wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2026 – 04:59 am BST

PDB ID	:	8RXU / pdb_00008rxu
Title	:	Crystal structure of octaheme nitrite reductase from Trichlorobacter ammonificans in space group P21
Authors	:	Polyakov, K.M.; Safonova, T.N.; Osipov, E.; Popov, A.N.; Tikhonova, T.V.; Popov, V.O.
Deposited on	:	2024-02-08
Resolution	:	1.74 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:

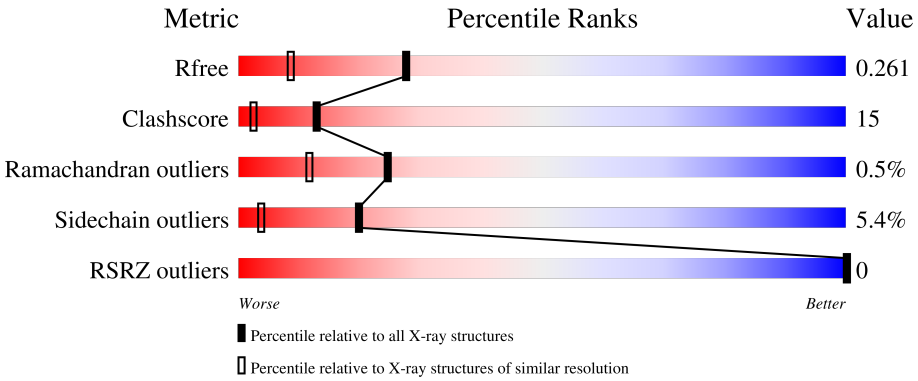
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	AAA	495	64% 31% 5%
1	MMM	495	66% 29% 5%
1	YYY	495	64% 31%

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
2	HEC	AAA	601	X	-	-	-
2	HEC	AAA	602	X	-	-	-
2	HEC	AAA	603	X	-	-	-
2	HEC	AAA	604	X	-	-	-
2	HEC	AAA	605	X	-	-	-
2	HEC	AAA	606	X	-	-	-
2	HEC	AAA	607[A]	X	-	-	-
2	HEC	AAA	607[B]	X	-	-	-
2	HEC	AAA	608	X	-	-	-
2	HEC	MMM	601	X	-	-	-
2	HEC	MMM	602	X	-	-	-
2	HEC	MMM	603	X	-	-	-
2	HEC	MMM	604	X	-	-	-
2	HEC	MMM	605	X	-	-	-
2	HEC	MMM	606	X	-	-	-
2	HEC	MMM	607	X	-	-	-
2	HEC	MMM	608	X	-	-	-
2	HEC	YYY	601	X	-	-	-
2	HEC	YYY	602	X	-	-	-
2	HEC	YYY	603	X	-	-	-
2	HEC	YYY	604	X	-	-	-
2	HEC	YYY	605	X	-	-	-
2	HEC	YYY	606	X	-	-	-
2	HEC	YYY	607	X	-	-	-
2	HEC	YYY	608	X	-	-	-
4	PO4	YYY	610	-	-	X	-

2 Entry composition (i)

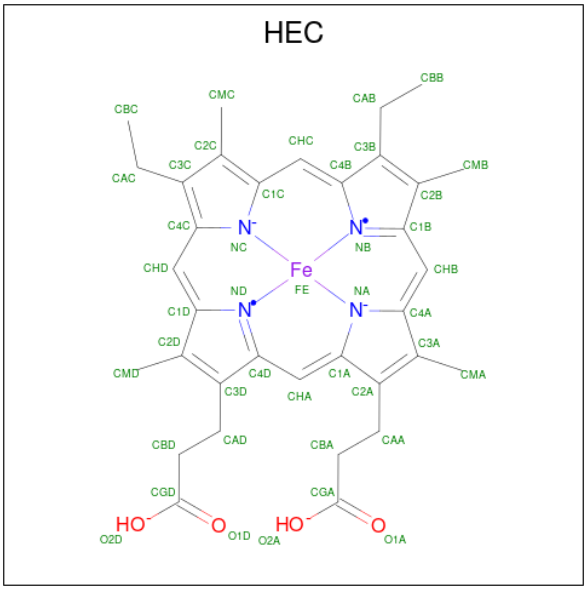
There are 5 unique types of molecules in this entry. The entry contains 13690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Octaheme nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	495	Total	C	N	O	S	0	2	0
			3895	2437	714	717	27			
1	MMM	495	Total	C	N	O	S	0	3	0
			3894	2438	714	715	27			
1	YYY	495	Total	C	N	O	S	0	2	0
			3898	2440	712	717	29			

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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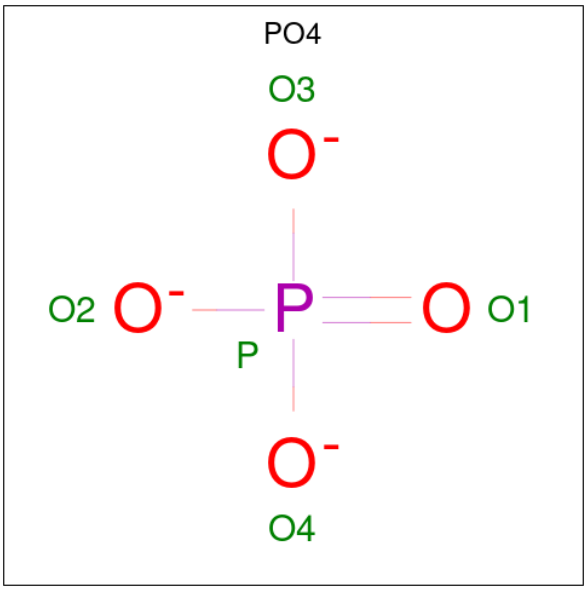
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	AAA	1	Total	C	Fe	N	O	0	1
			46	35	1	4	6		
2	AAA	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	MMM	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	MMM	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	MMM	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	MMM	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	MMM	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	MMM	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	MMM	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	YYY	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total Ca 1 1	0	0
3	MMM	1	Total Ca 1 1	0	0
3	YYY	1	Total Ca 1 1	0	0

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total O P 5 4 1	0	0
4	MMM	1	Total O P 5 4 1	0	0
4	YYY	1	Total O P 5 4 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	AAA	323	Total O 323 323	0	0
5	MMM	308	Total O 308 308	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	YYY	319	Total 319	O 319	0	0

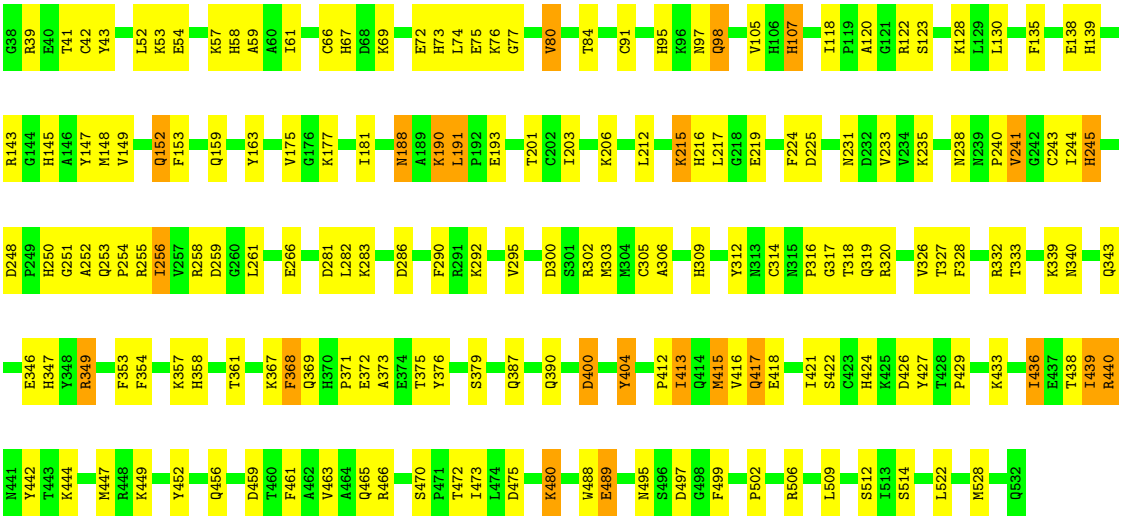
3 Residue-property plots (i)

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: Octaheme nitrite reductase

Chain AAA:

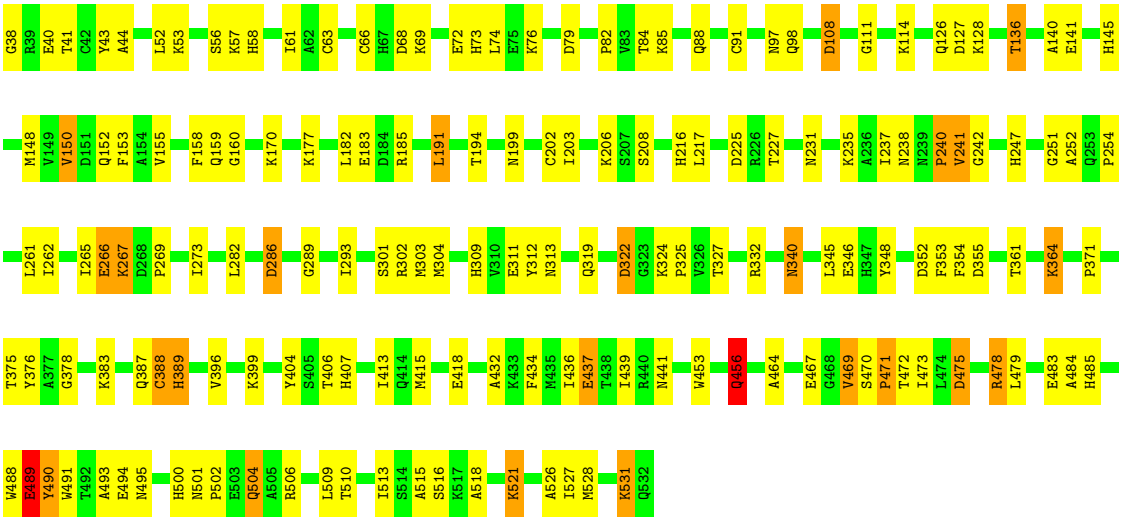




- Molecule 1: Octaheme nitrite reductase

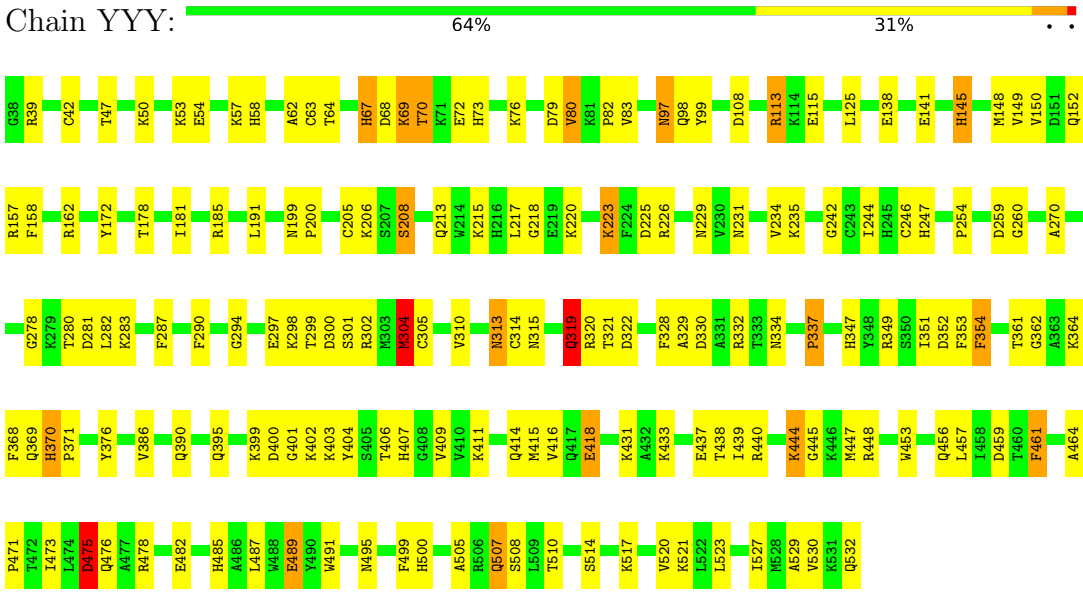
Chain MMM:





• Molecule 1: Octaheme nitrite reductase

Chain YYY:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	114.20Å 64.80Å 114.20Å 90.00° 119.90° 90.00°	Depositor
Resolution (Å)	42.88 – 1.74 42.88 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.8 (42.88-1.74) 97.8 (42.88-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.191 , 0.254 0.196 , 0.261	Depositor DCC
R_{free} test set	7348 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	22.0	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 14.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.457 for -h-l,k,h 0.457 for l,k,-h-l 0.023 for h,-k,-h-l 0.029 for -h-l,-k,l 0.024 for l,-k,h	Xtriage
Reported twinning fraction	0.400 for H, K, L 0.290 for L, K, -H-L 0.310 for -H-L, K, H	Depositor
Outliers	0 of 145920 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13690	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: HEC, PO4, CA

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	AAA	1.23	13/4002 (0.3%)	1.70	30/5390 (0.6%)
1	MMM	1.24	8/4003 (0.2%)	1.66	39/5391 (0.7%)
1	YYY	1.24	12/4000 (0.3%)	1.66	36/5388 (0.7%)
All	All	1.24	33/12005 (0.3%)	1.67	105/16169 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	YYY	0	1

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	MMM	432	ALA	C-O	8.07	1.33	1.24
1	YYY	507	GLN	C-O	7.76	1.33	1.24
1	YYY	453	TRP	C-O	6.55	1.31	1.24
1	AAA	357	LYS	C-O	6.26	1.31	1.24
1	AAA	120	ALA	C-O	6.15	1.32	1.24

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	YYY	406	THR	CA-CB-OG1	-9.73	95.00	109.60
1	MMM	325	PRO	N-CA-C	7.68	123.25	111.19
1	MMM	153	PHE	CA-C-O	-7.65	112.79	120.82
1	AAA	120	ALA	CA-C-N	7.32	131.83	121.30
1	AAA	120	ALA	C-N-CA	7.32	131.83	121.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	YYY	310	VAL	Peptide

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	AAA	3895	0	3804	125	0
1	MMM	3894	0	3811	112	0
1	YYY	3898	0	3812	127	0
2	AAA	347	0	214	34	0
2	MMM	344	0	240	25	0
2	YYY	344	0	240	26	0
3	AAA	1	0	0	0	0
3	MMM	1	0	0	0	0
3	YYY	1	0	0	0	0
4	AAA	5	0	0	1	0
4	MMM	5	0	0	0	0
4	YYY	5	0	0	2	0
5	AAA	323	0	0	13	1
5	MMM	308	0	0	9	0
5	YYY	319	0	0	13	1
All	All	13690	0	12121	374	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 374 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)
2:AAA:603:HEC:HBC3	5:AAA:1015:HOH:O	1.56	1.05
1:YYY:319:GLN:NE2	1:YYY:322:ASP:OD2	1.98	0.97
1:MMM:456:GLN:HE21	1:MMM:456:GLN:HA	1.30	0.95
1:MMM:415:MET:SD	1:MMM:418:GLU:HG3	2.14	0.88
1:YYY:495:ASN:HB3	2:YYY:607:HEC:HAA1	1.59	0.84

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:AAA:1019:HOH:O	5:YYY:1013:HOH:O[2_546]	2.12	0.08

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	AAA	495/495 (100%)	459 (93%)	33 (7%)	3 (1%)	21 8
1	MMM	496/495 (100%)	453 (91%)	41 (8%)	2 (0%)	30 16
1	YYY	495/495 (100%)	448 (90%)	45 (9%)	2 (0%)	30 16
All	All	1486/1485 (100%)	1360 (92%)	119 (8%)	7 (0%)	24 12

