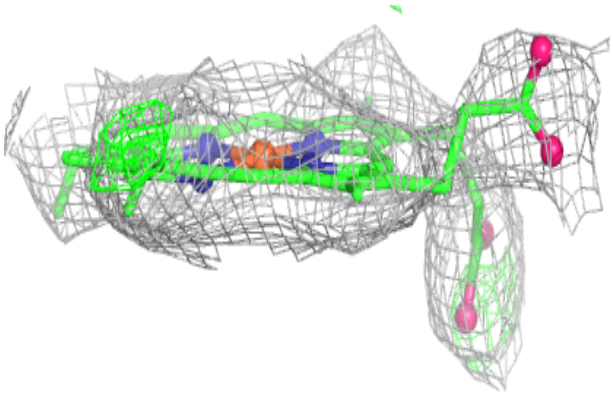


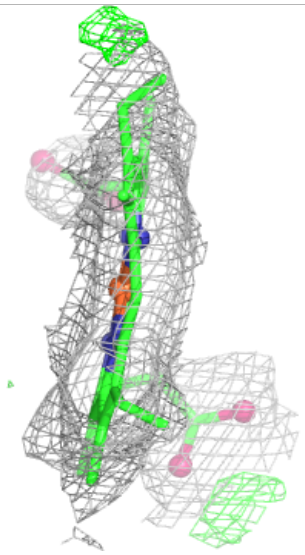


Electron density around HEC V 601:

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

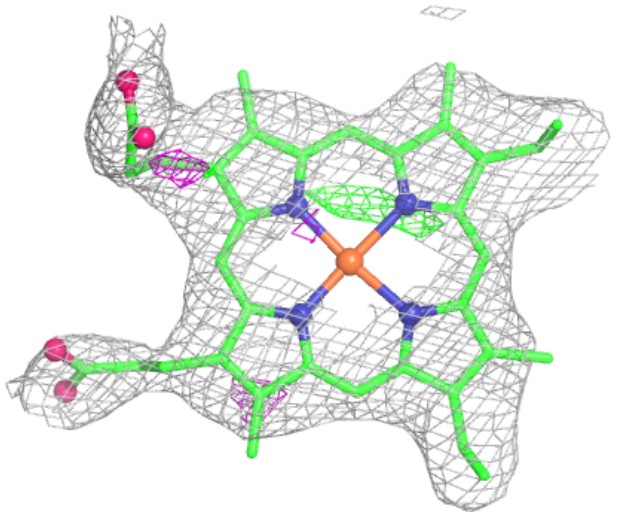


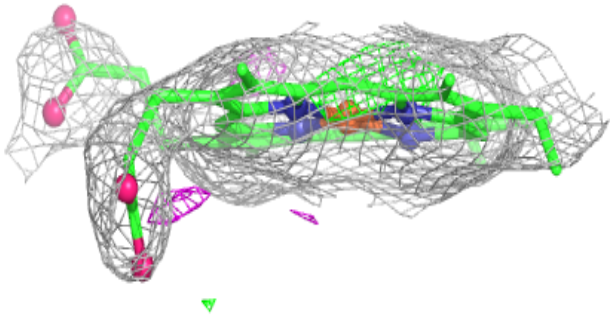


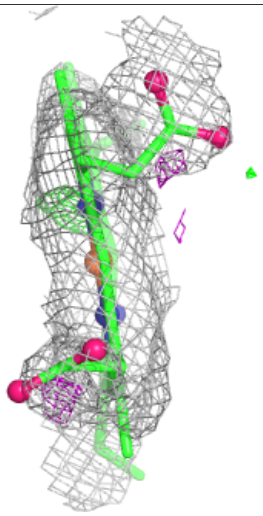


Electron density around HEC F 601:

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

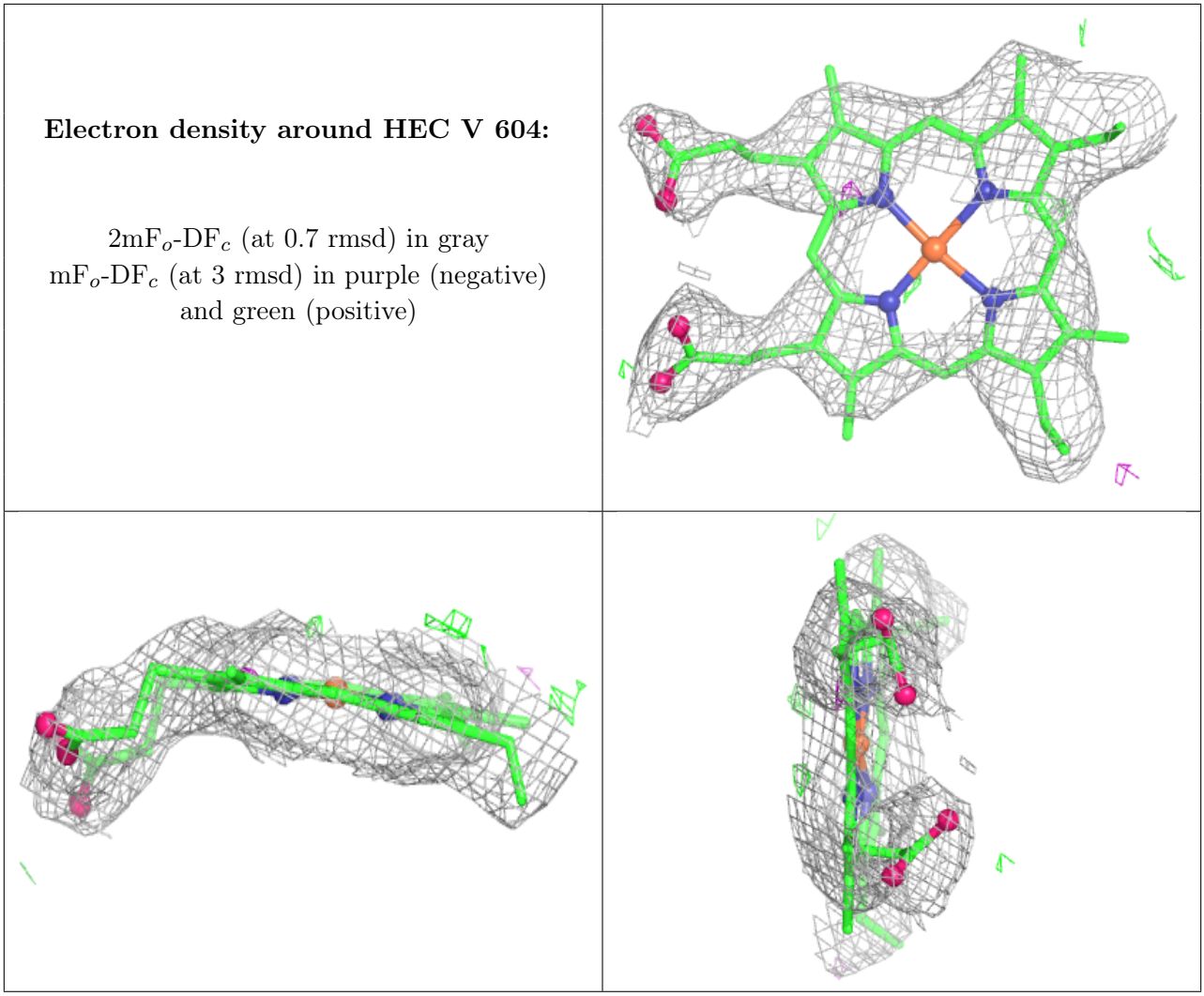






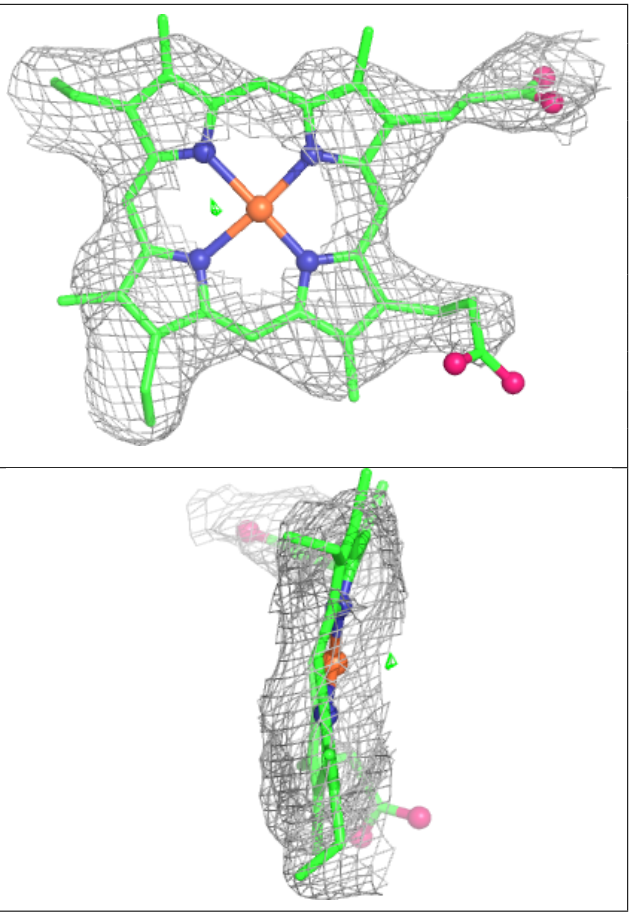
Electron density around HEC V 604:

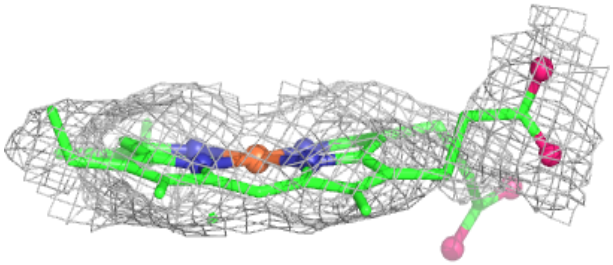
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC F 602:

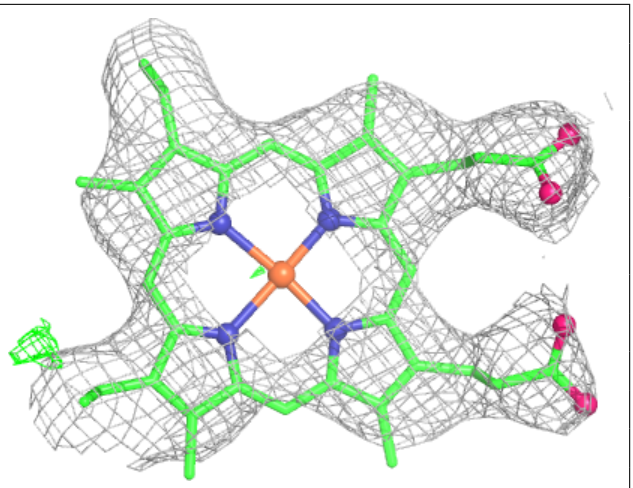
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

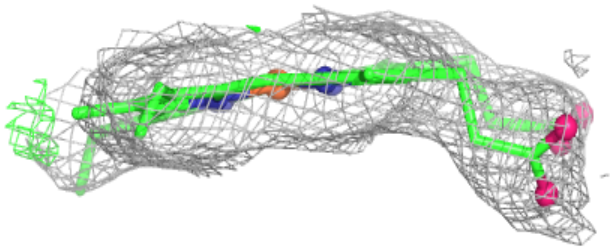


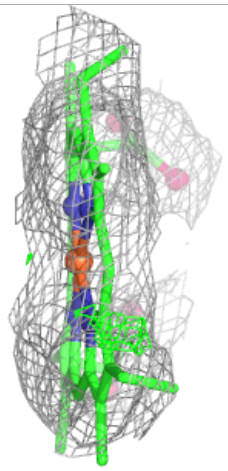


Electron density around HEC F 604:

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

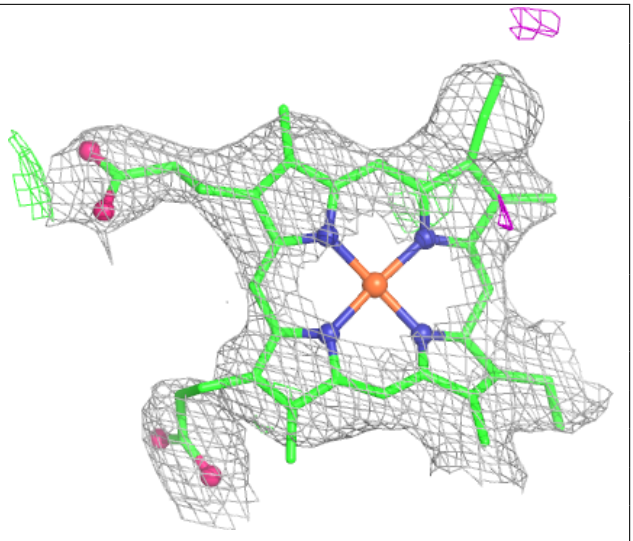


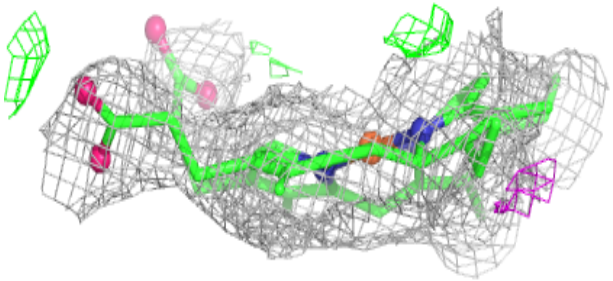


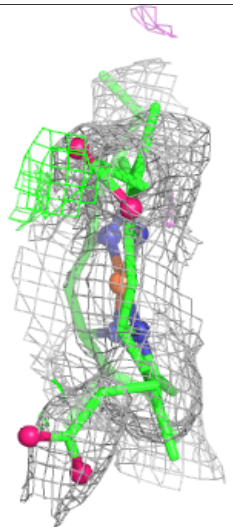


Electron density around HEC A 603:

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

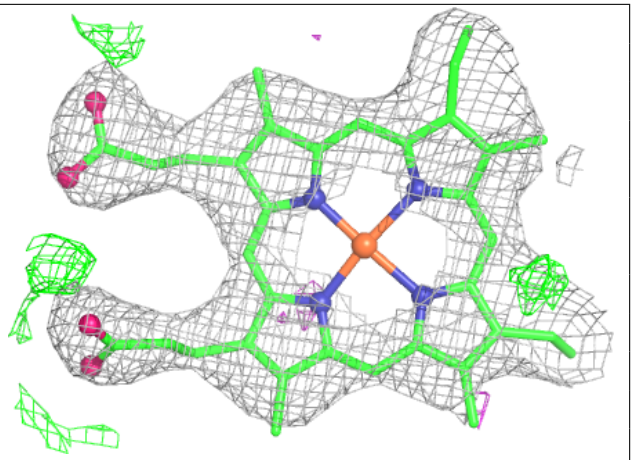


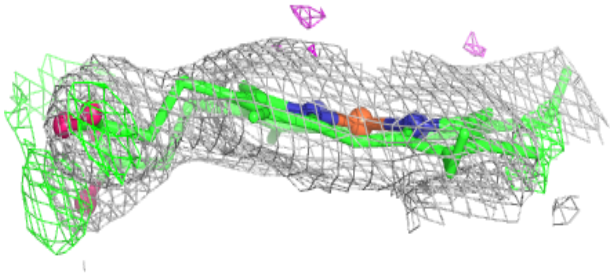


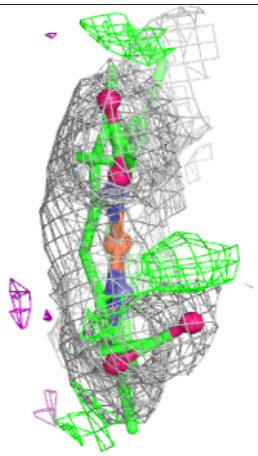


Electron density around HEC F 606:

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

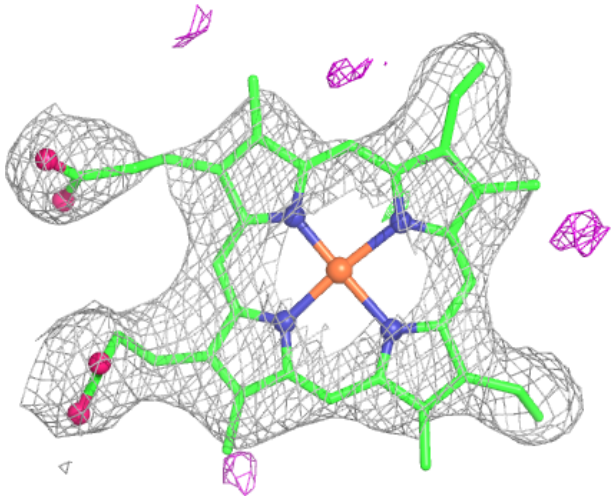


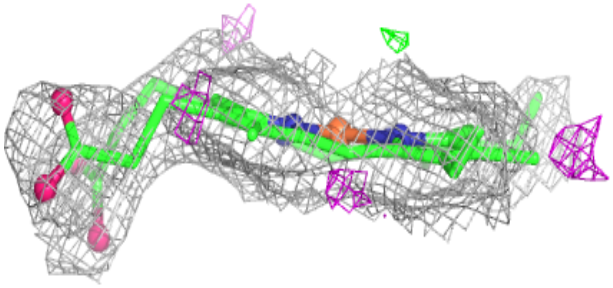


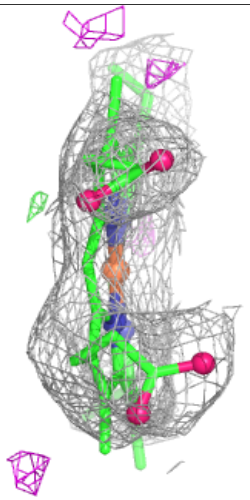


Electron density around HEC F 607:

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

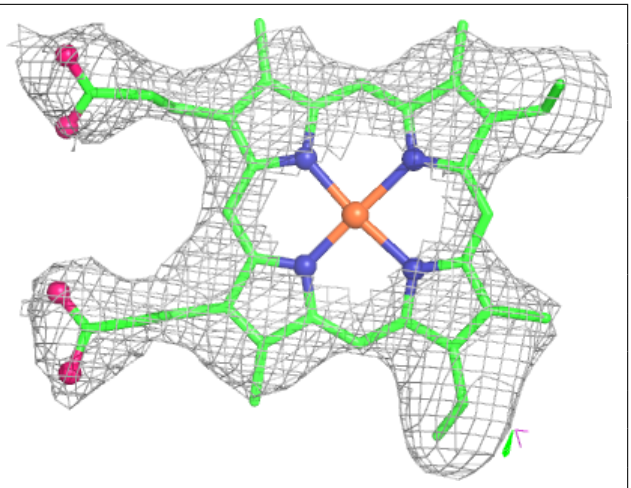


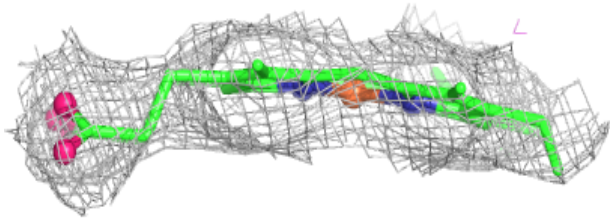


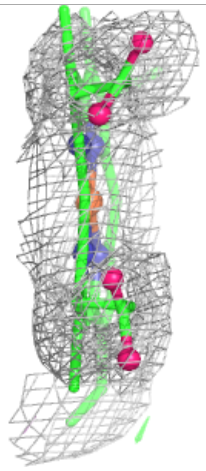


Electron density around HEC W 600:

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

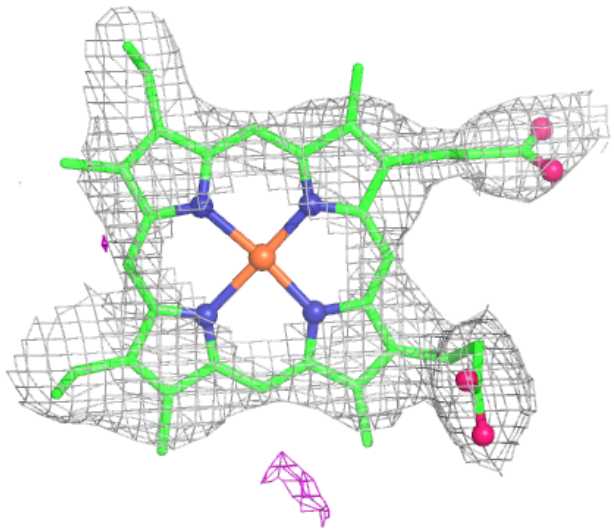


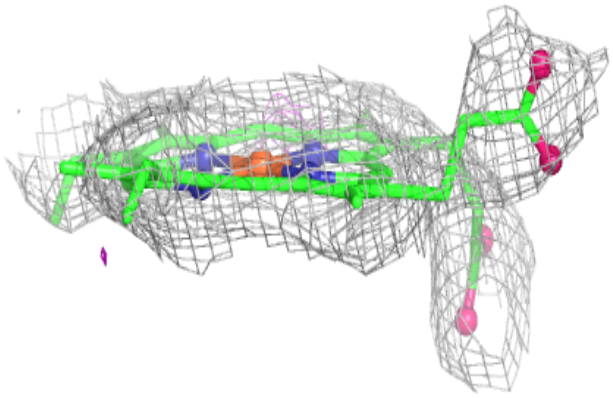


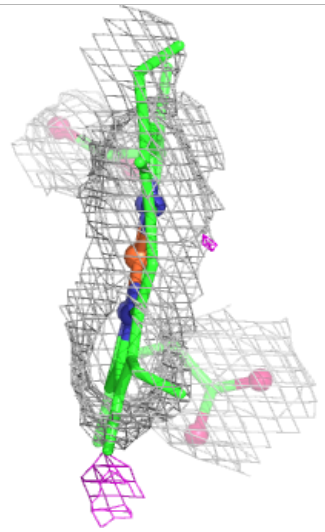


Electron density around HEC W 601:

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

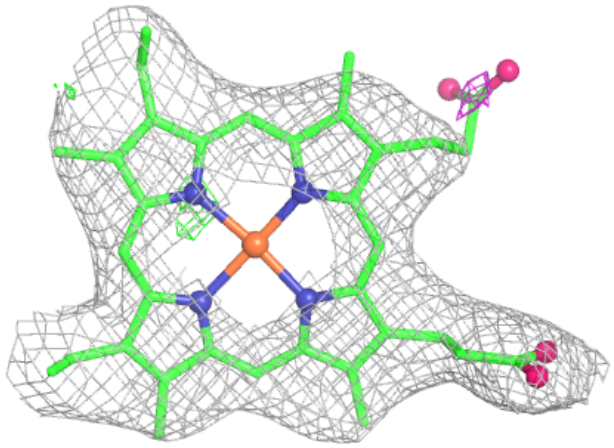


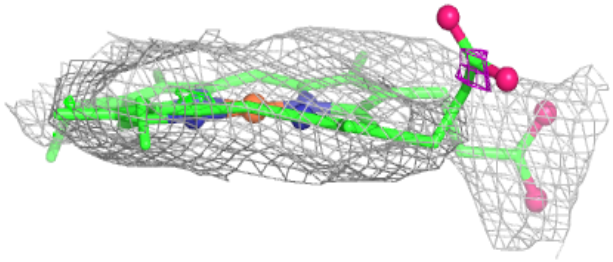


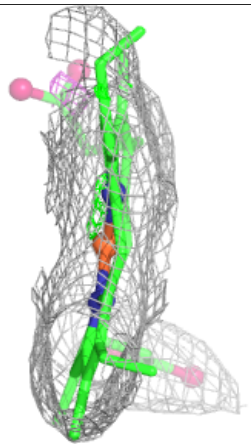


Electron density around HEC W 602:

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

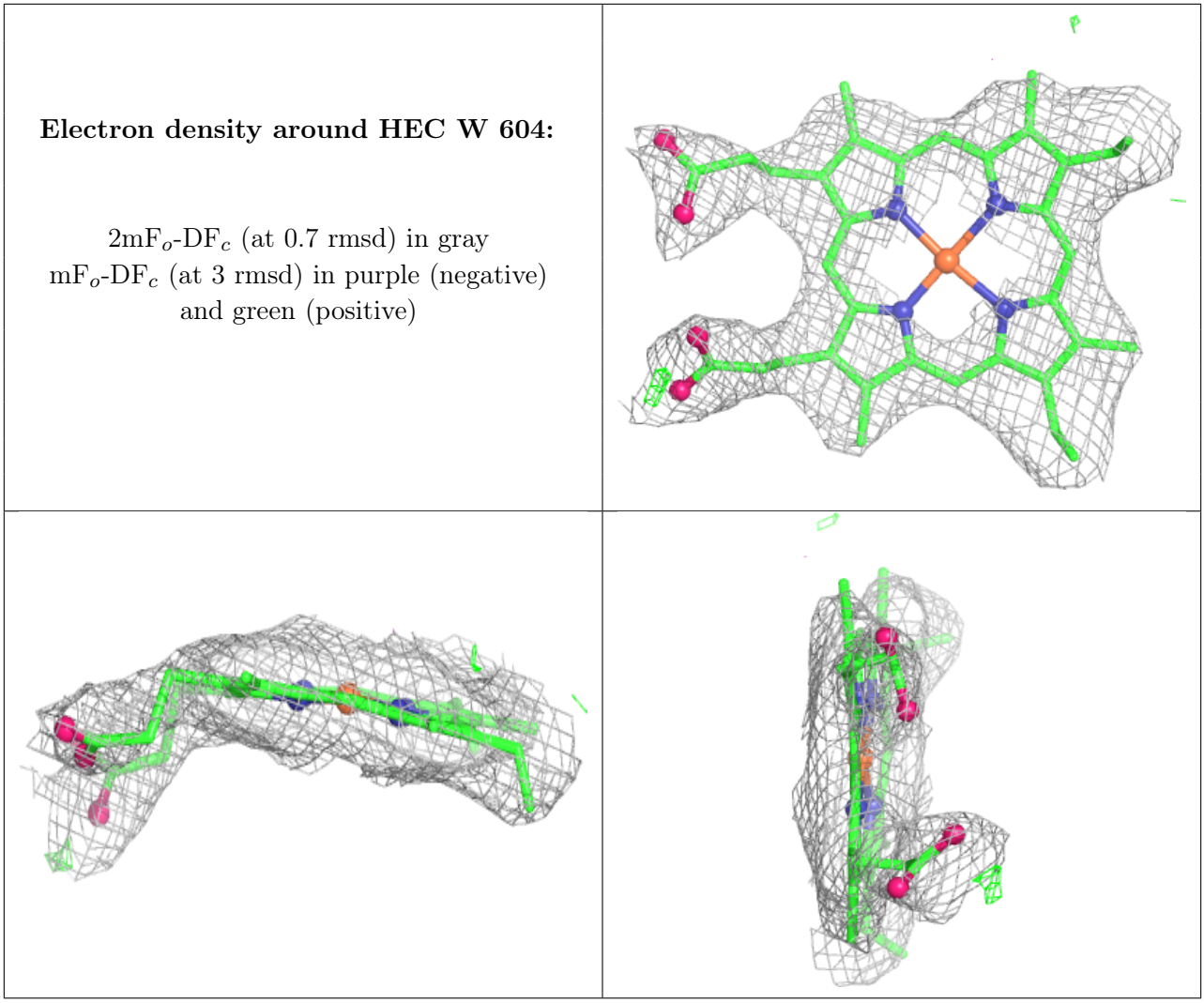






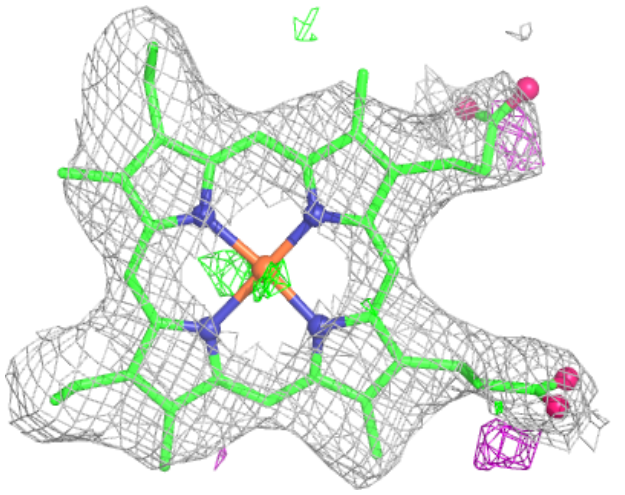
Electron density around HEC W 604:

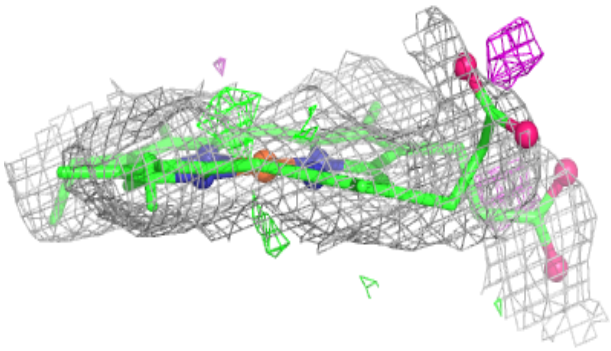
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC H 602:

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

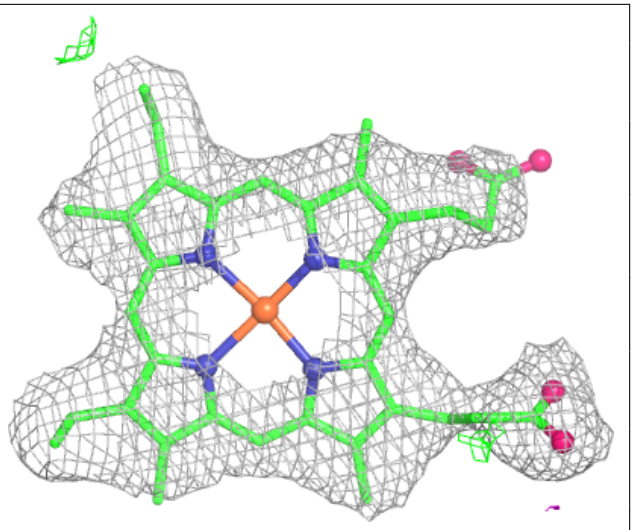


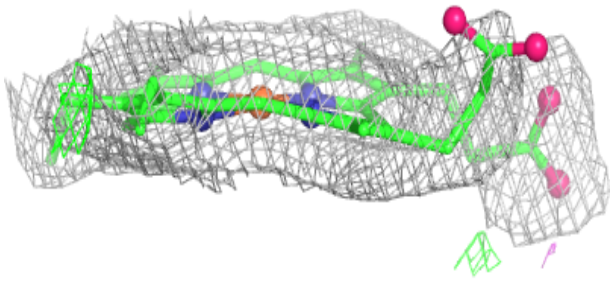


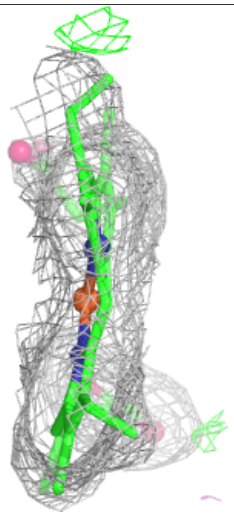


Electron density around HEC I 602:

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

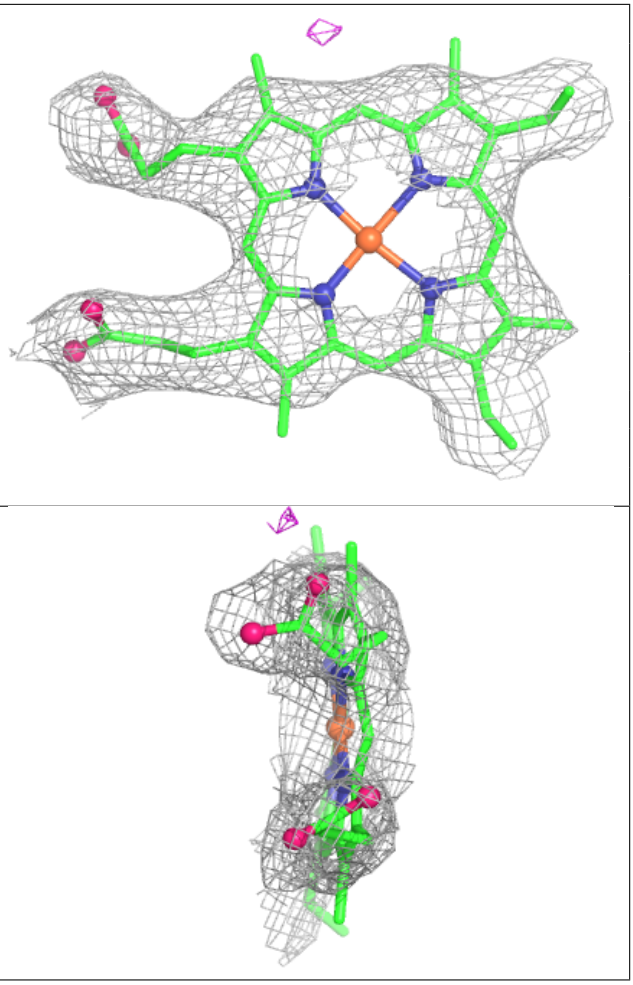






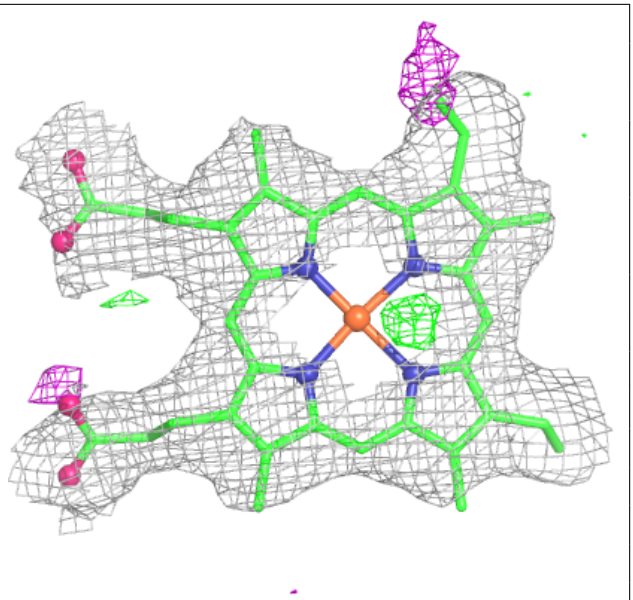
Electron density around HEC W 607:

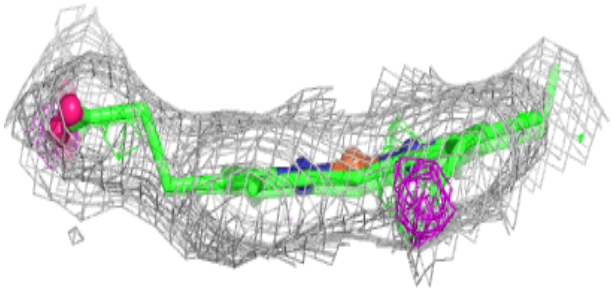
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

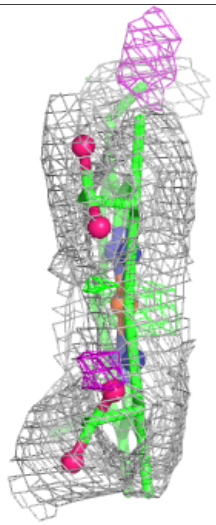


Electron density around HEC J 600:

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

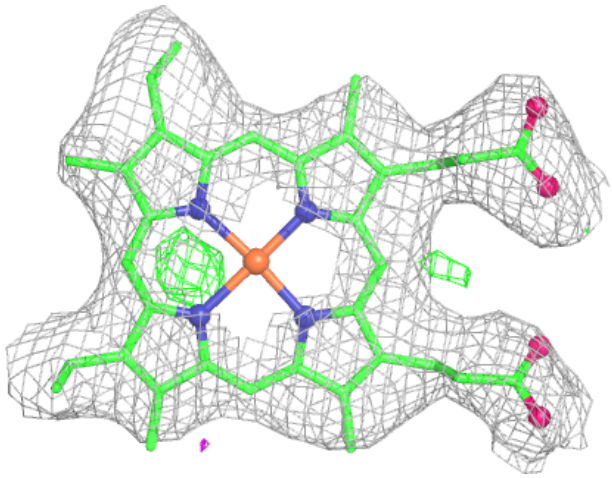


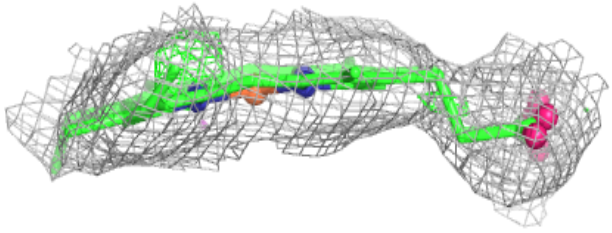


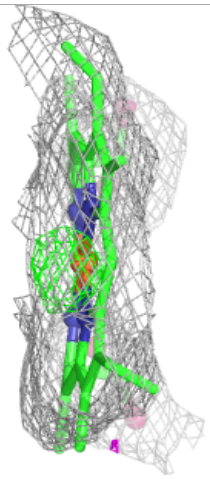


Electron density around HEC X 600:

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

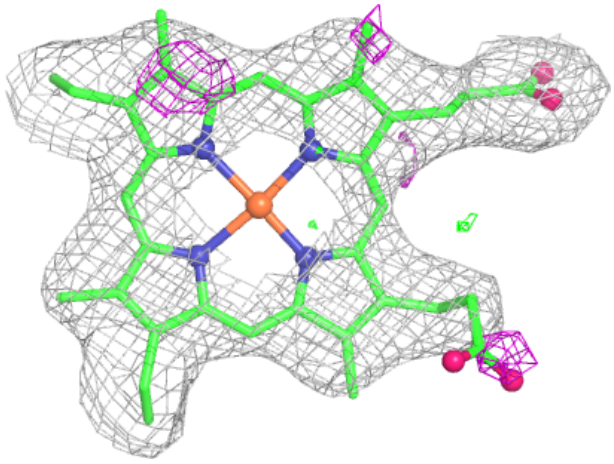


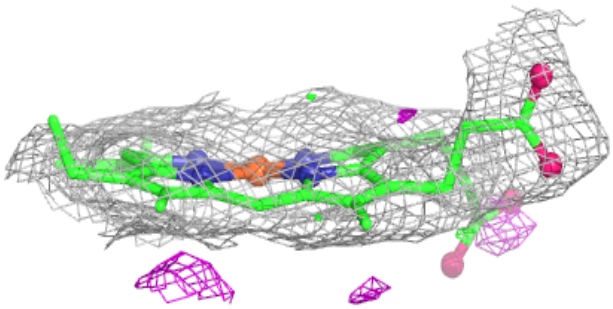


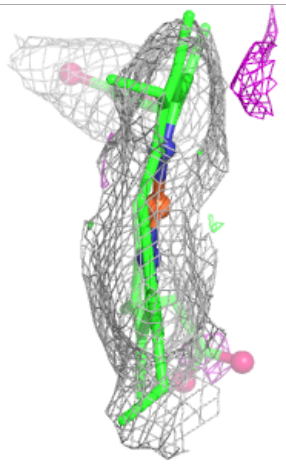


Electron density around HEC J 602:

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

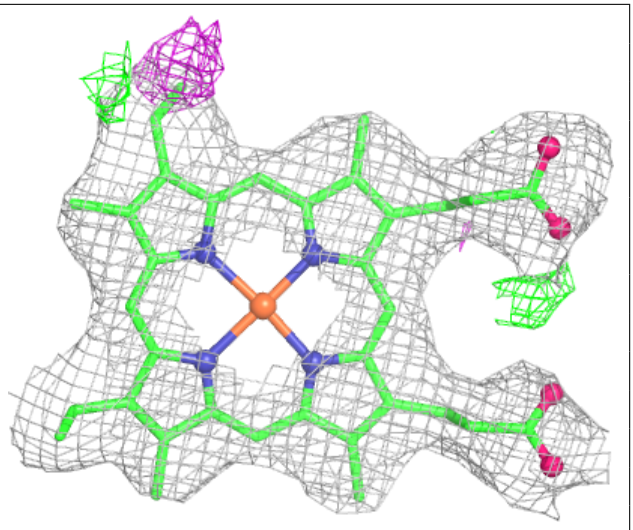


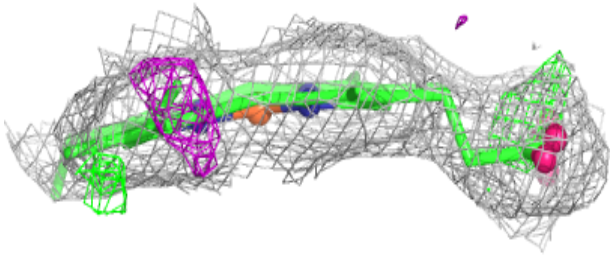


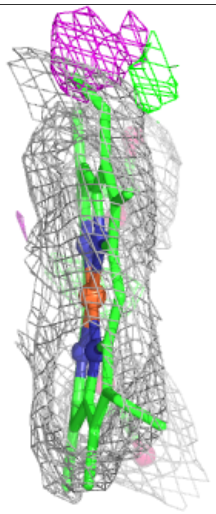


Electron density around HEC K 600:

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

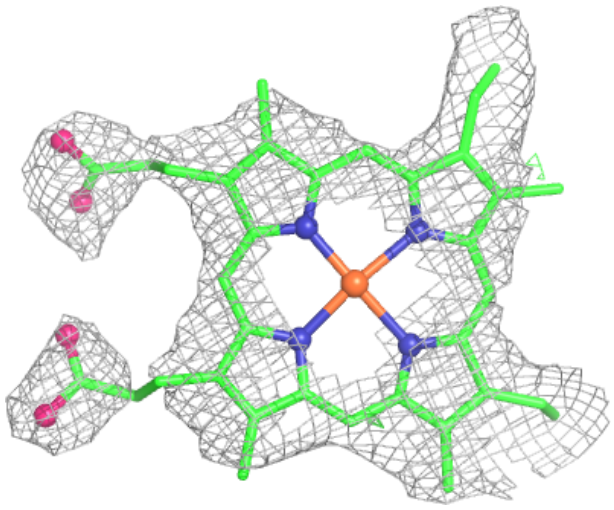


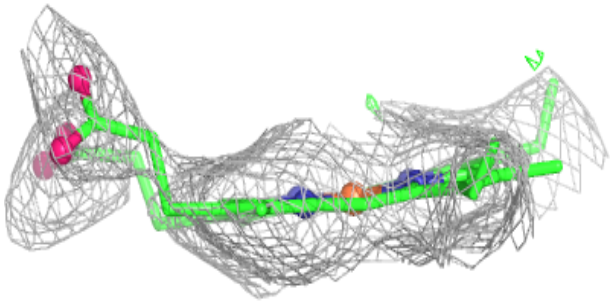


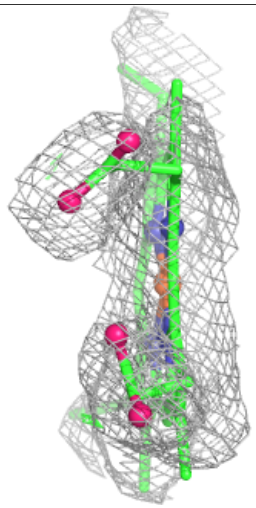


Electron density around HEC X 604:

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

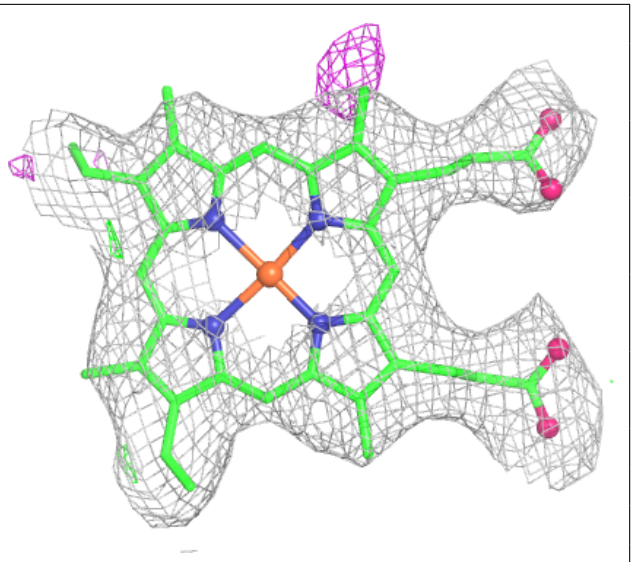


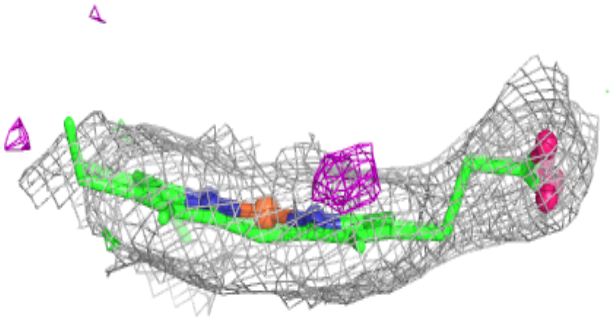


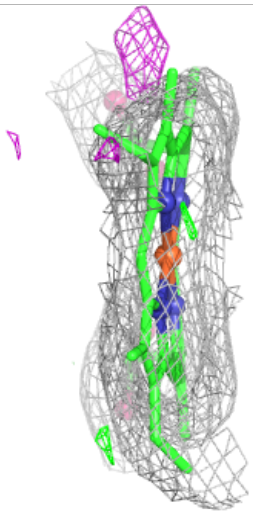


Electron density around HEC L 600:

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

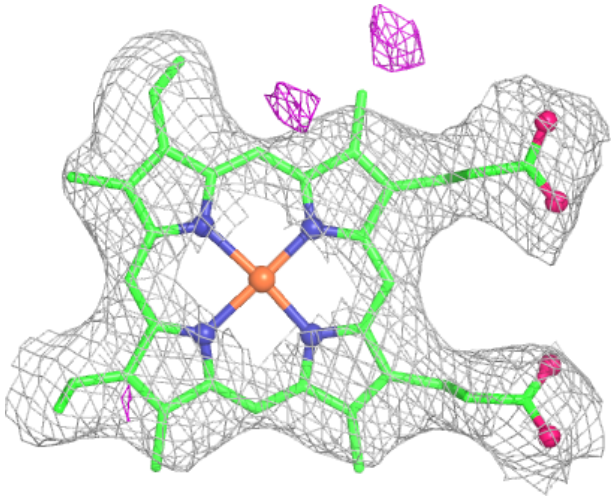


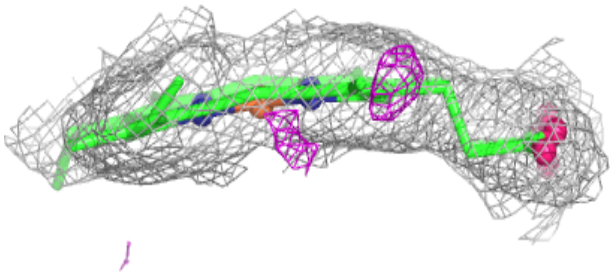


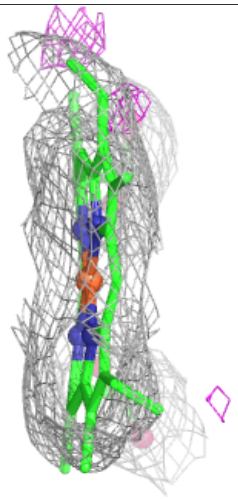


Electron density around HEC M 600:

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

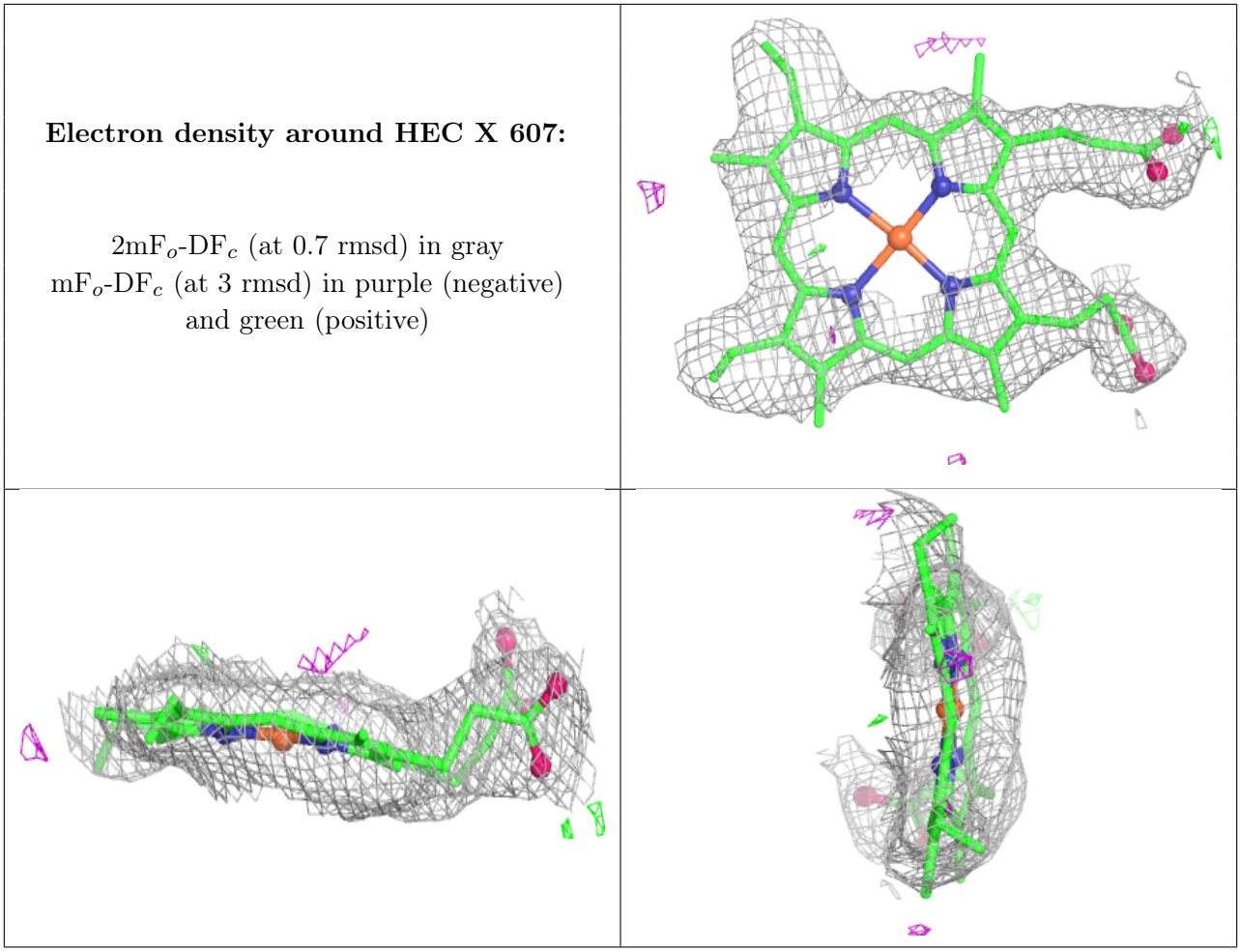






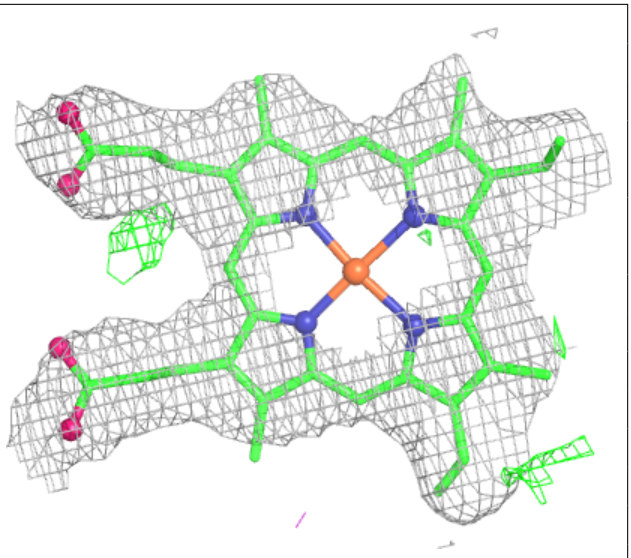
Electron density around HEC X 607:

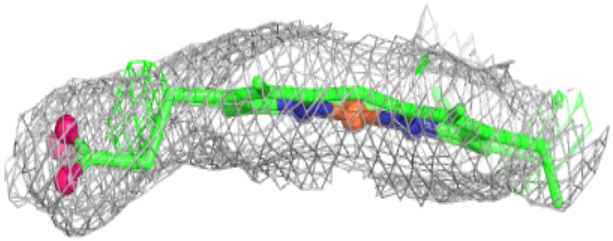
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

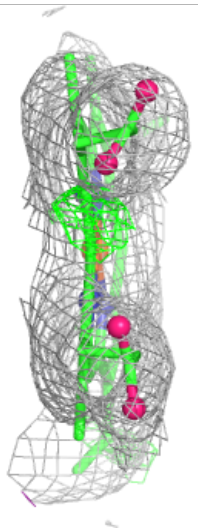


Electron density around HEC N 600:

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

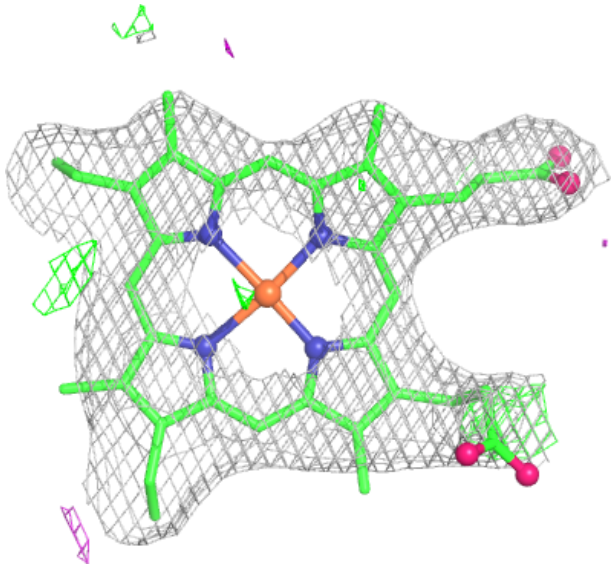


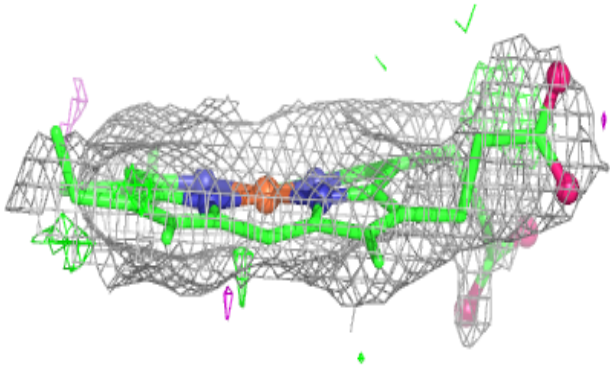




Electron density around HEC B 602:

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

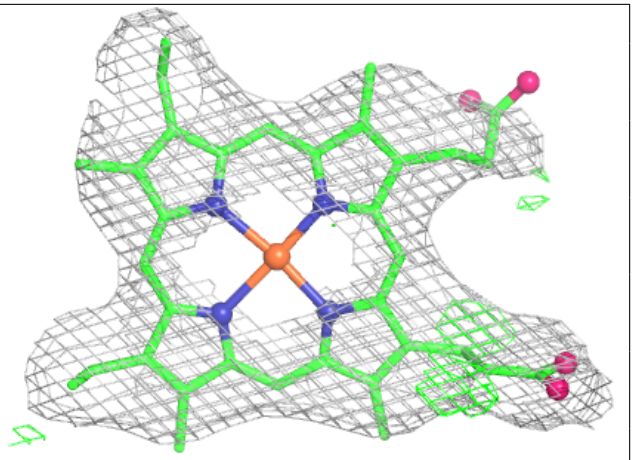


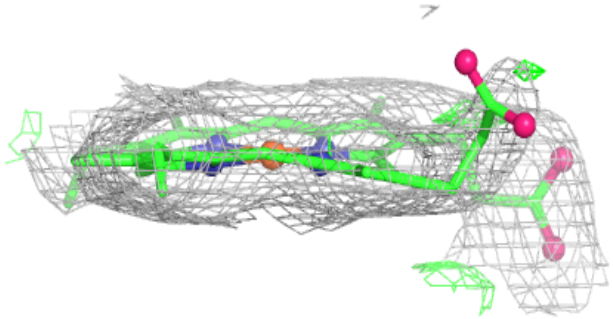


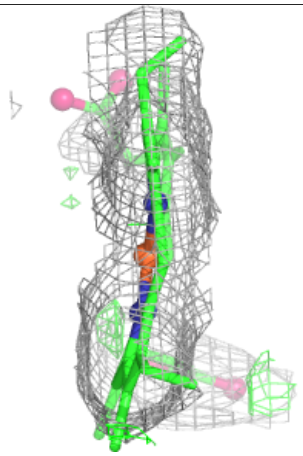


Electron density around HEC N 602:

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

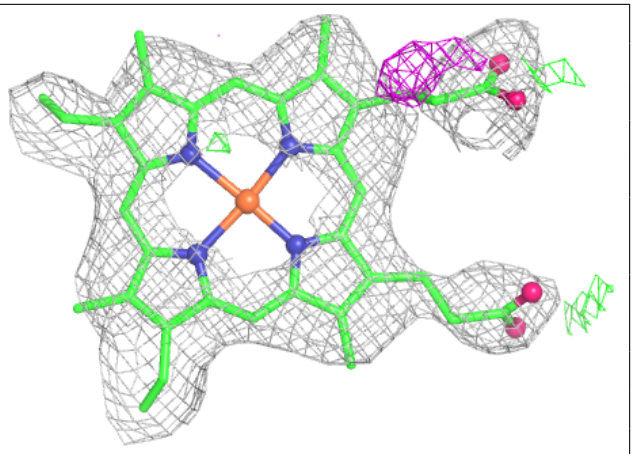


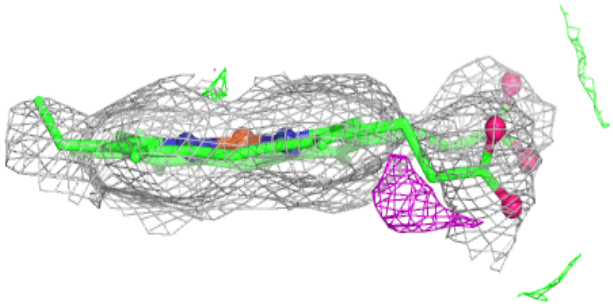


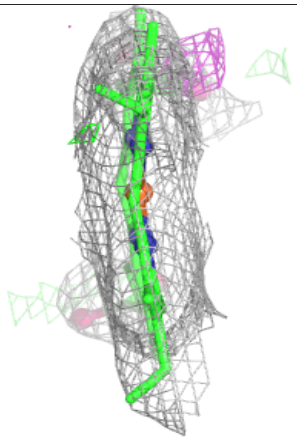


Electron density around HEC N 605:

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

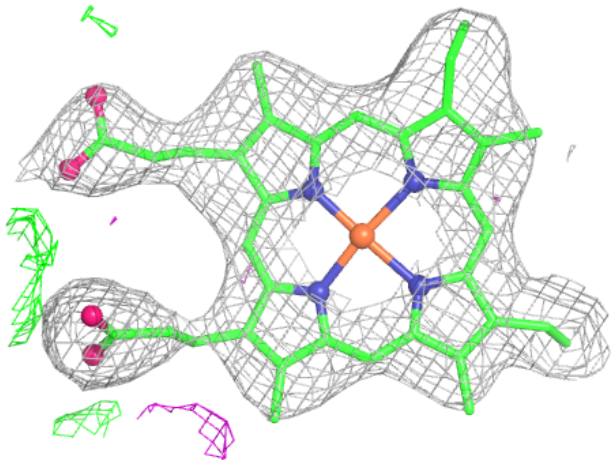


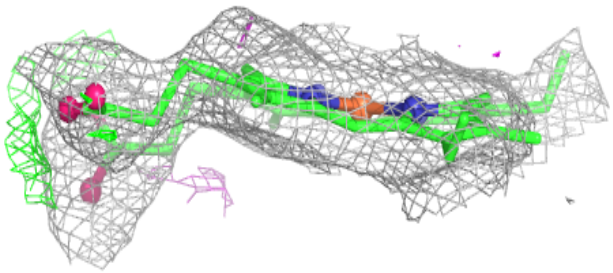


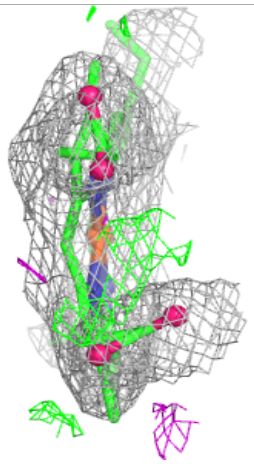


Electron density around HEC N 606:

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

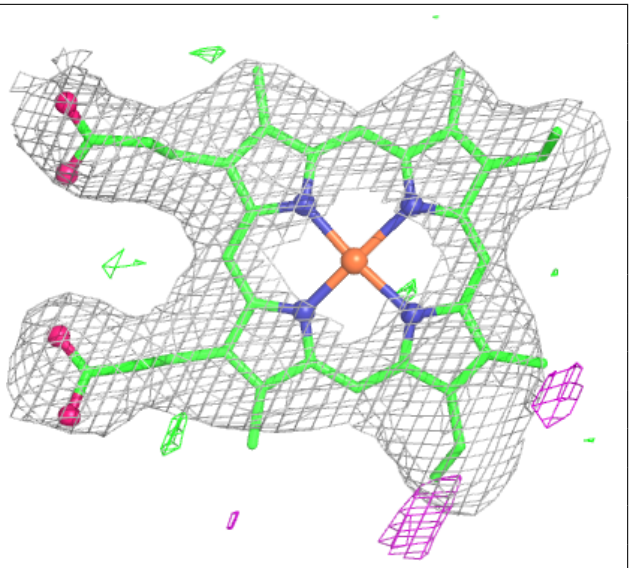


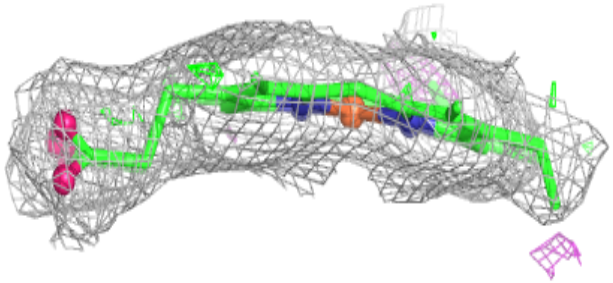


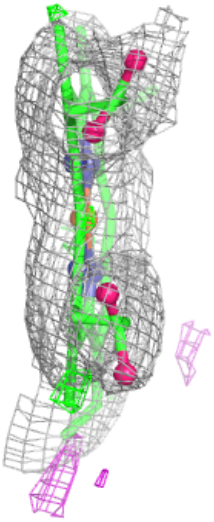


Electron density around HEC O 600:

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

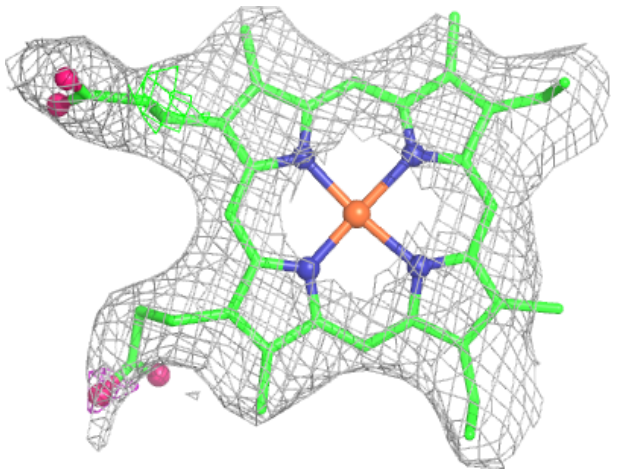


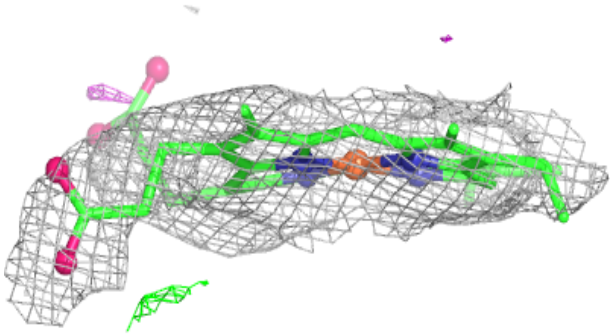


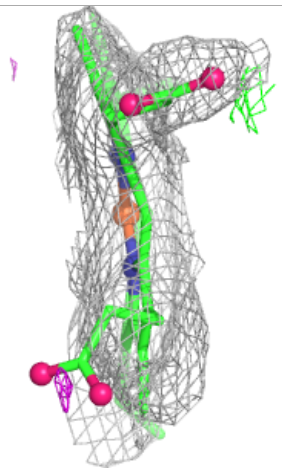


Electron density around HEC O 602:

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

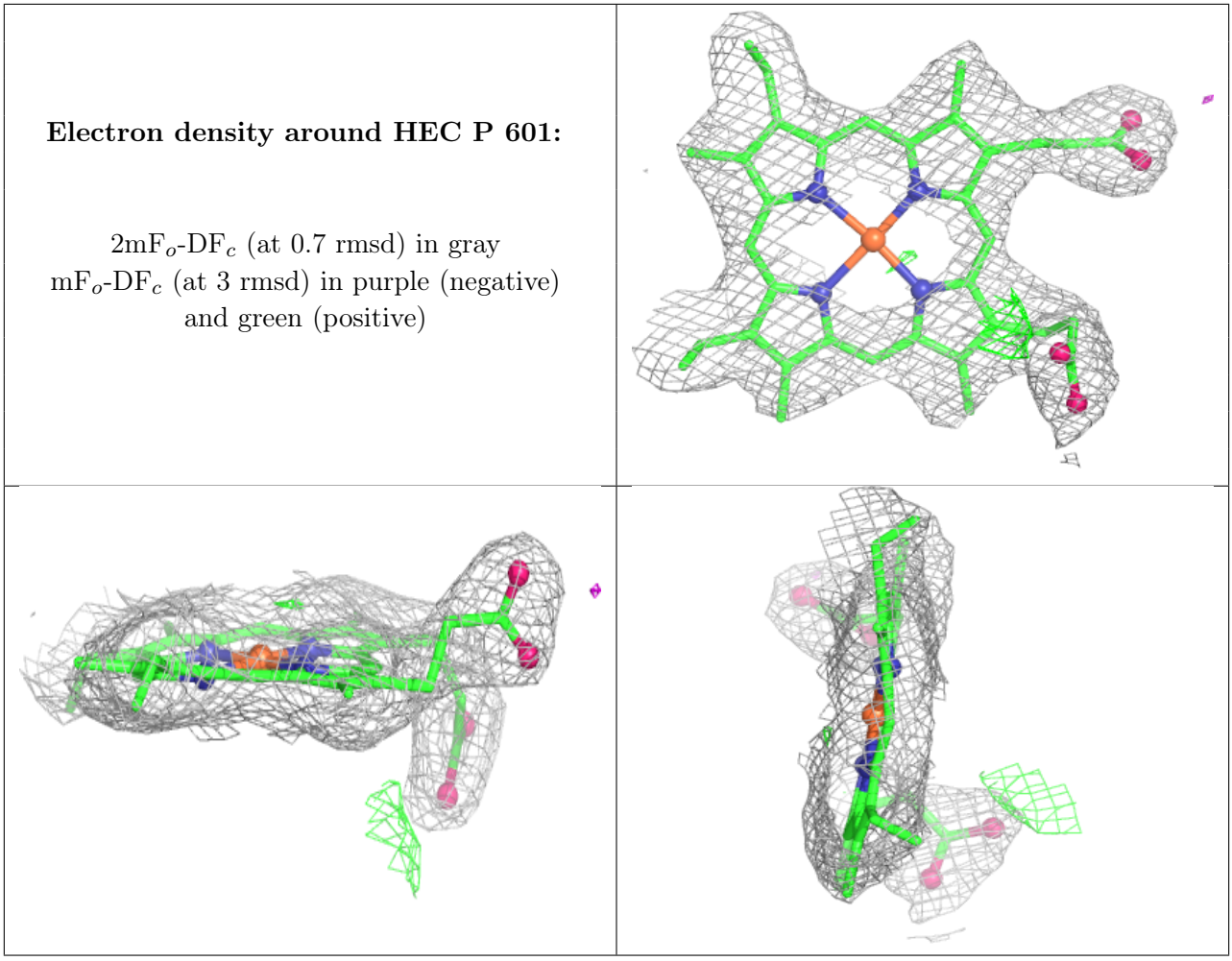






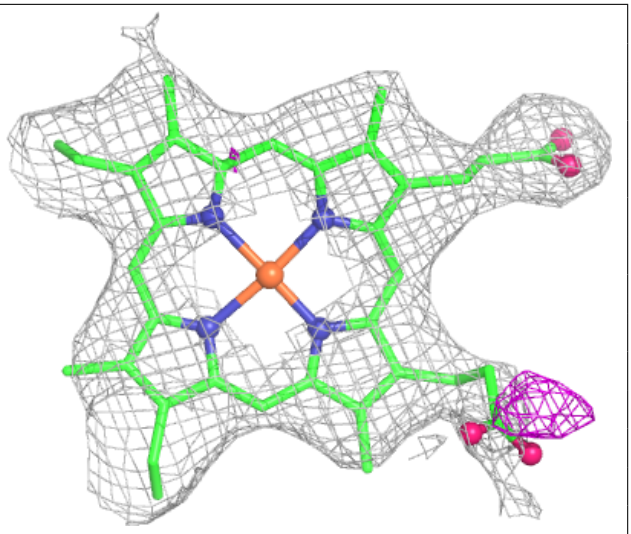
Electron density around HEC P 601:

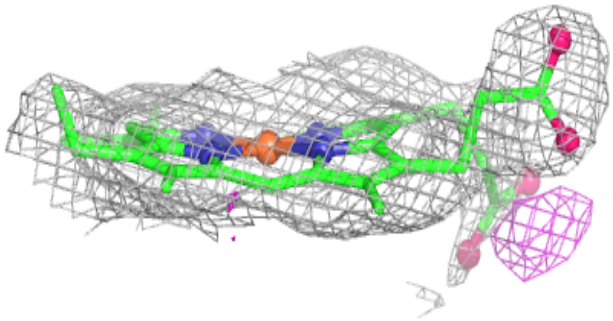
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

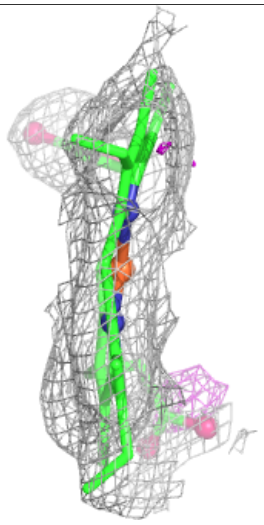


Electron density around HEC P 602:

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

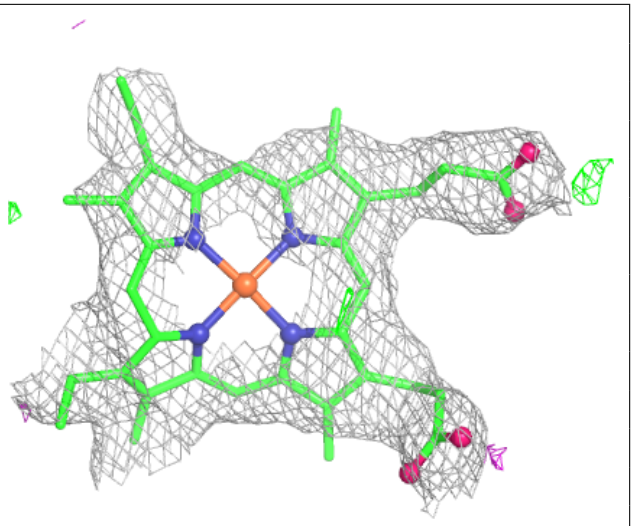


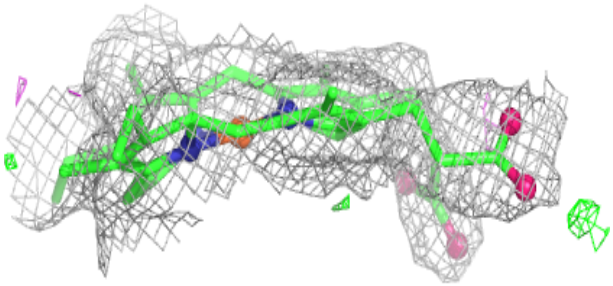


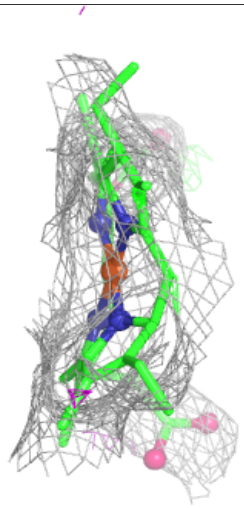


Electron density around HEC Q 603:

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

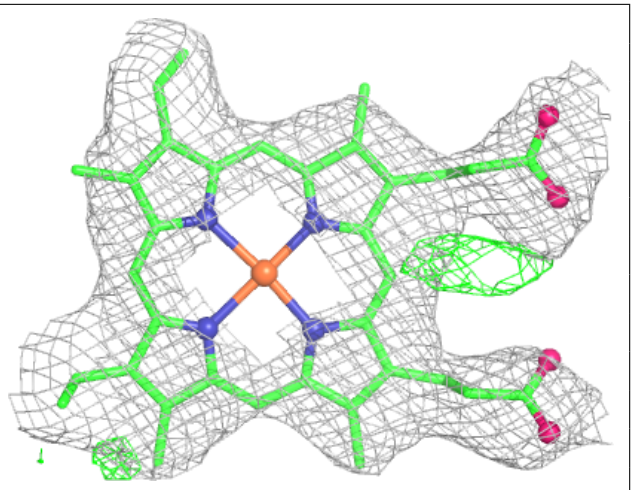


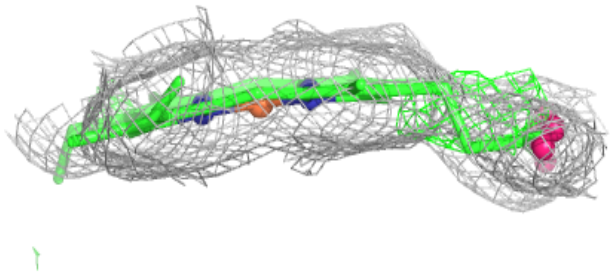


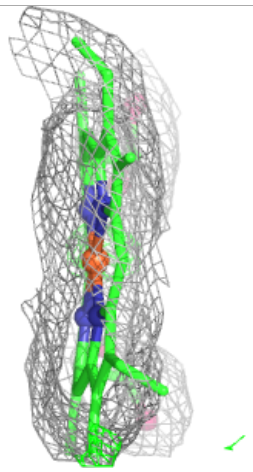


Electron density around HEC Q 600:

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

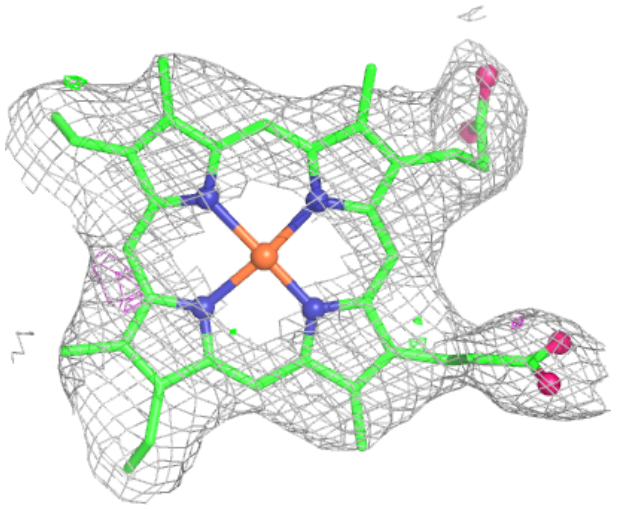


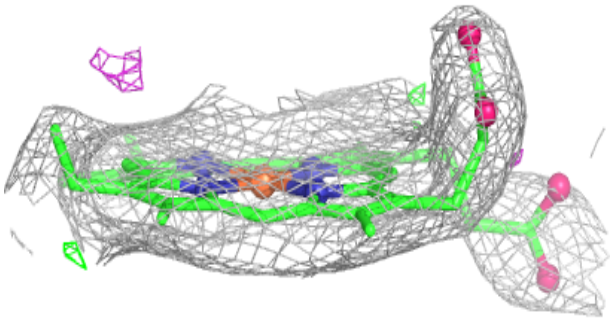




Electron density around HEC Q 601:

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

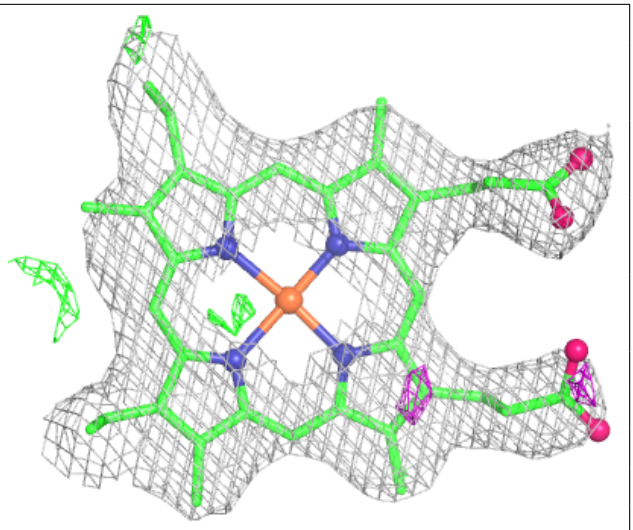


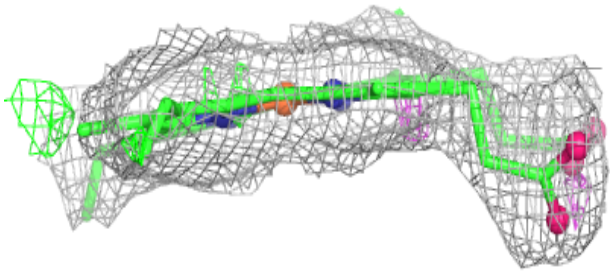


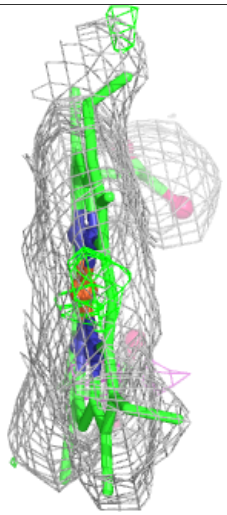


Electron density around HEC B 604:

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

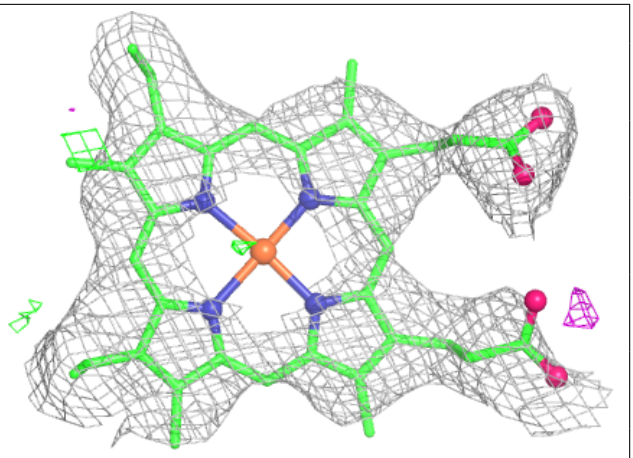


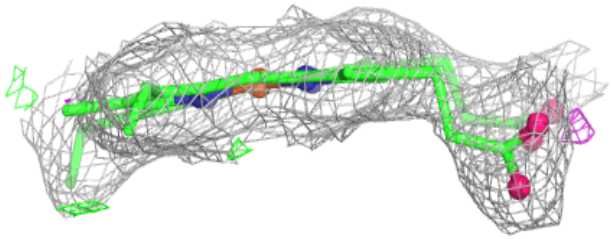


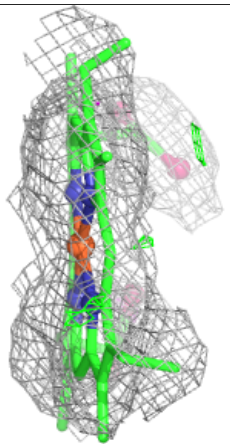


Electron density around HEC Q 604:

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

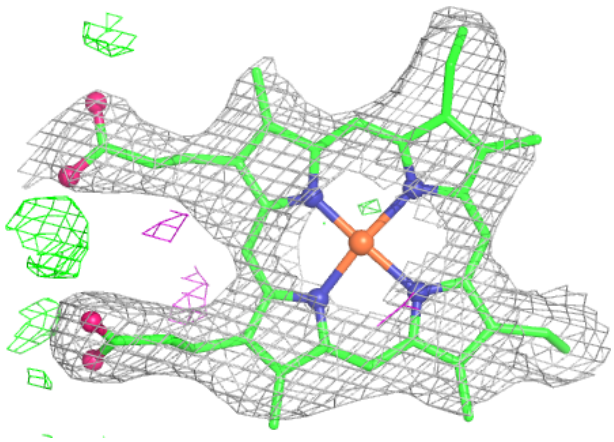


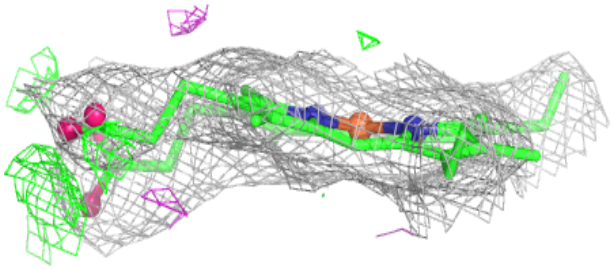


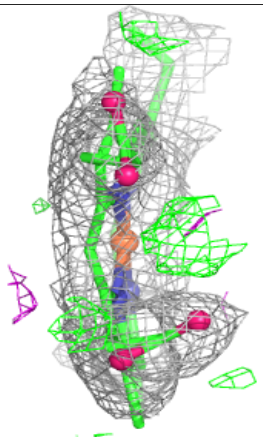


Electron density around HEC Q 606:

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

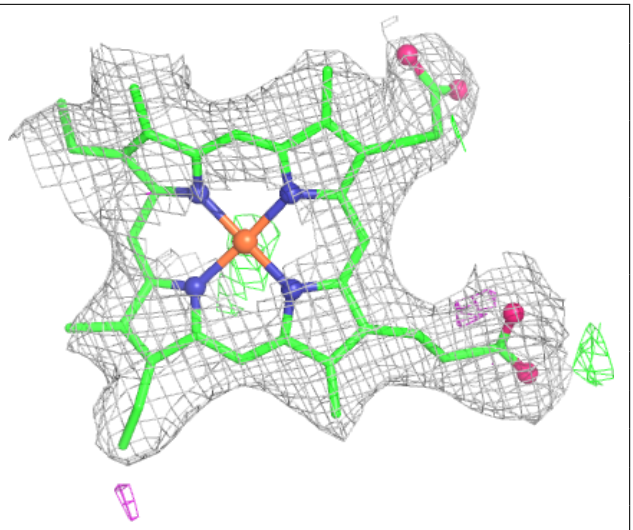


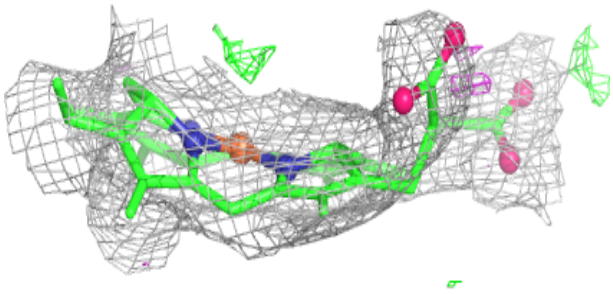


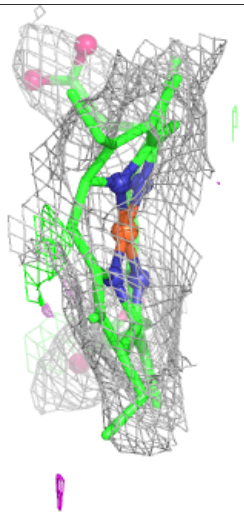


Electron density around HEC R 603:

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

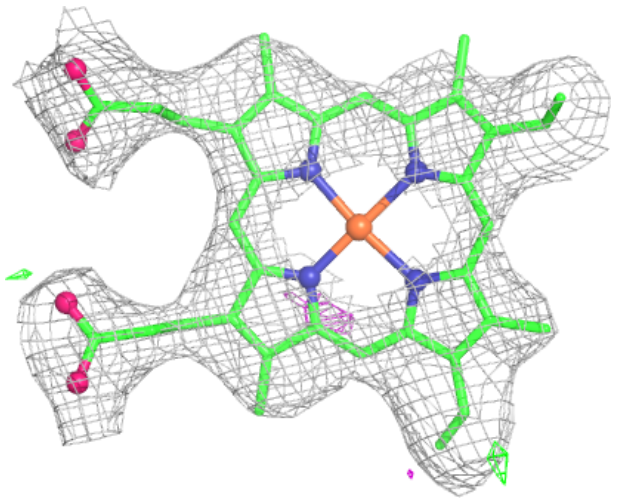


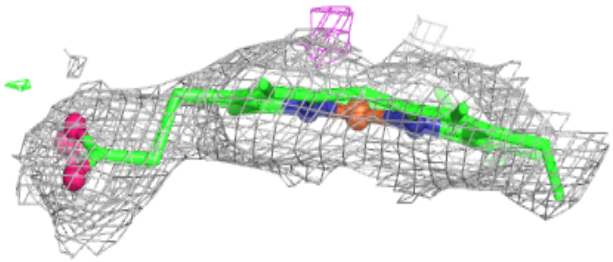


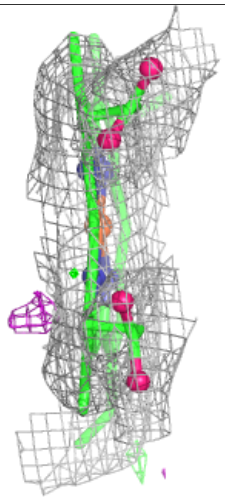


Electron density around HEC R 600:

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

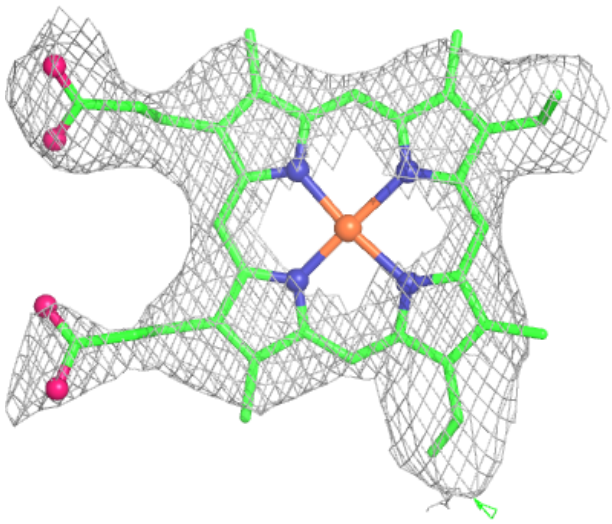


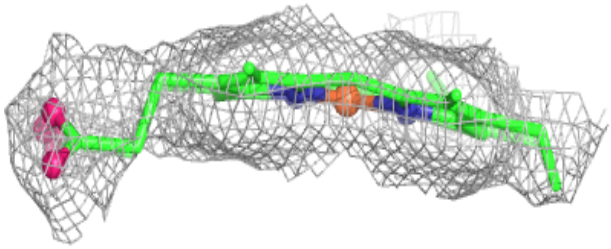


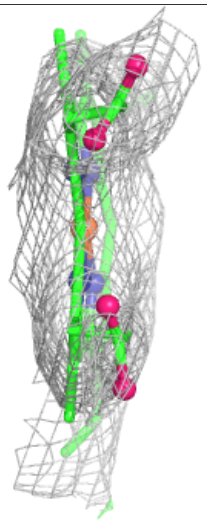


Electron density around HEC S 600:

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

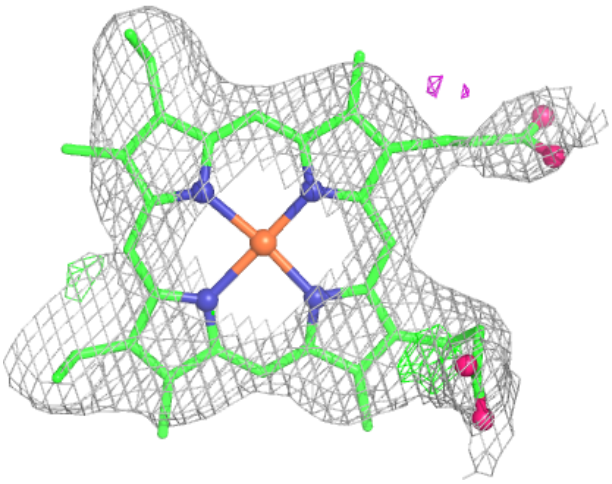


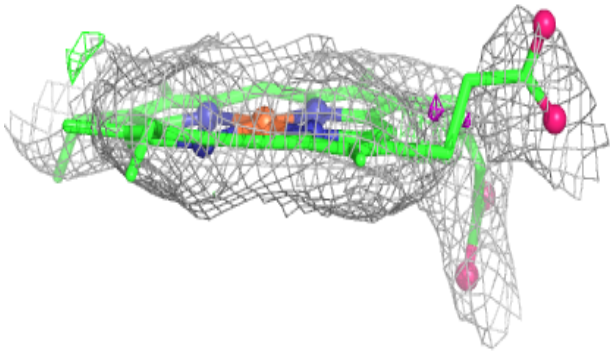


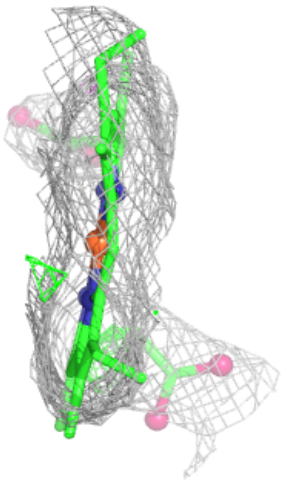


Electron density around HEC S 601:

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

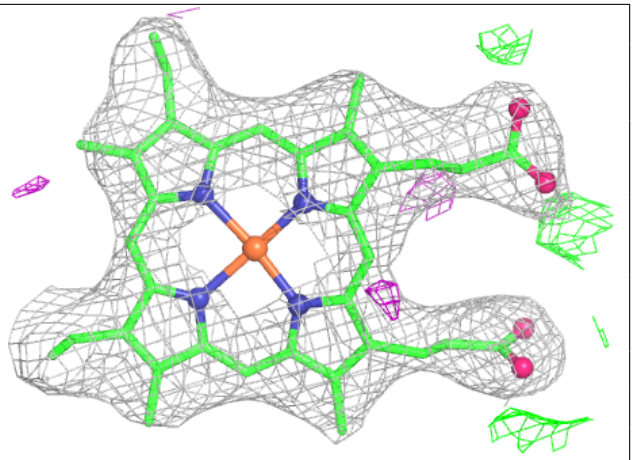


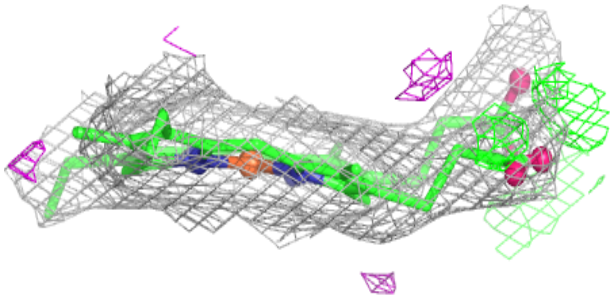


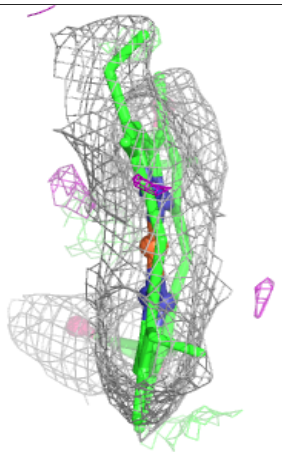


Electron density around HEC C 606:

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

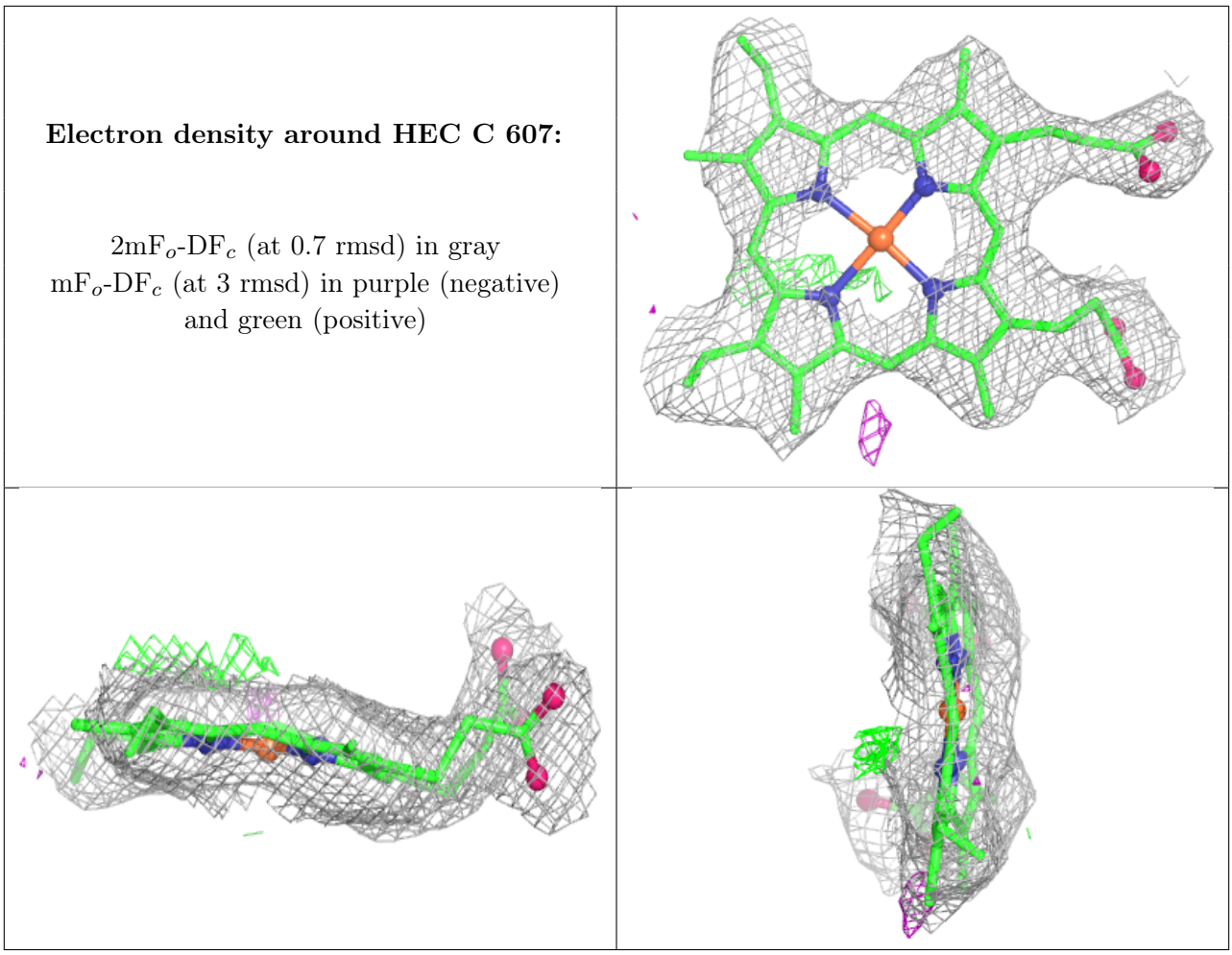






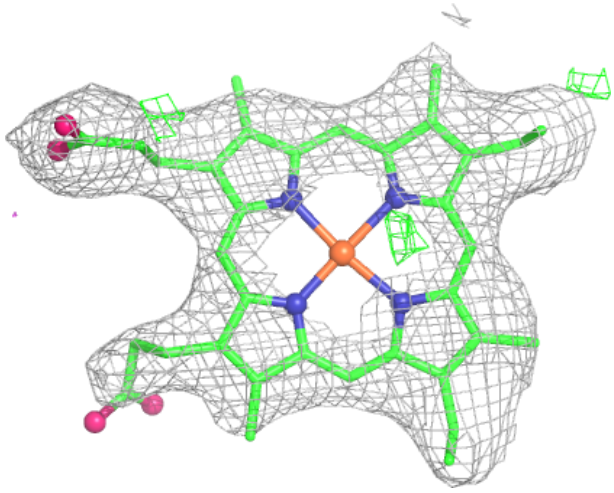
Electron density around HEC C 607:

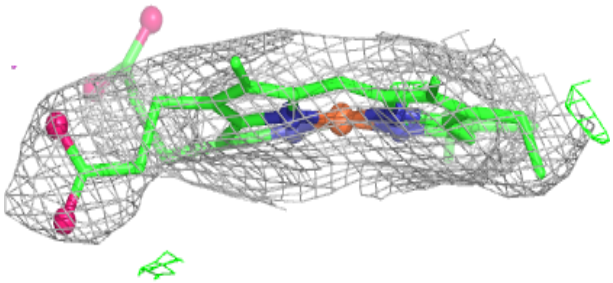
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

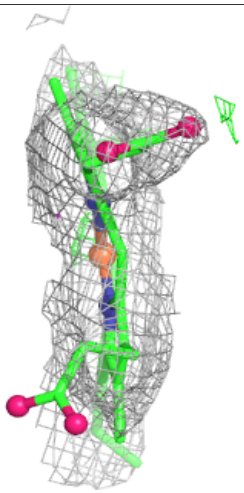


Electron density around HEC A 602:

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

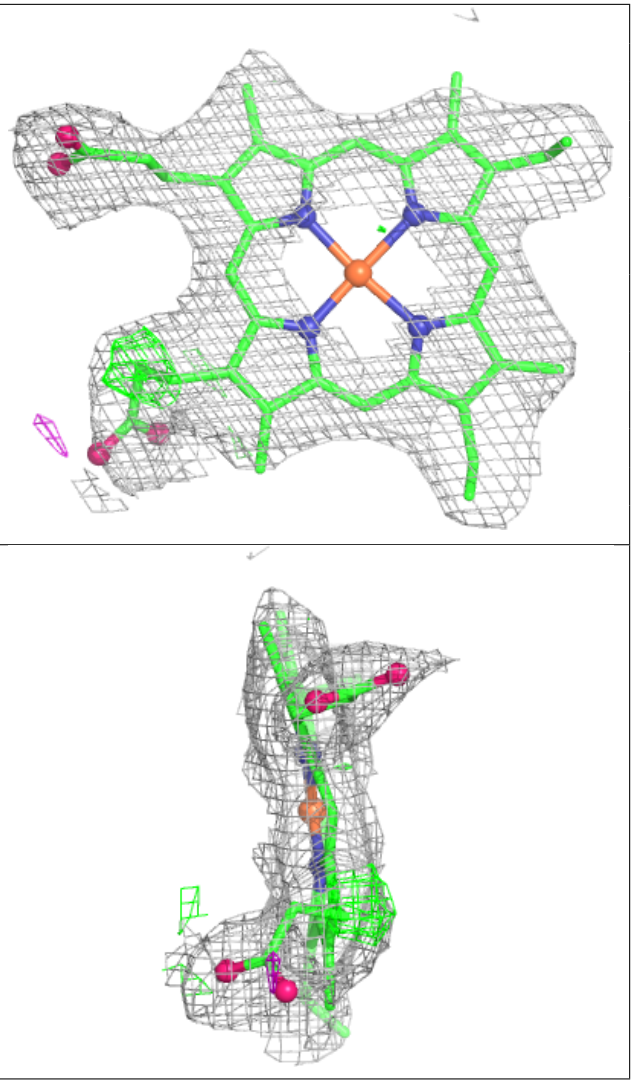






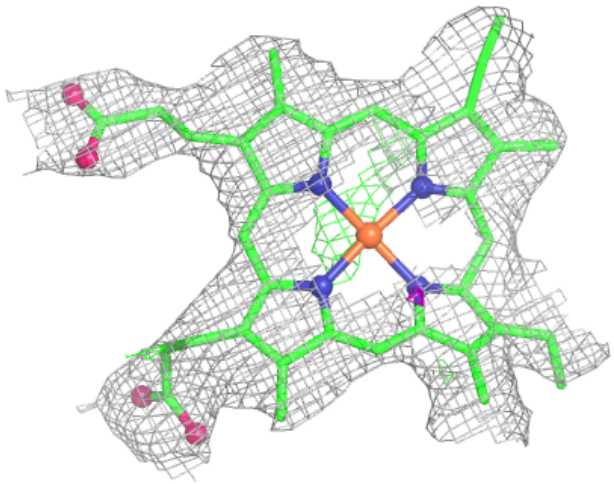
Electron density around HEC G 602:

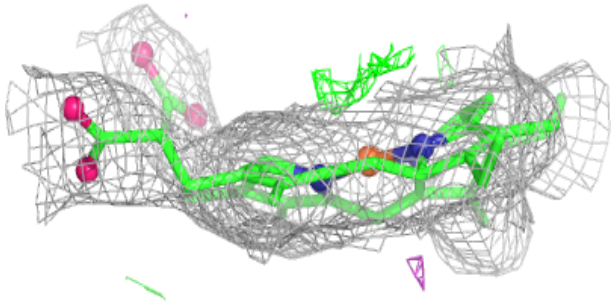
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

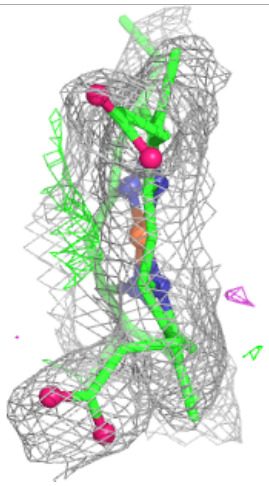


Electron density around HEC B 603:

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

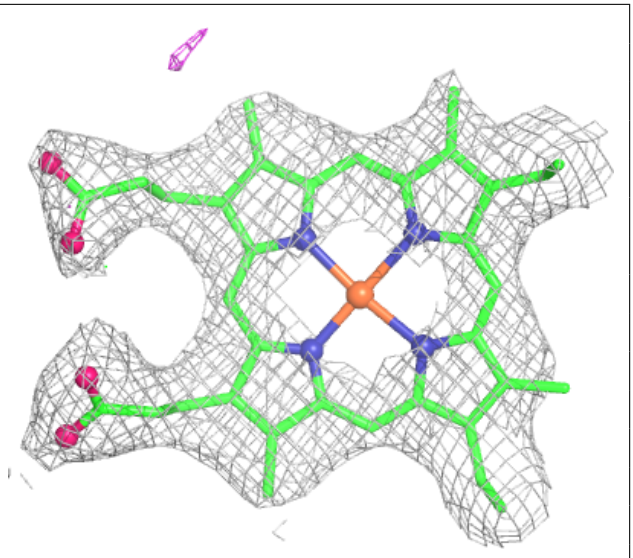


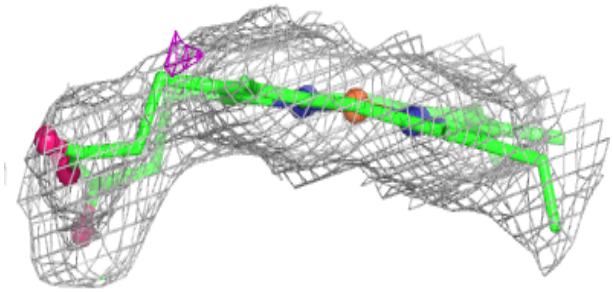


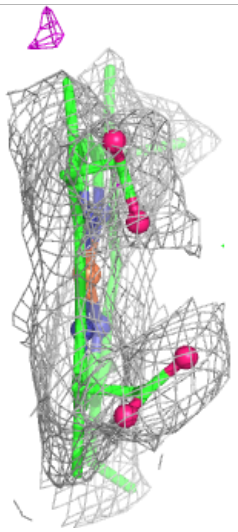


Electron density around HEC H 604:

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

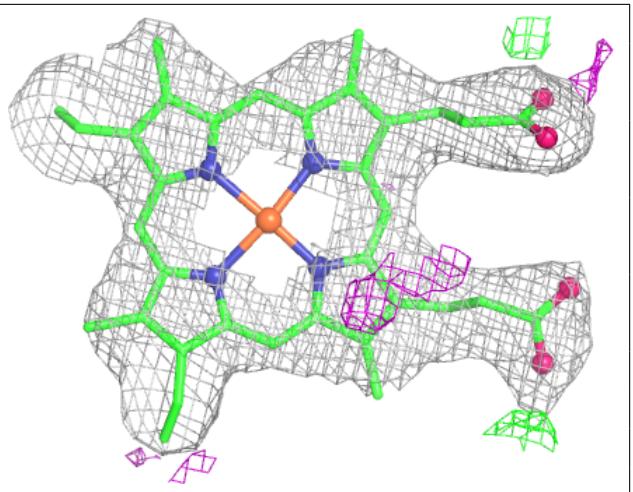


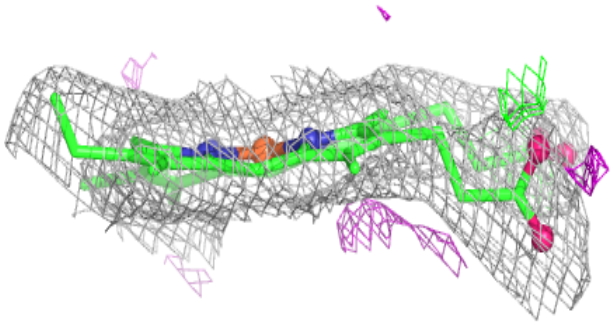


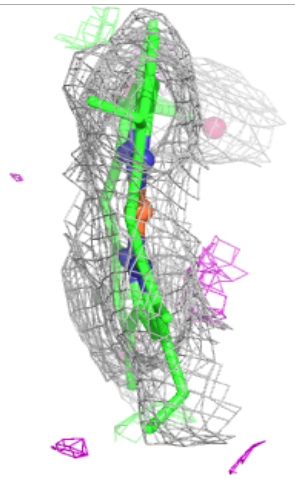


Electron density around HEC H 606:

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

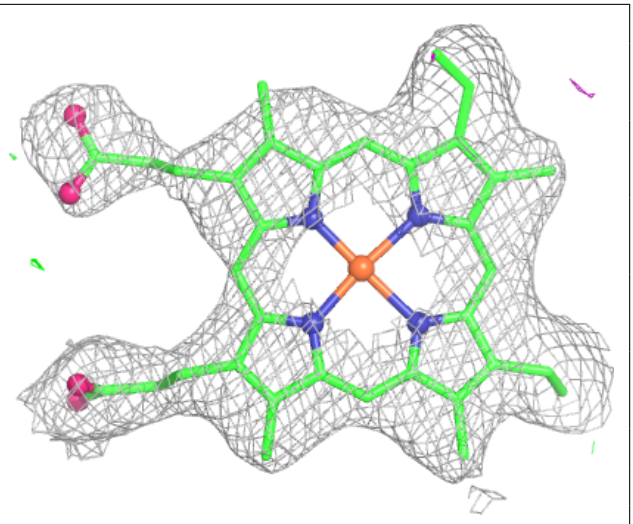


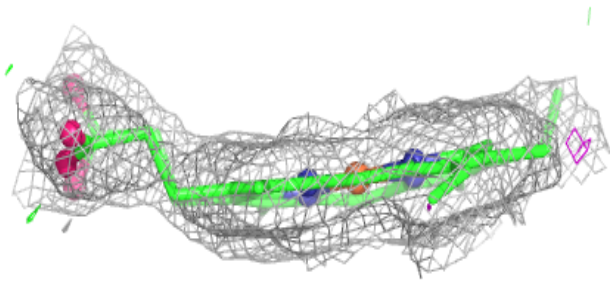


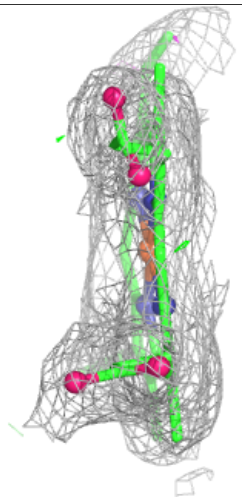


Electron density around HEC I 600:

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

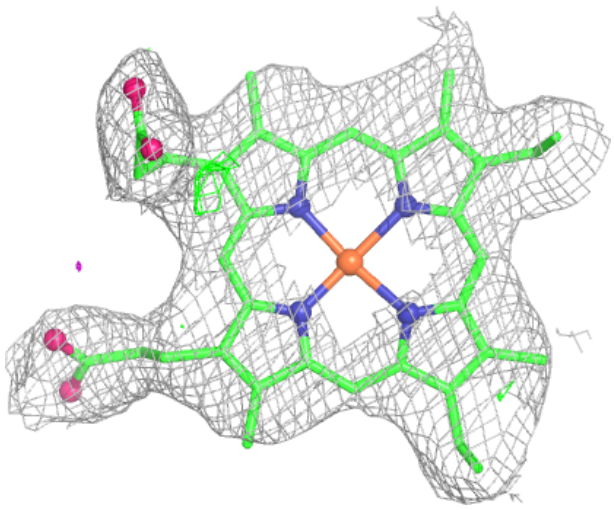


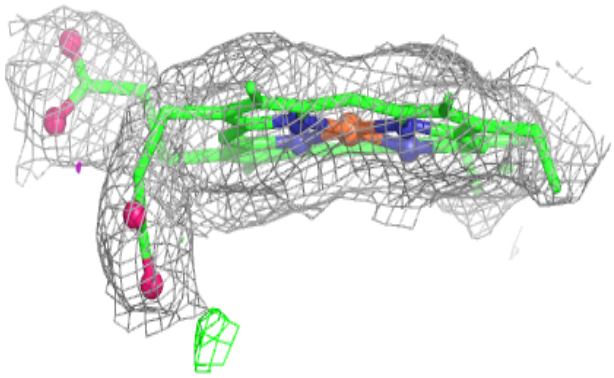


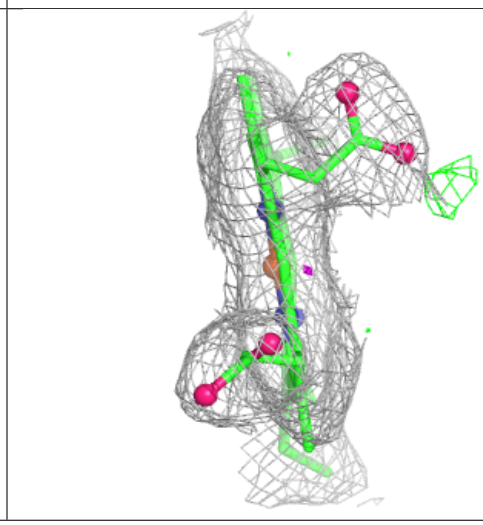


Electron density around HEC I 601:

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

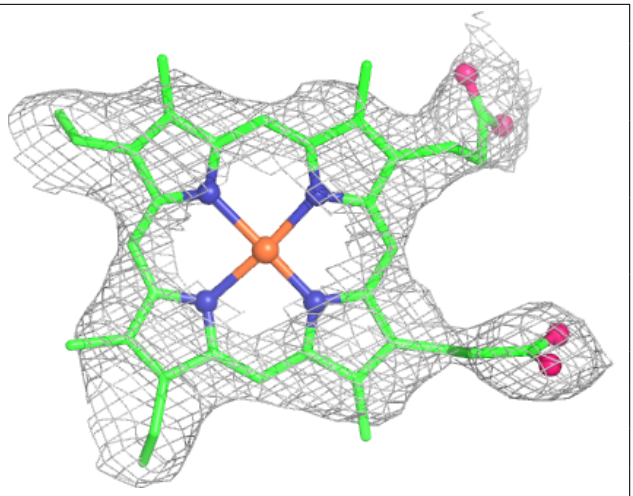


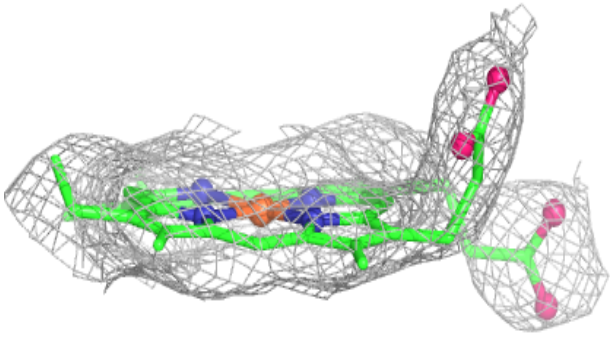


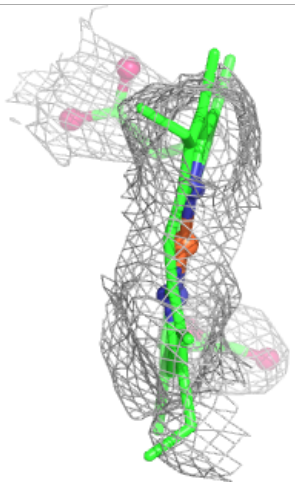


Electron density around HEC D 601:

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

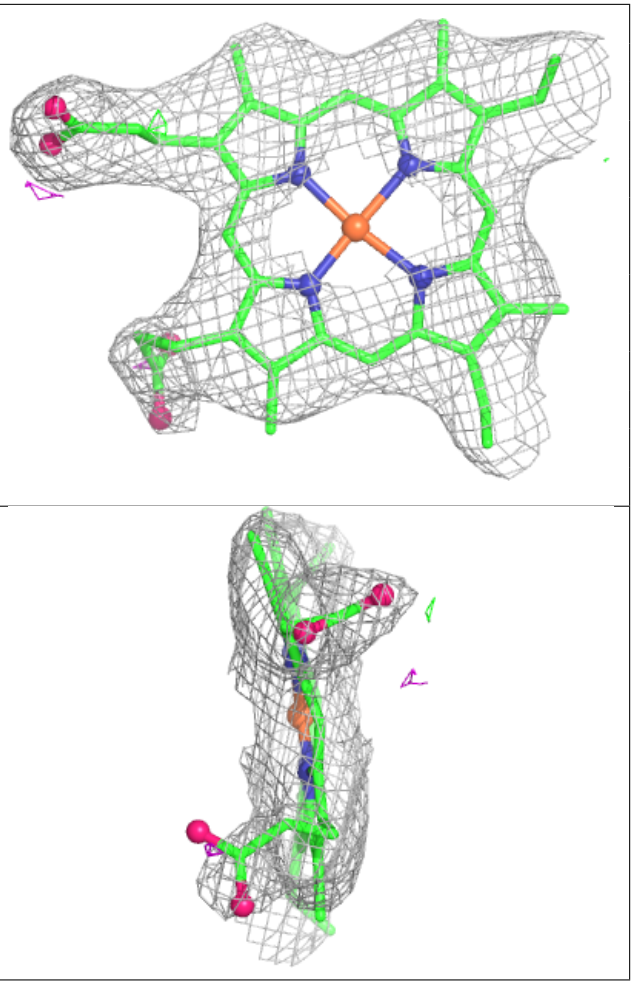






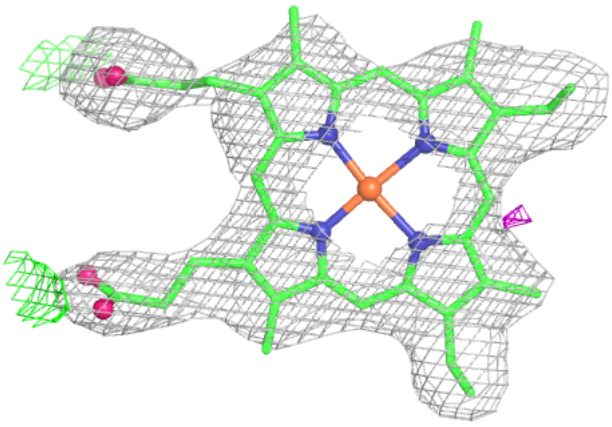
Electron density around HEC D 602:

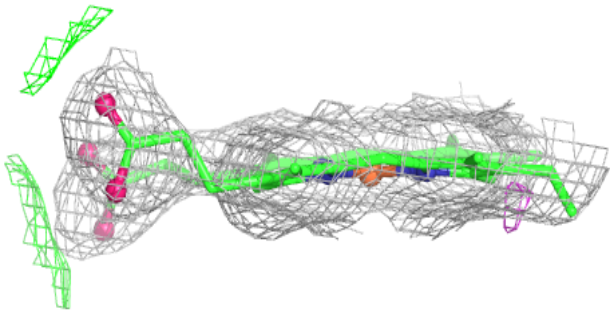
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC D 605:

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

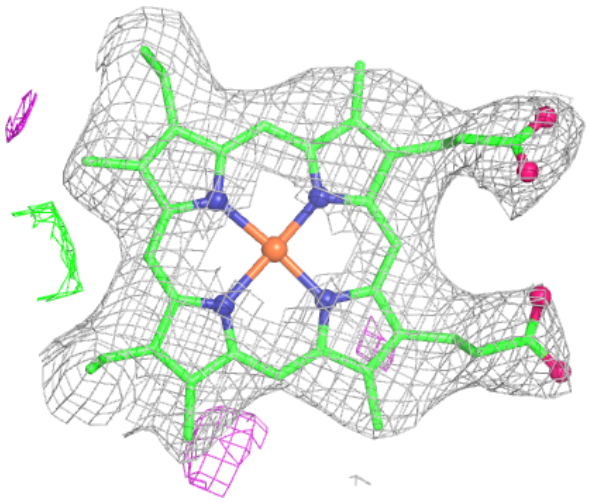


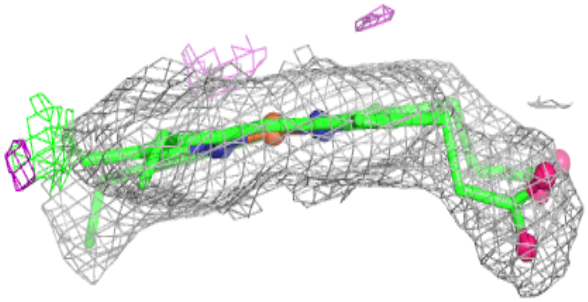


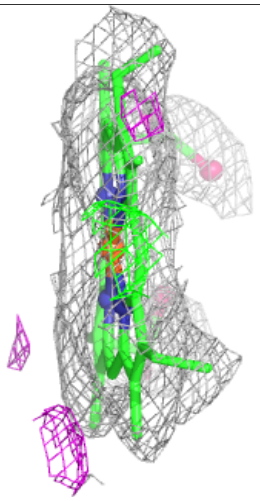


Electron density around HEC J 604:

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

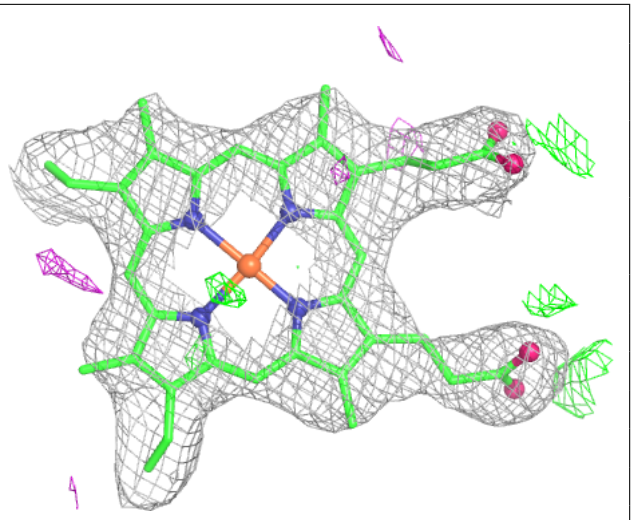


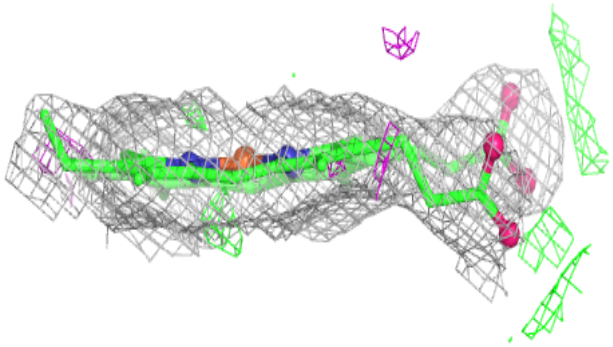


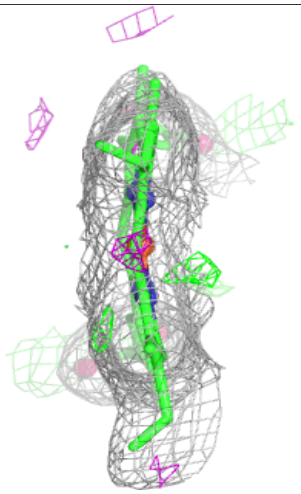


Electron density around HEC J 605:

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

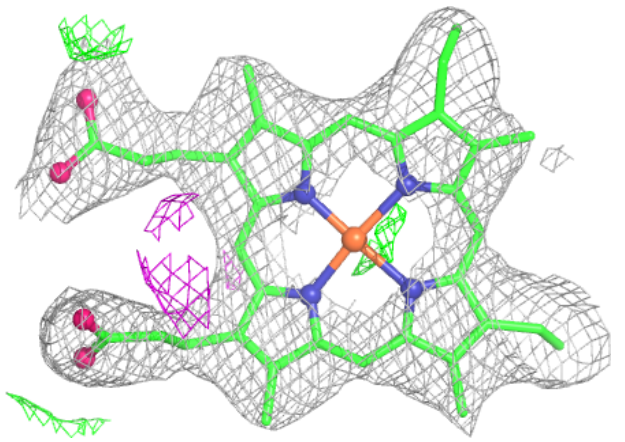


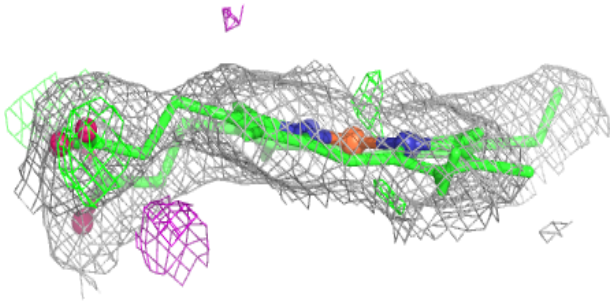


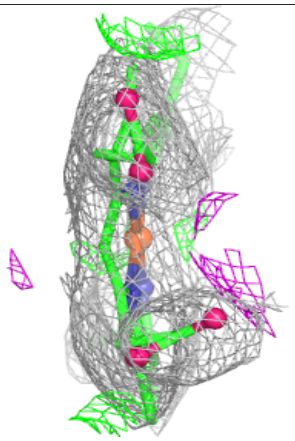


Electron density around HEC J 606:

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

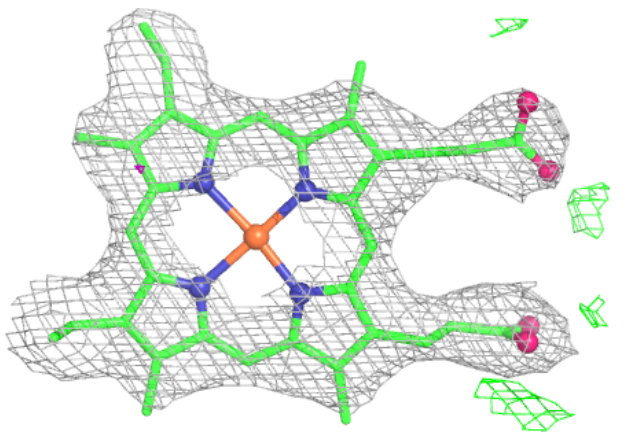


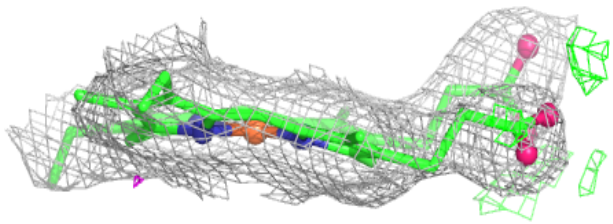


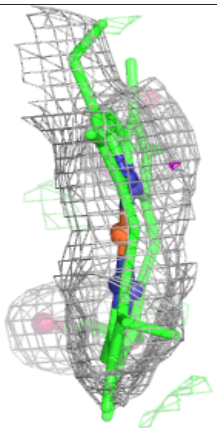


Electron density around HEC D 606:

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

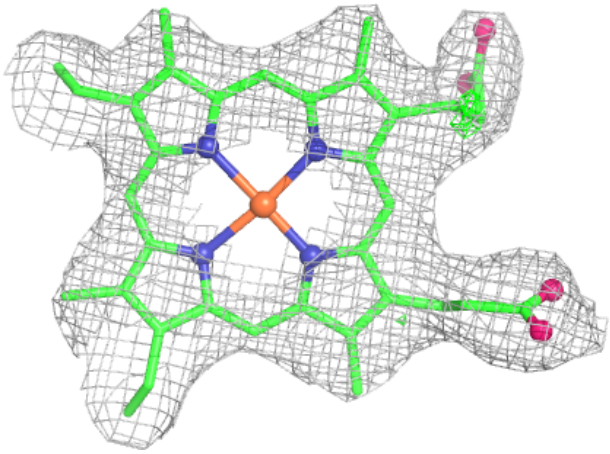


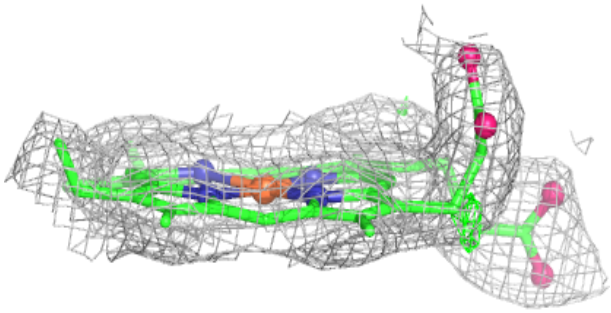


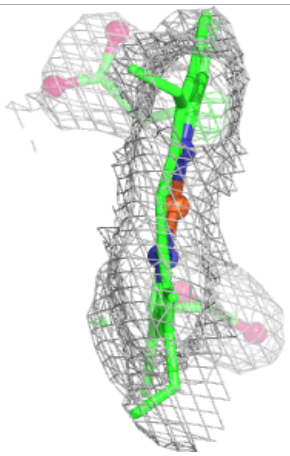


Electron density around HEC K 601:

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

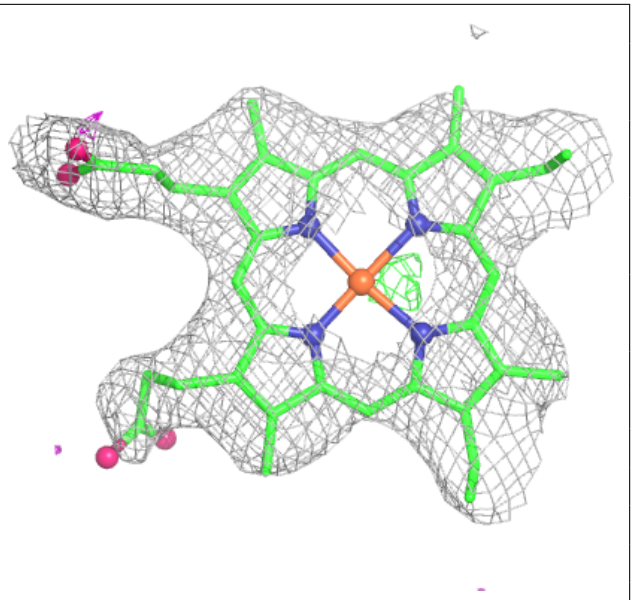


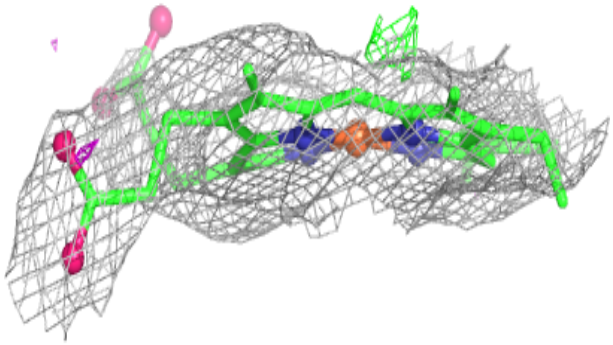


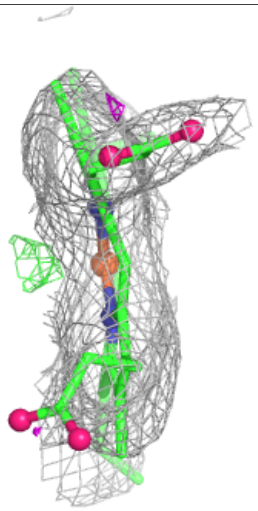


Electron density around HEC K 602:

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

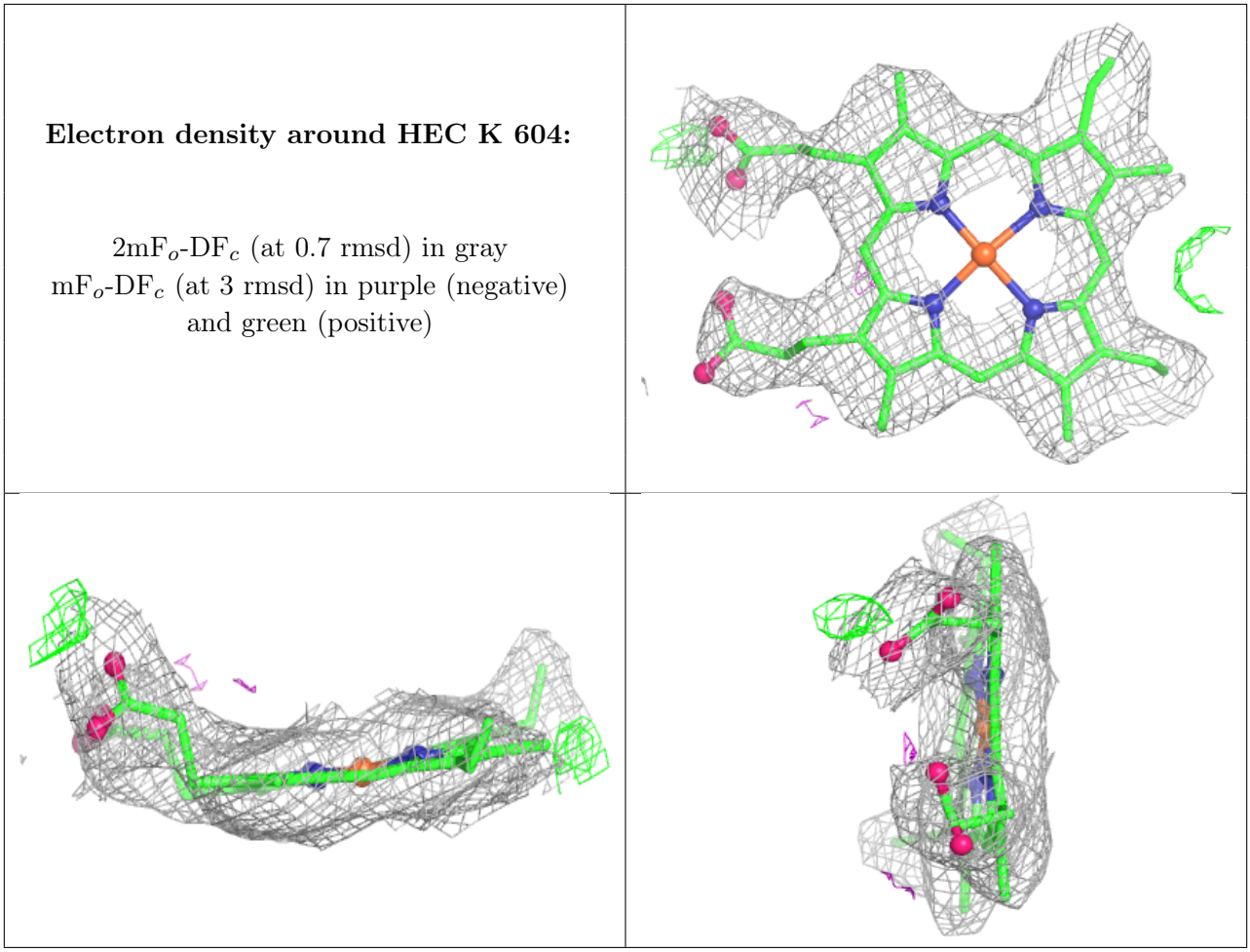






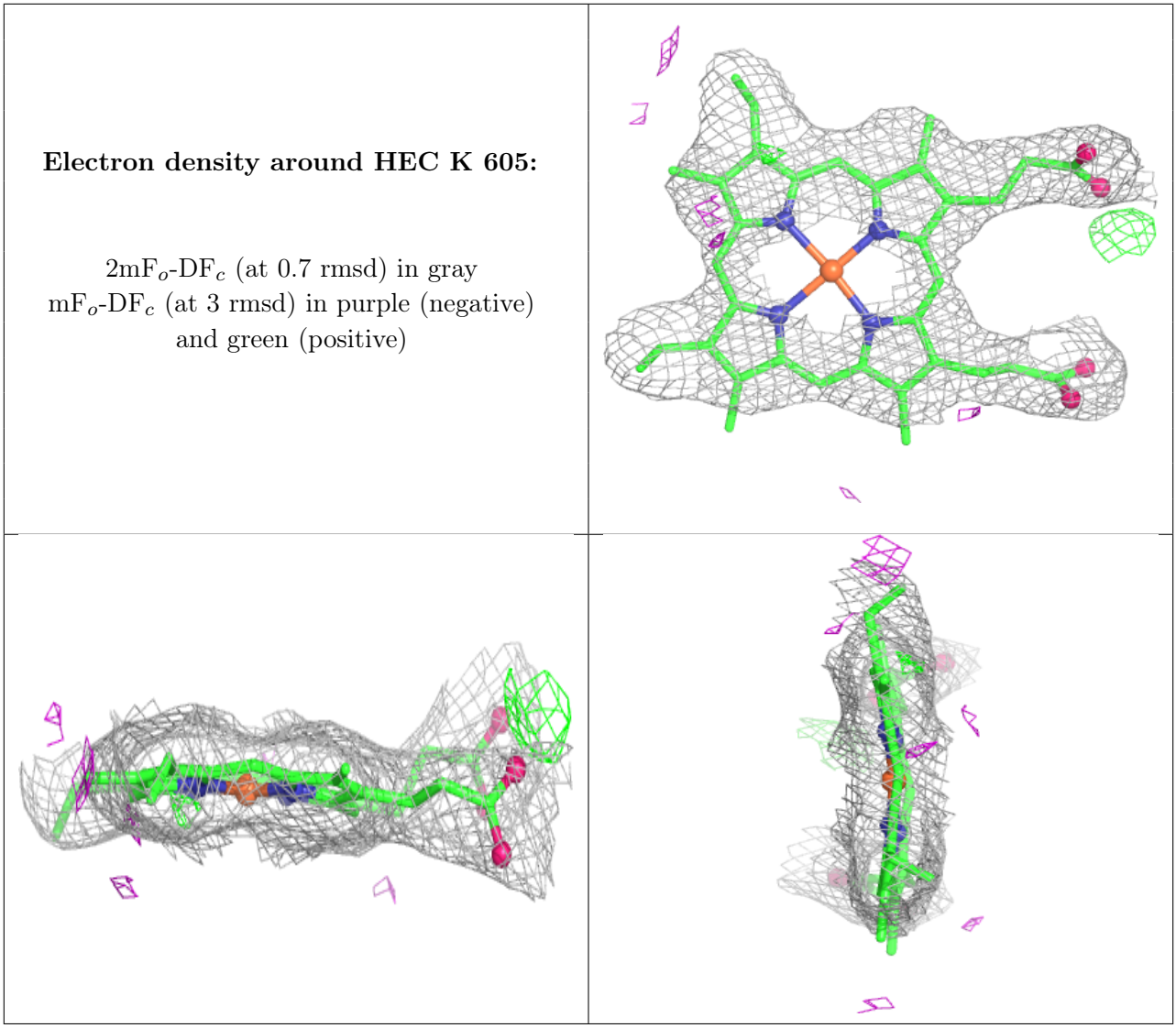
Electron density around HEC K 604:

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



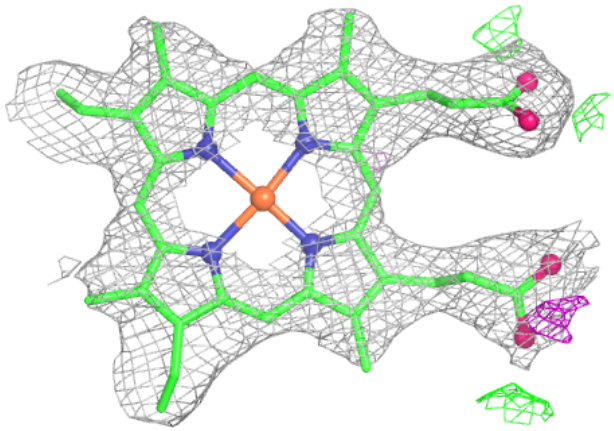
Electron density around HEC K 605:

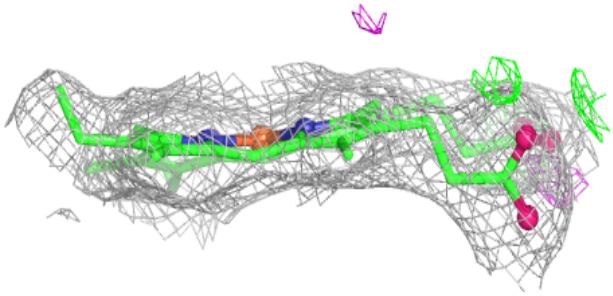
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

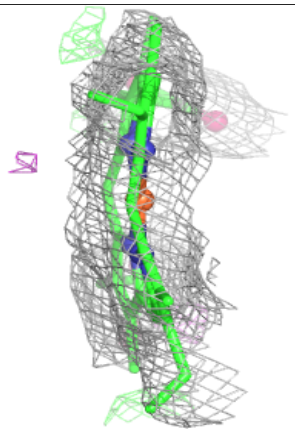


Electron density around HEC K 606:

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

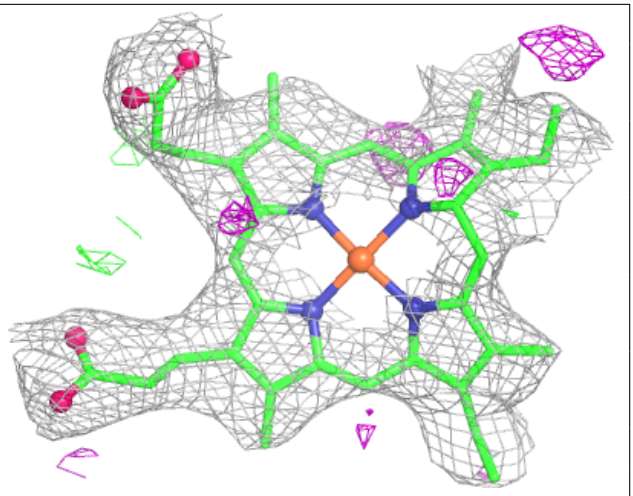


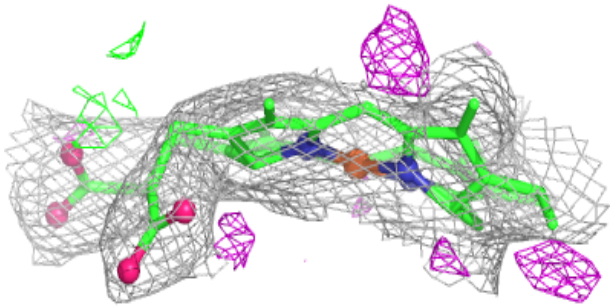


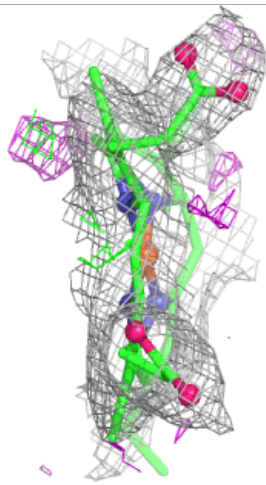


Electron density around HEC L 603:

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

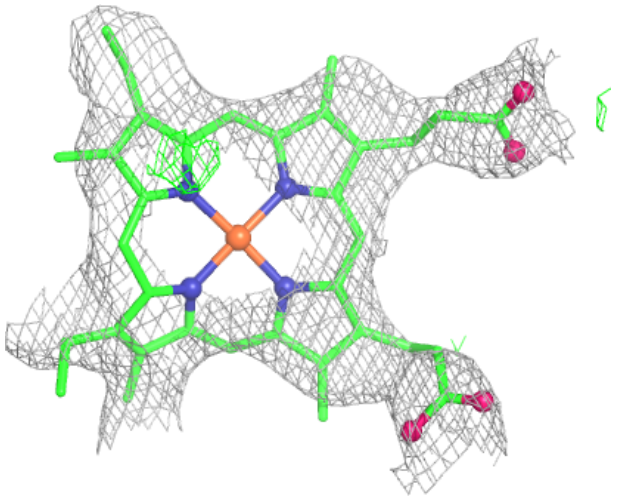


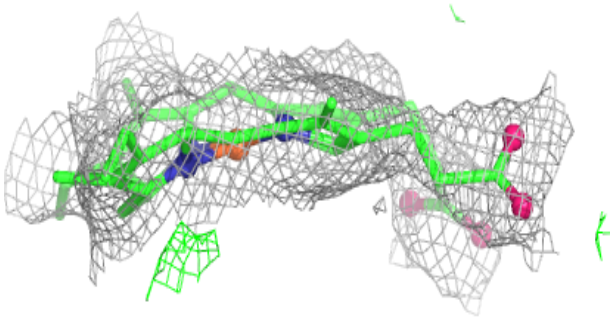


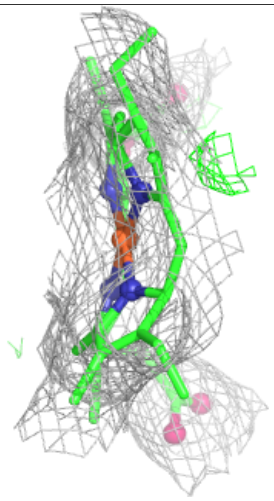


Electron density around HEC D 603:

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

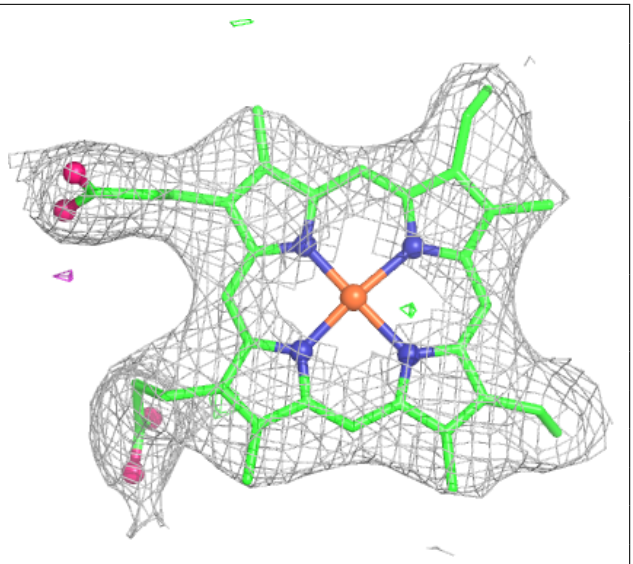


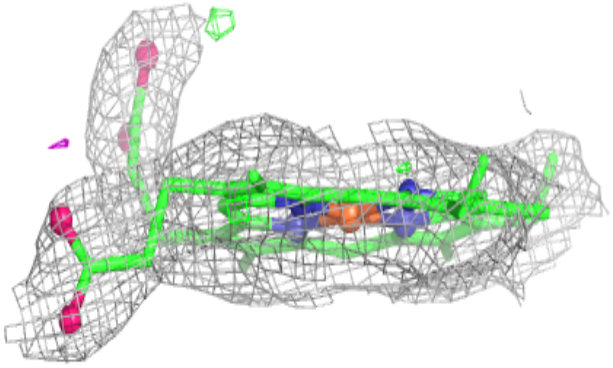


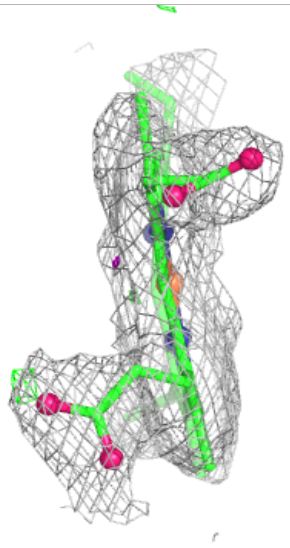


Electron density around HEC L 601:

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

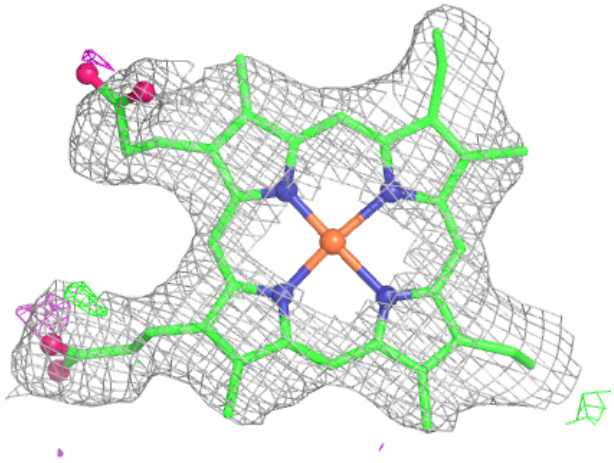


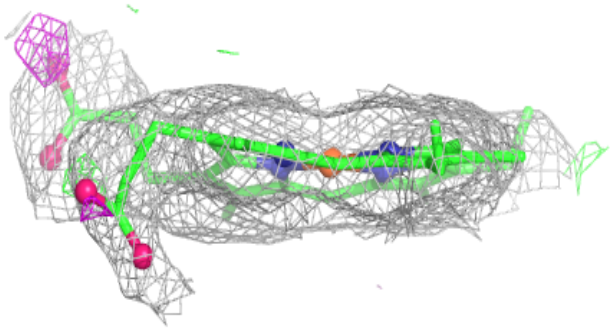


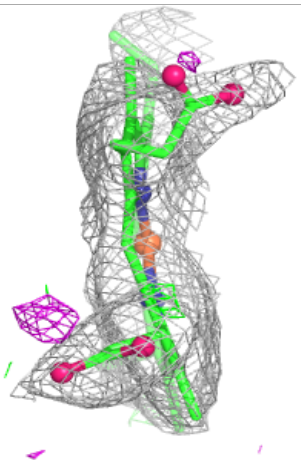


Electron density around HEC L 602:

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

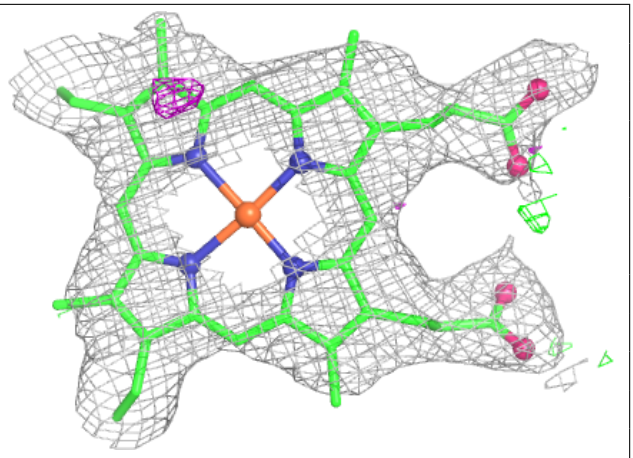


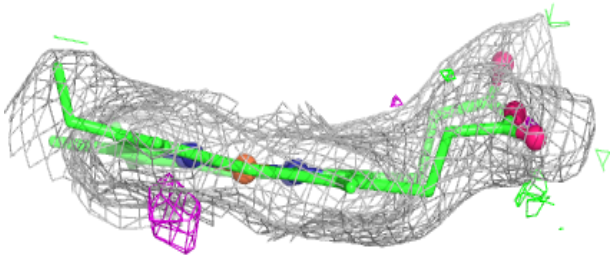


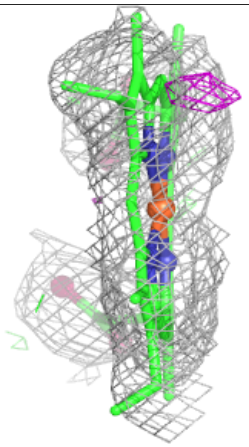


Electron density around HEC L 604:

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

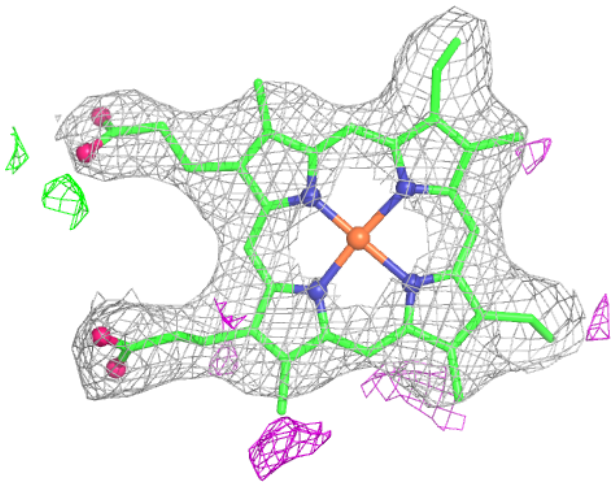


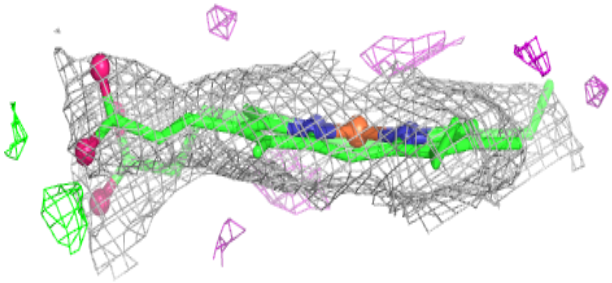


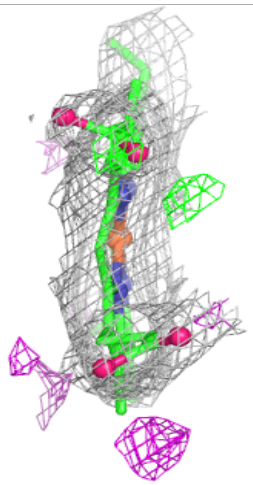


Electron density around HEC L 605:

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

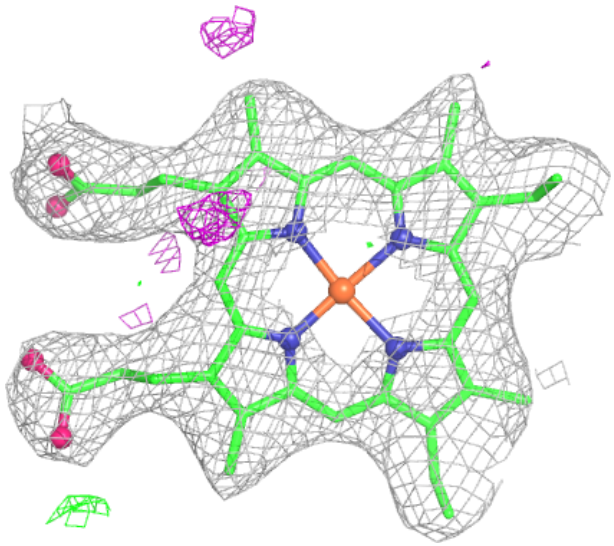


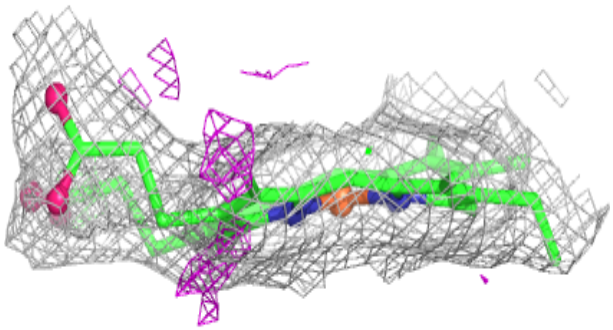


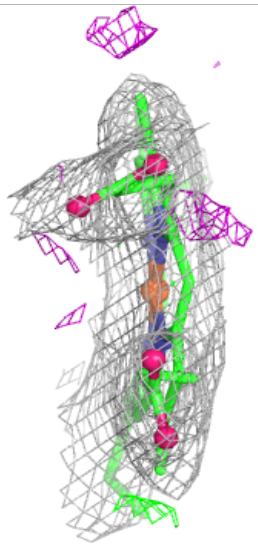


Electron density around HEC L 606:

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

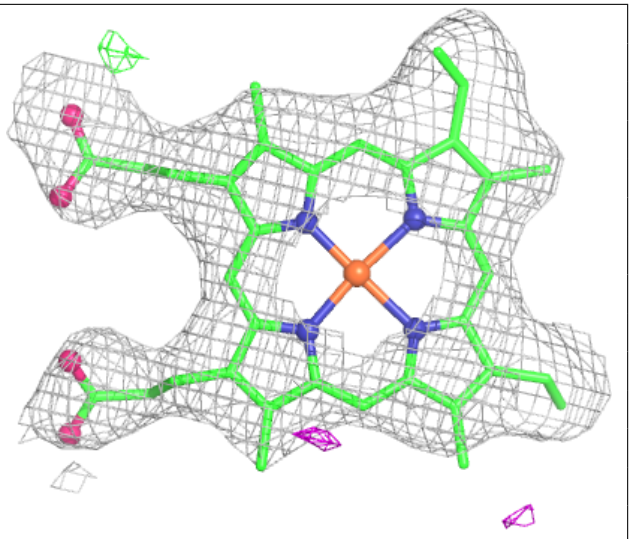


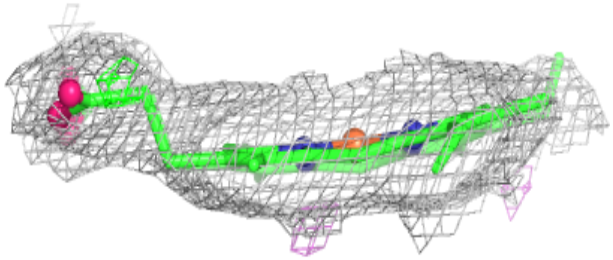


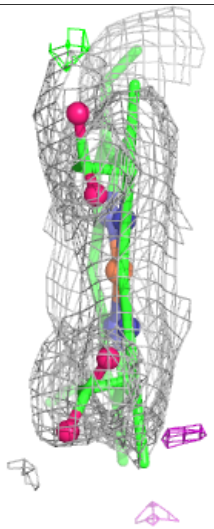


Electron density around HEC B 600:

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

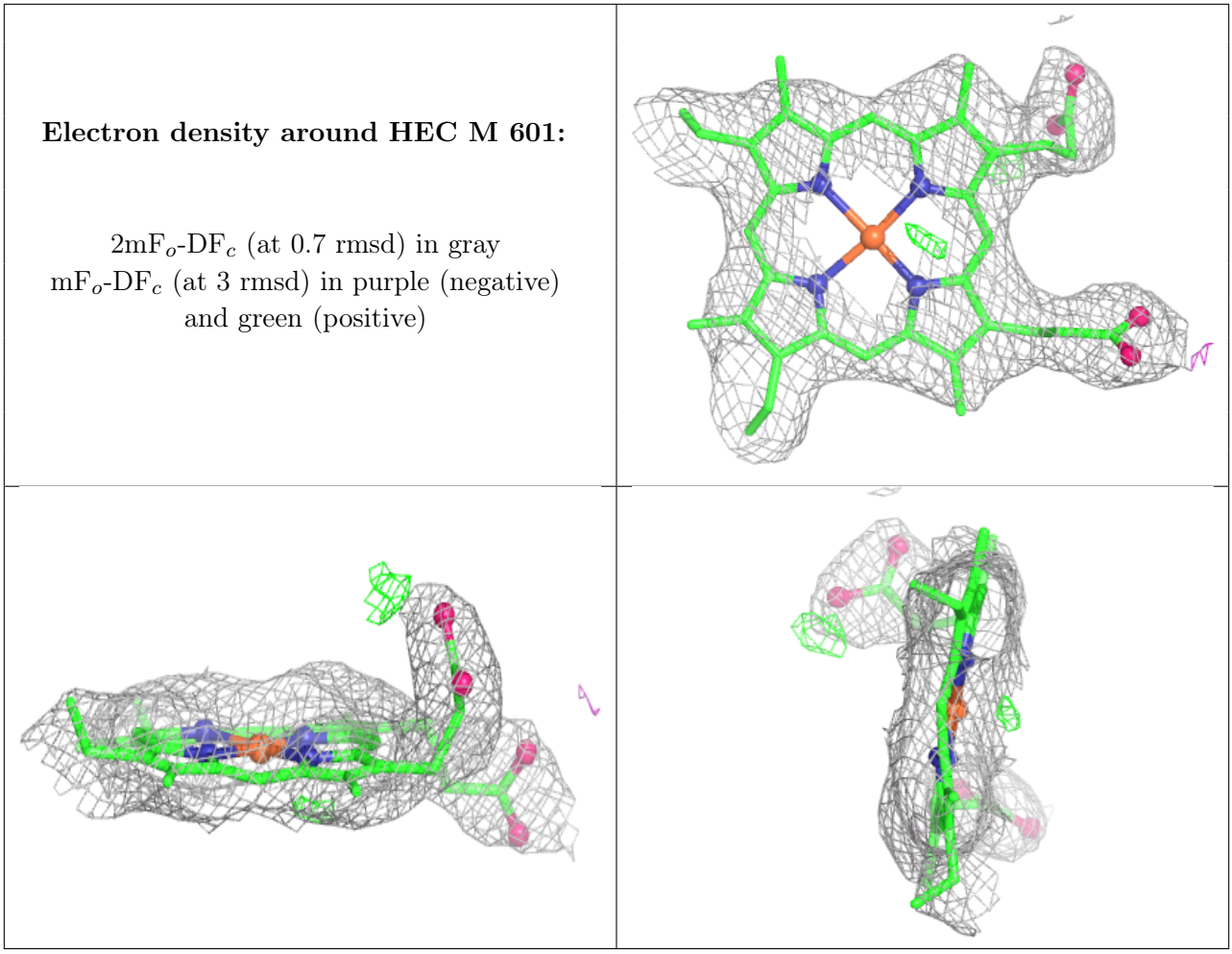






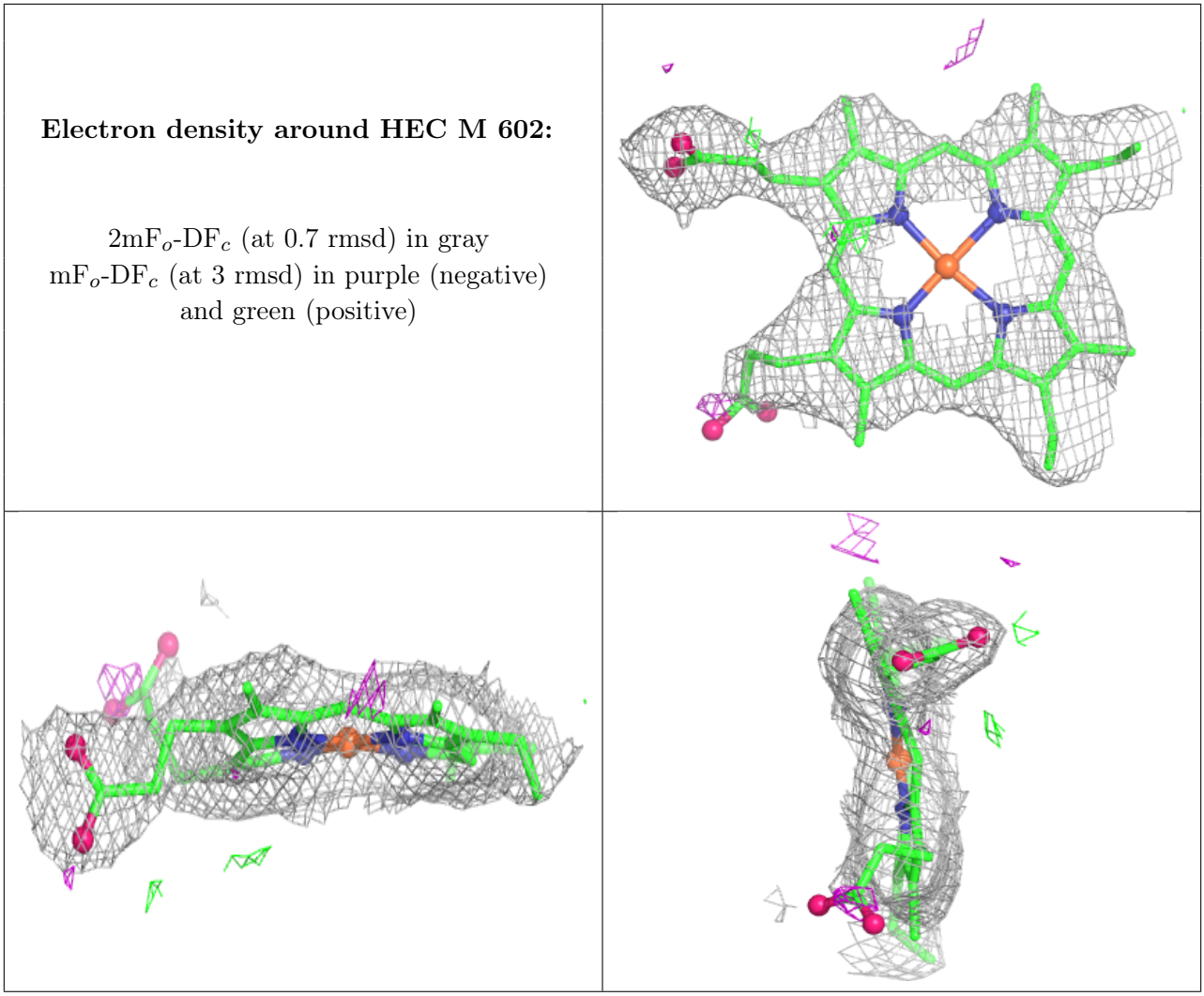
Electron density around HEC M 601:

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



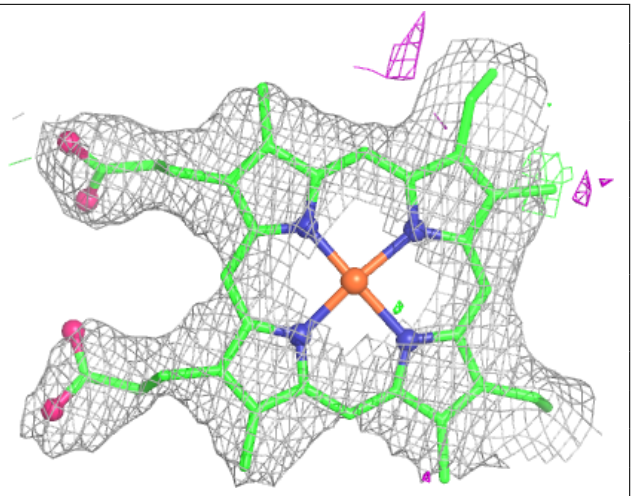
Electron density around HEC M 602:

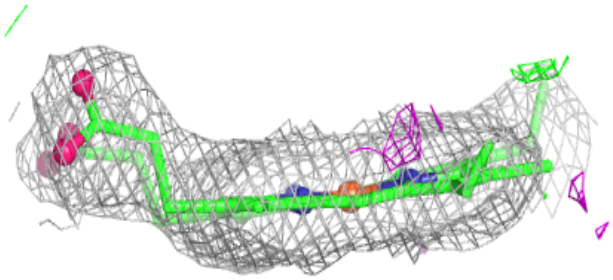
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

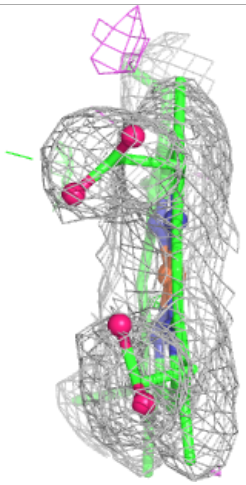


Electron density around HEC M 604:

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

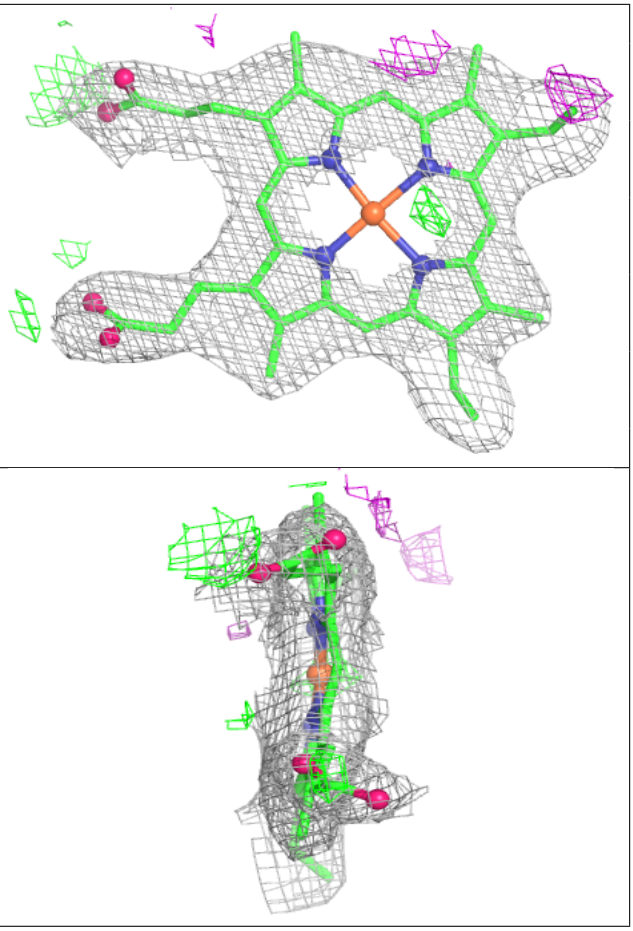


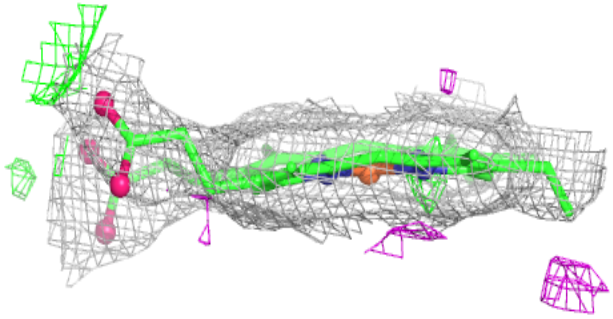




Electron density around HEC M 605:

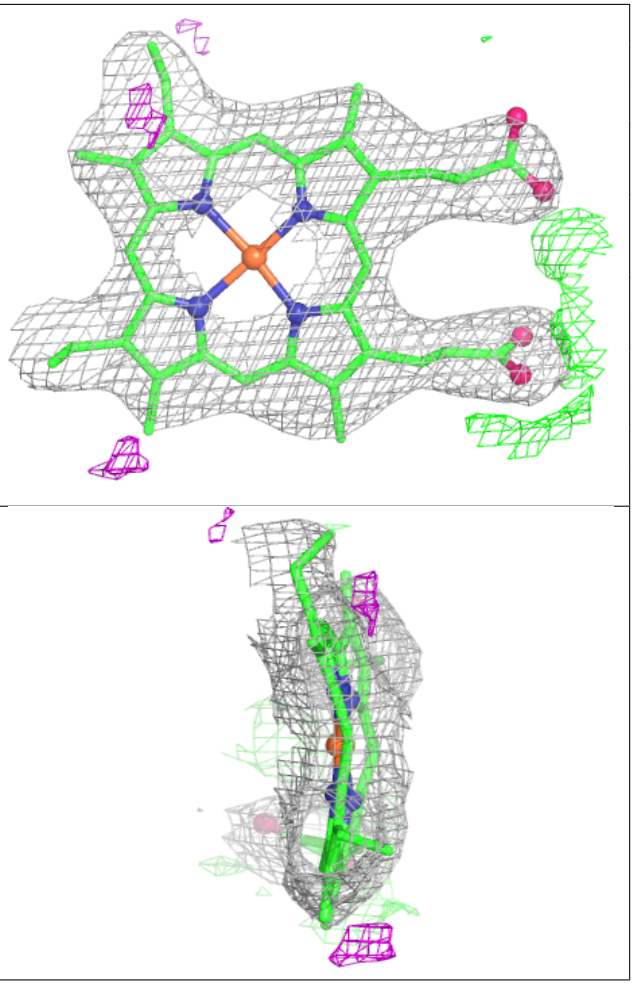
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





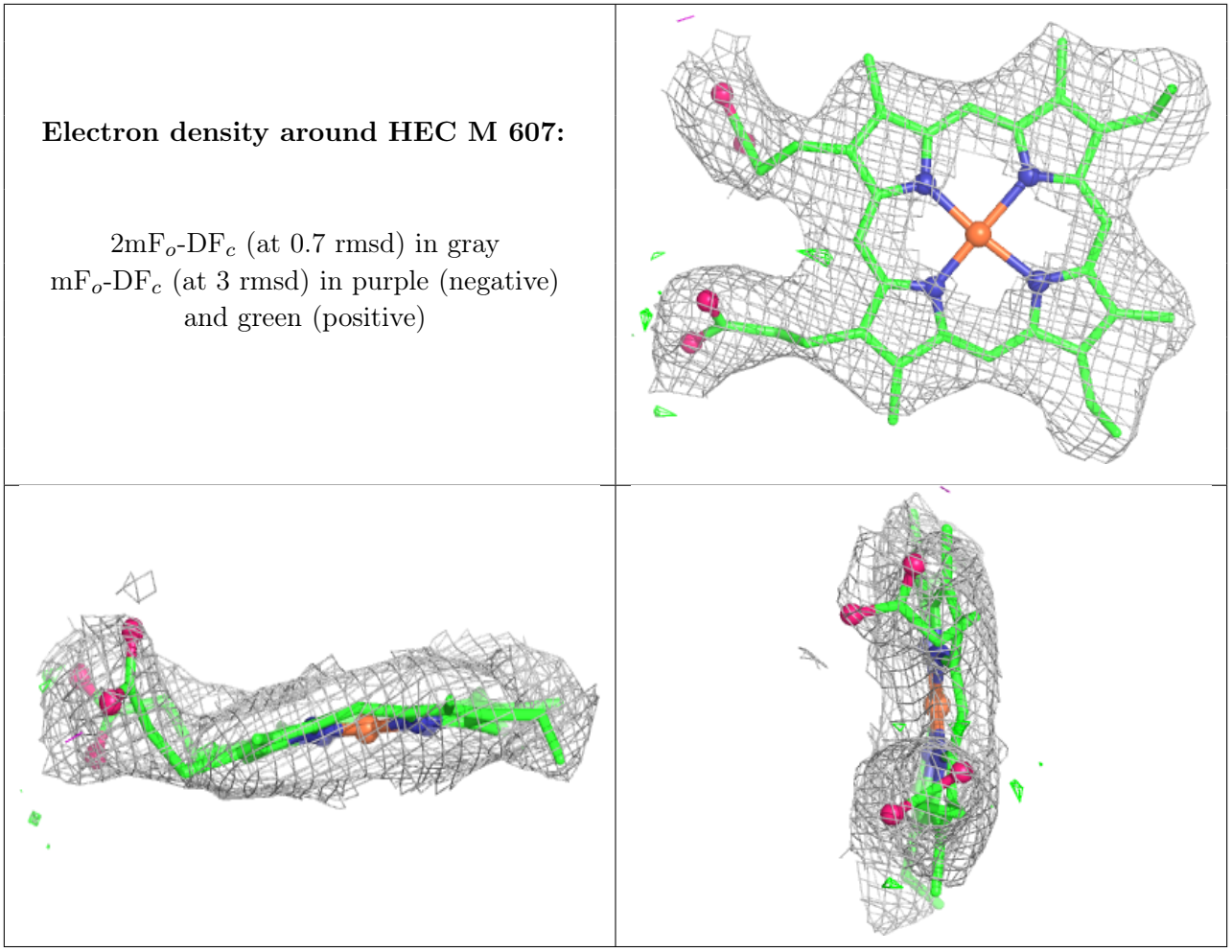
Electron density around HEC M 606:

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



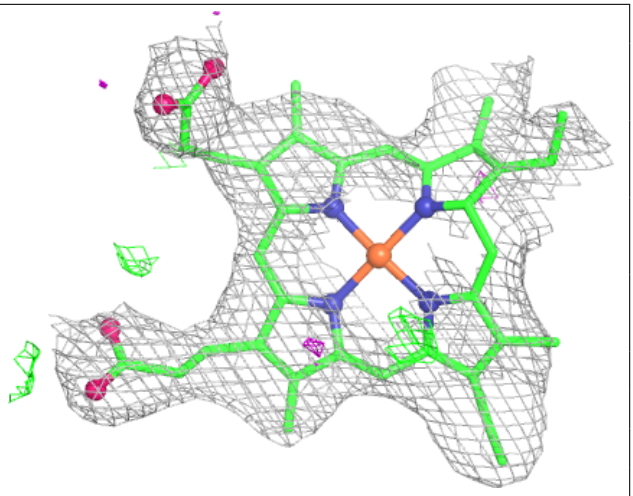
Electron density around HEC M 607:

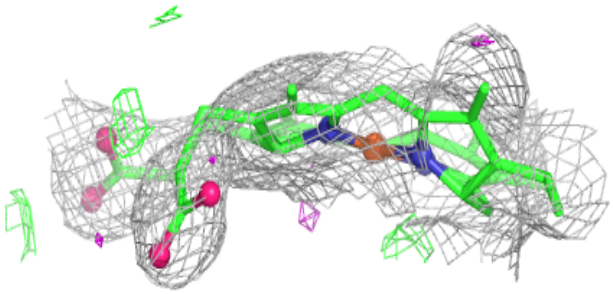
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

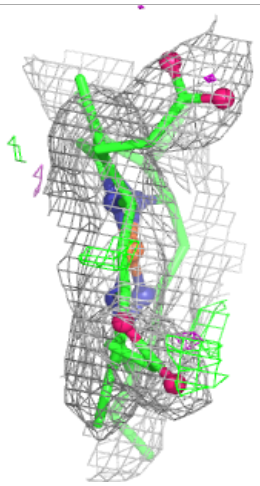


Electron density around HEC M 603:

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

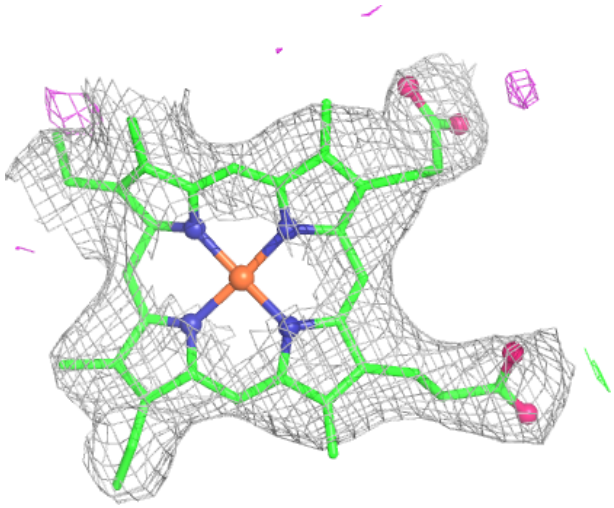


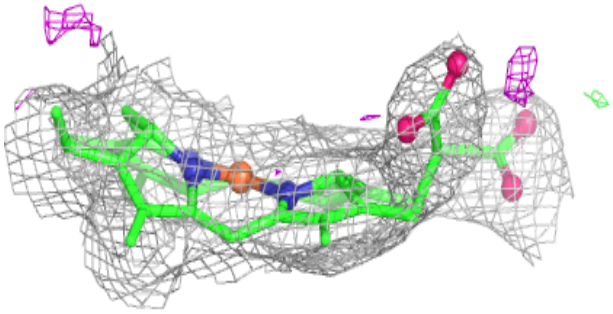


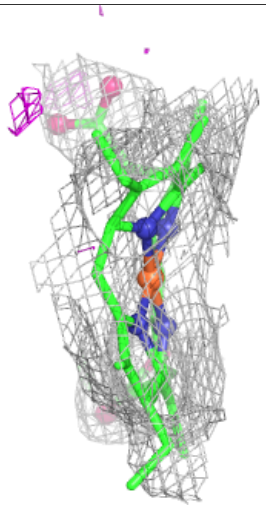


Electron density around HEC N 603:

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

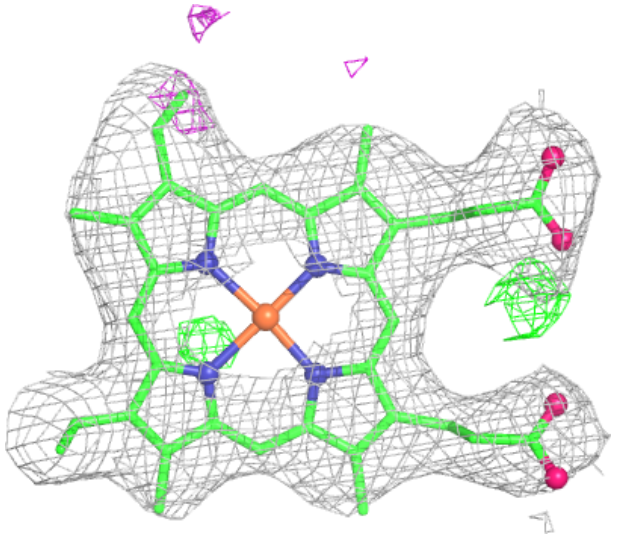


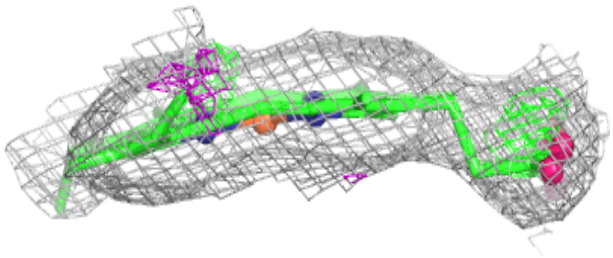


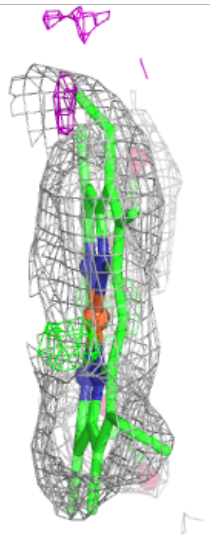


Electron density around HEC E 600:

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

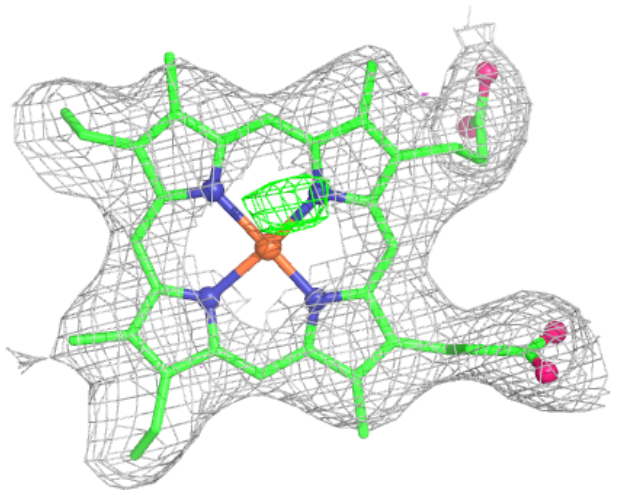


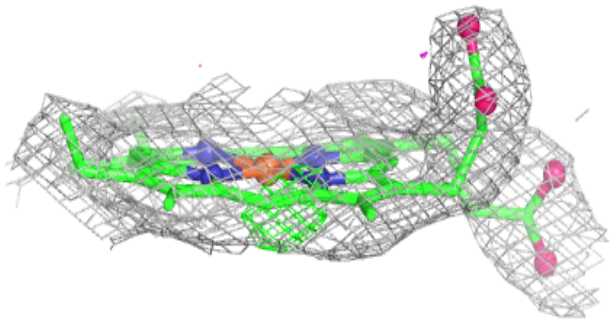


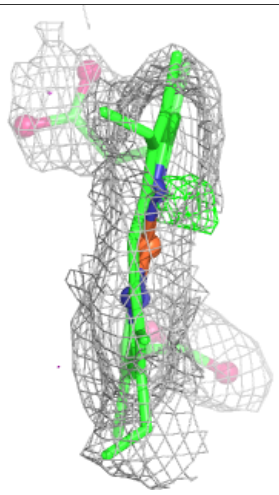


Electron density around HEC E 601:

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

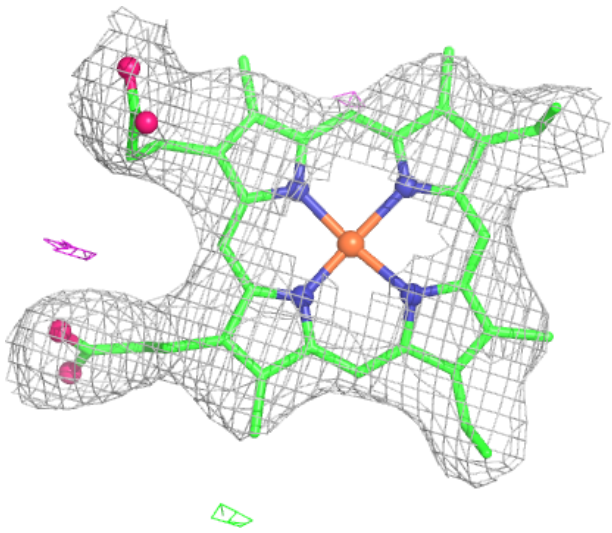


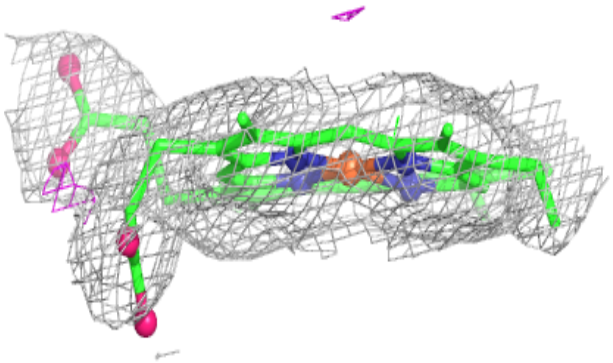


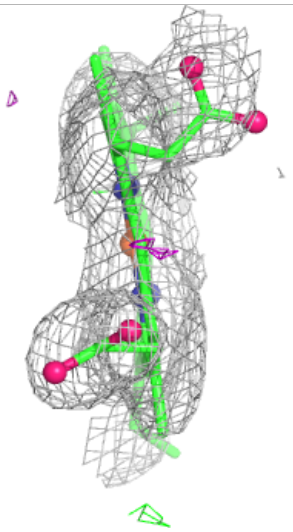


Electron density around HEC B 601:

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

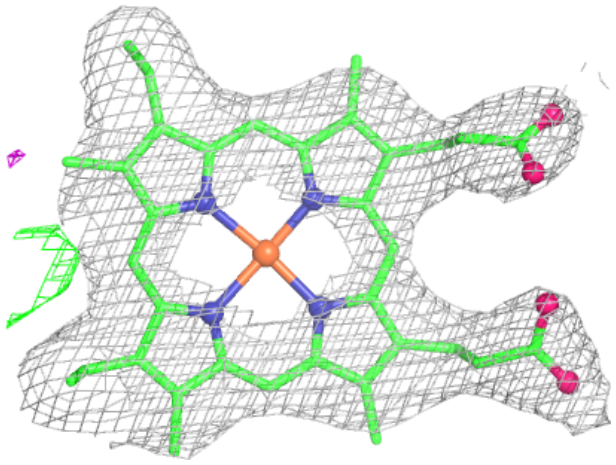


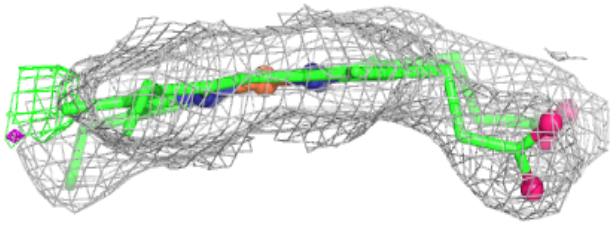


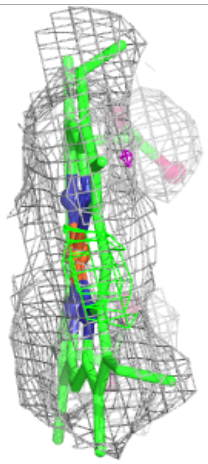


Electron density around HEC N 604:

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

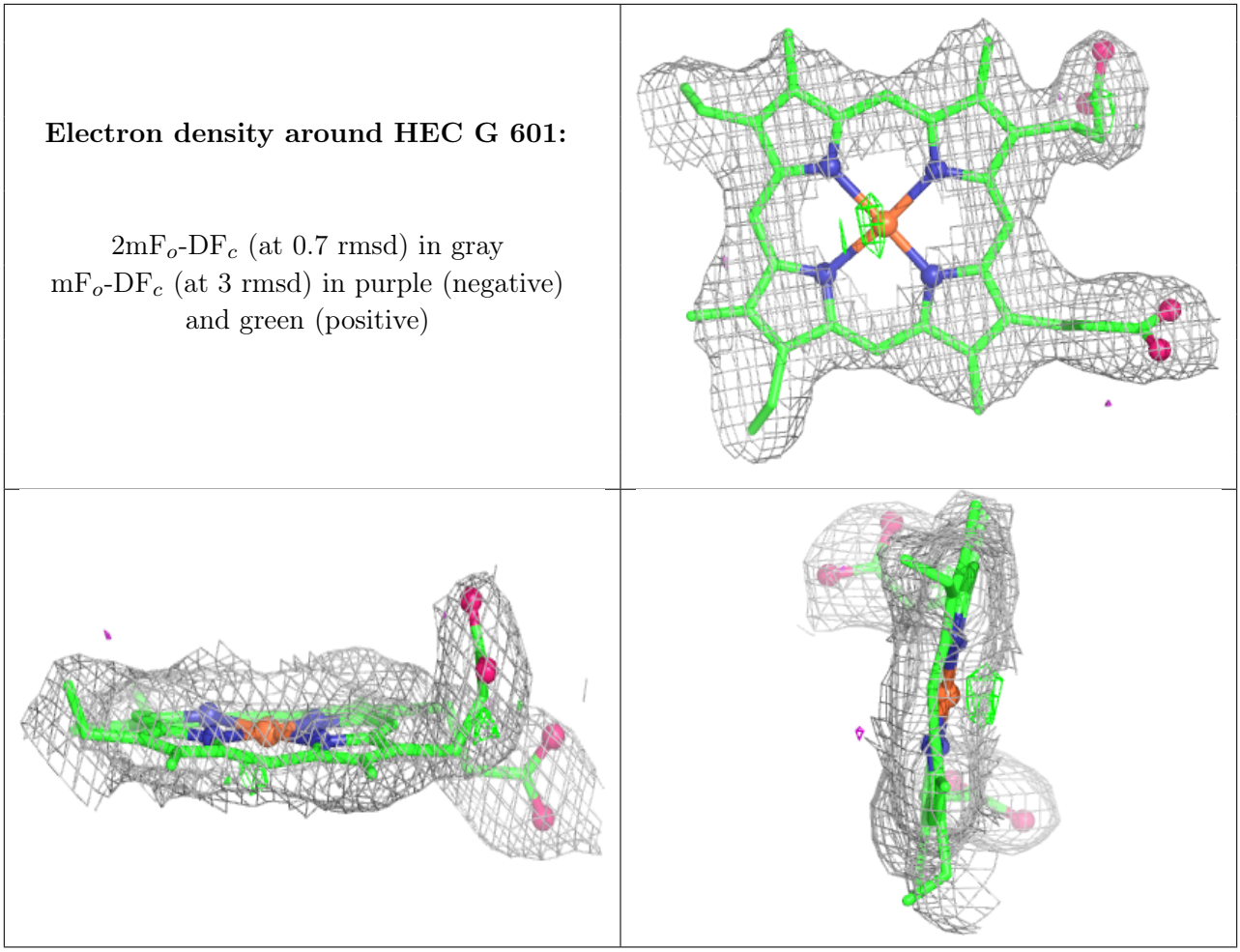






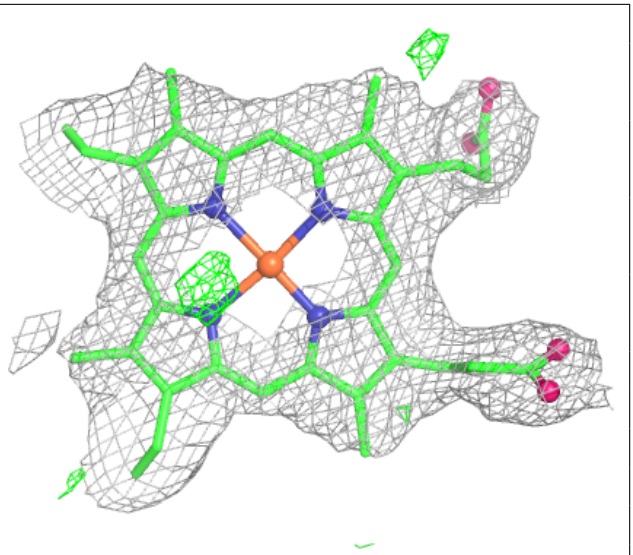
Electron density around HEC G 601:

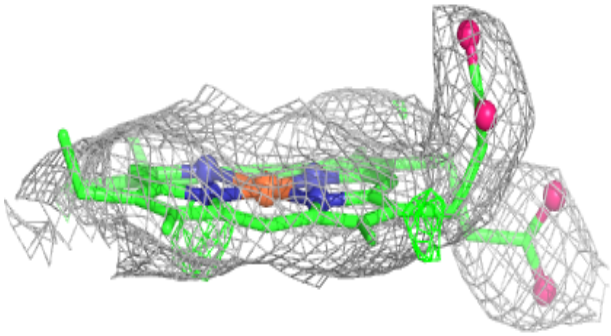
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

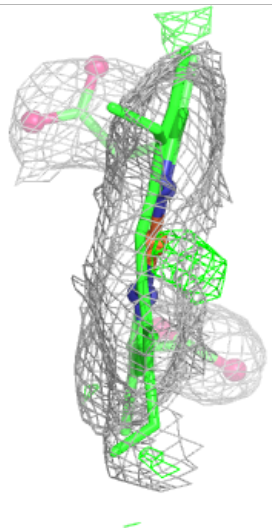


Electron density around HEC A 601:

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

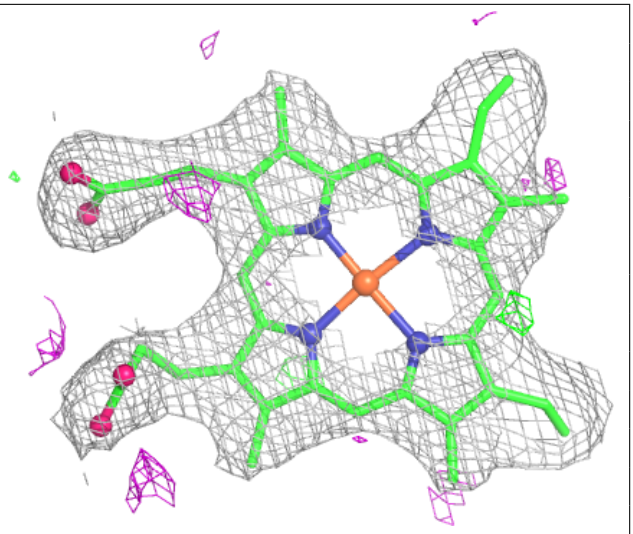


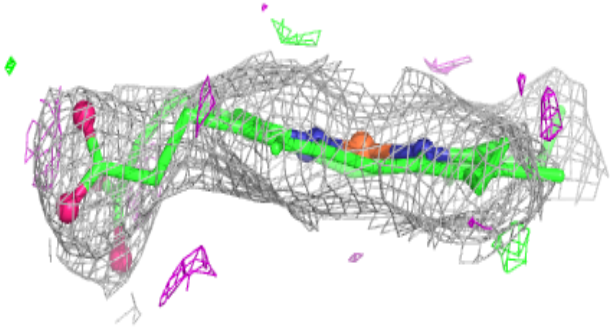


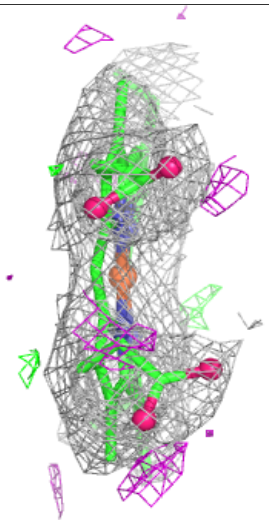


Electron density around HEC N 607:

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

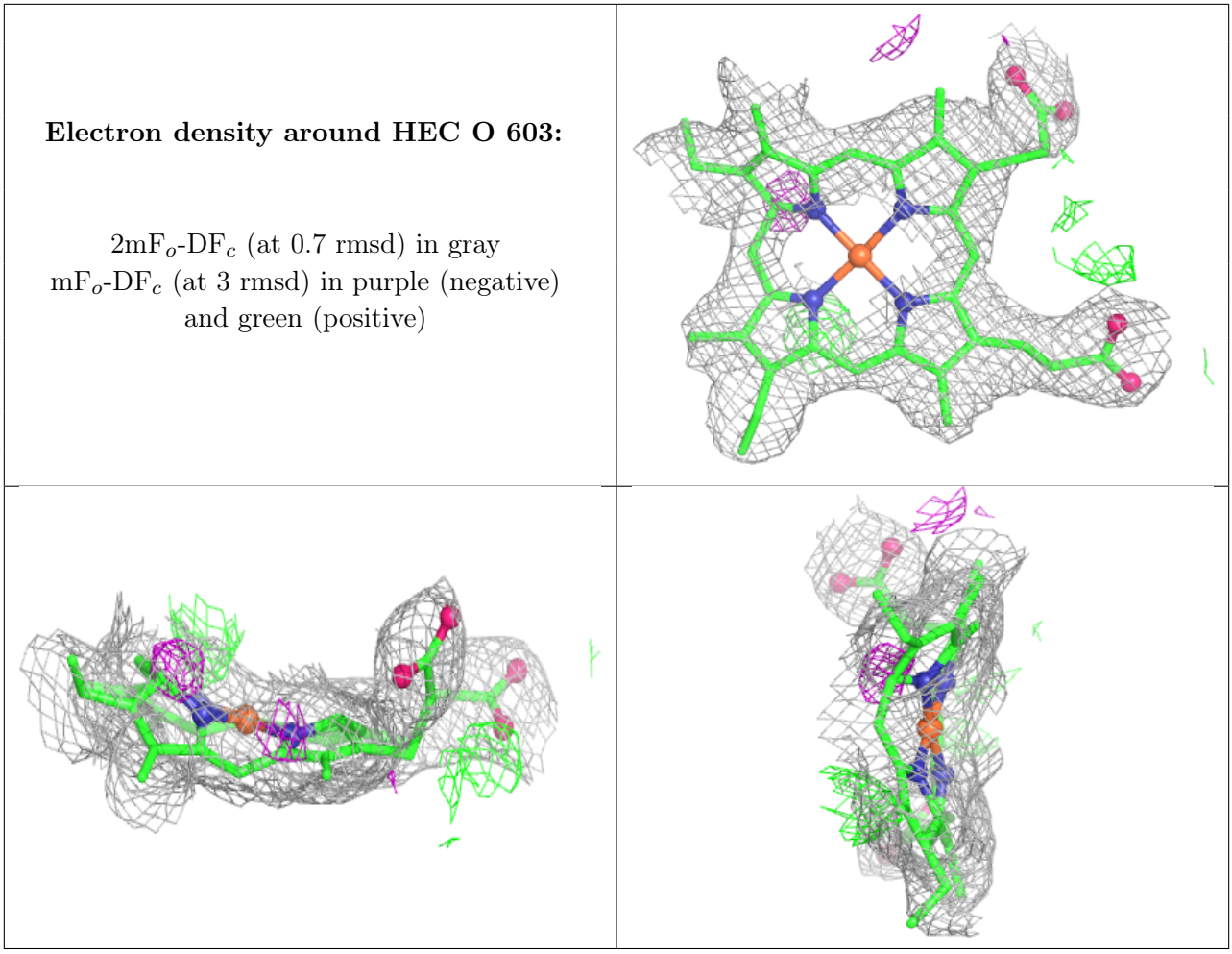






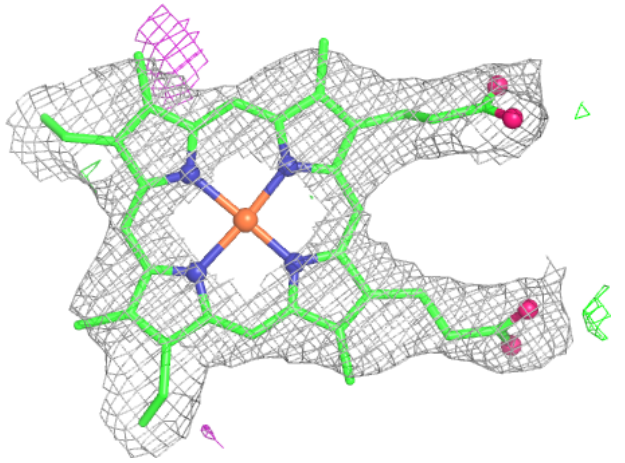
Electron density around HEC O 603:

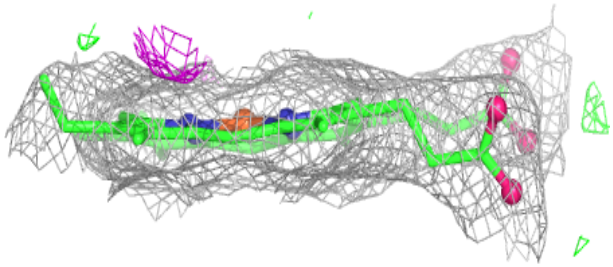
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

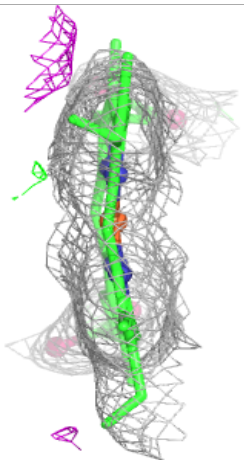


Electron density around HEC B 605:

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

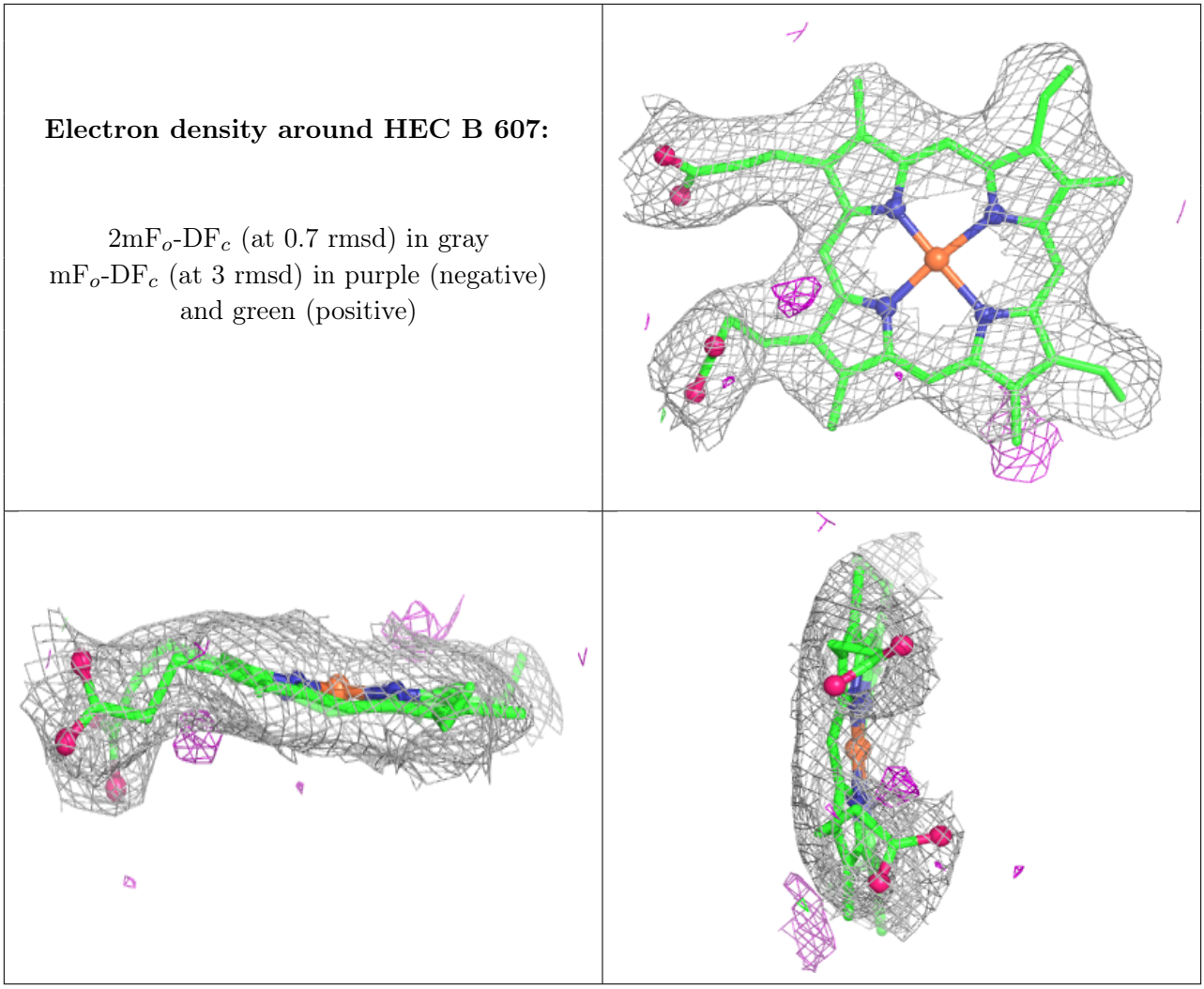






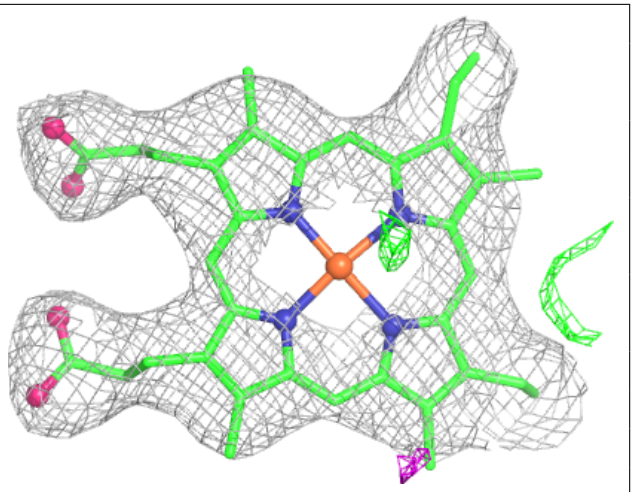
Electron density around HEC B 607:

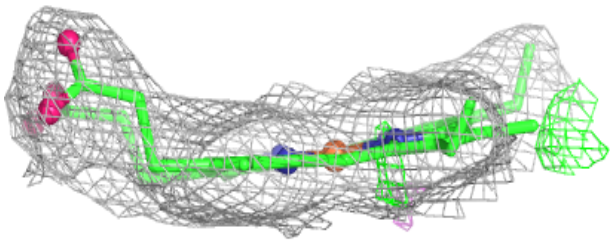
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

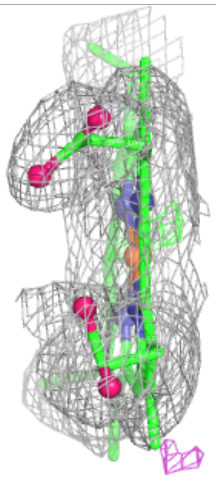


Electron density around HEC O 604:

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

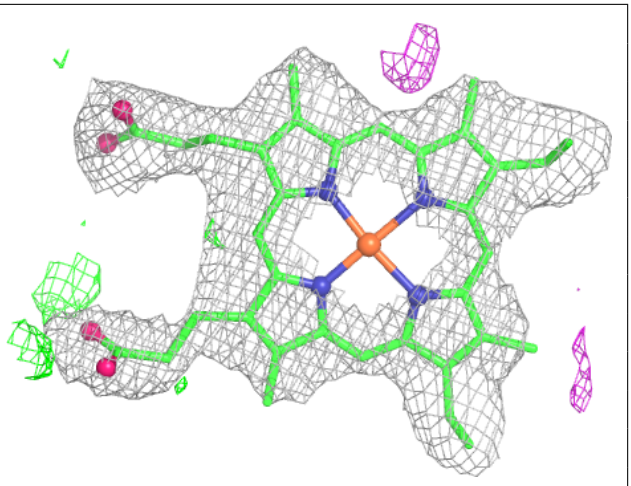


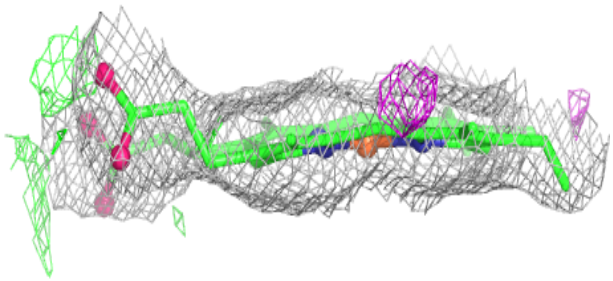




Electron density around HEC O 605:

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

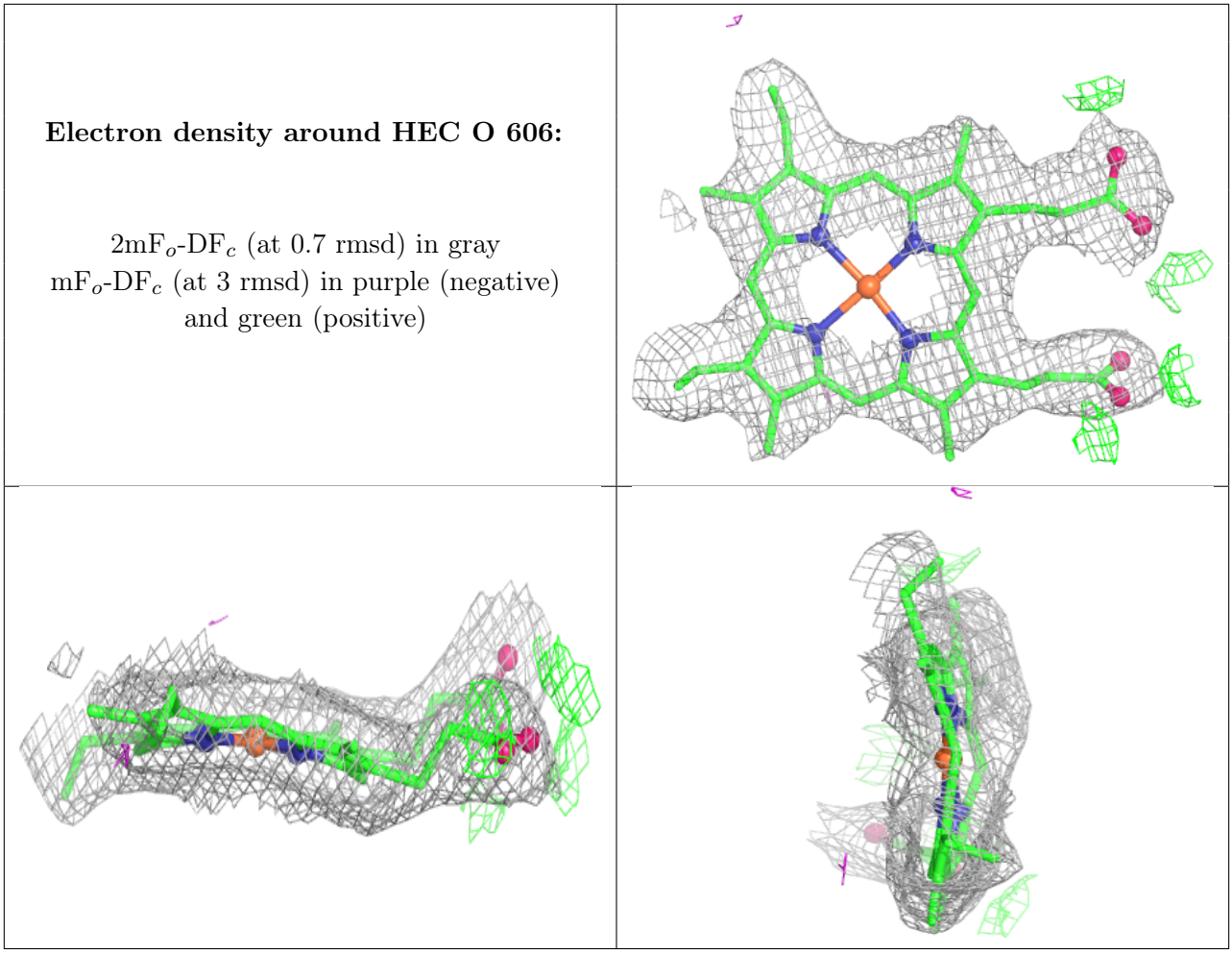






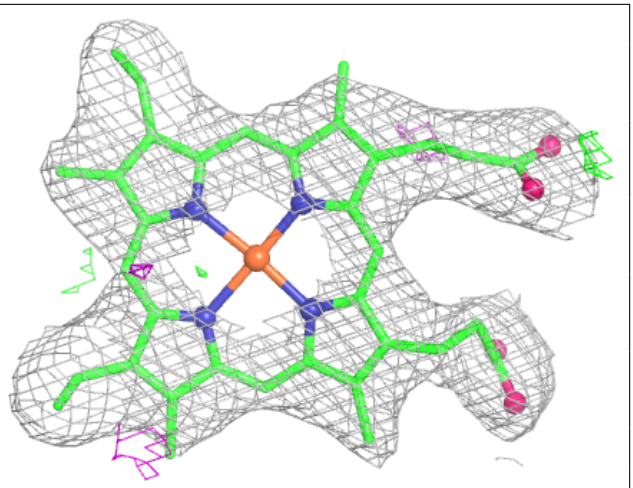
Electron density around HEC O 606:

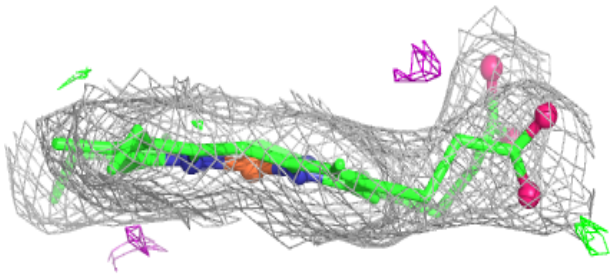
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

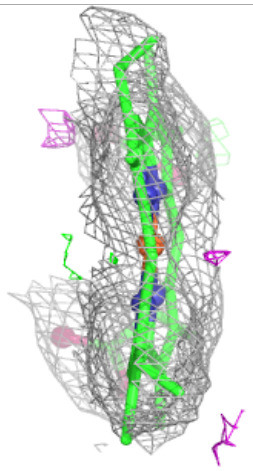


Electron density around HEC O 607:

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

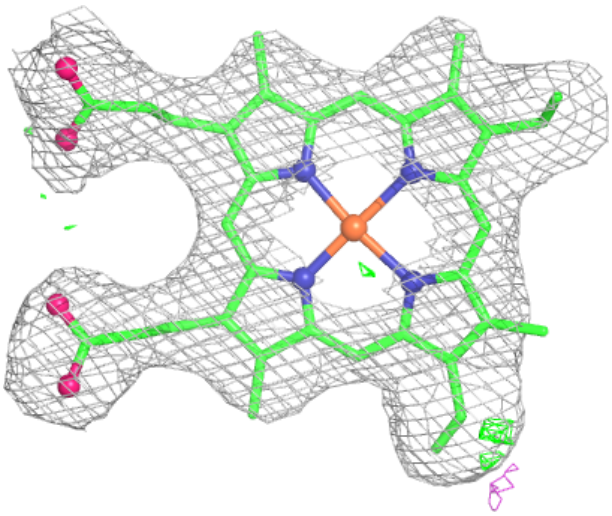


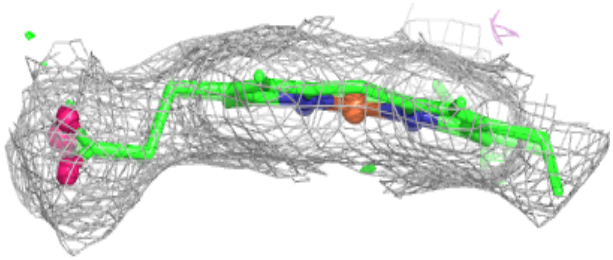


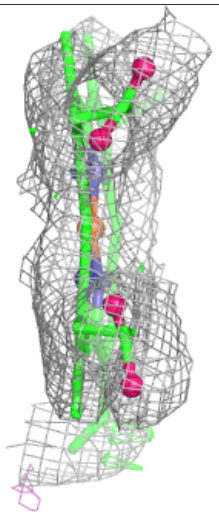


Electron density around HEC P 600:

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

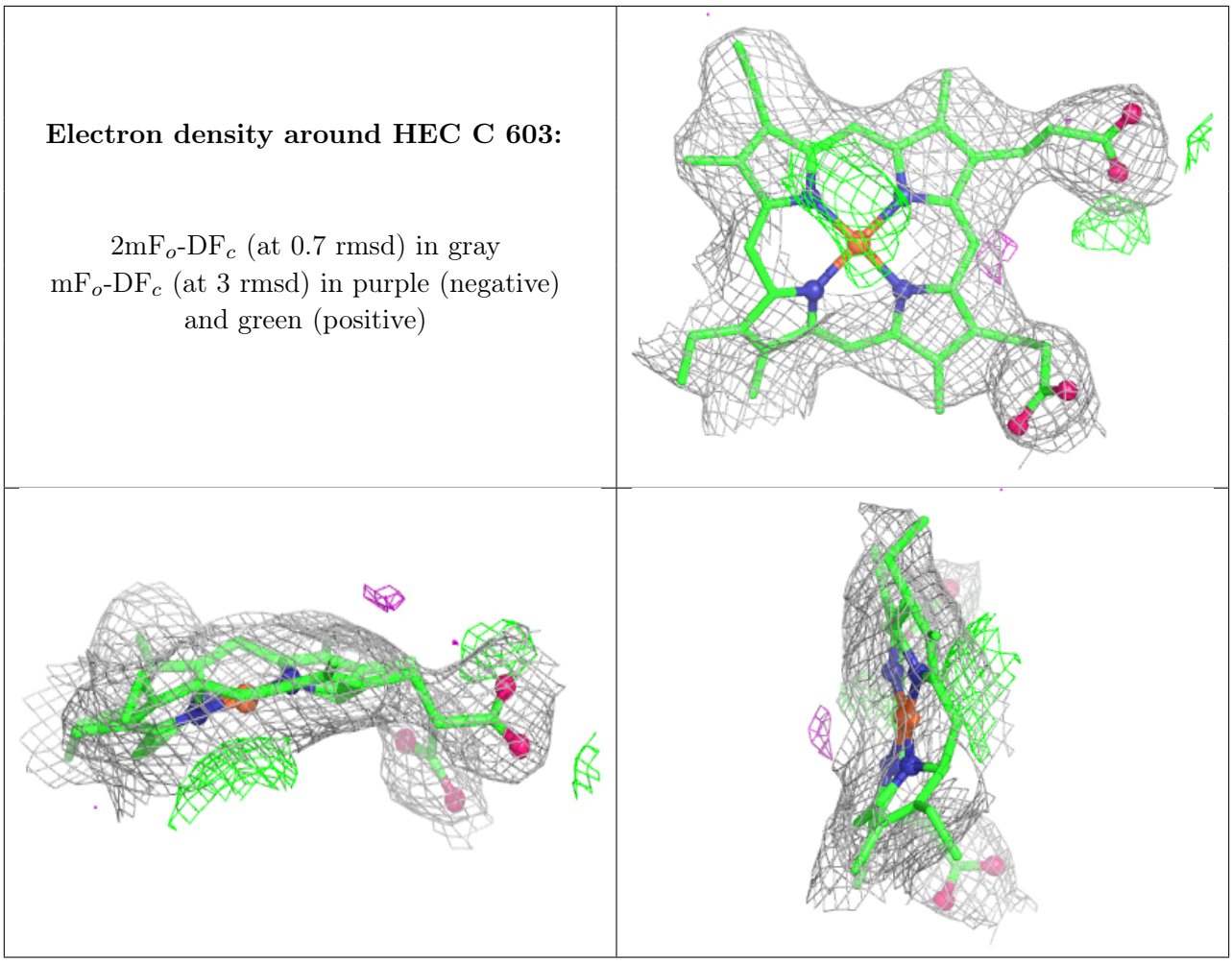






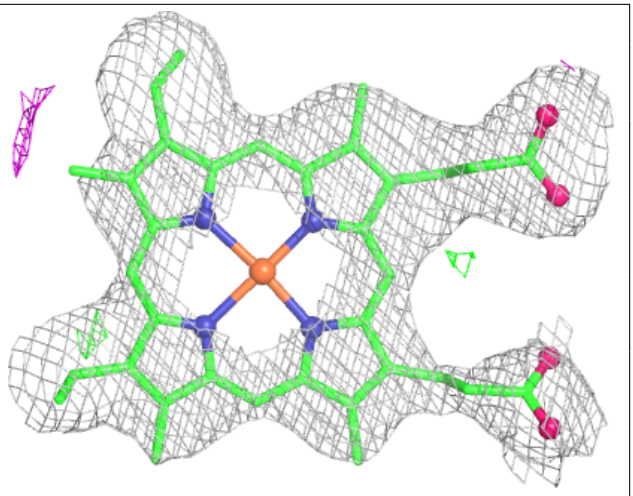
Electron density around HEC C 603:

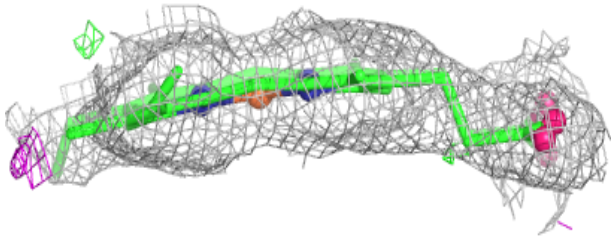
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

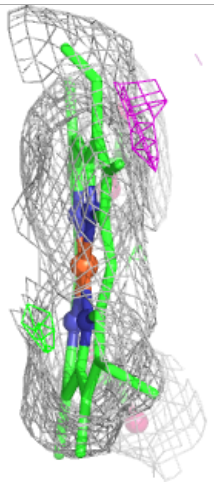


Electron density around HEC C 600:

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

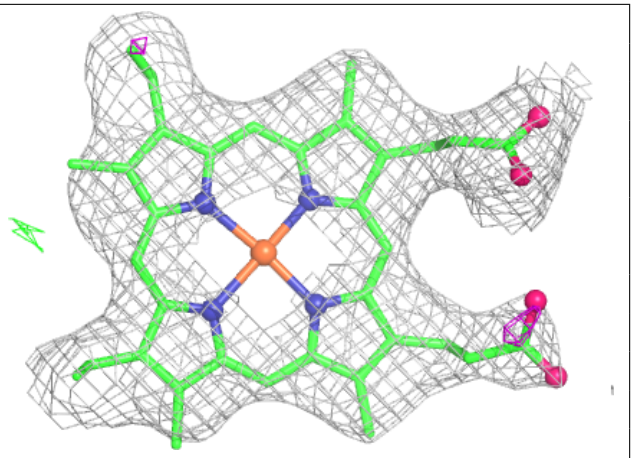


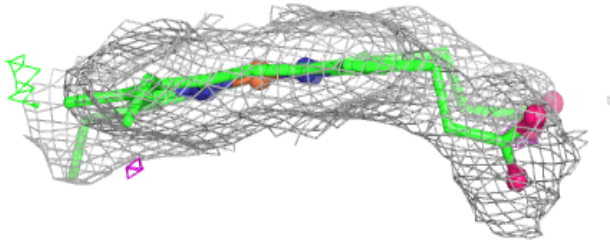


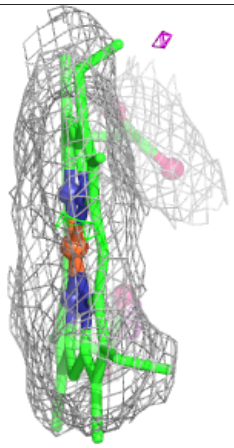


Electron density around HEC P 604:

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

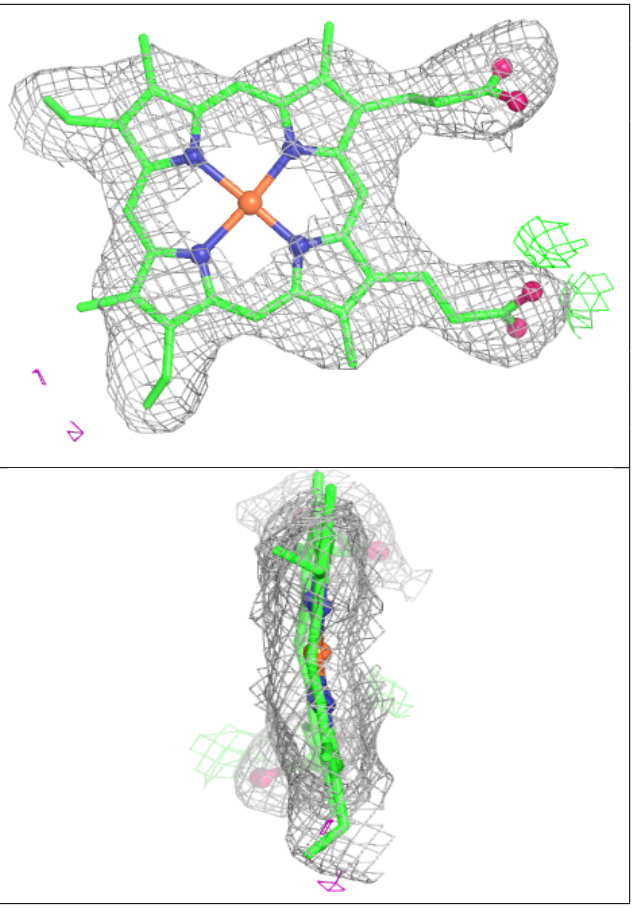


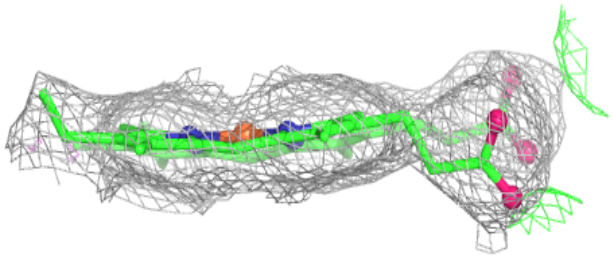




Electron density around HEC P 605:

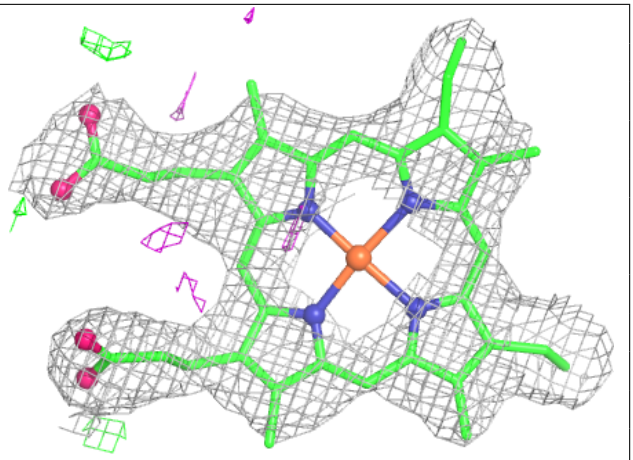
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

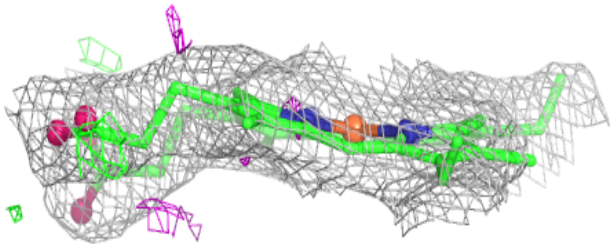


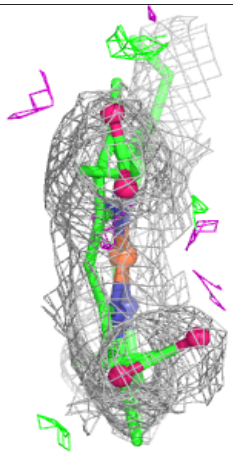


Electron density around HEC P 606:

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

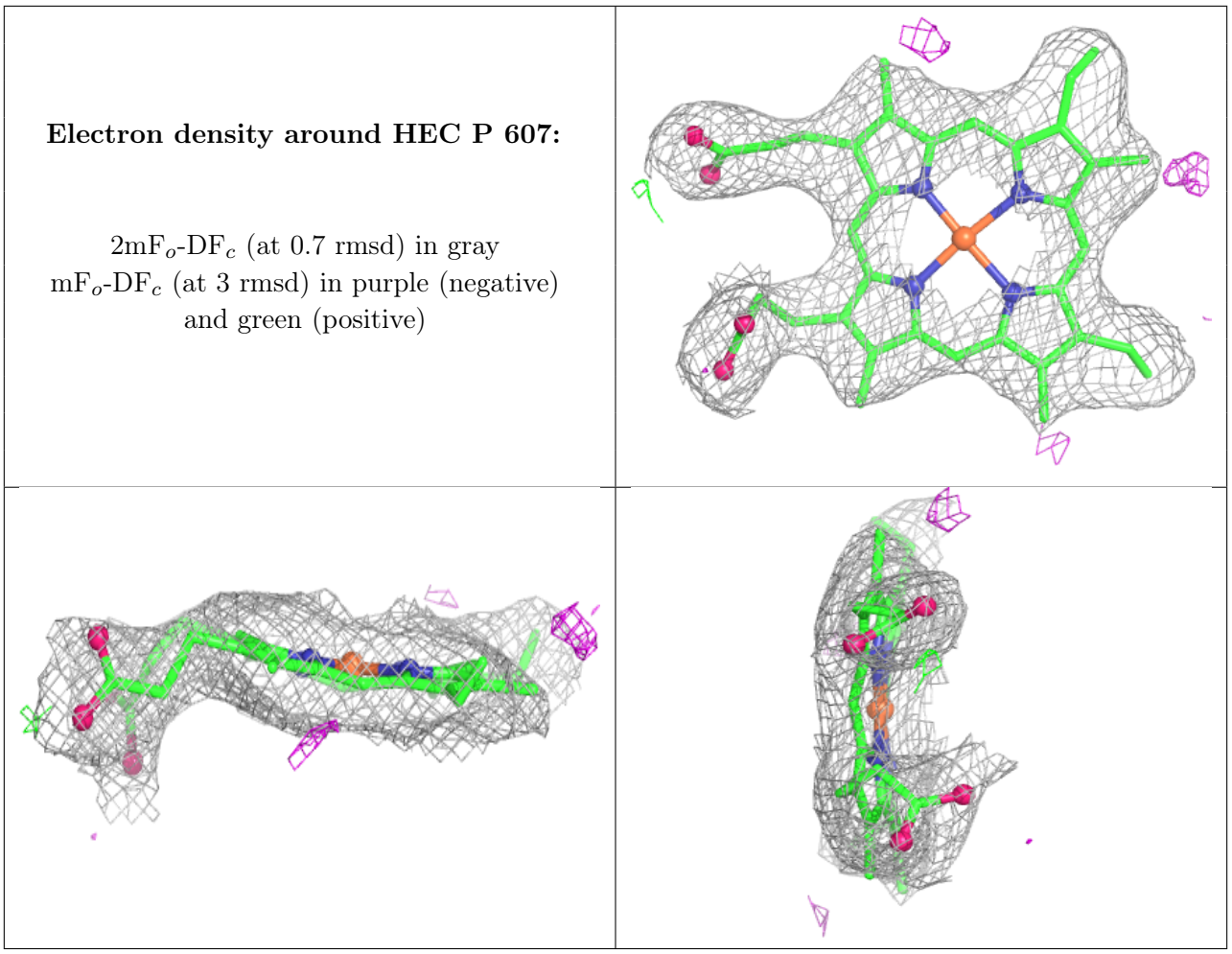






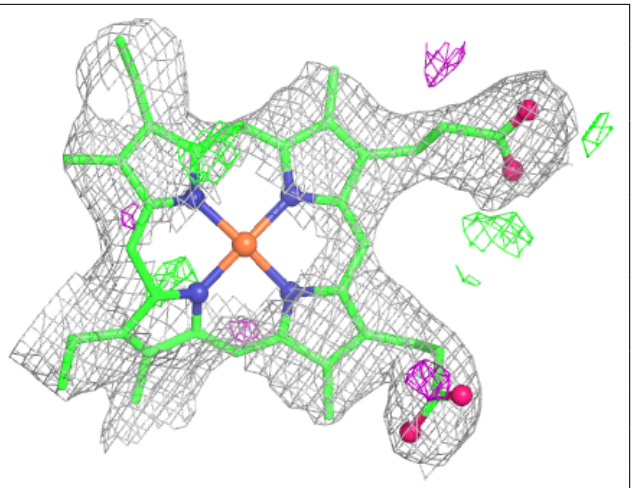
Electron density around HEC P 607:

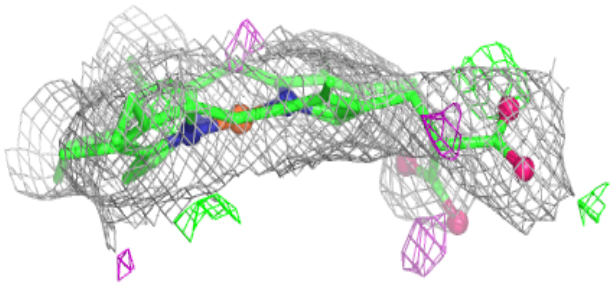
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

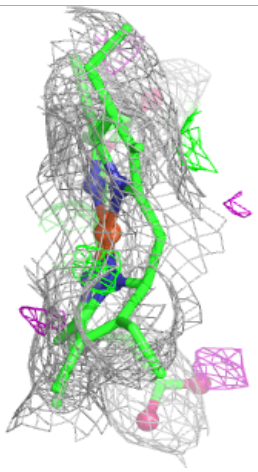


Electron density around HEC P 603:

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

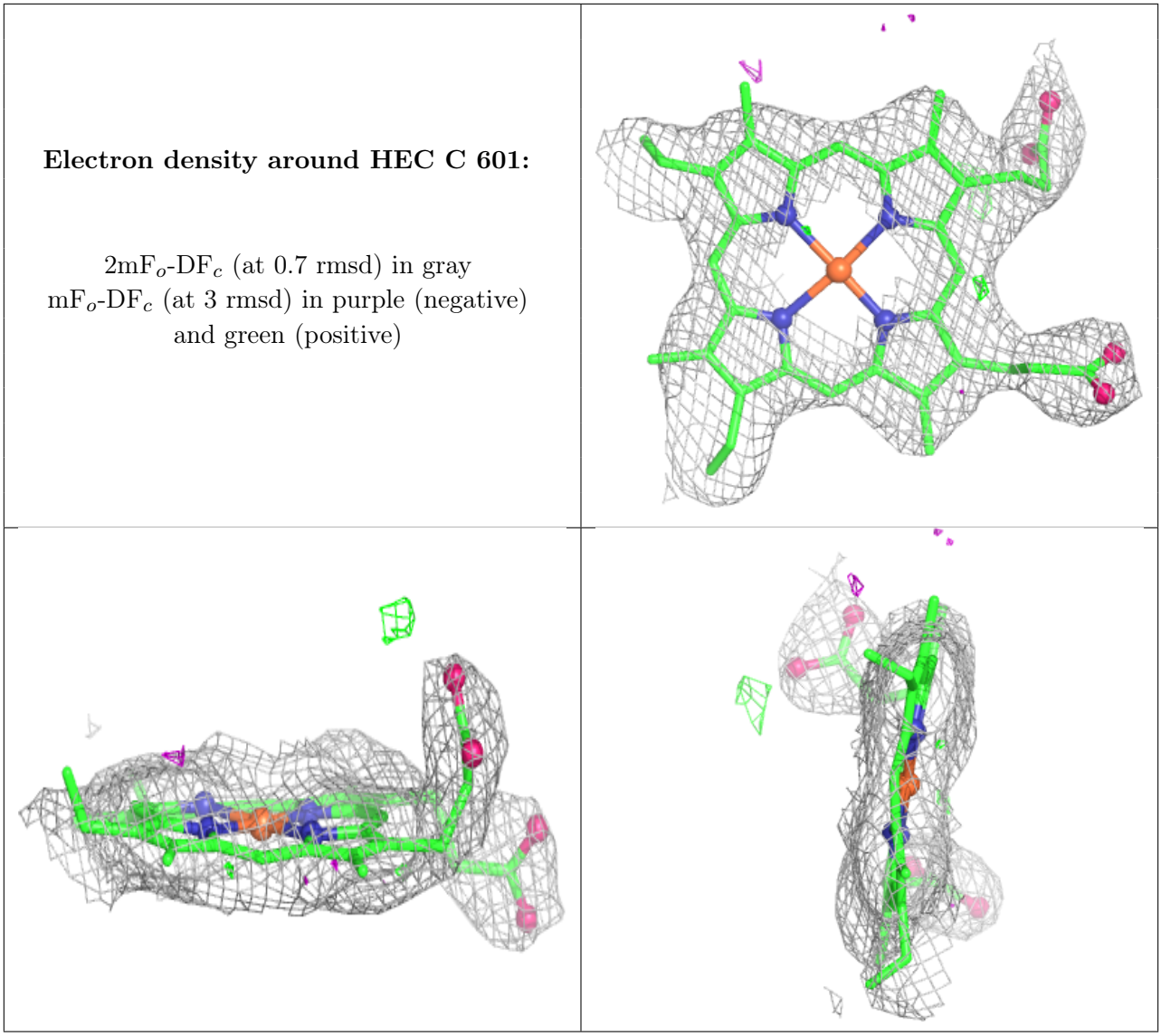






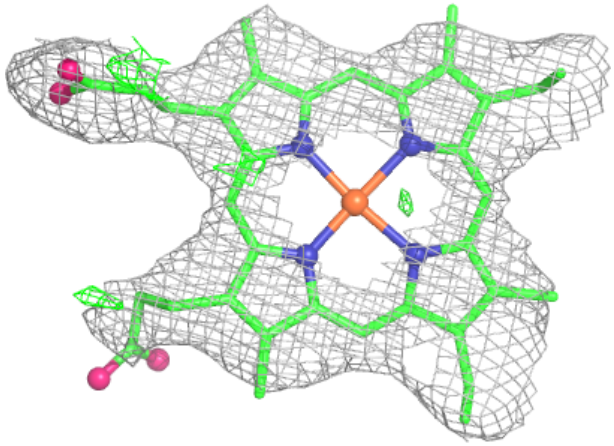
Electron density around HEC C 601:

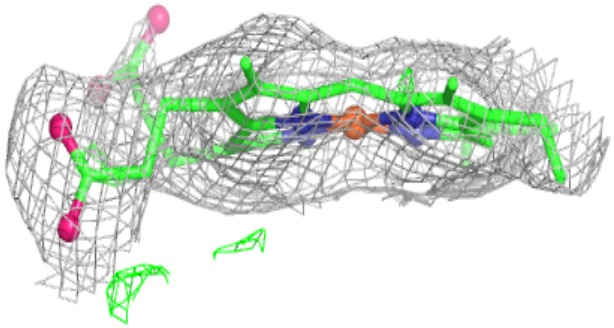
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

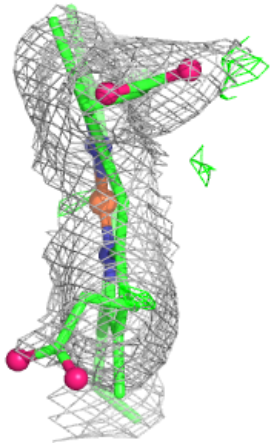


Electron density around HEC C 602:

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

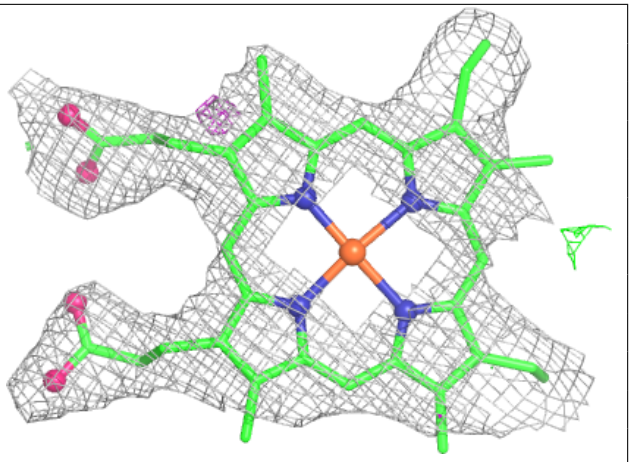


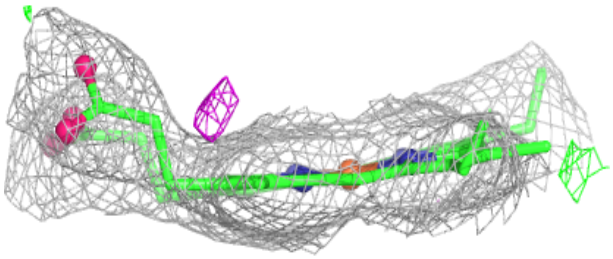


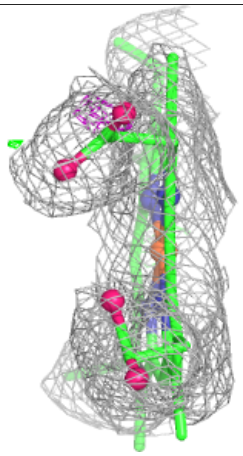


Electron density around HEC C 604:

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

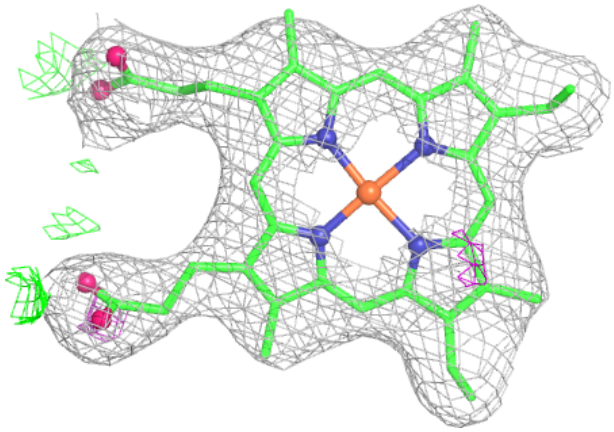


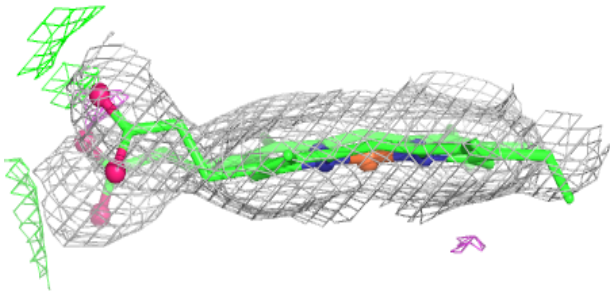


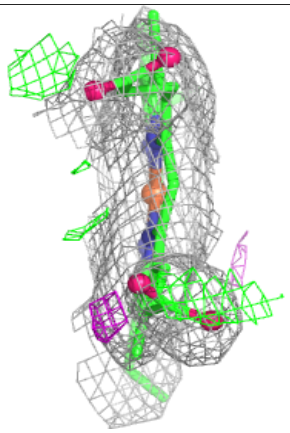


Electron density around HEC C 605:

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

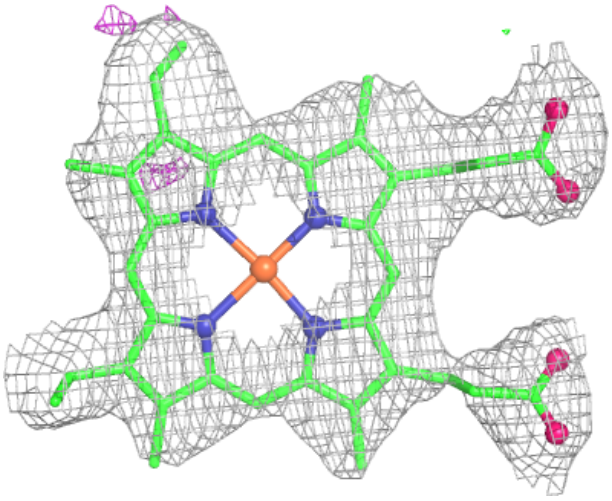


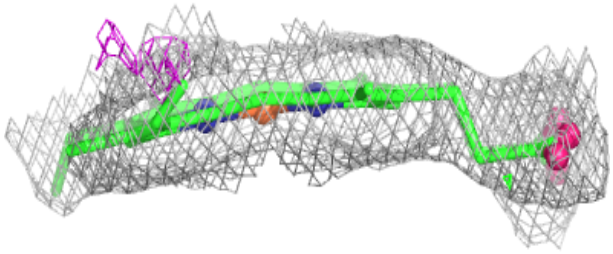


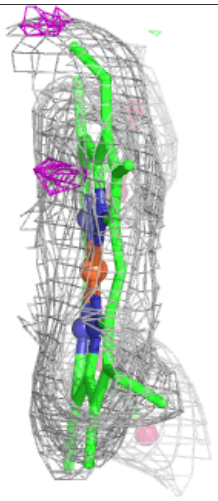


Electron density around HEC G 600:

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

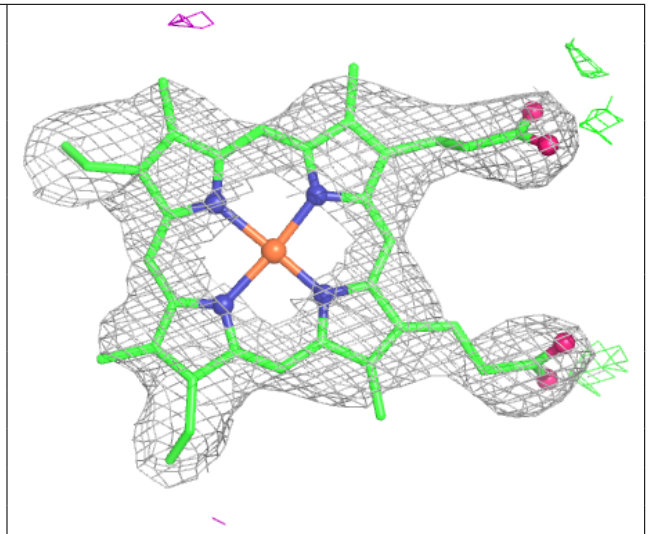


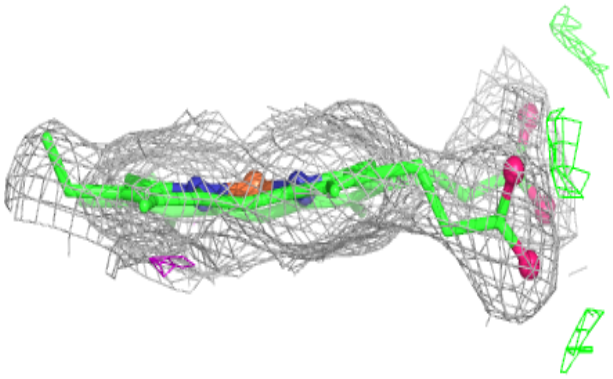


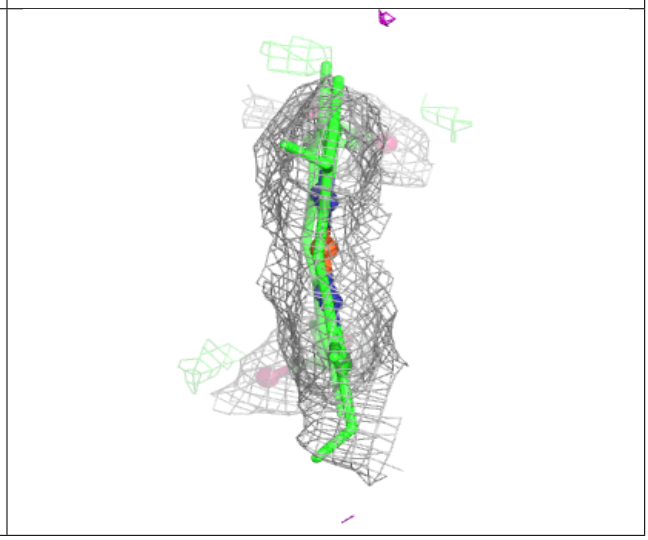


Electron density around HEC Q 605:

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

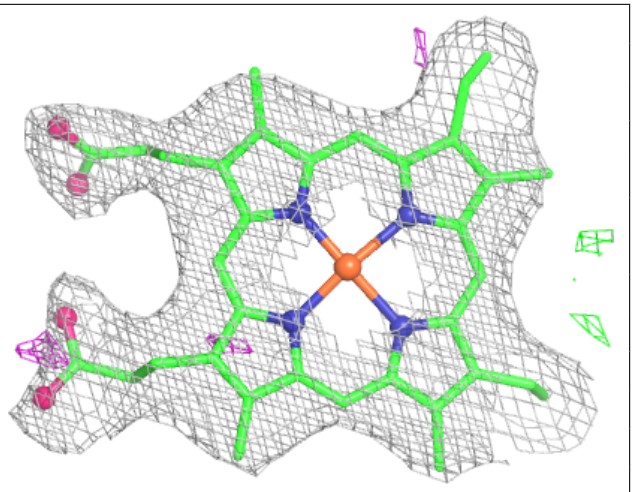


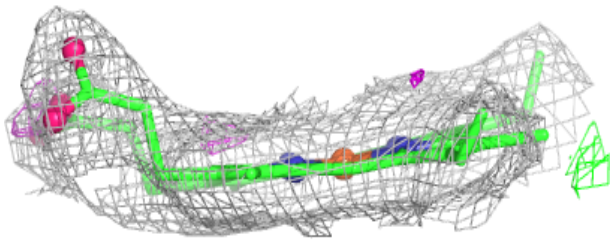


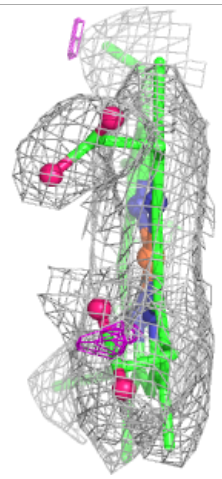


Electron density around HEC G 604:

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

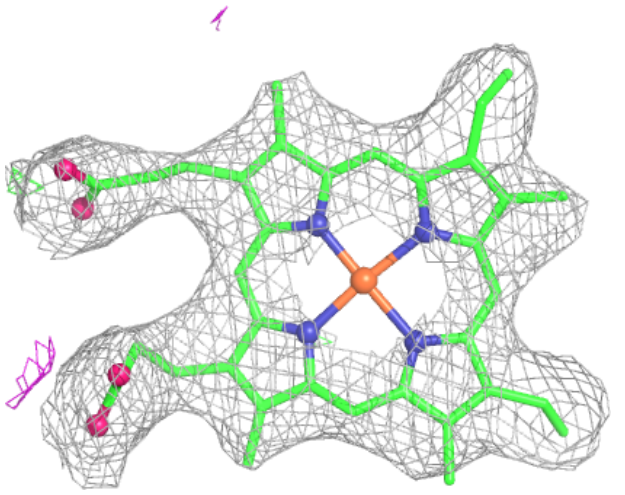


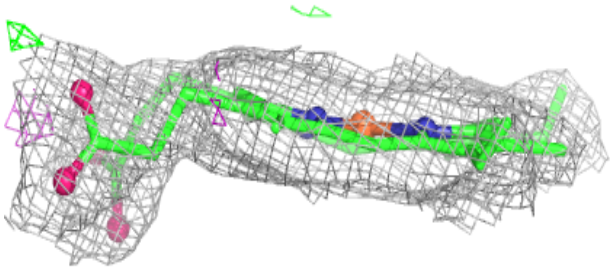


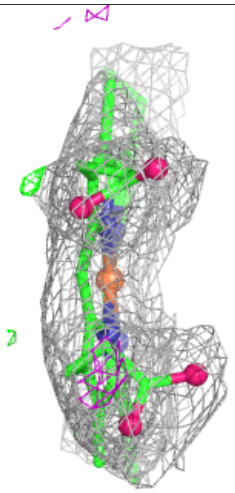


Electron density around HEC Q 607:

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

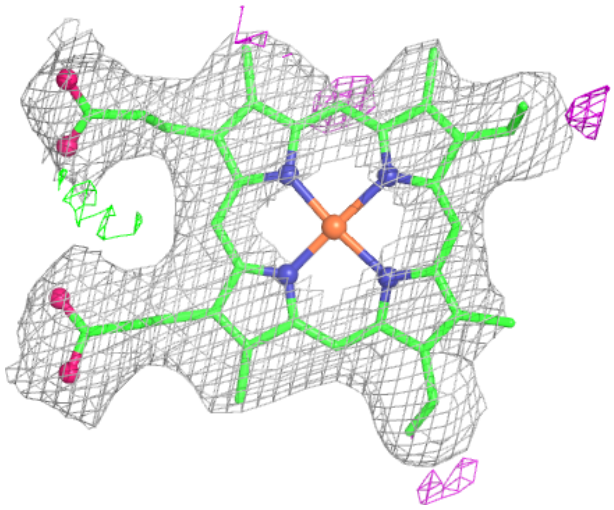


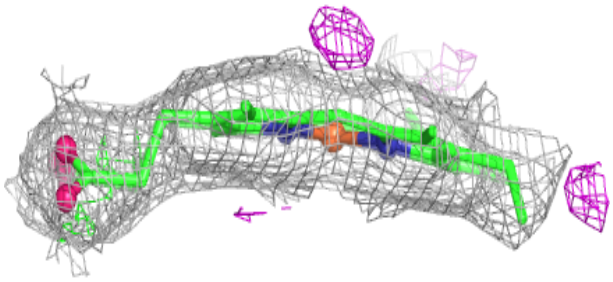


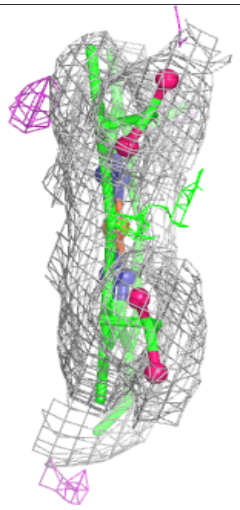


Electron density around HEC H 600:

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

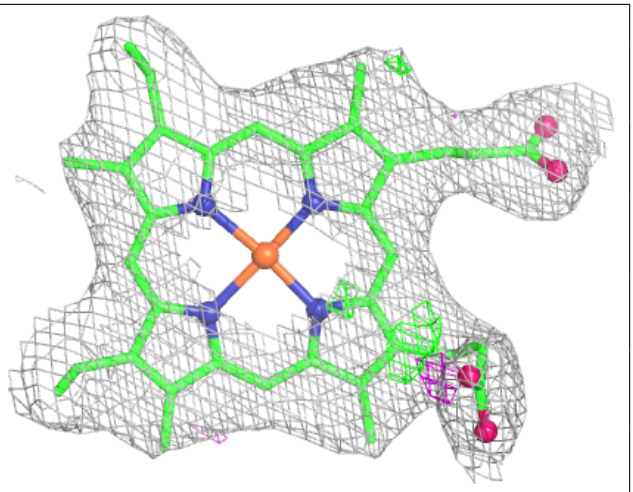


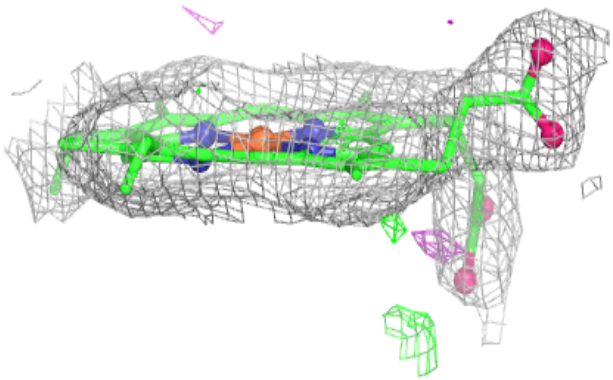


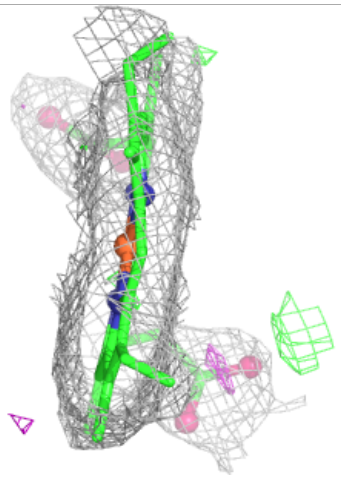


Electron density around HEC H 601:

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

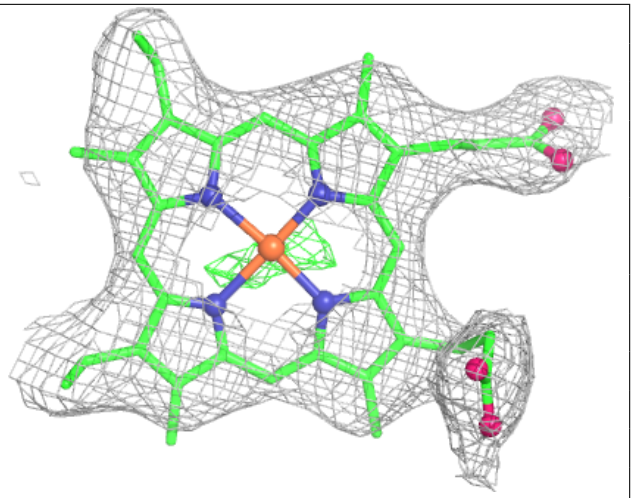


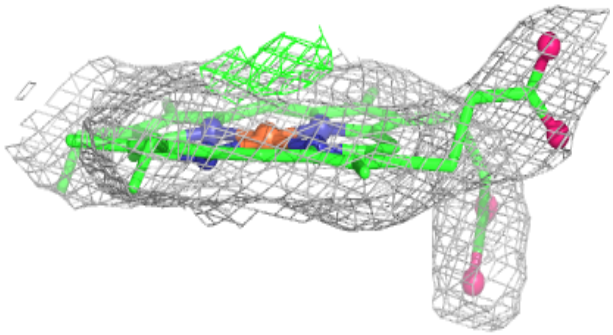


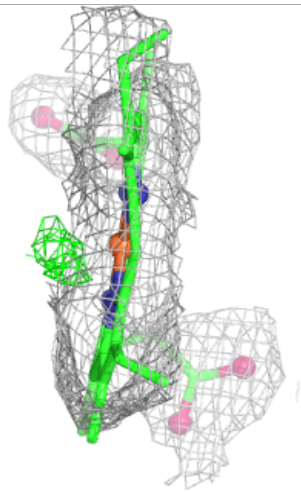


Electron density around HEC R 601:

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

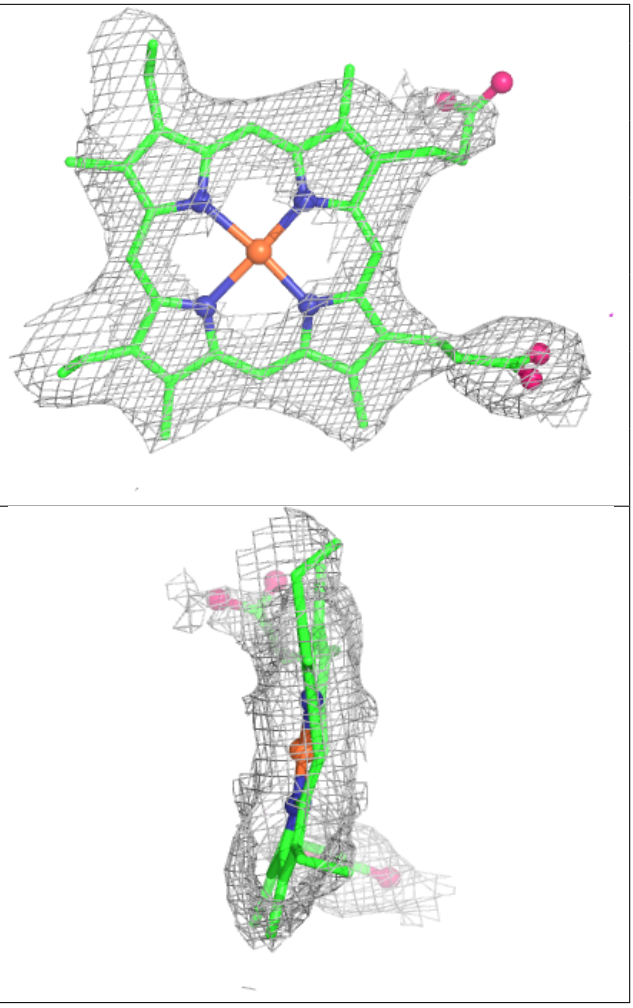






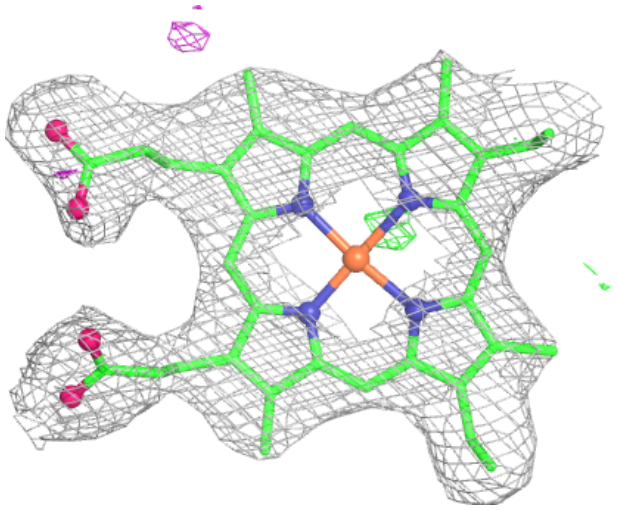
Electron density around HEC R 602:

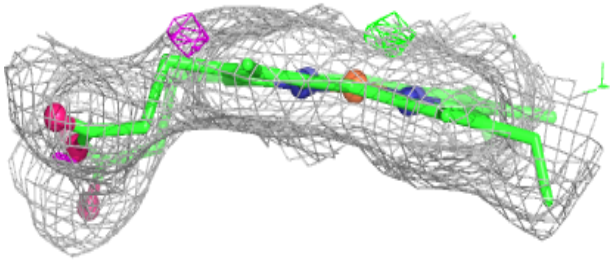
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

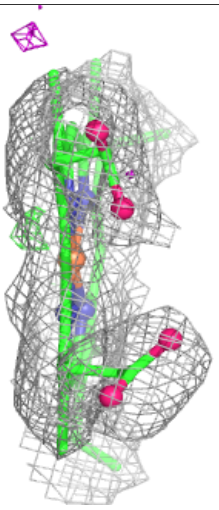


Electron density around HEC R 604:

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

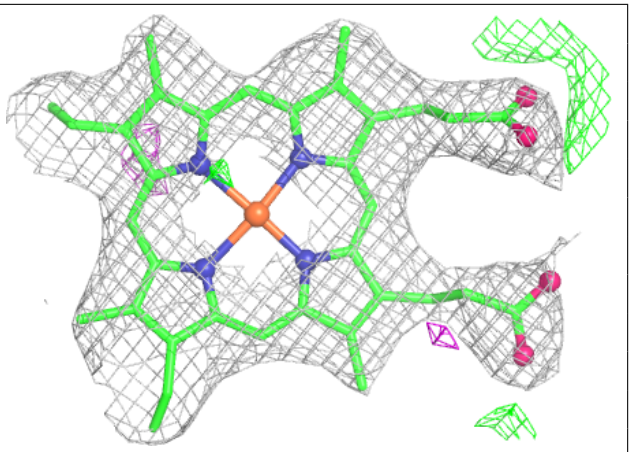


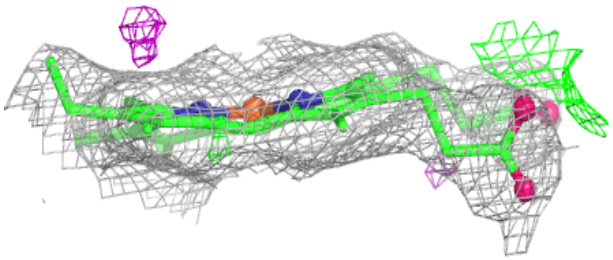


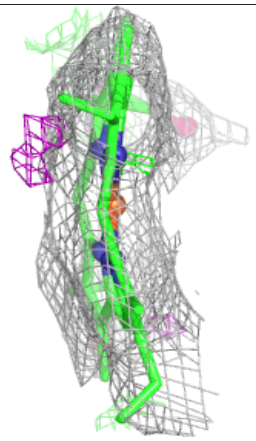


Electron density around HEC R 606:

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

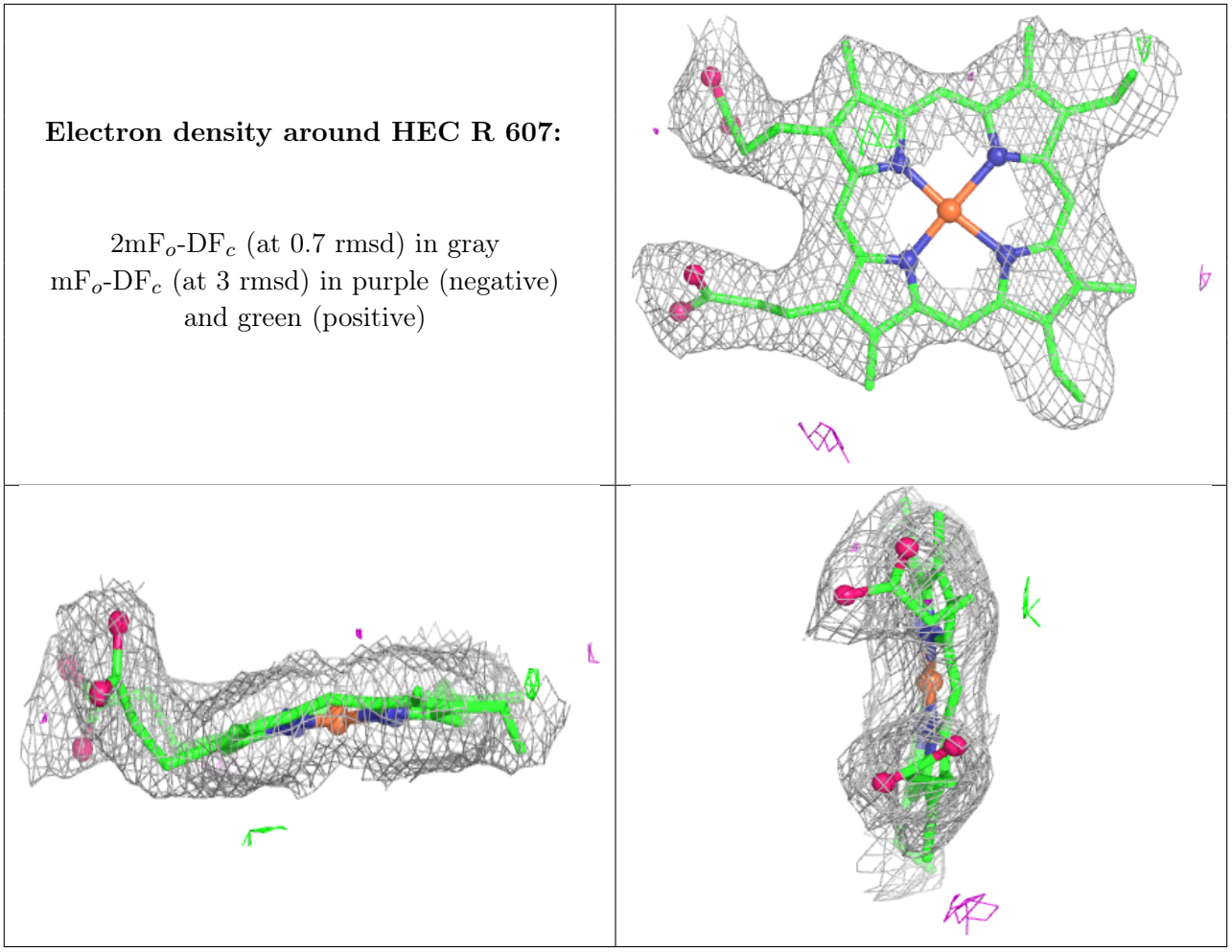






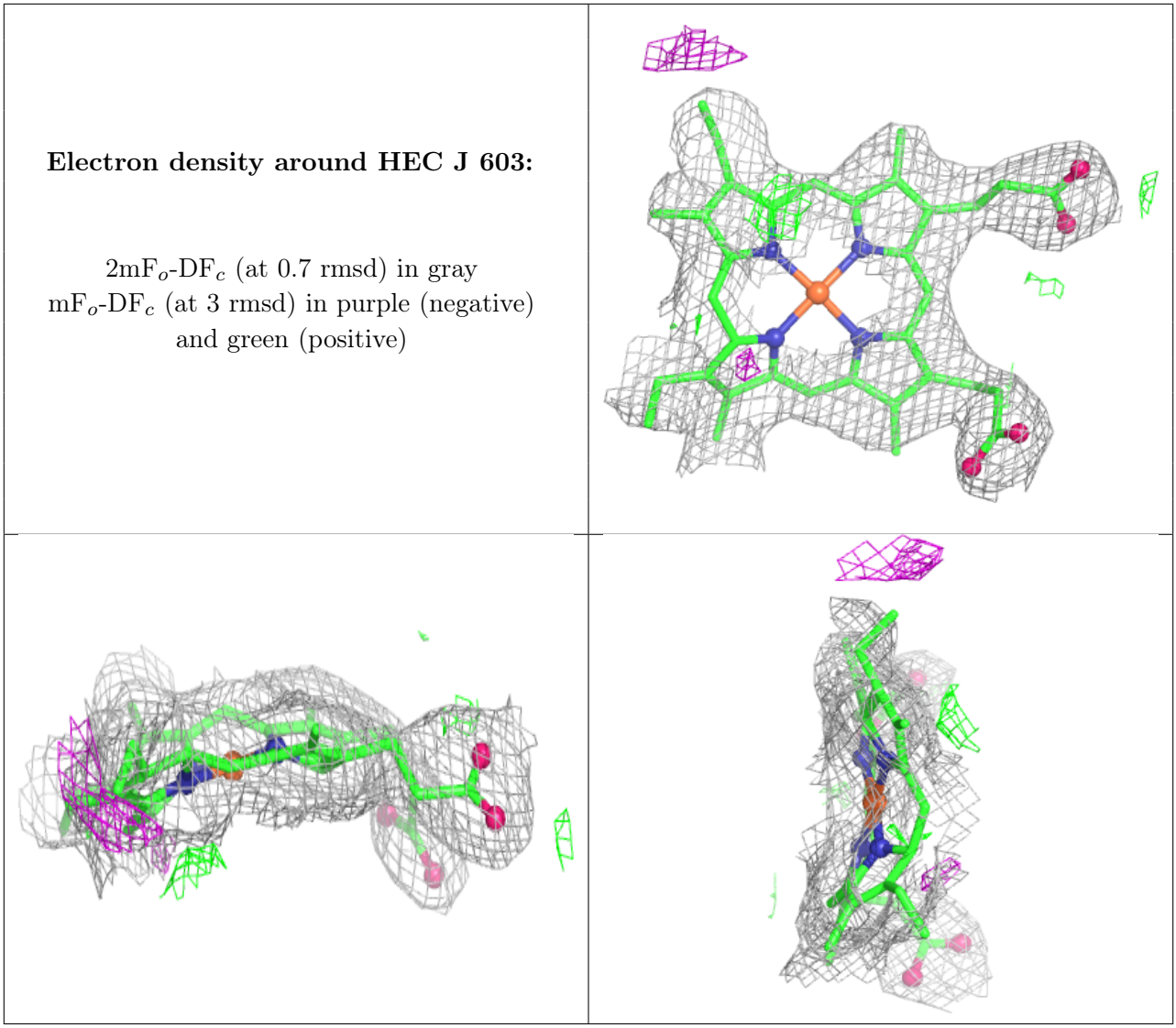
Electron density around HEC R 607:

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



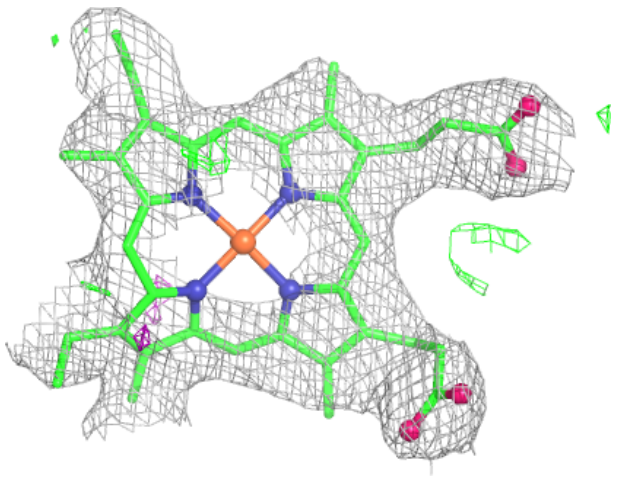
Electron density around HEC J 603:

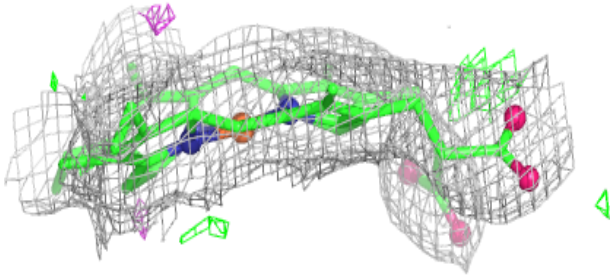
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

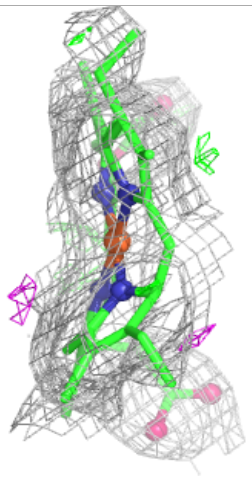


Electron density around HEC K 603:

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

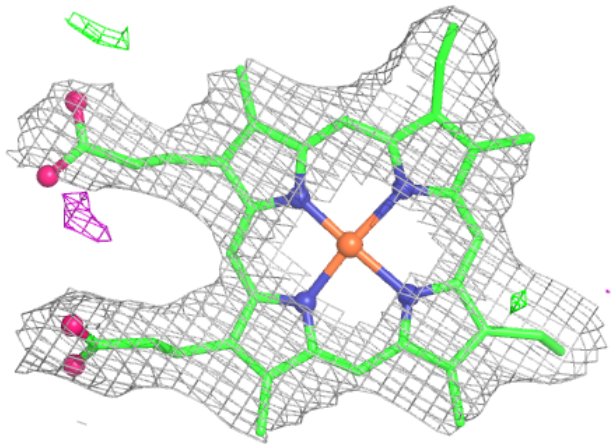


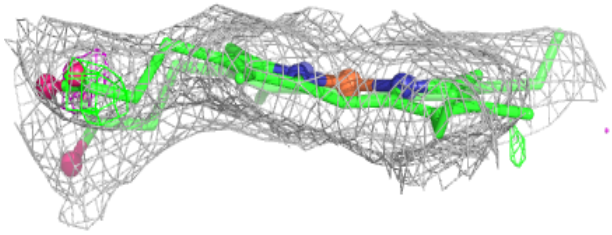


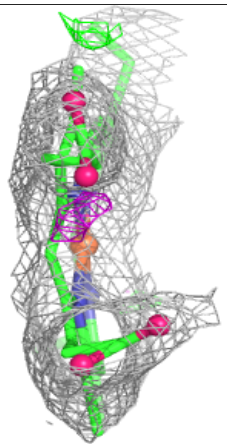


Electron density around HEC B 606:

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

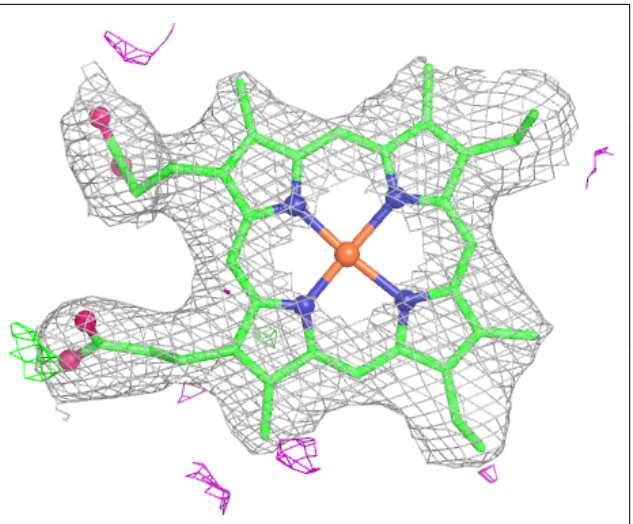


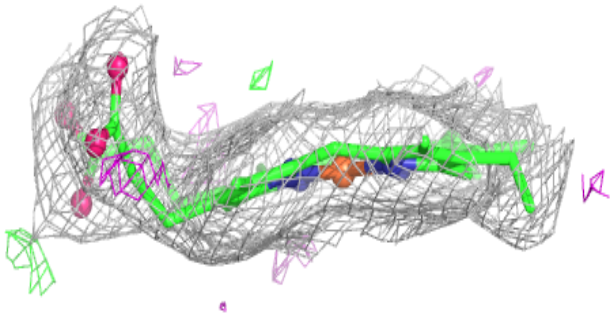




Electron density around HEC H 607:

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

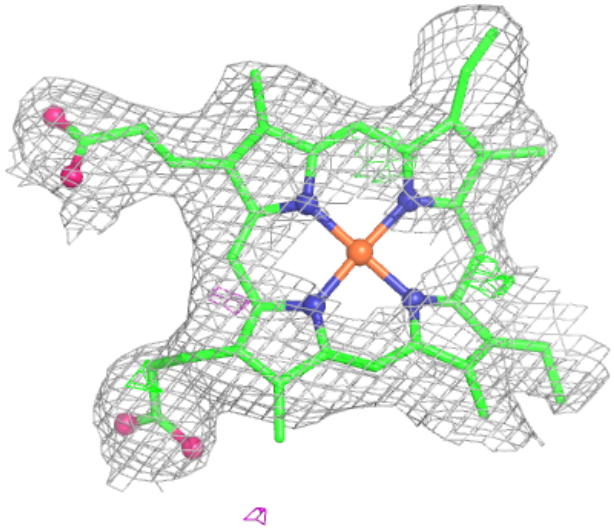


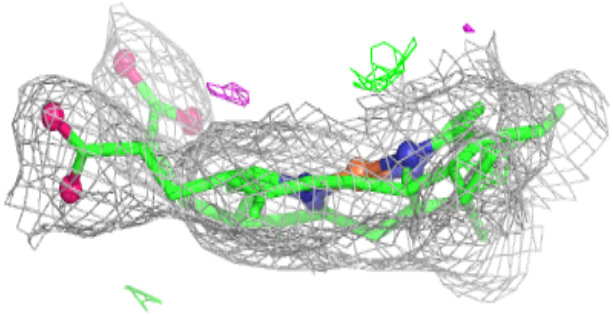


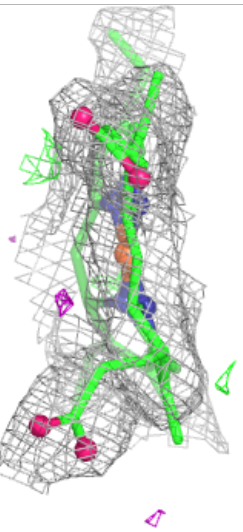


Electron density around HEC I 603:

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

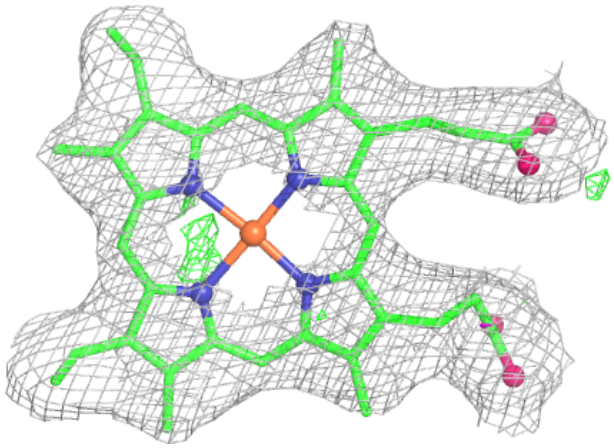


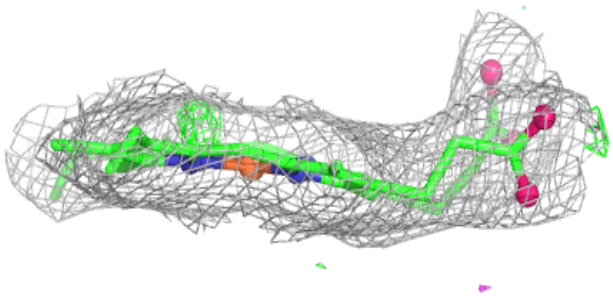


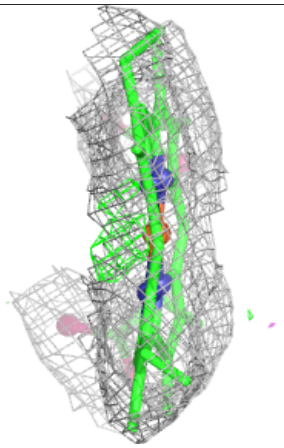


Electron density around HEC G 607:

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

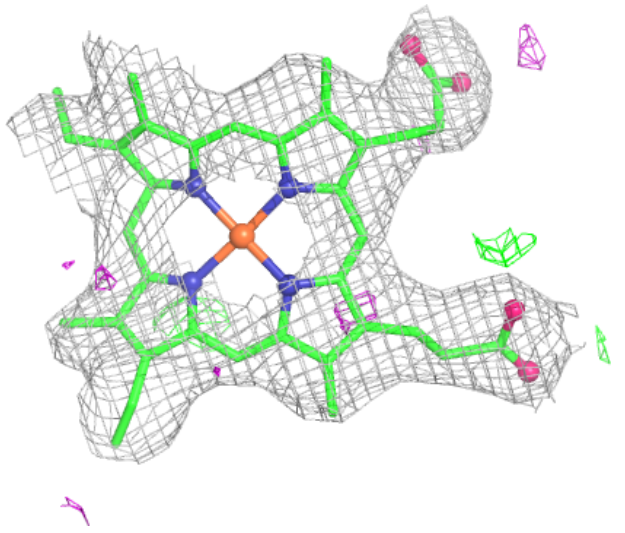


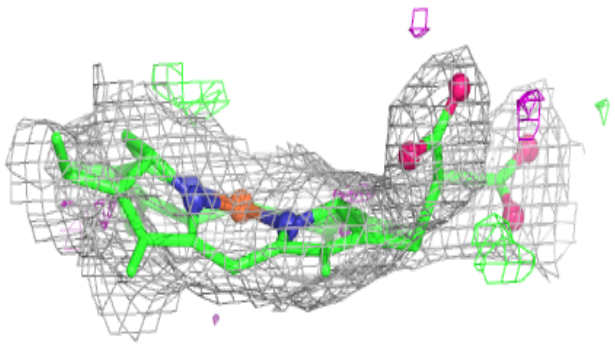


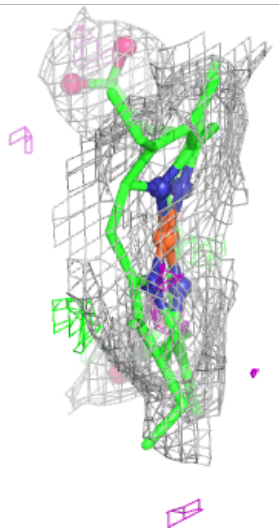


Electron density around HEC G 603:

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

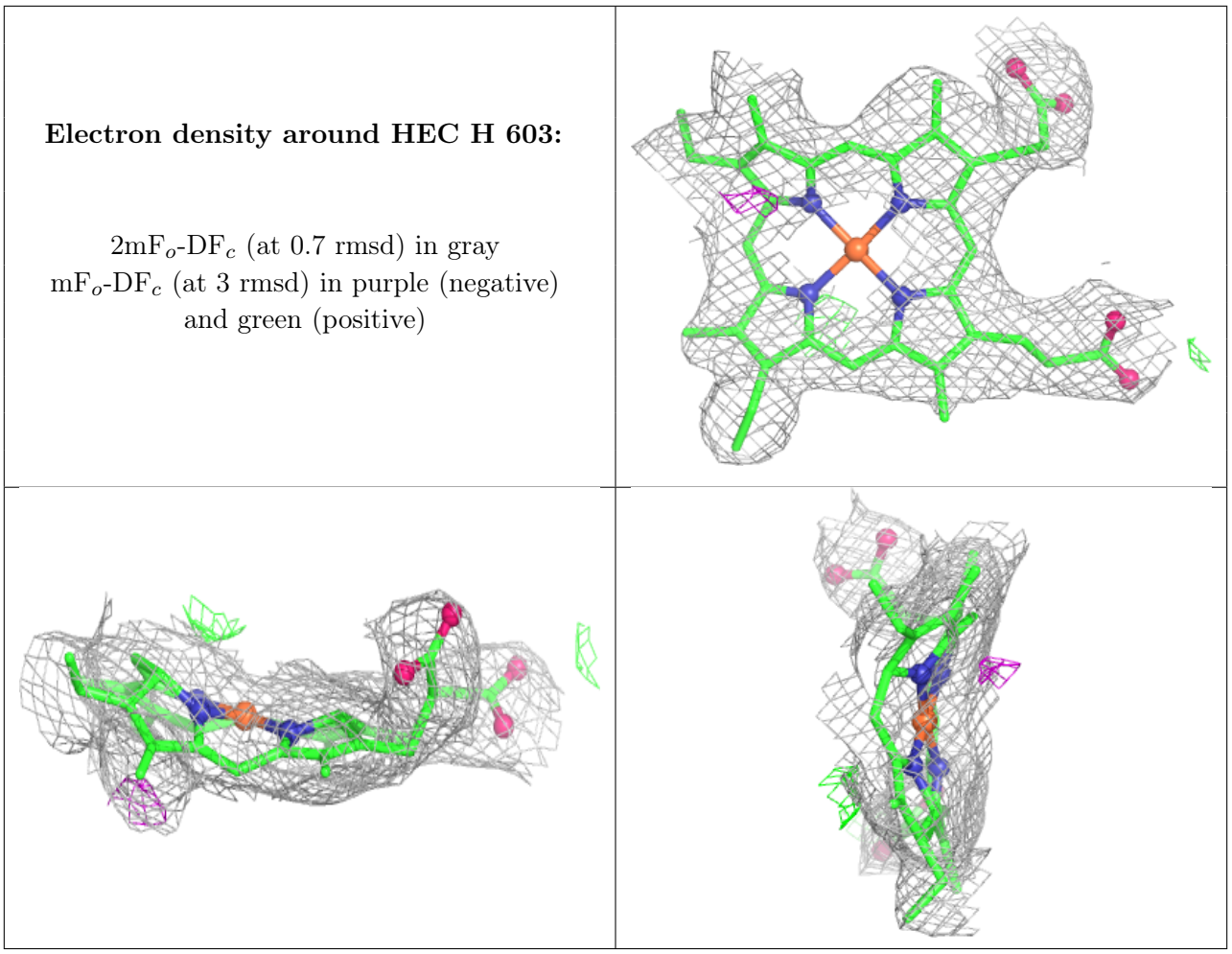






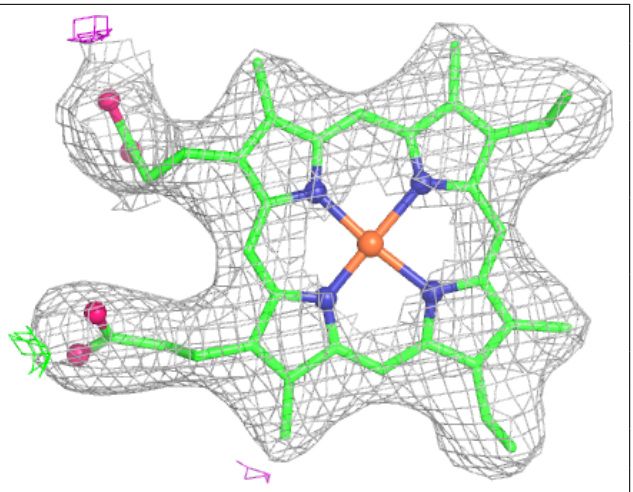
Electron density around HEC H 603:

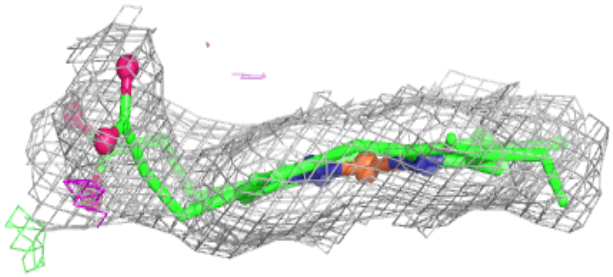
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

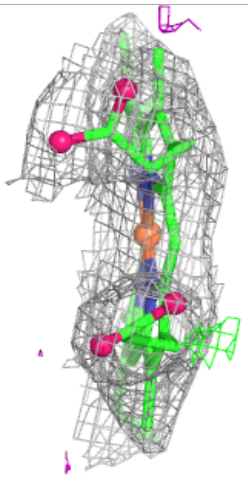


Electron density around HEC K 607:

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

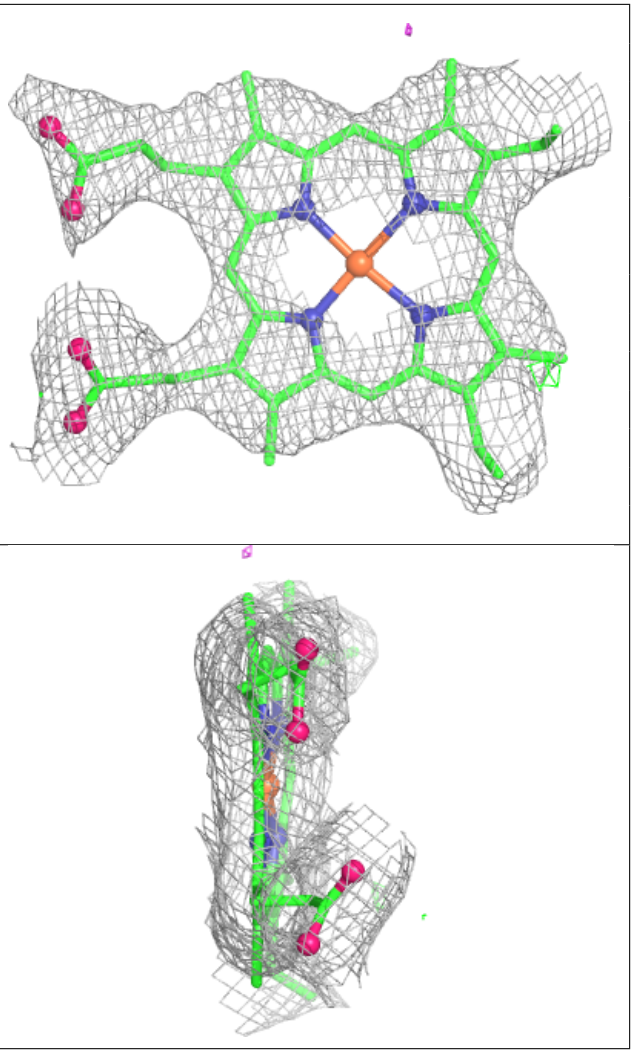






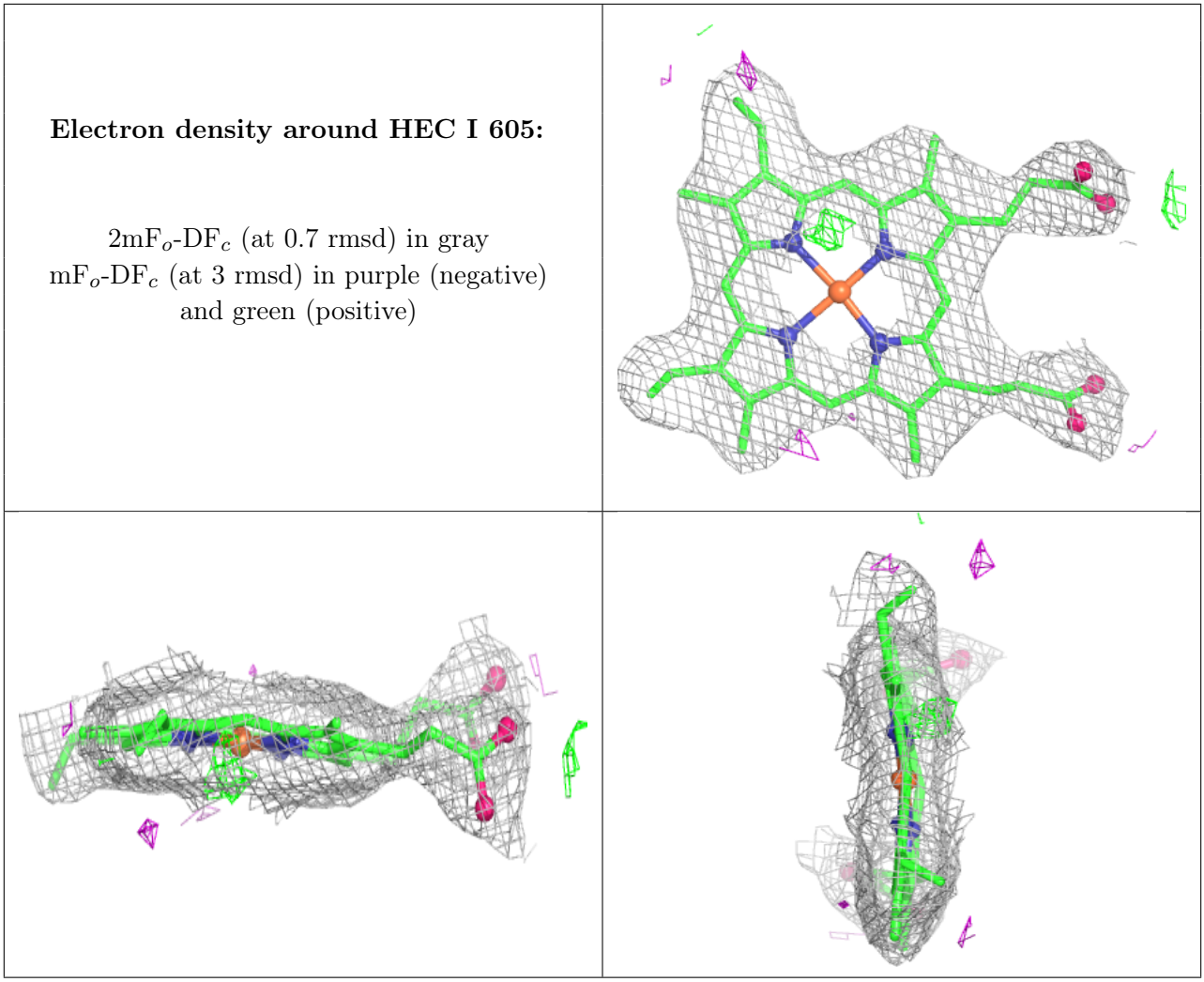
Electron density around HEC I 604:

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



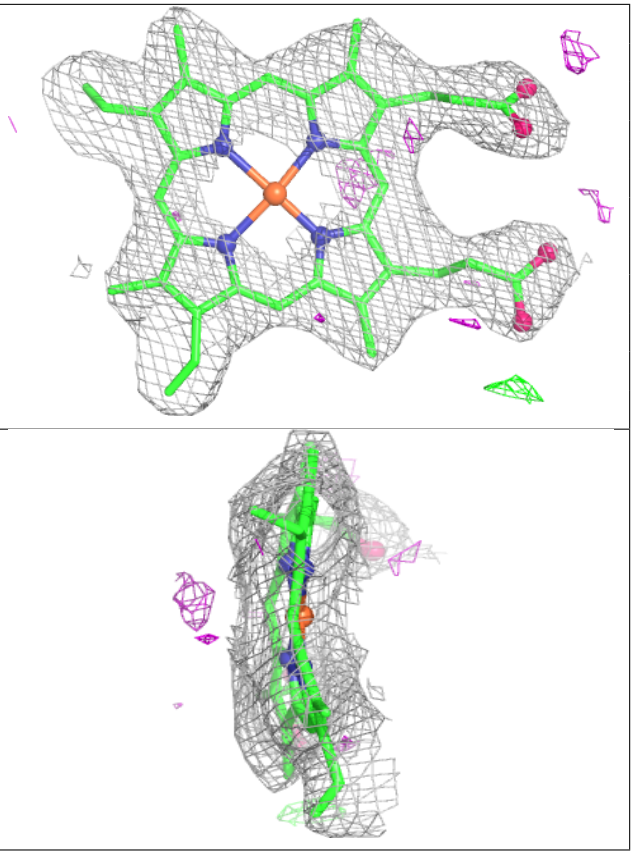
Electron density around HEC I 605:

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



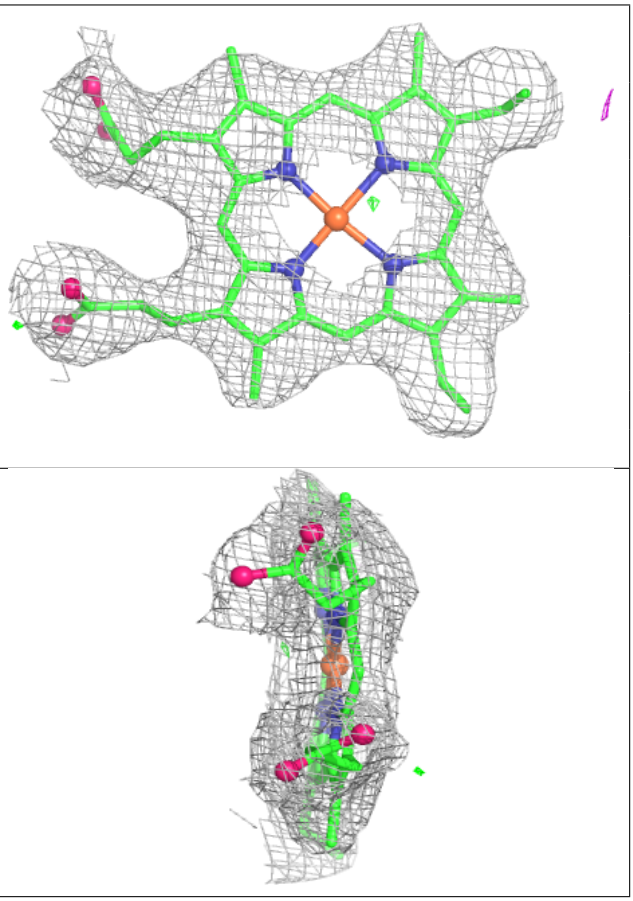
Electron density around HEC I 606:

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



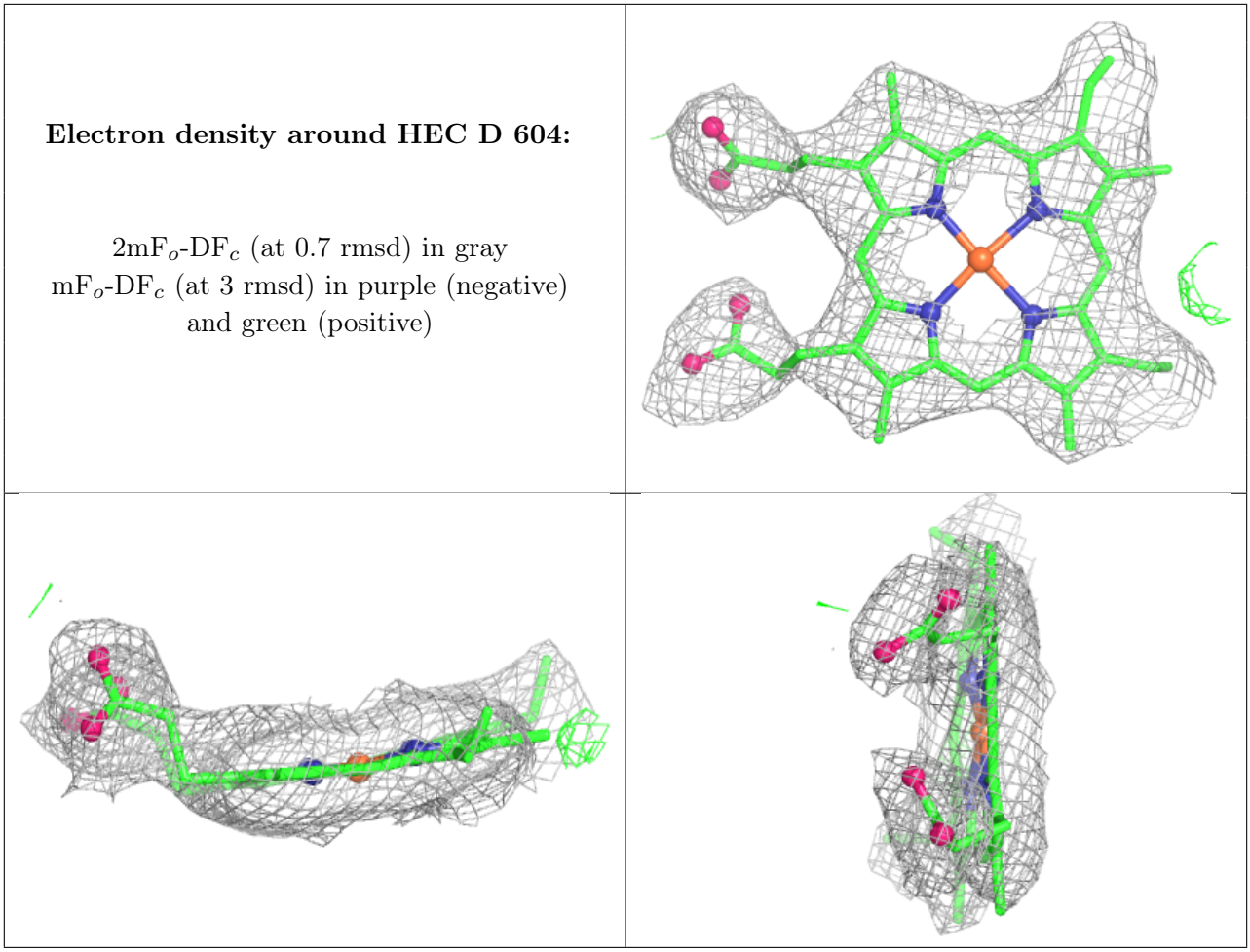
Electron density around HEC I 607:

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



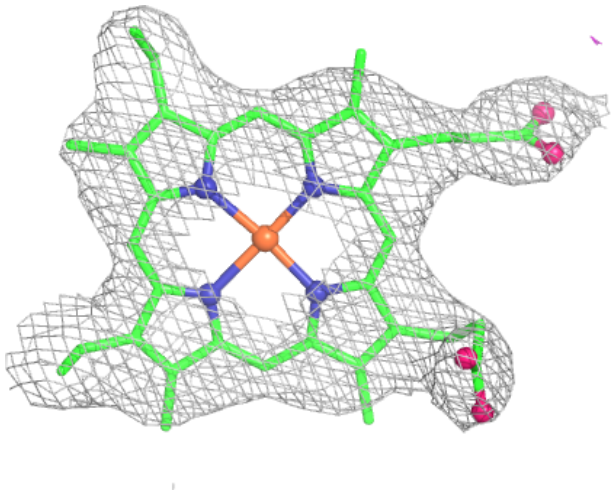
Electron density around HEC D 604:

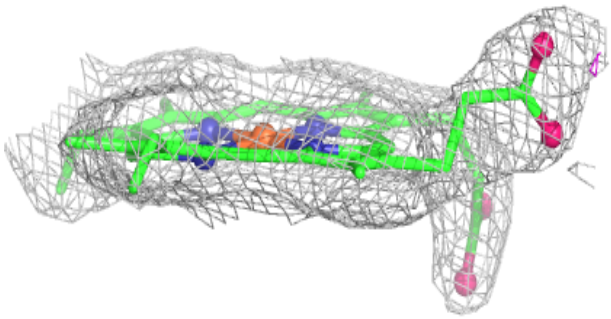
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC O 601:

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

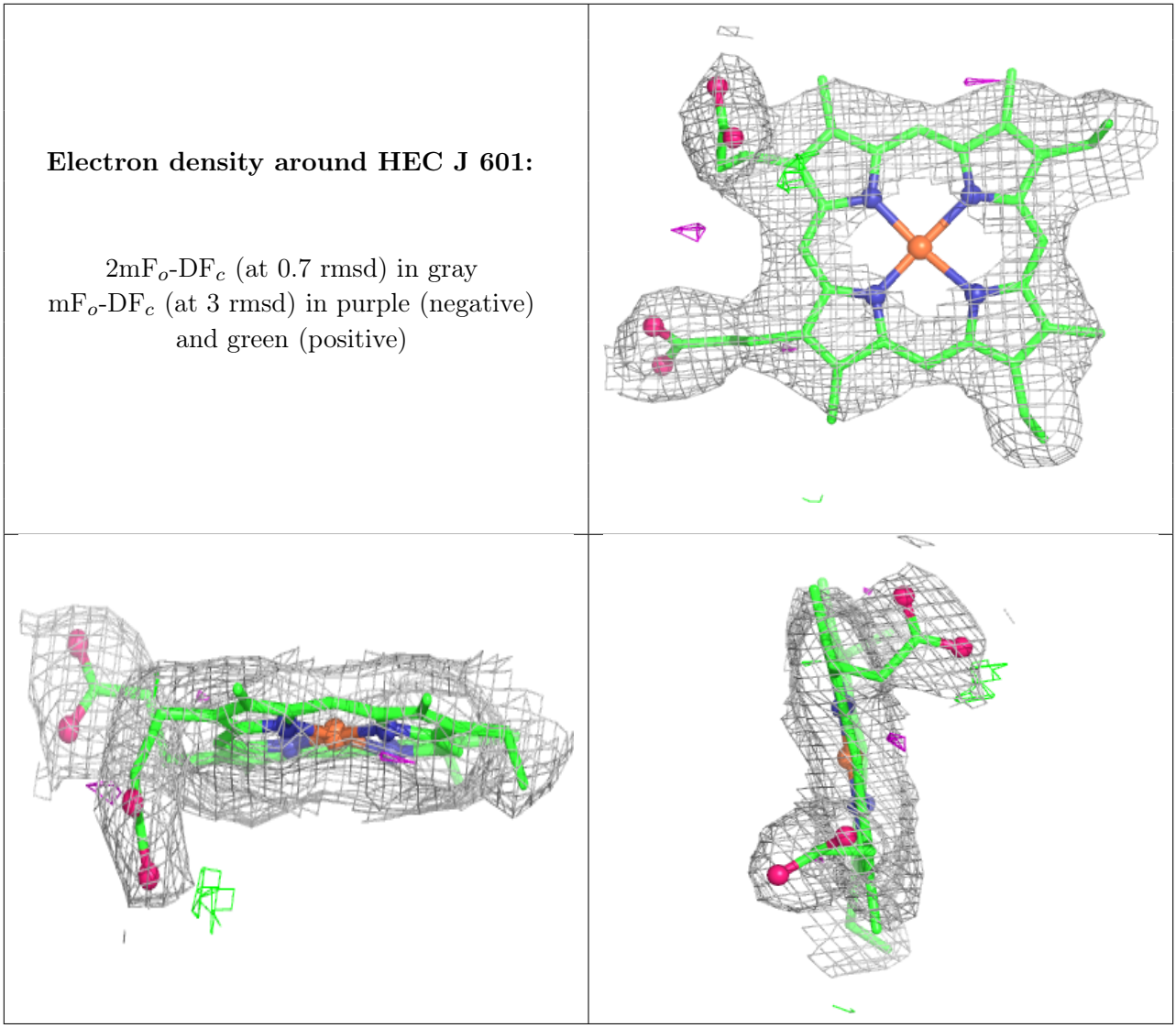






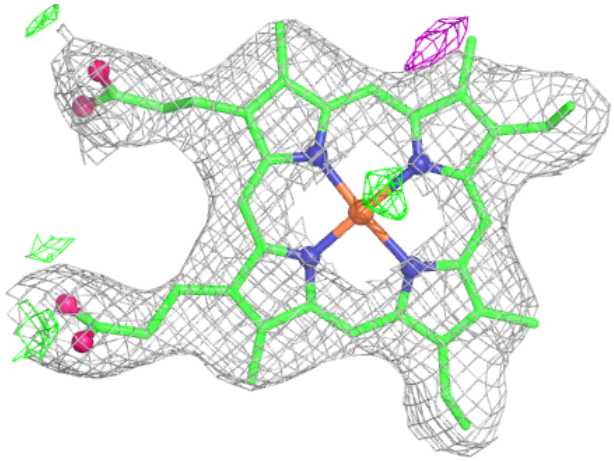
Electron density around HEC J 601:

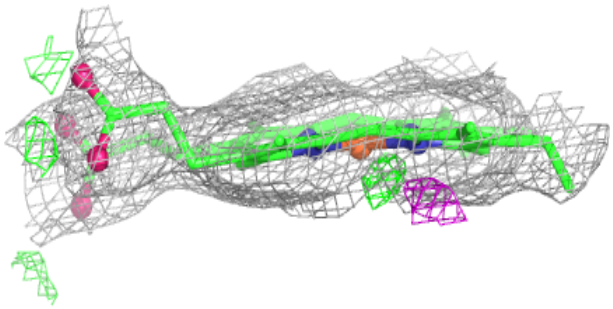
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEC G 605:

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

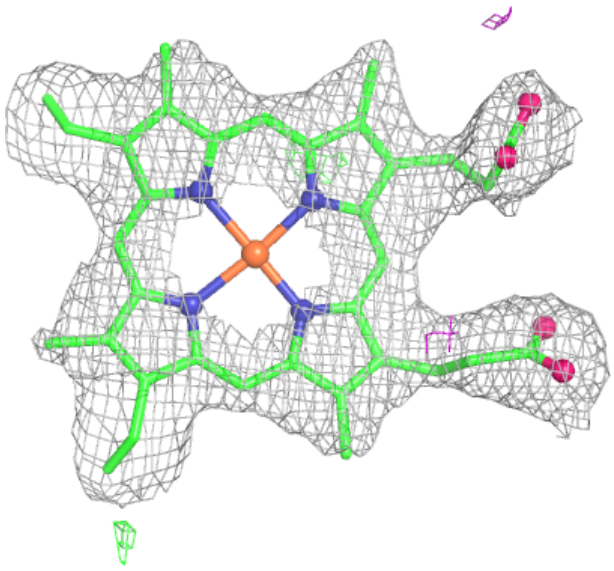


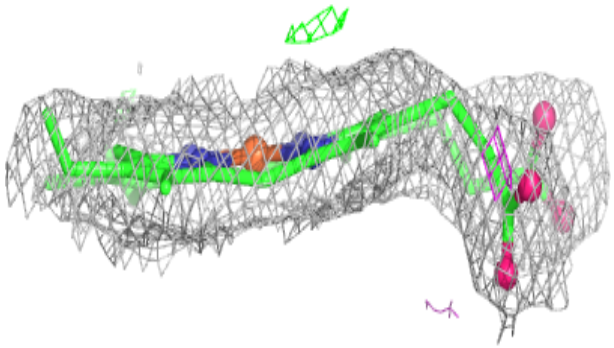


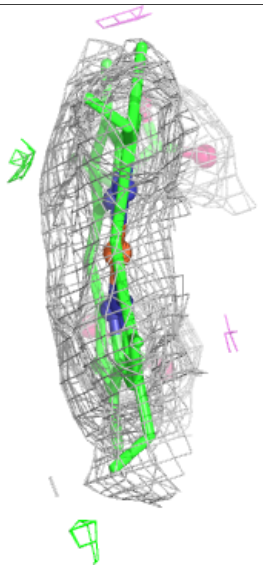


Electron density around HEC L 607:

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

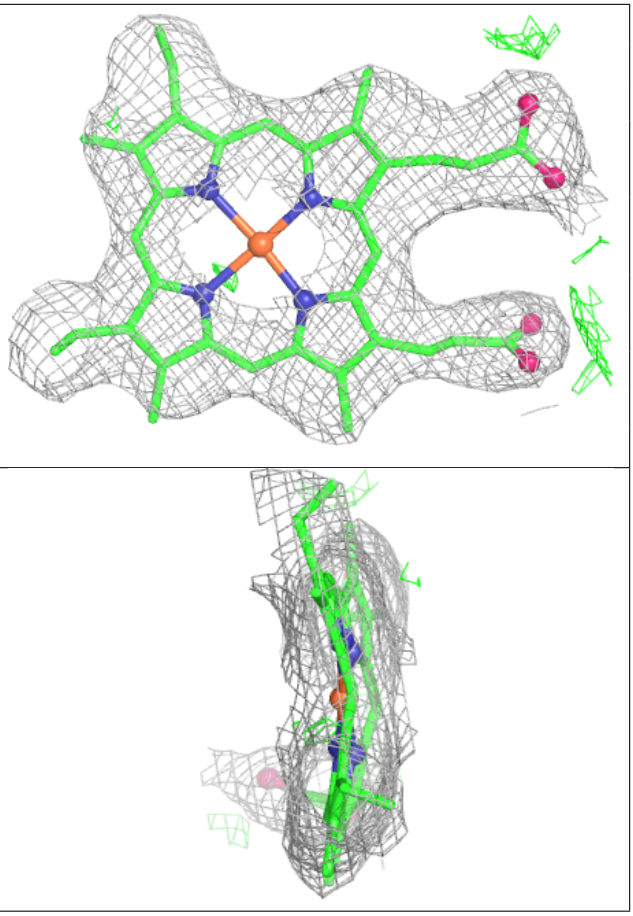


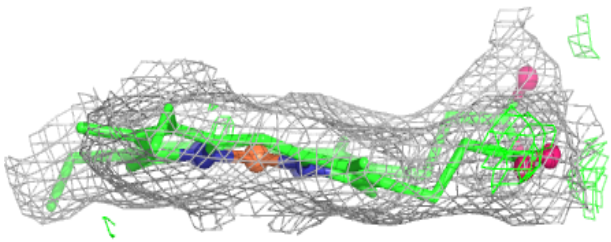




Electron density around HEC G 606:

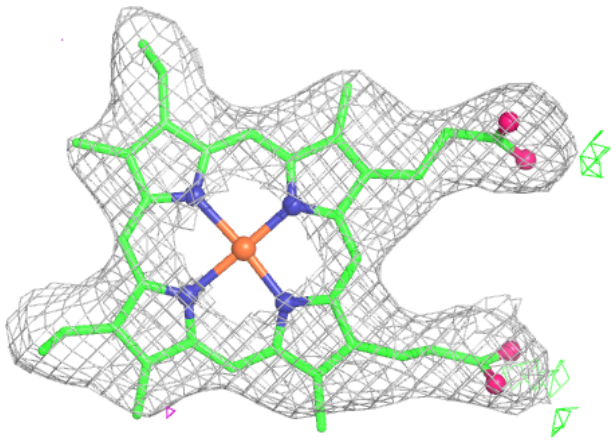
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

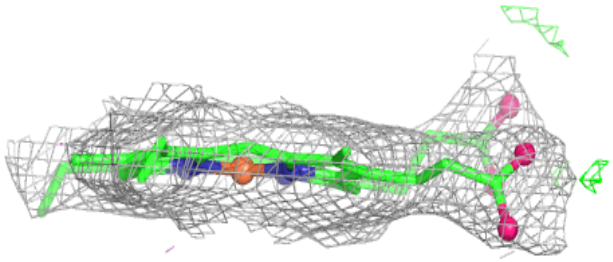


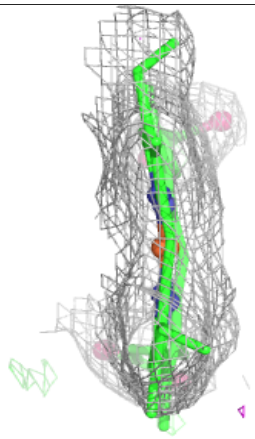


Electron density around HEC R 605:

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

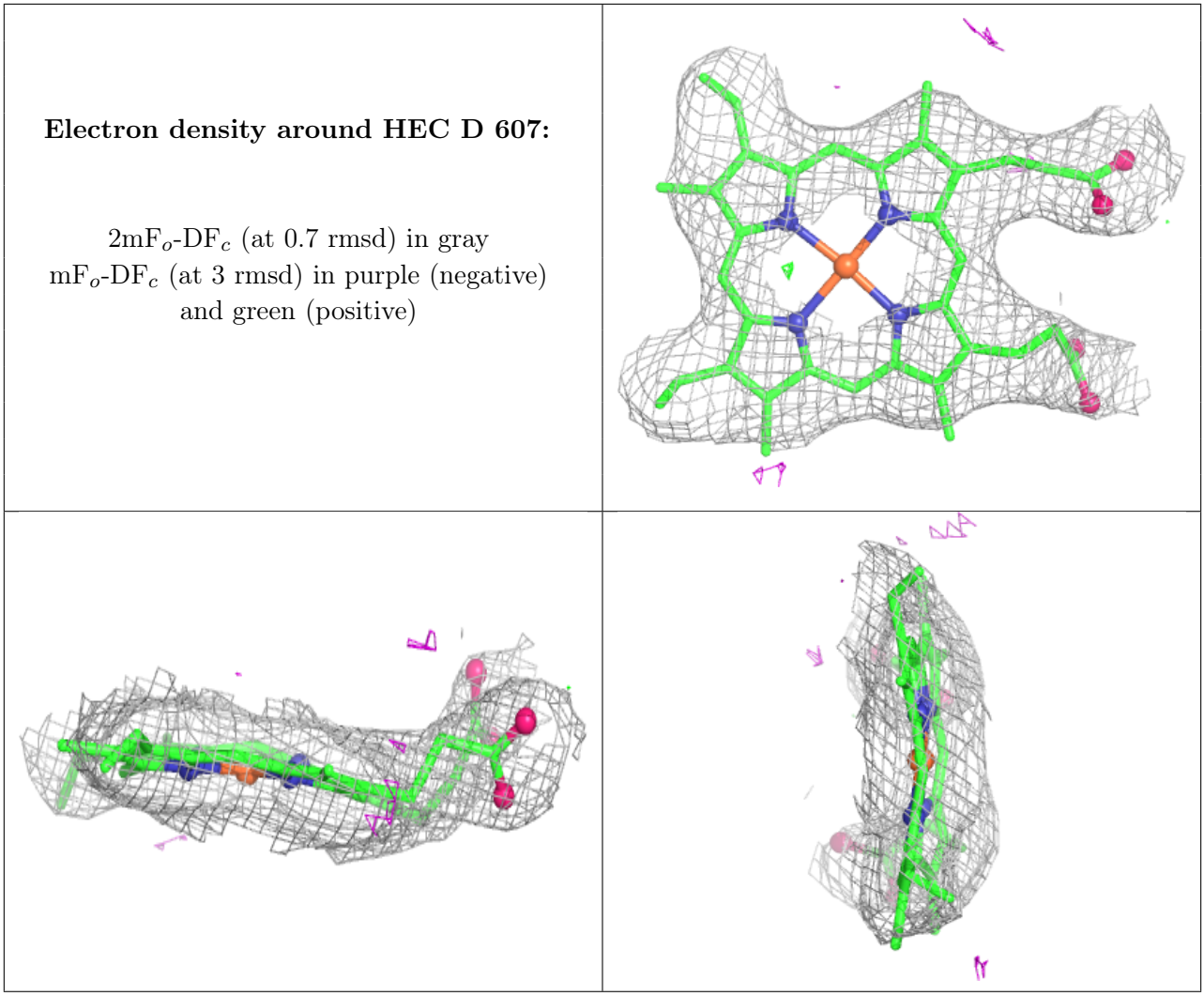






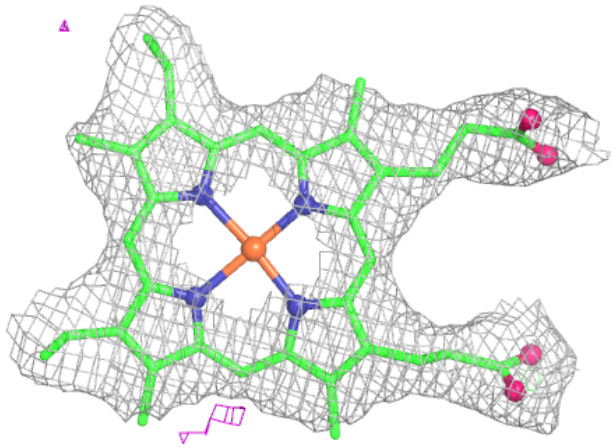
Electron density around HEC D 607:

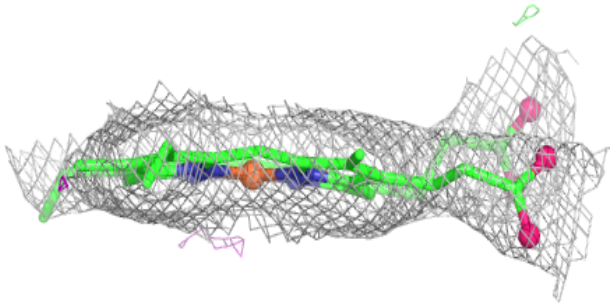
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

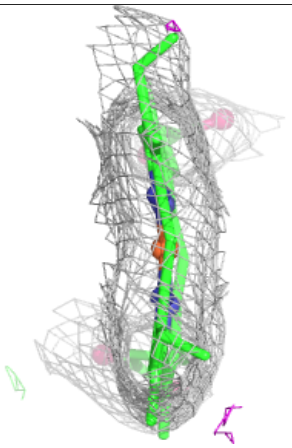


Electron density around HEC H 605:

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

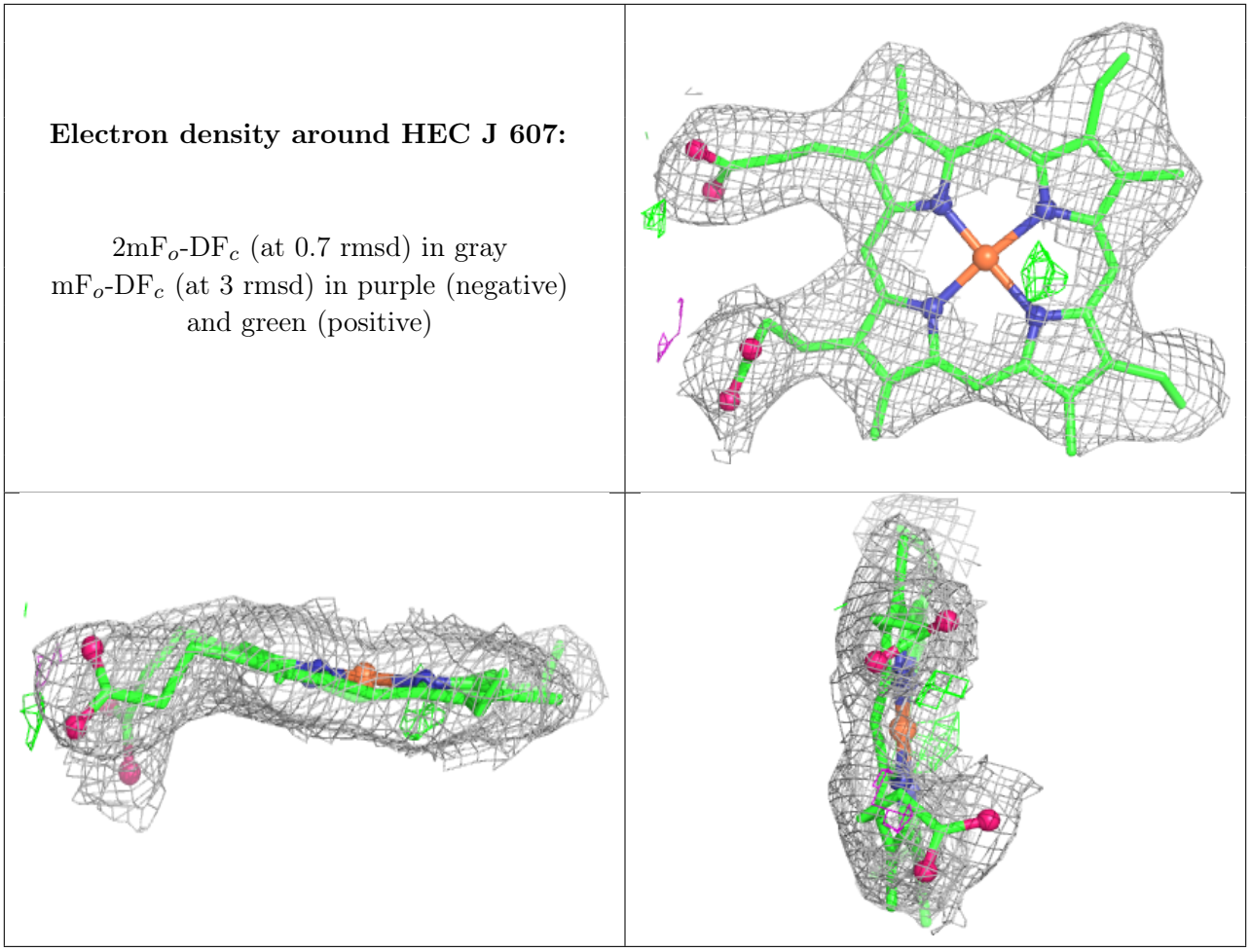






Electron density around HEC J 607:

$2mF_o$-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.