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	138	GLU
1	AAA	241	VAL
1	AAA	282	LEU
1	YYY	475	ASP
1	MMM	241	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	AAA	416/414 (100%)	393 (94%)	23 (6%)	19 3
1	MMM	415/414 (100%)	390 (94%)	25 (6%)	17 3
1	YYY	416/414 (100%)	395 (95%)	21 (5%)	22 4
All	All	1247/1242 (100%)	1178 (94%)	69 (6%)	20 3

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

Mol	Chain	Res	Type
1	YYY	283	LYS
1	YYY	304	MET
1	YYY	489	GLU
1	MMM	108	ASP
1	MMM	85	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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	$\#\|Z\|>2$
2	HEC	MMM	602	1	50,50,50	2.45	22 (44%)	68,82,82	3.04	33 (48%)
2	HEC	AAA	608	1	50,50,50	2.66	25 (50%)	68,82,82	2.29	23 (33%)
2	HEC	MMM	604	1,4	50,50,50	2.42	24 (48%)	68,82,82	2.96	27 (39%)
2	HEC	YYY	608	1	50,50,50	2.59	26 (52%)	68,82,82	2.14	21 (30%)
2	HEC	MMM	605	1	50,50,50	2.71	25 (50%)	68,82,82	2.72	27 (39%)
2	HEC	YYY	606	1	50,50,50	2.66	26 (52%)	68,82,82	2.69	31 (45%)
2	HEC	AAA	601	1	50,50,50	2.60	24 (48%)	68,82,82	3.14	38 (55%)
2	HEC	AAA	603	1	50,50,50	2.71	27 (54%)	68,82,82	2.58	28 (41%)
2	HEC	MMM	606	1	50,50,50	2.60	29 (58%)	68,82,82	2.90	33 (48%)
2	HEC	YYY	603	1	50,50,50	2.70	26 (52%)	68,82,82	2.51	26 (38%)
2	HEC	YYY	607	1	50,50,50	2.69	25 (50%)	68,82,82	2.78	29 (42%)
2	HEC	AAA	602	1	50,50,50	2.53	26 (52%)	68,82,82	2.65	36 (52%)
2	HEC	AAA	607[A]	-	50,50,50	2.51	21 (42%)	68,82,82	3.61	36 (52%)
2	HEC	YYY	602	1	50,50,50	2.43	23 (46%)	68,82,82	2.62	33 (48%)
2	HEC	YYY	604	1,4	50,50,50	2.48	22 (44%)	68,82,82	2.62	28 (41%)
4	PO4	MMM	610	2	4,4,4	1.76	2 (50%)	6,6,6	1.27	0
4	PO4	YYY	610	2	4,4,4	0.45	0	6,6,6	0.91	0
2	HEC	YYY	605	1	50,50,50	2.69	25 (50%)	68,82,82	2.57	28 (41%)
2	HEC	AAA	606	1	50,50,50	2.70	22 (44%)	68,82,82	2.82	36 (52%)
2	HEC	AAA	605	1	50,50,50	2.61	26 (52%)	68,82,82	2.43	28 (41%)
2	HEC	AAA	607[B]	-	50,50,50	2.50	21 (42%)	68,82,82	3.55	34 (50%)
2	HEC	MMM	603	1	50,50,50	2.59	21 (42%)	68,82,82	2.86	33 (48%)
2	HEC	AAA	604	1,4	50,50,50	2.48	27 (54%)	68,82,82	2.57	24 (35%)
2	HEC	MMM	607	1	50,50,50	2.67	22 (44%)	68,82,82	2.97	31 (45%)
2	HEC	YYY	601	1	50,50,50	2.54	25 (50%)	68,82,82	2.78	32 (47%)
2	HEC	MMM	608	1	50,50,50	2.53	21 (42%)	68,82,82	2.45	24 (35%)
2	HEC	MMM	601	1	50,50,50	2.55	27 (54%)	68,82,82	2.86	35 (51%)
4	PO4	AAA	610	2	4,4,4	1.94	2 (50%)	6,6,6	0.93	0

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
2	HEC	MMM	602	1	1/1/3/7	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	AAA	608	1	1/1/3/7	4/14/54/54	-
2	HEC	MMM	604	1,4	1/1/3/7	6/14/54/54	-
2	HEC	YYY	608	1	1/1/3/7	4/14/54/54	-
2	HEC	MMM	605	1	1/1/3/7	6/14/54/54	-
2	HEC	YYY	606	1	1/1/3/7	3/14/54/54	-
2	HEC	AAA	601	1	1/1/3/7	6/14/54/54	-
2	HEC	AAA	603	1	1/1/3/7	7/14/54/54	-
2	HEC	MMM	606	1	1/1/3/7	4/14/54/54	-
2	HEC	YYY	603	1	1/1/3/7	8/14/54/54	-
2	HEC	YYY	607	1	1/1/3/7	7/14/54/54	-
2	HEC	AAA	602	1	1/1/3/7	7/14/54/54	-
2	HEC	AAA	607[A]	-	1/1/3/7	8/14/54/54	-
2	HEC	YYY	602	1	1/1/3/7	8/14/54/54	-
2	HEC	YYY	604	1,4	1/1/3/7	5/14/54/54	-
2	HEC	YYY	605	1	1/1/3/7	4/14/54/54	-
2	HEC	AAA	606	1	1/1/3/7	3/14/54/54	-
2	HEC	AAA	605	1	1/1/3/7	4/14/54/54	-
2	HEC	AAA	607[B]	-	1/1/3/7	9/14/54/54	-
2	HEC	MMM	603	1	1/1/3/7	5/14/54/54	-
2	HEC	AAA	604	1,4	1/1/3/7	6/14/54/54	-
2	HEC	MMM	607	1	1/1/3/7	8/14/54/54	-
2	HEC	YYY	601	1	1/1/3/7	11/14/54/54	-
2	HEC	MMM	608	1	1/1/3/7	5/14/54/54	-
2	HEC	MMM	601	1	1/1/3/7	5/14/54/54	-

The worst 5 of 612 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	MMM	607	HEC	C4B-NB	-6.92	1.28	1.40
2	MMM	604	HEC	C4B-NB	-6.85	1.28	1.40
2	YYY	607	HEC	CHA-C1A	6.56	1.51	1.38
2	AAA	604	HEC	C4B-NB	-6.10	1.29	1.40
2	AAA	606	HEC	C1D-ND	-6.02	1.29	1.40

The worst 5 of 754 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	607[A]	HEC	C3D-C4D-ND	11.53	121.52	110.36
2	AAA	607[B]	HEC	C3D-C4D-ND	11.53	121.52	110.36
2	MMM	601	HEC	CAA-CBA-CGA	-8.53	95.26	113.60
2	MMM	603	HEC	C1B-C2B-C3B	-8.32	98.21	106.96
2	MMM	603	HEC	C1C-C2C-C3C	-8.22	97.22	106.83

5 of 25 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	AAA	601	HEC	NA
2	AAA	602	HEC	NA
2	AAA	603	HEC	NA
2	AAA	604	HEC	NA
2	AAA	605	HEC	NA

5 of 150 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	608	HEC	C2C-C3C-CAC-CBC
2	MMM	608	HEC	C2C-C3C-CAC-CBC
2	YYY	601	HEC	C4D-C3D-CAD-CBD
2	YYY	608	HEC	C2C-C3C-CAC-CBC
2	MMM	601	HEC	C4C-C3C-CAC-CBC

There are no ring outliers.

26 monomers are involved in 88 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	MMM	602	HEC	3	0
2	AAA	608	HEC	3	0
2	MMM	604	HEC	5	0
2	YYY	608	HEC	1	0
2	MMM	605	HEC	3	0
2	YYY	606	HEC	2	0
2	AAA	601	HEC	4	0
2	AAA	603	HEC	8	0
2	MMM	606	HEC	4	0
2	YYY	603	HEC	1	0
2	YYY	607	HEC	5	0
2	AAA	602	HEC	7	0
2	AAA	607[A]	HEC	1	0
2	YYY	602	HEC	2	0
2	YYY	604	HEC	3	0

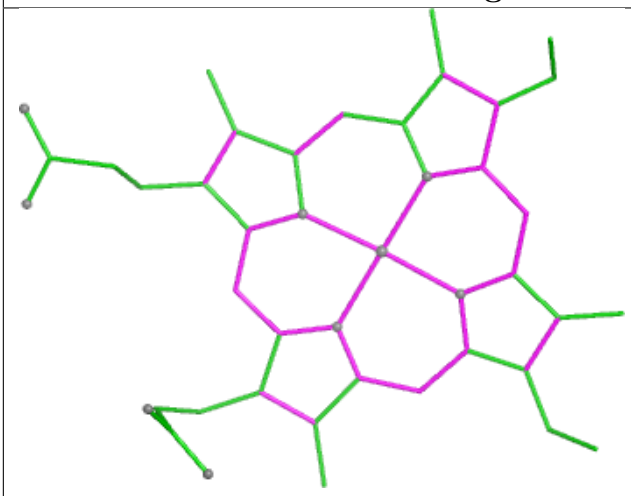
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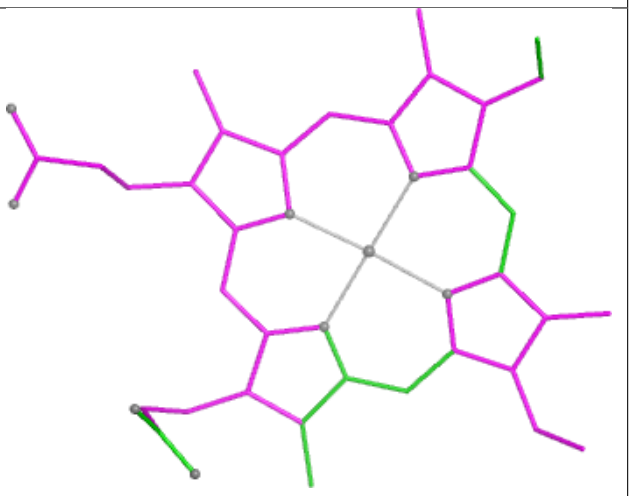
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	YYY	610	PO4	2	0
2	YYY	605	HEC	4	0
2	AAA	606	HEC	5	0
2	AAA	605	HEC	7	0
2	MMM	603	HEC	3	0
2	AAA	604	HEC	3	0
2	MMM	607	HEC	4	0
2	YYY	601	HEC	8	0
2	MMM	608	HEC	1	0
2	MMM	601	HEC	2	0
4	AAA	610	PO4	1	0

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

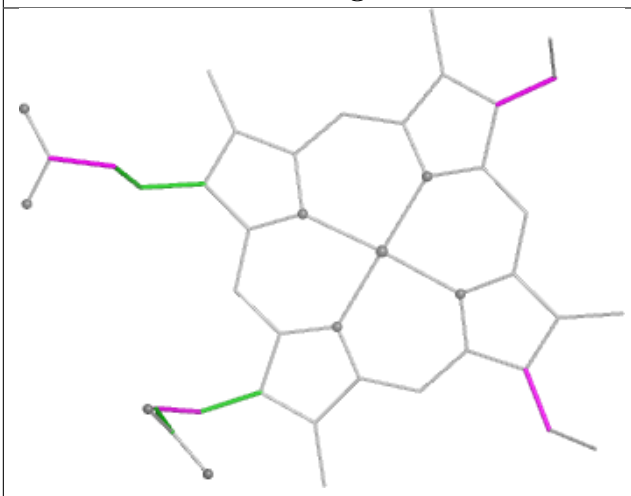
Ligand HEC MMM 602



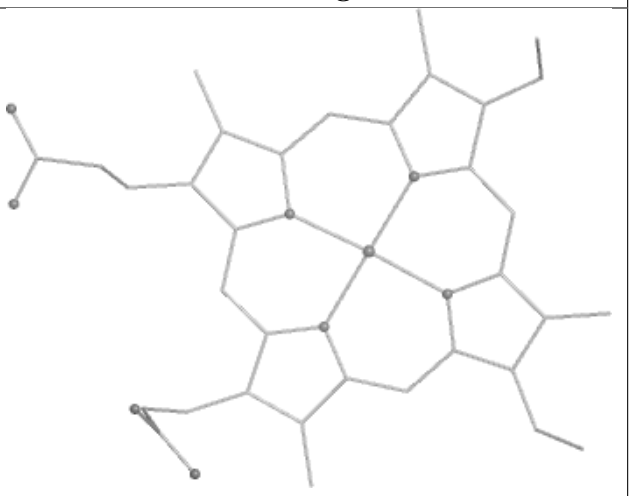
Bond lengths



Bond angles

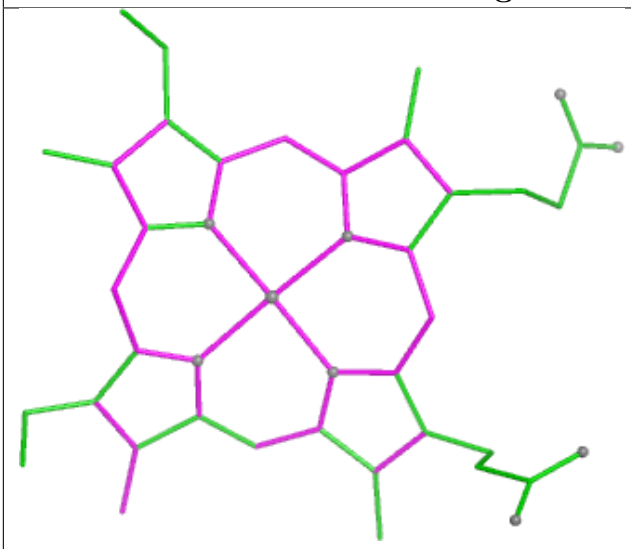


Torsions

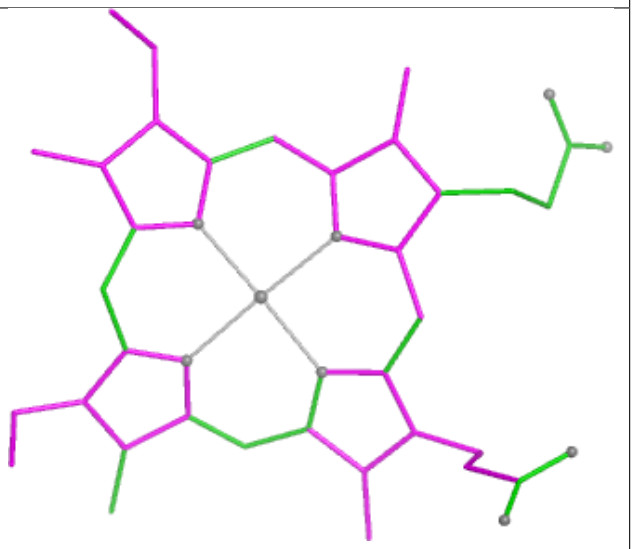


Rings

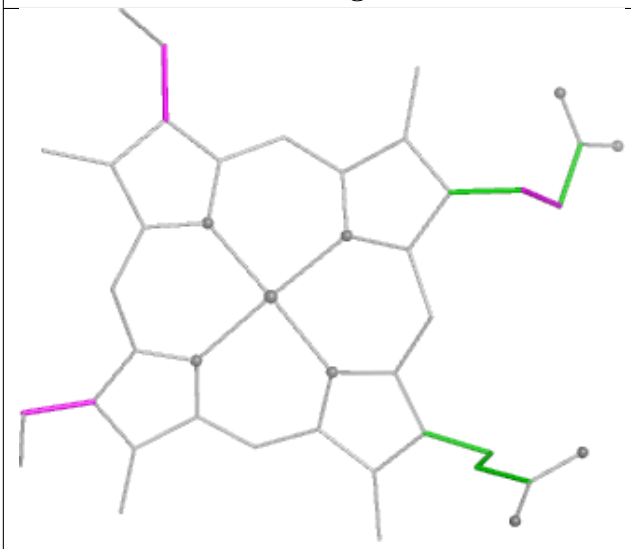
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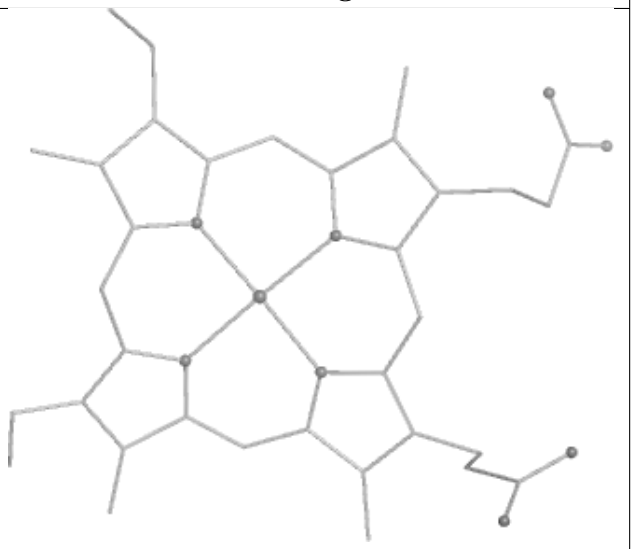
Bond lengths



Bond angles

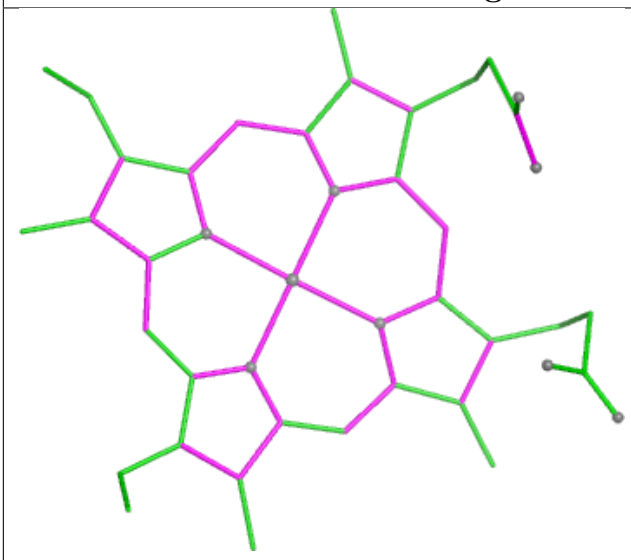


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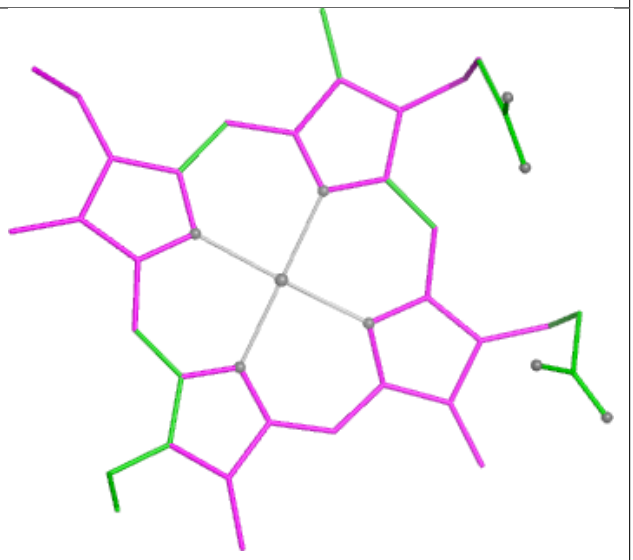


Rings

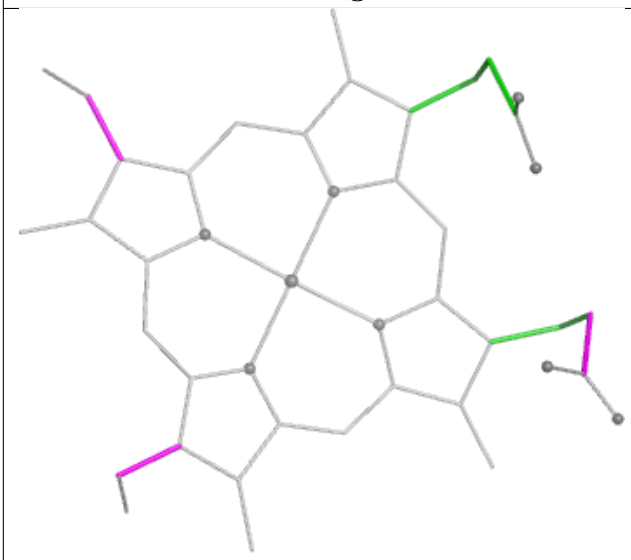
Ligand HEC MMM 604



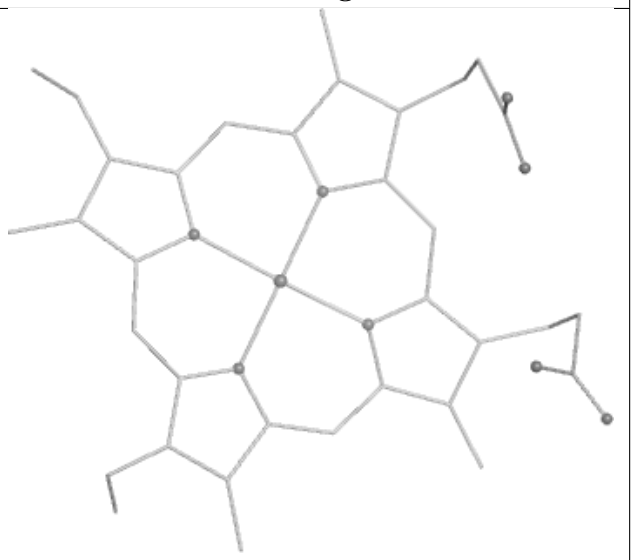
Bond lengths



Bond angles

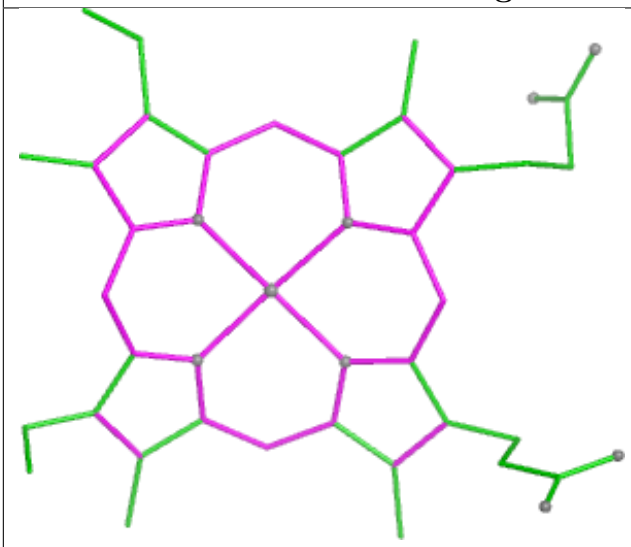


Torsions

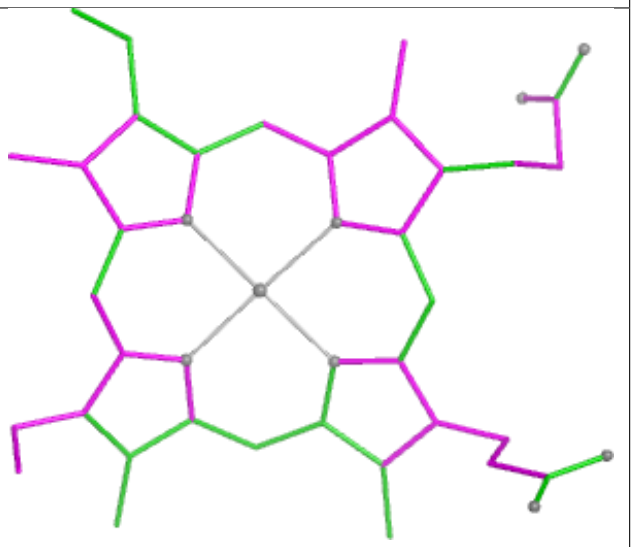


Rings

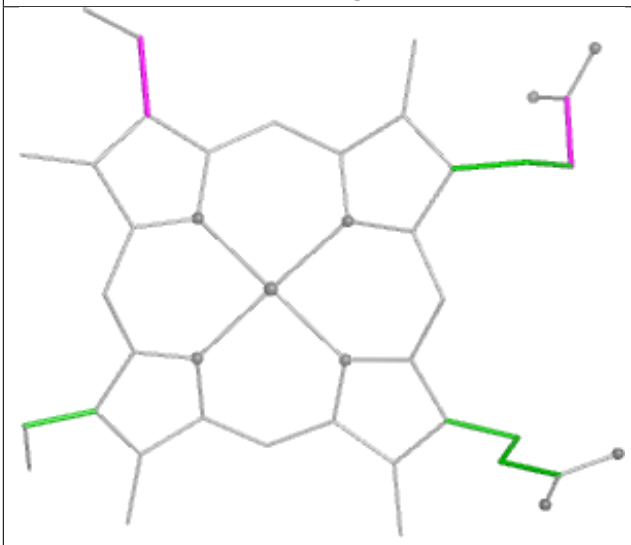
Ligand HEC YYY 608



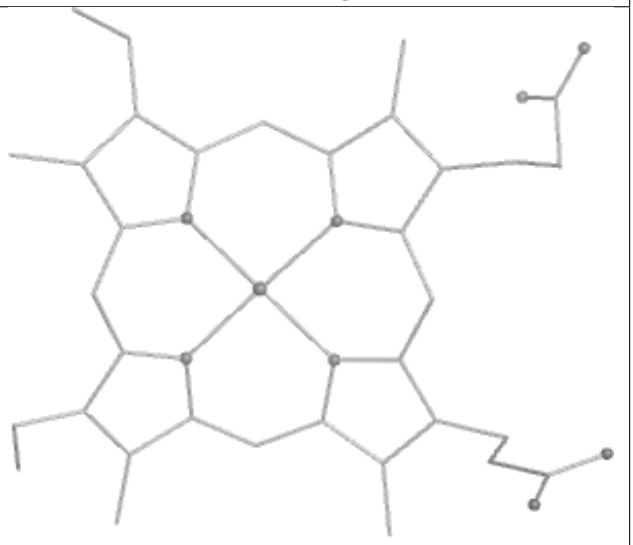
Bond lengths



Bond angles

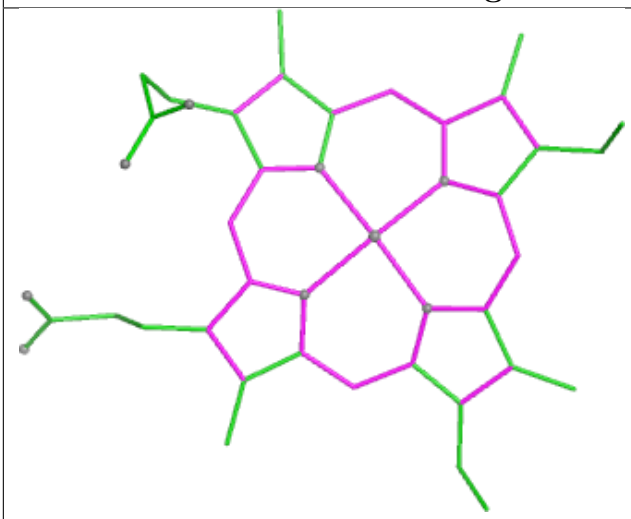


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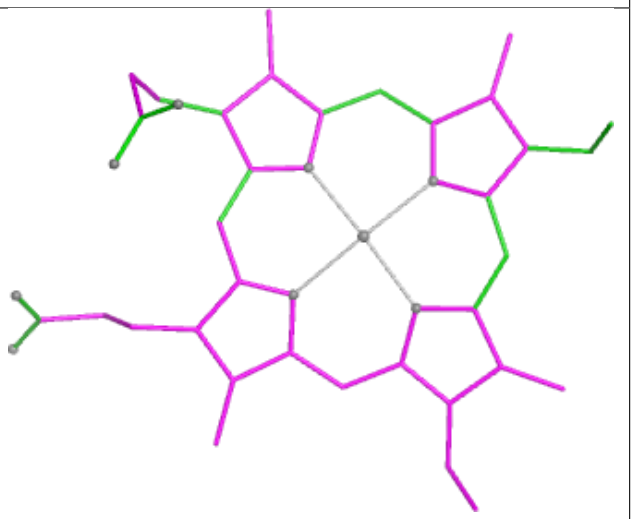


Rings

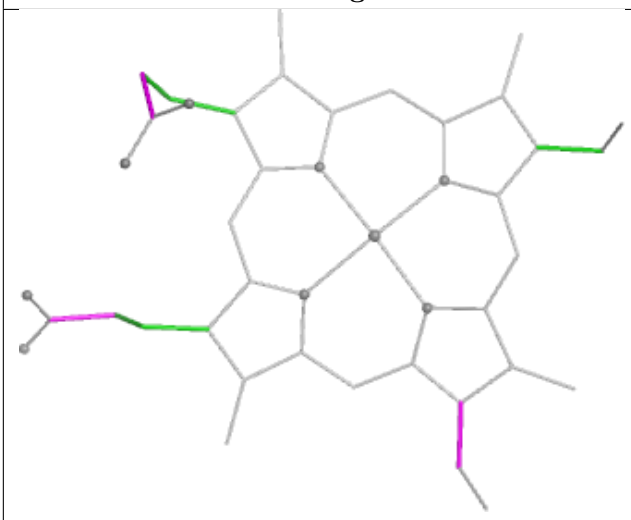
Ligand HEC MMM 605



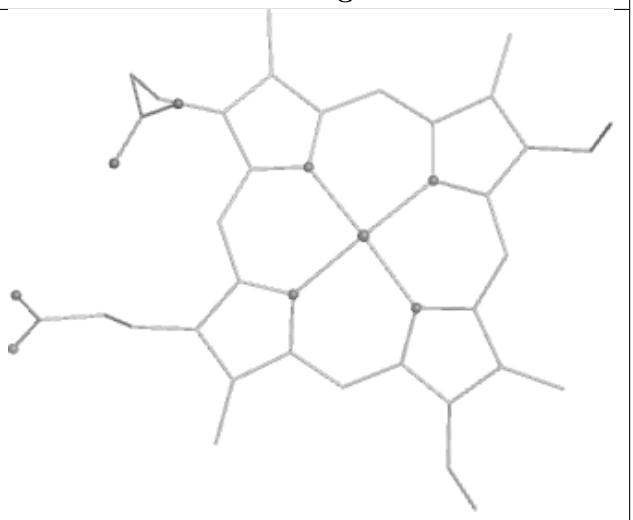
Bond lengths



Bond angles

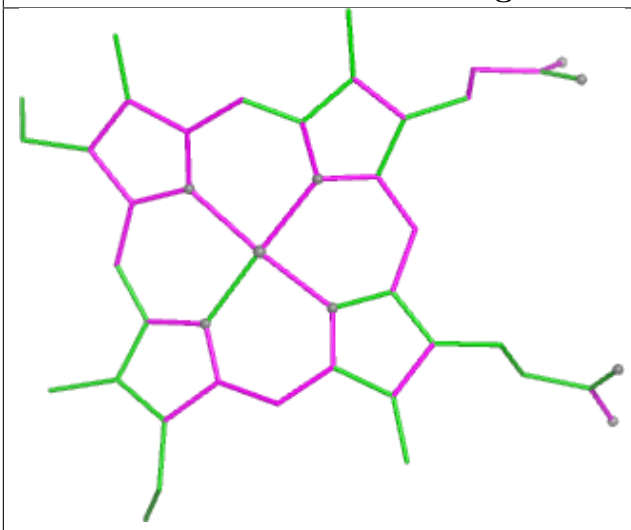


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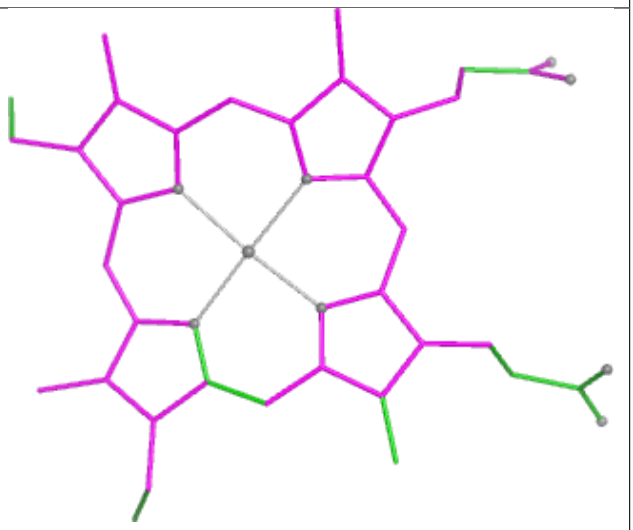


Rings

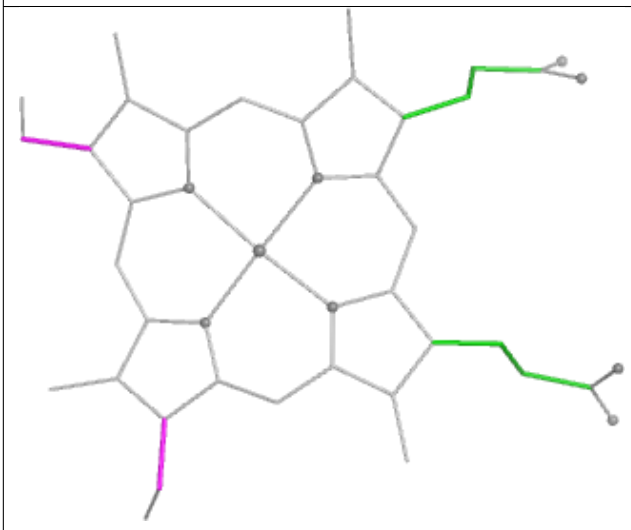
Ligand HEC YYY 606



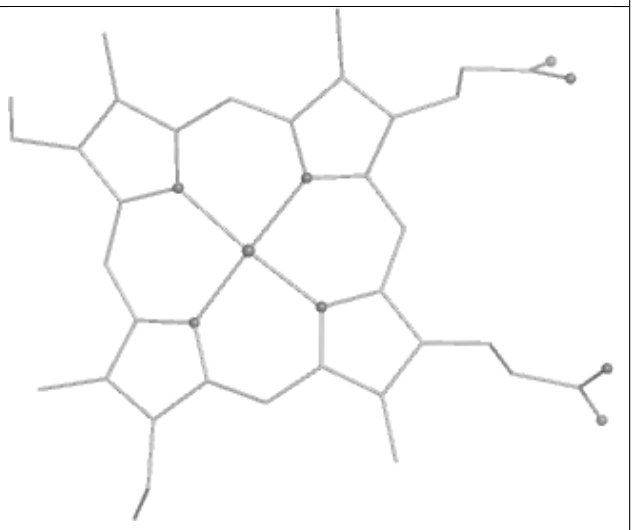
Bond lengths



Bond angles

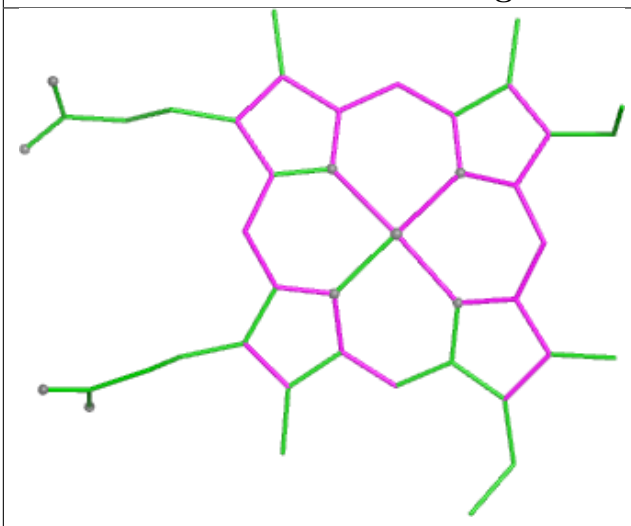


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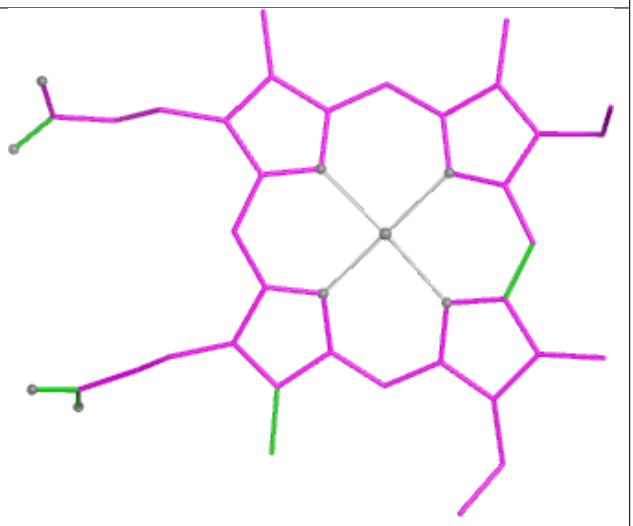


Rings

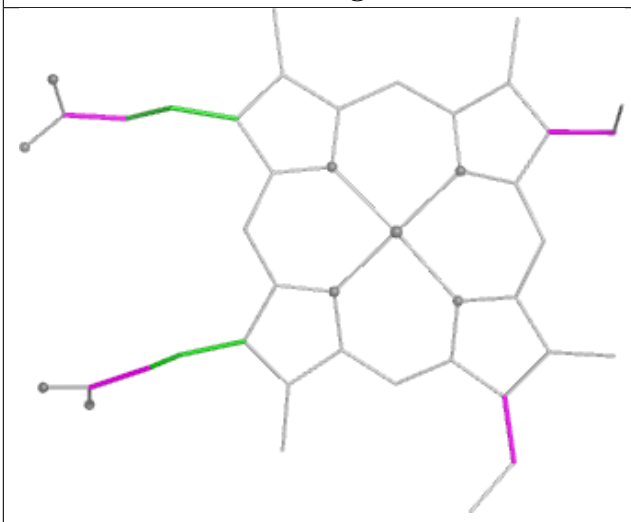
Ligand HEC AAA 601



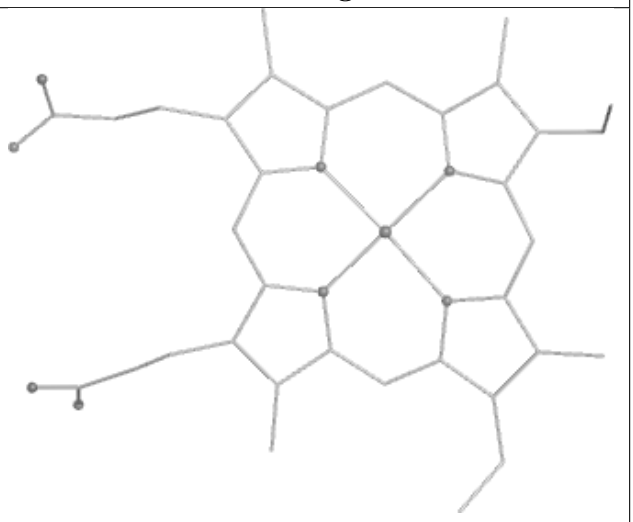
Bond lengths



Bond angles

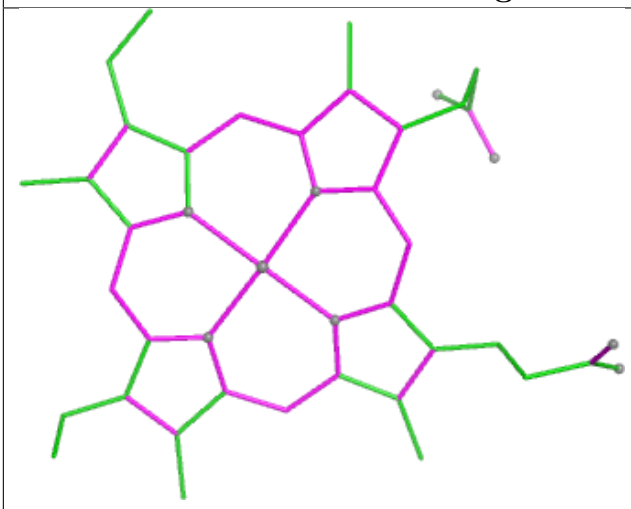


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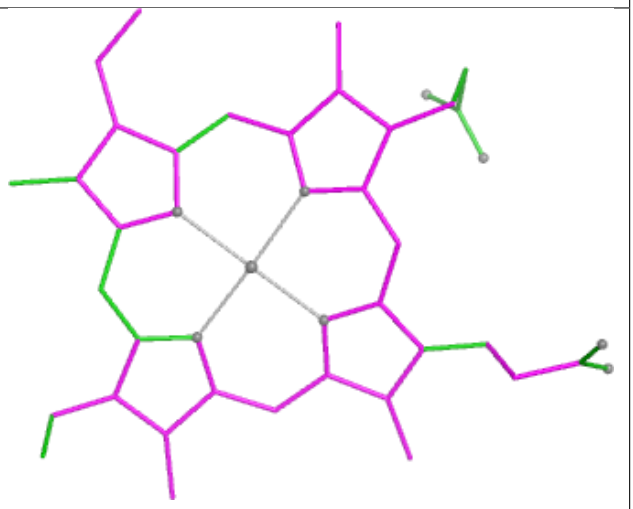


Rings

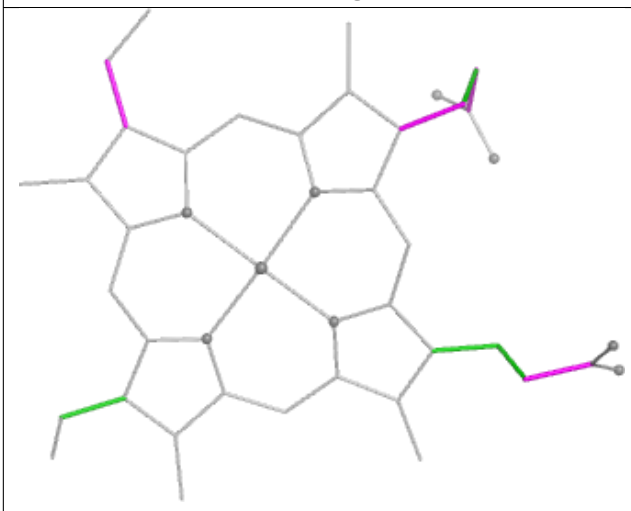
Ligand HEC AAA 603



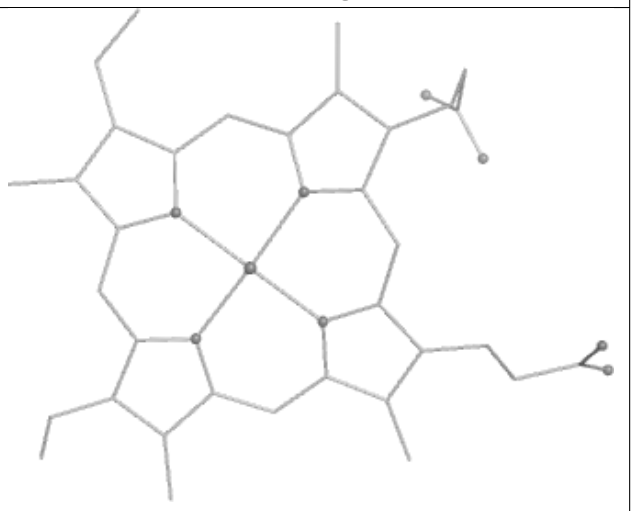
Bond lengths



Bond angles

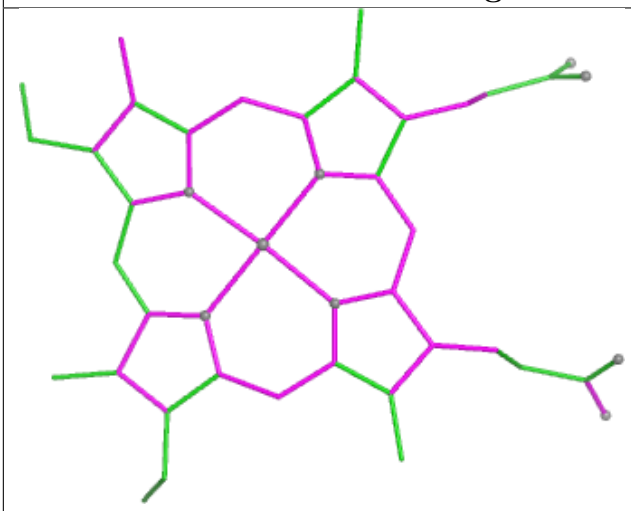


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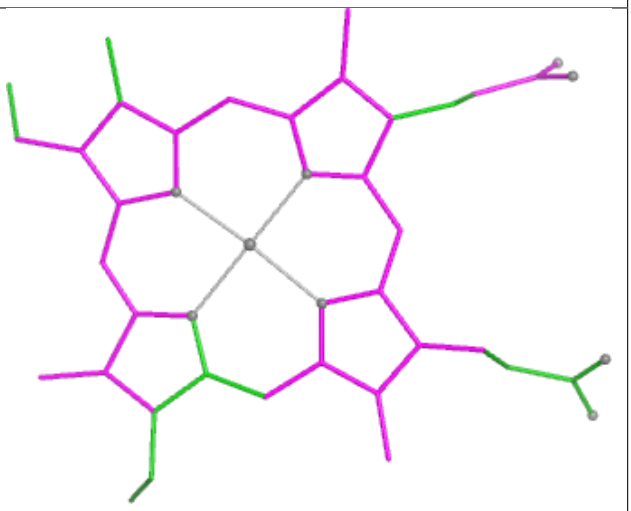


Rings

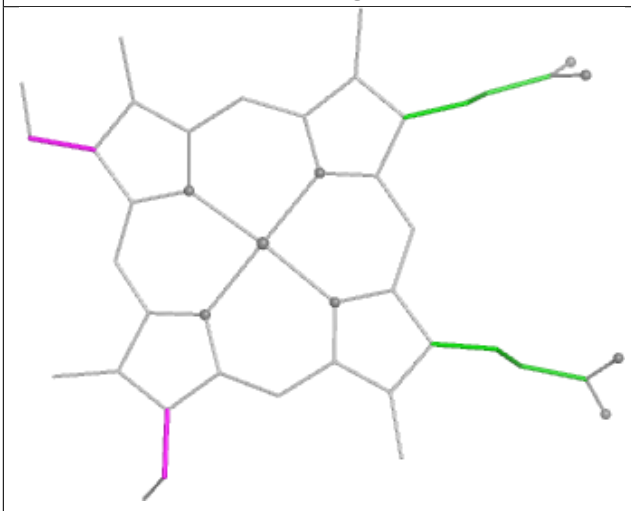
Ligand HEC MMM 606



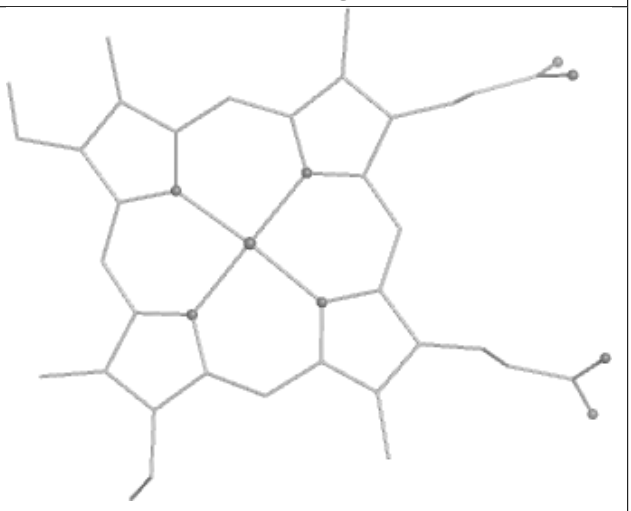
Bond lengths



Bond angles

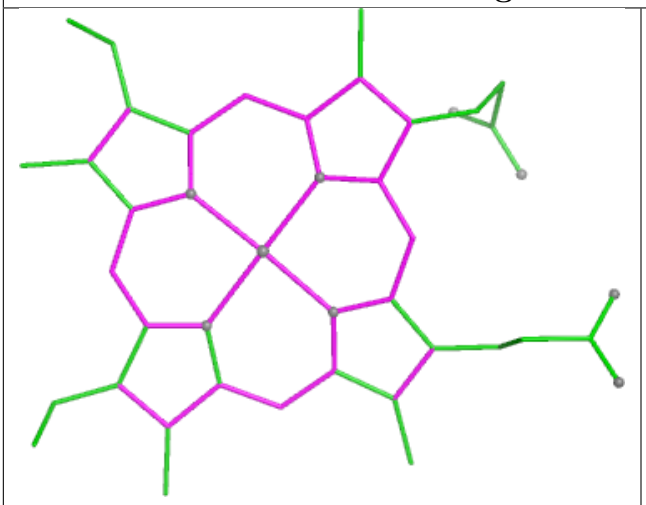


Torsions

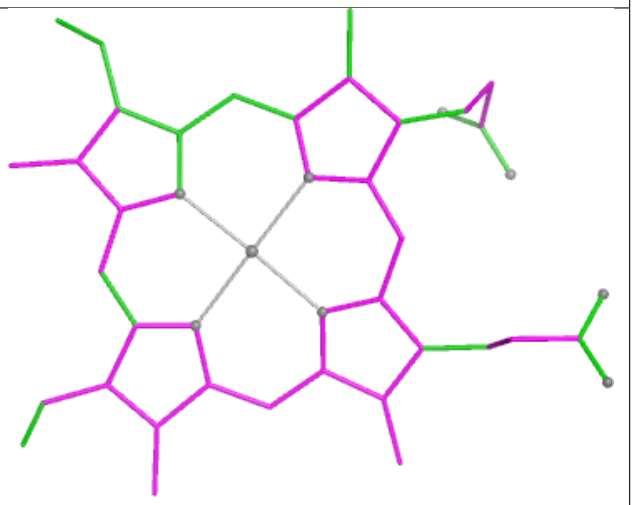


Rings

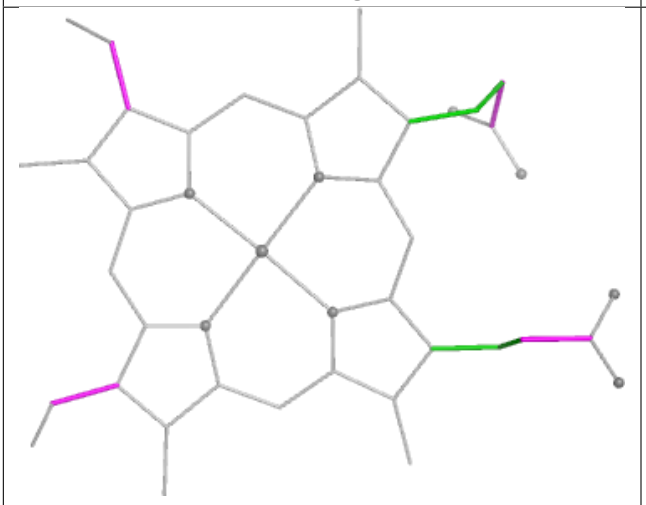
Ligand HEC YYY 603



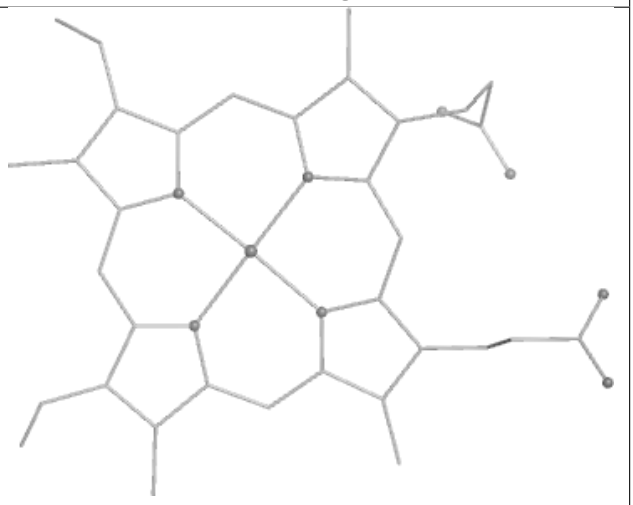
Bond lengths



Bond angles

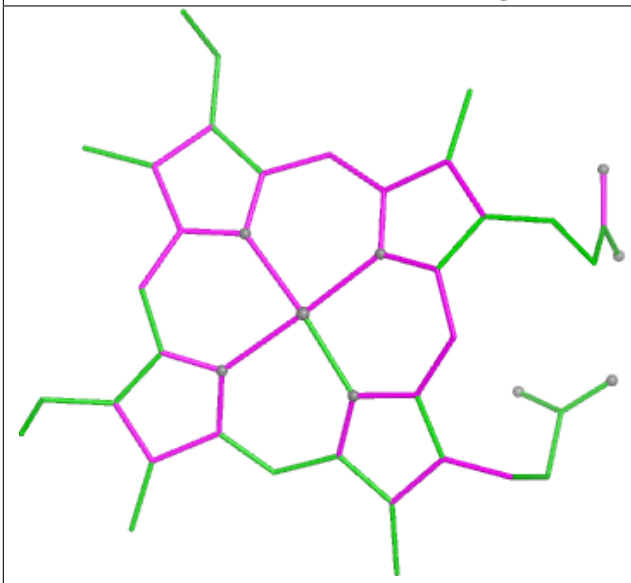


Torsions

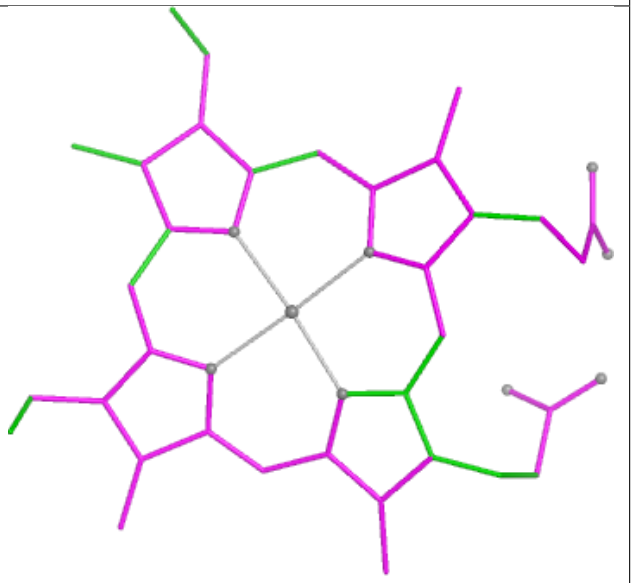


Rings

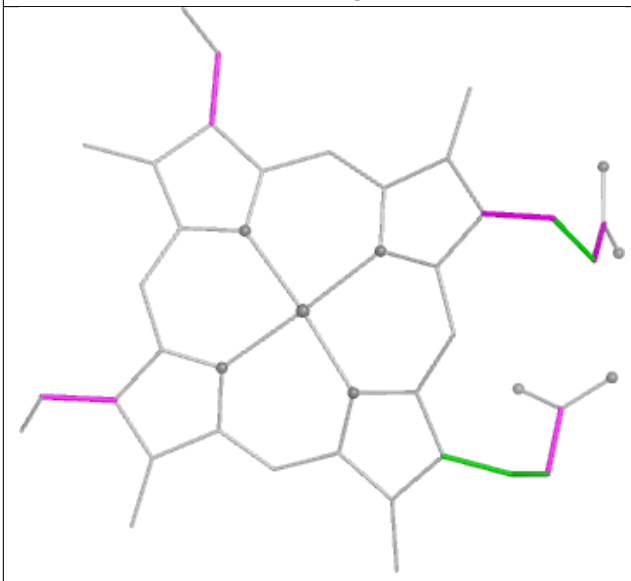
Ligand HEC YYY 607



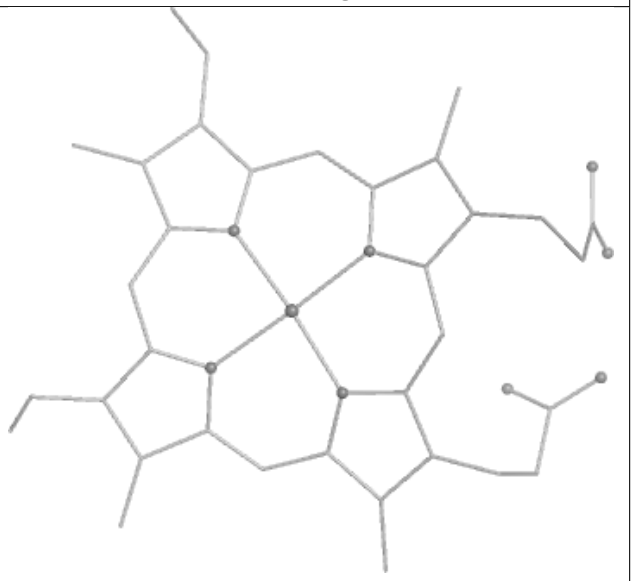
Bond lengths



Bond angles

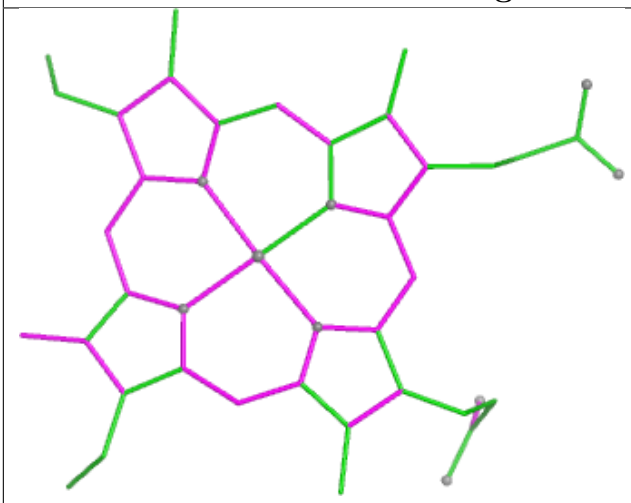


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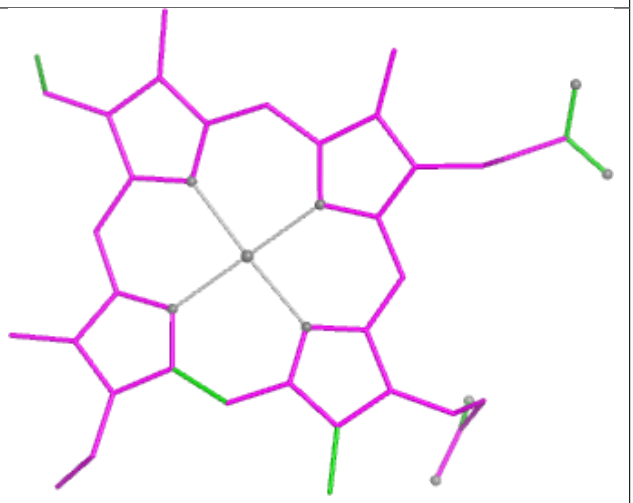


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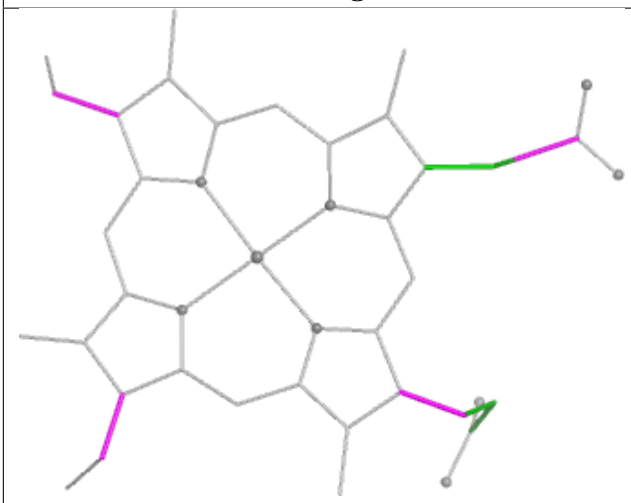
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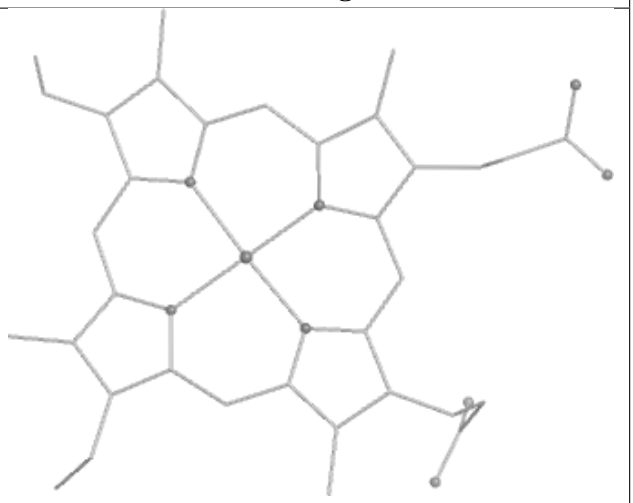
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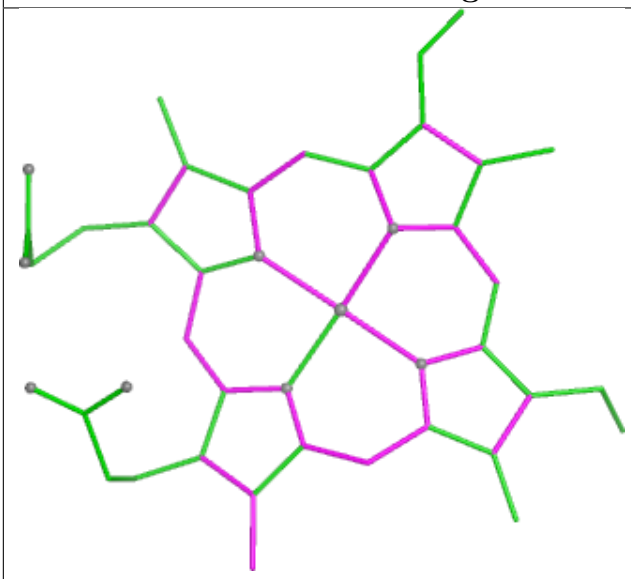


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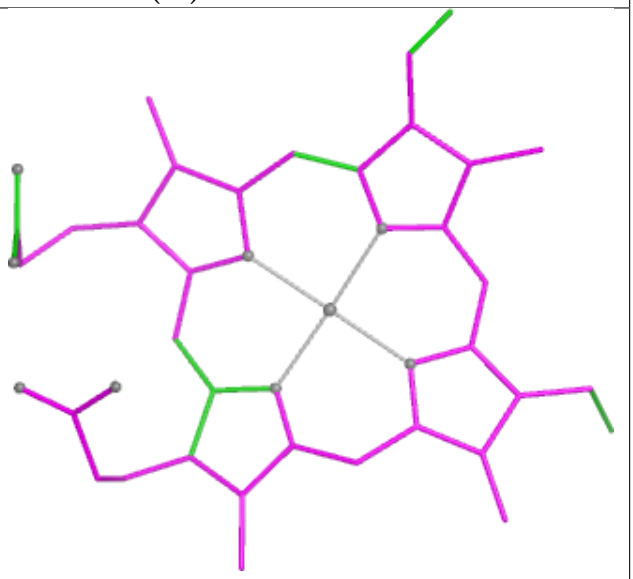


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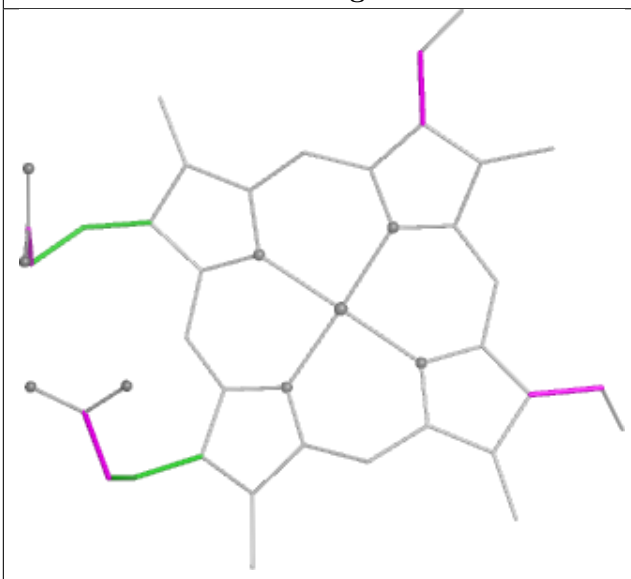
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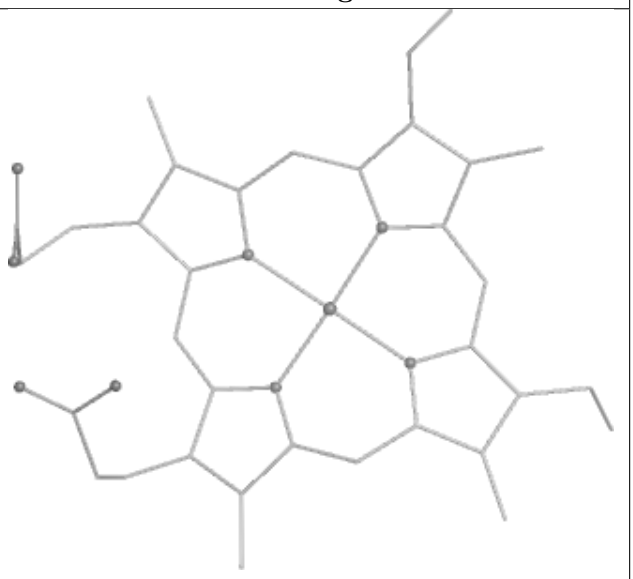
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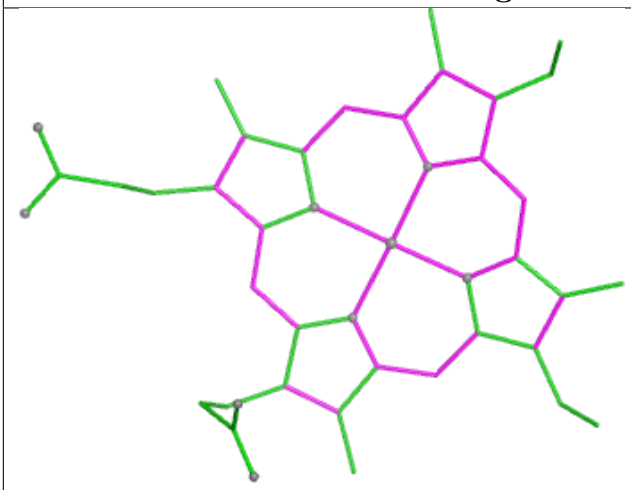


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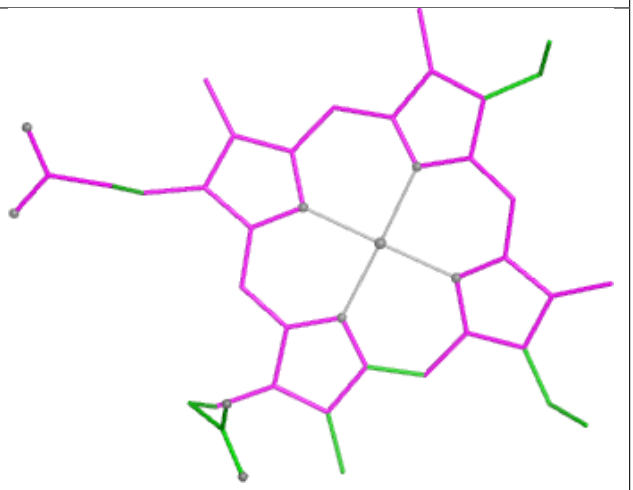


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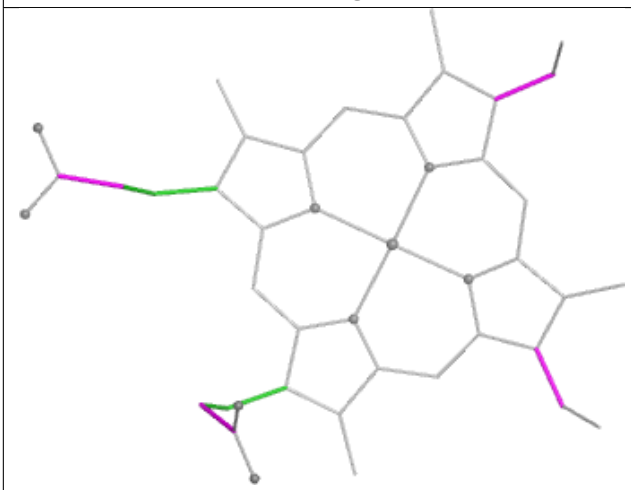
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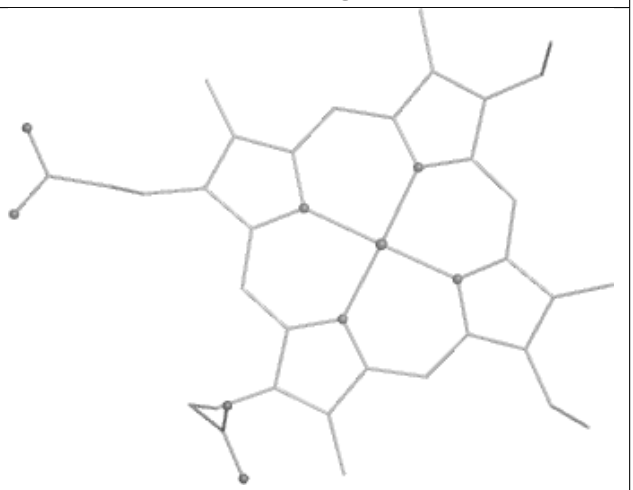
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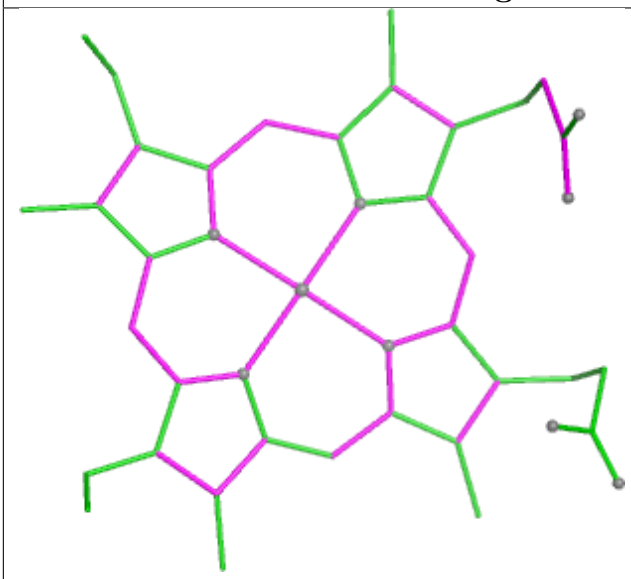


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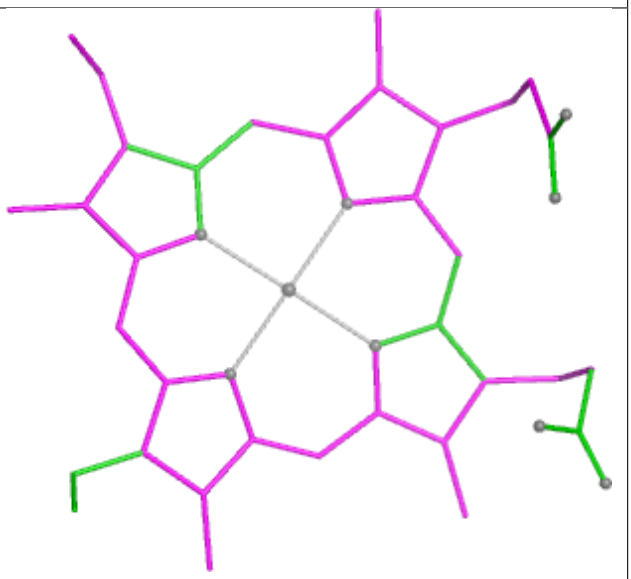


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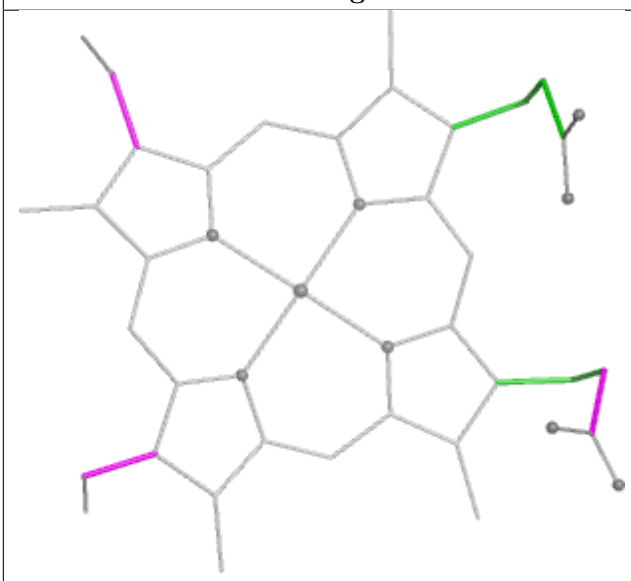
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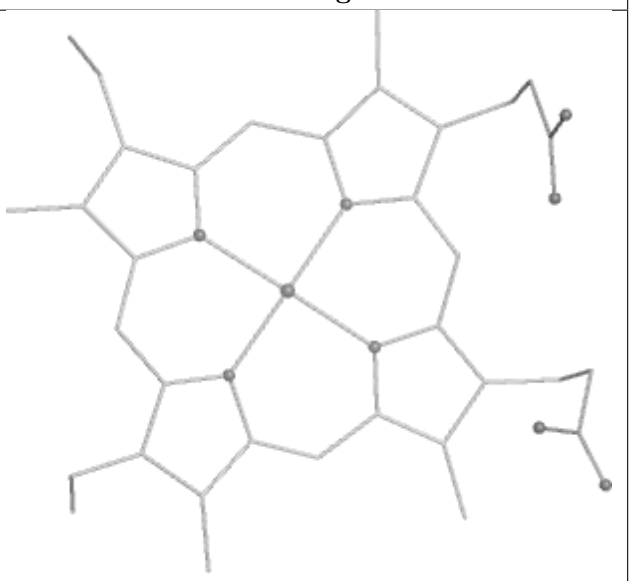
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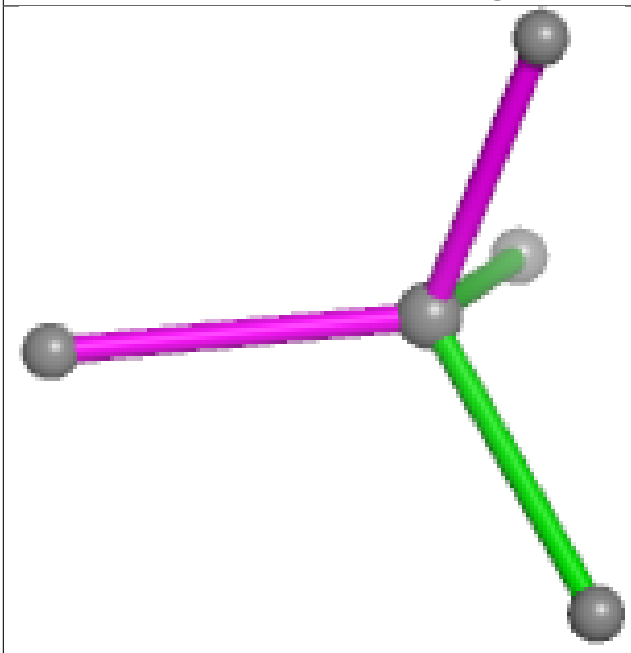


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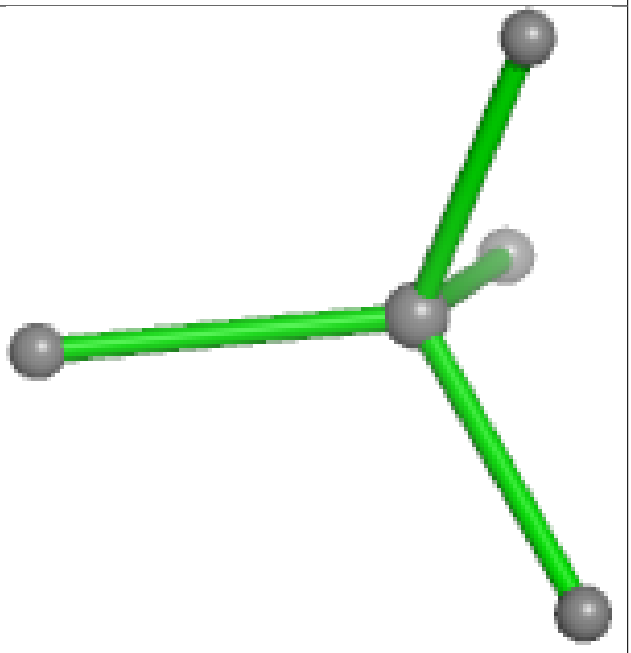


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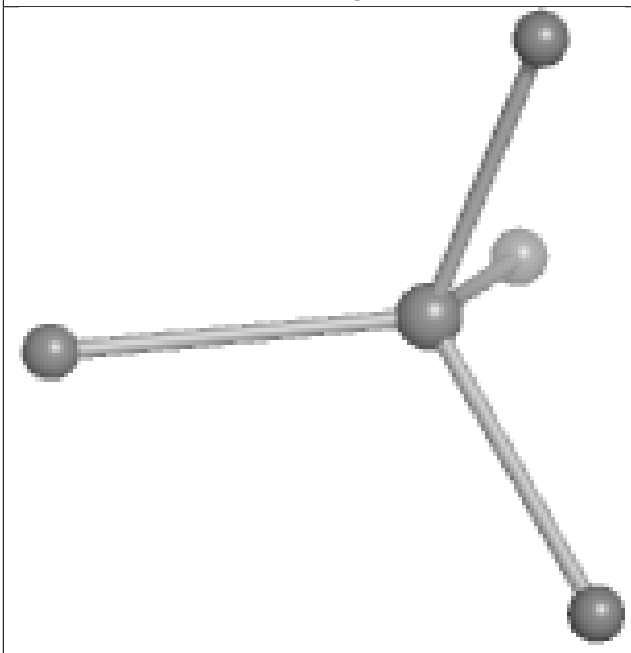
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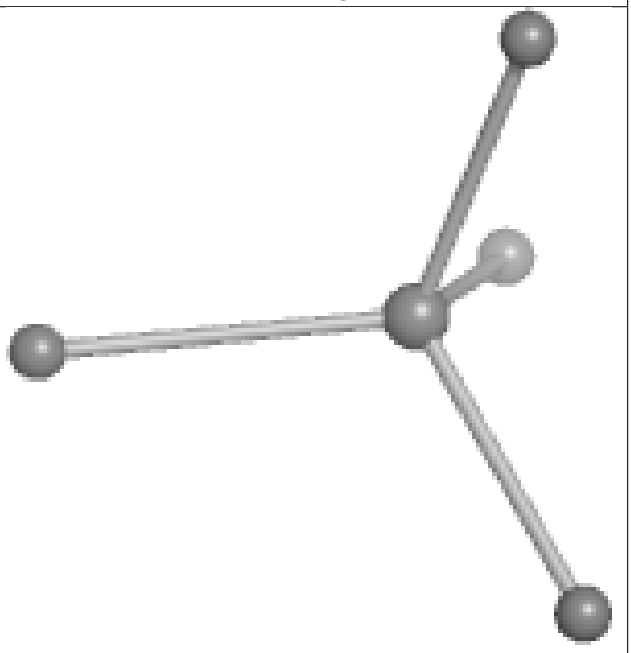
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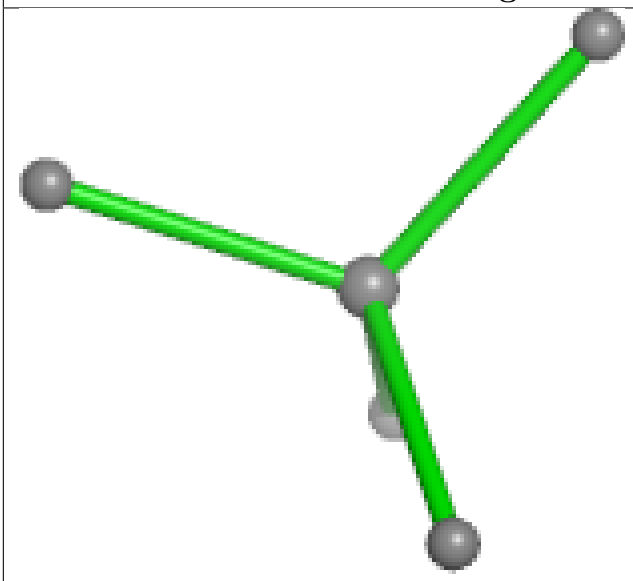


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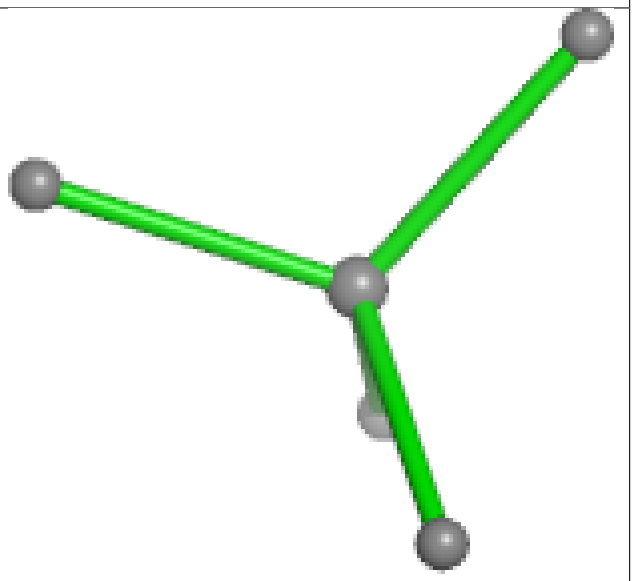


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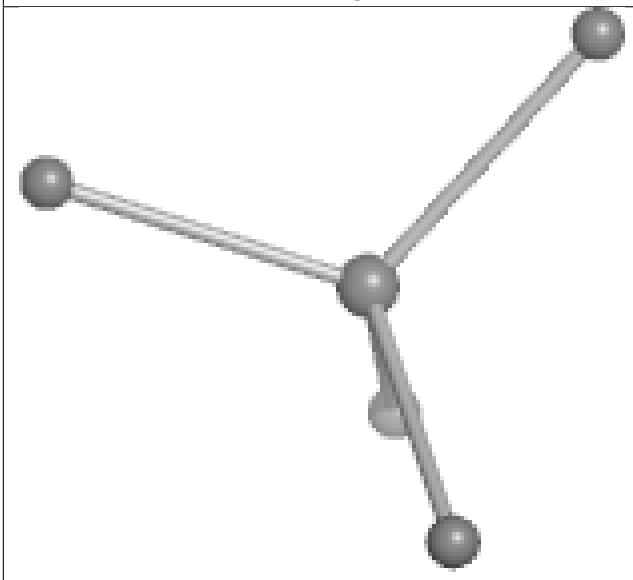
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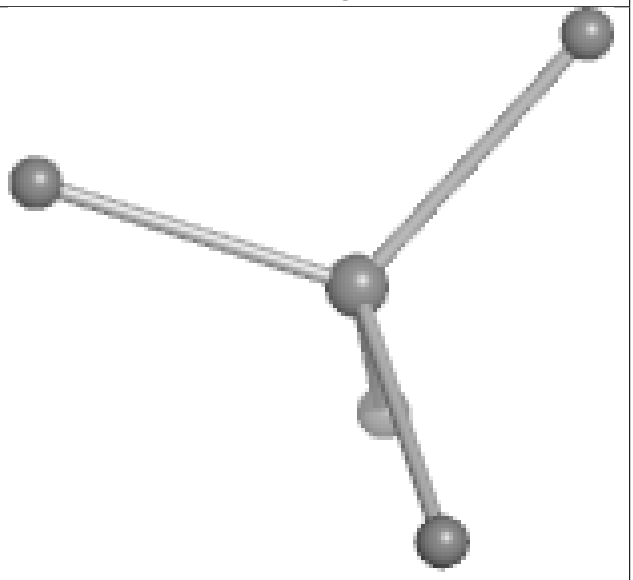
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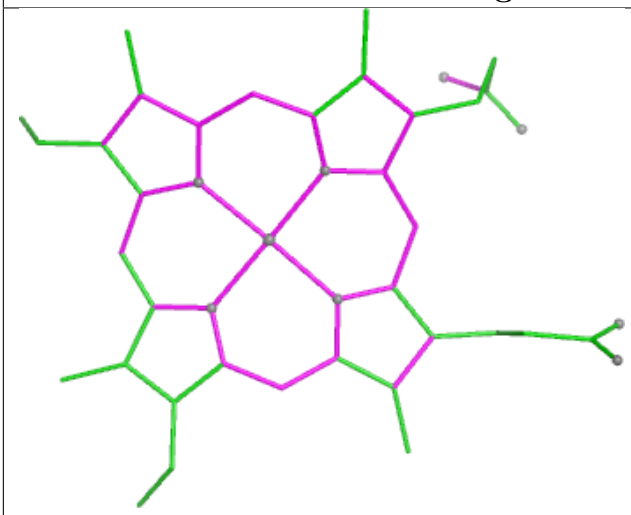


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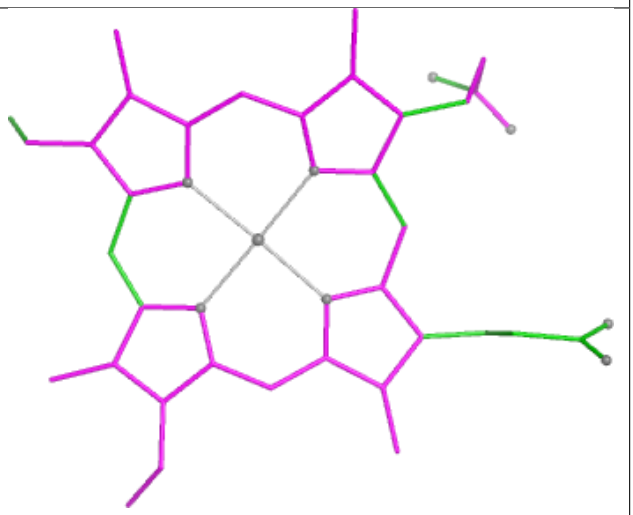


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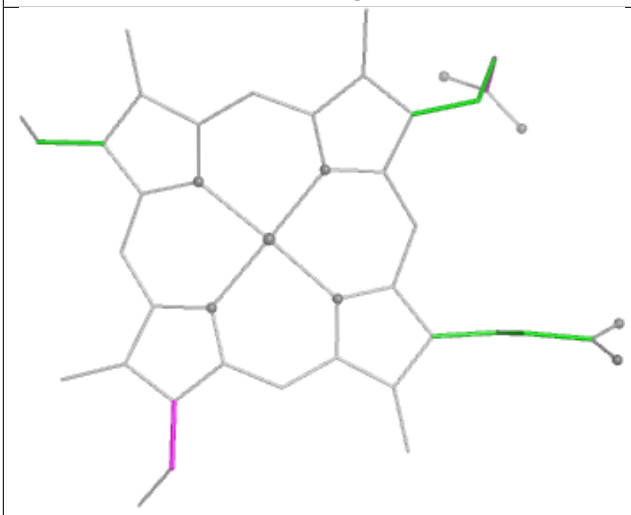
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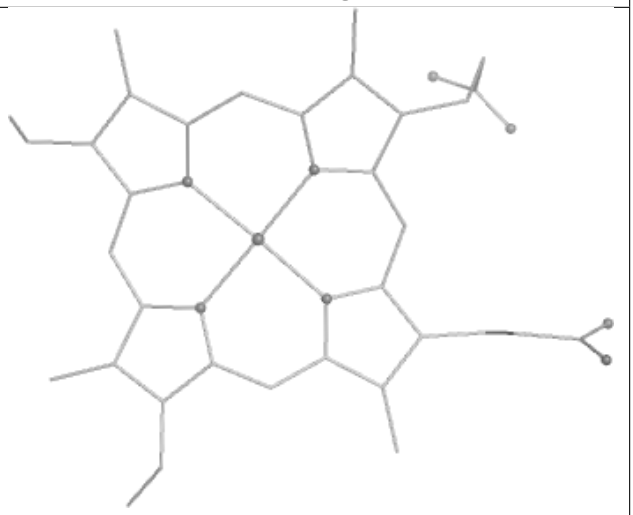
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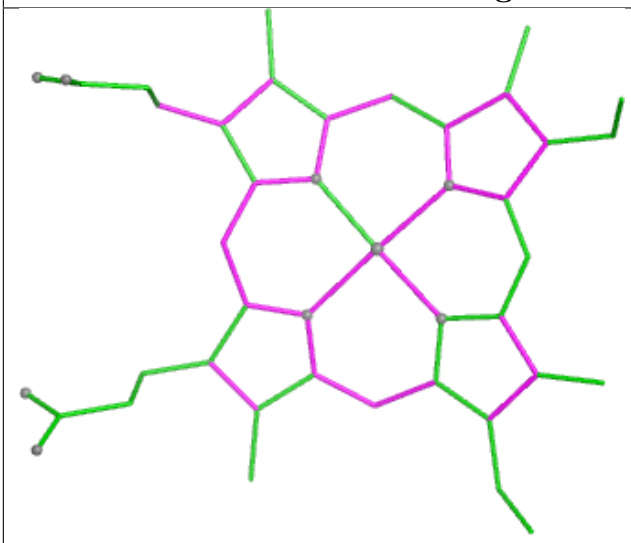


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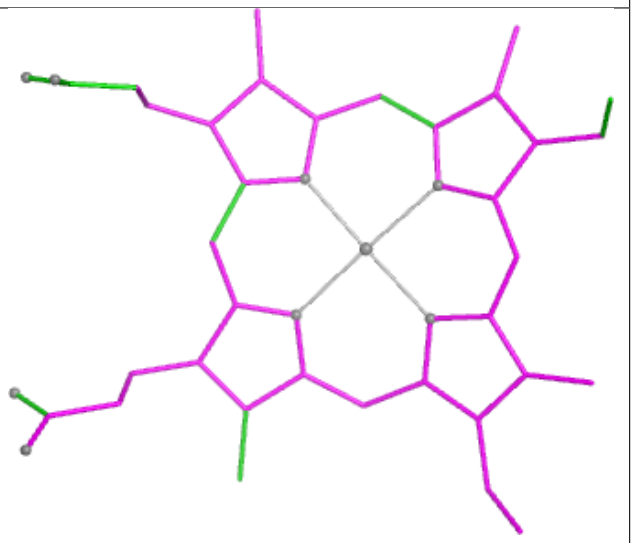


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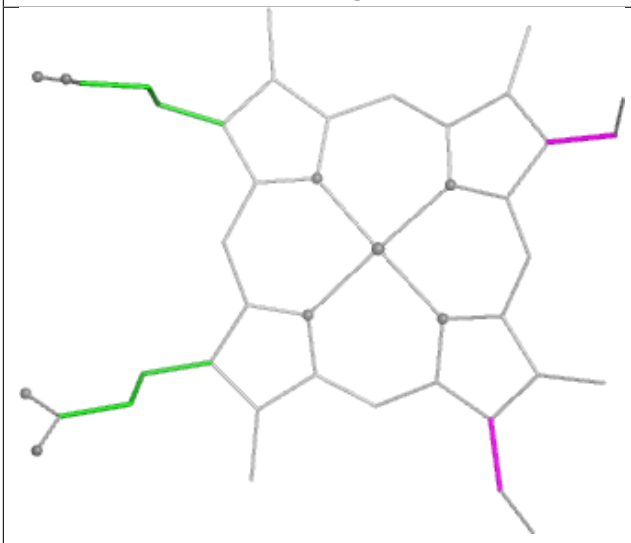
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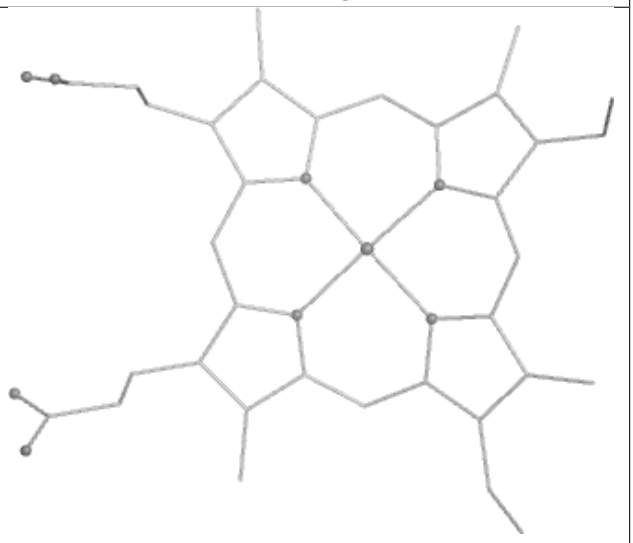
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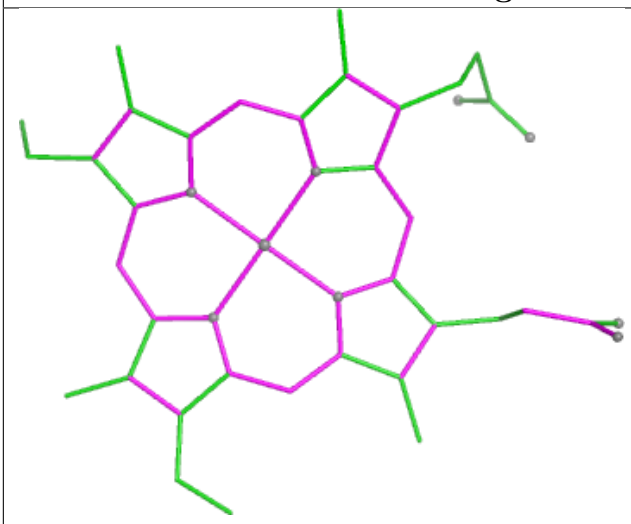


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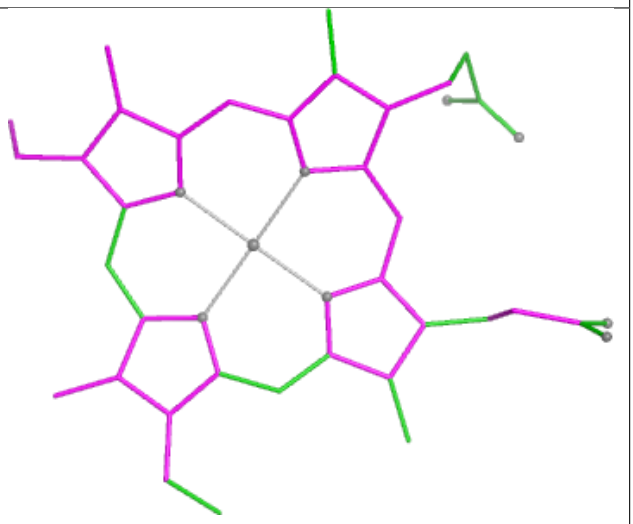


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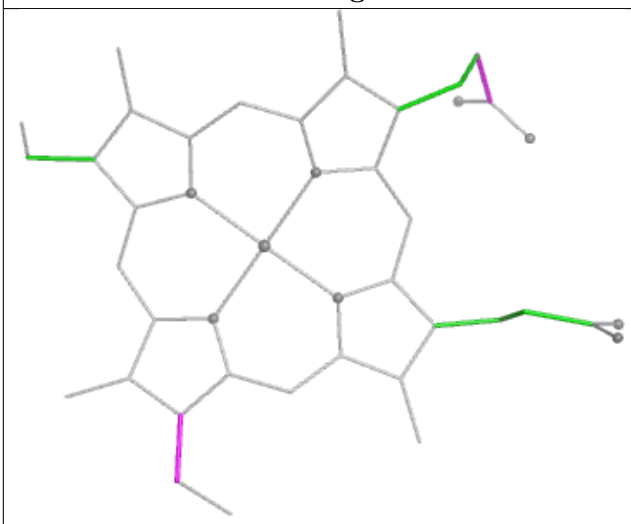
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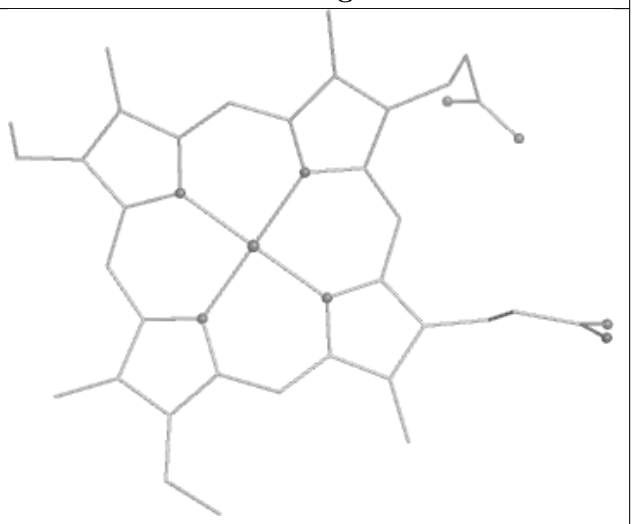
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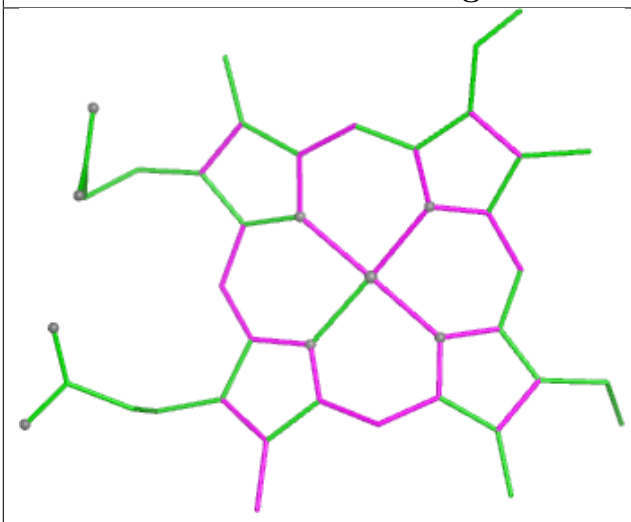


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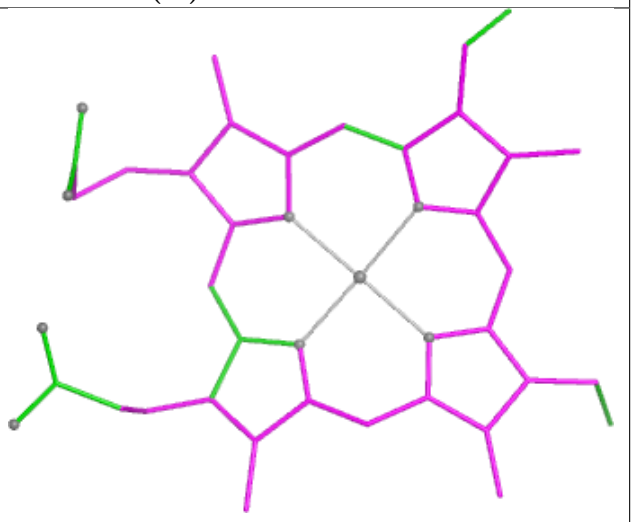


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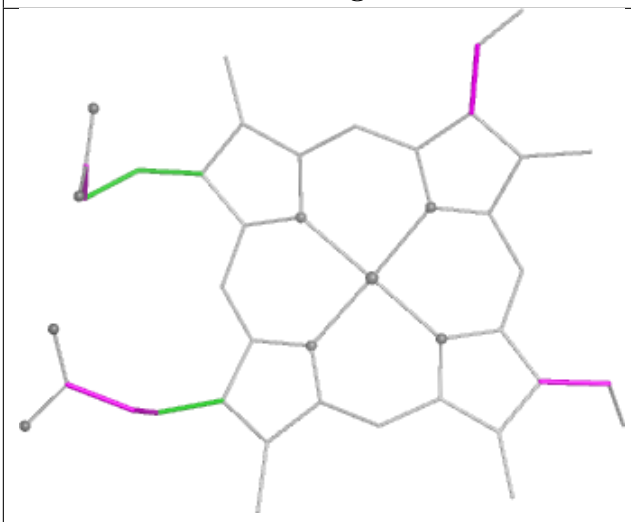
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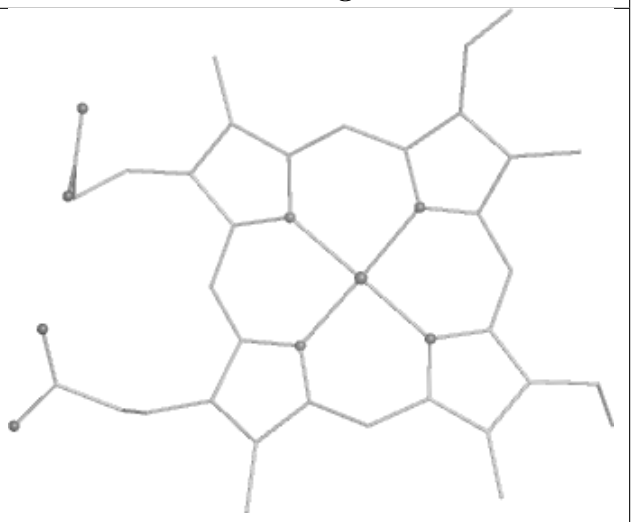
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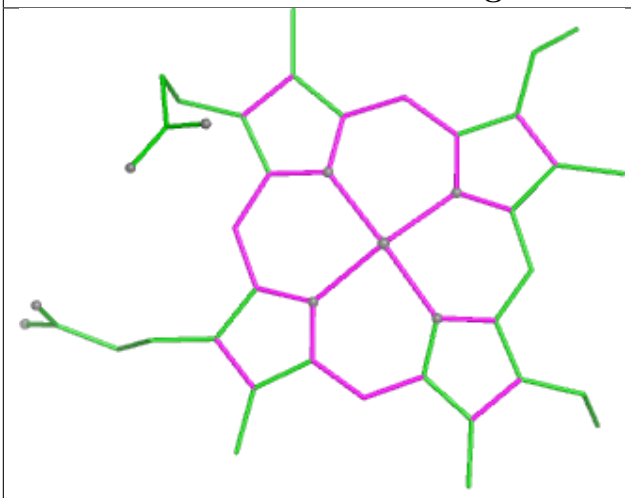


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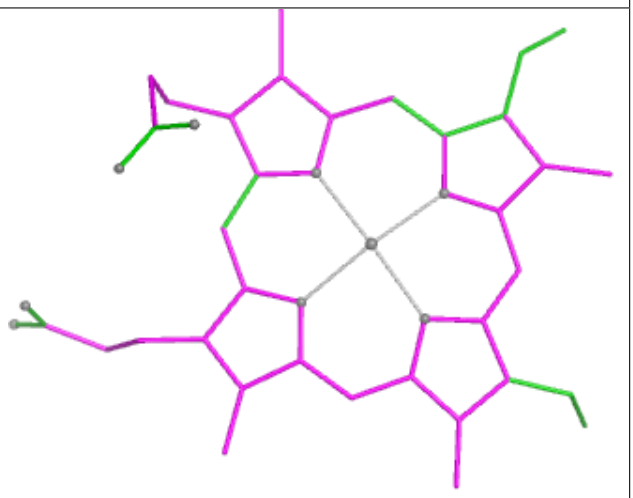


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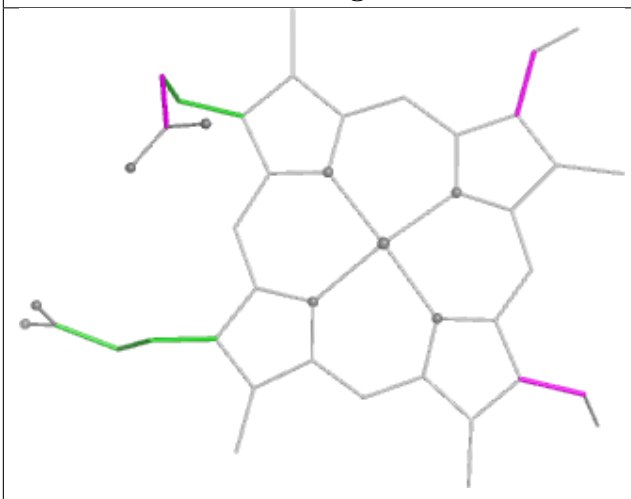
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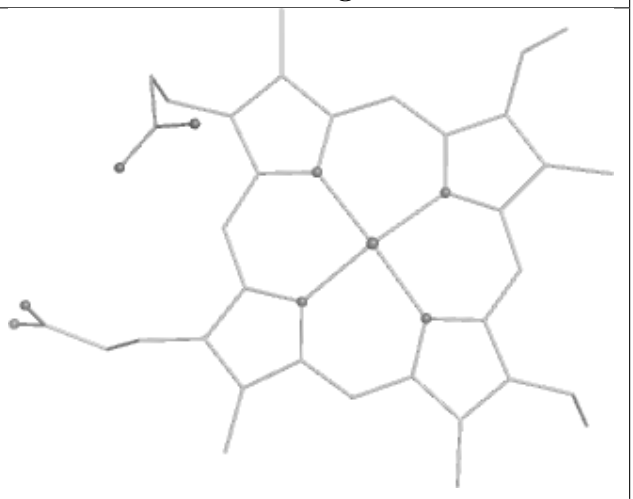
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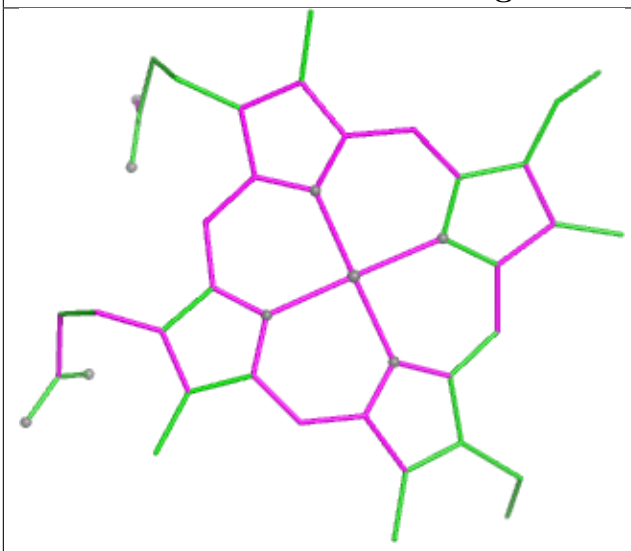


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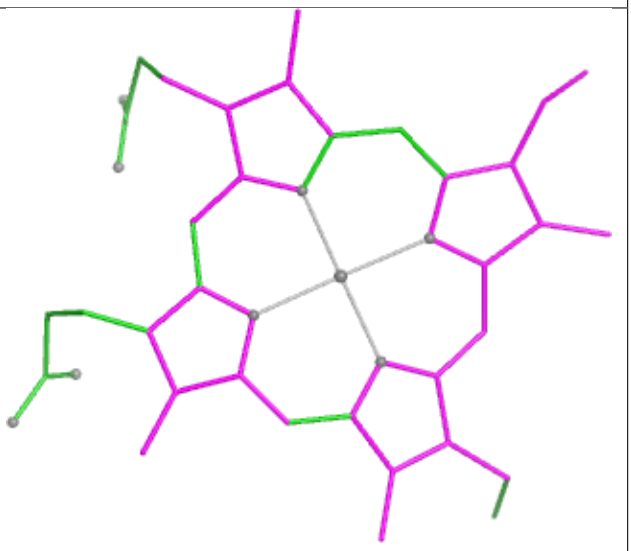


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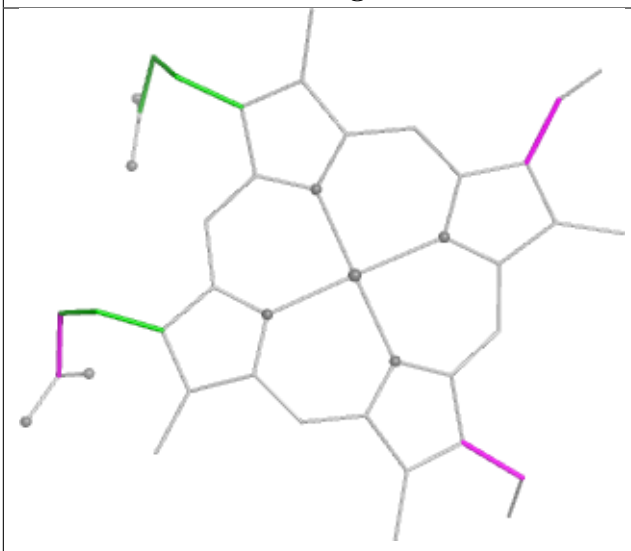
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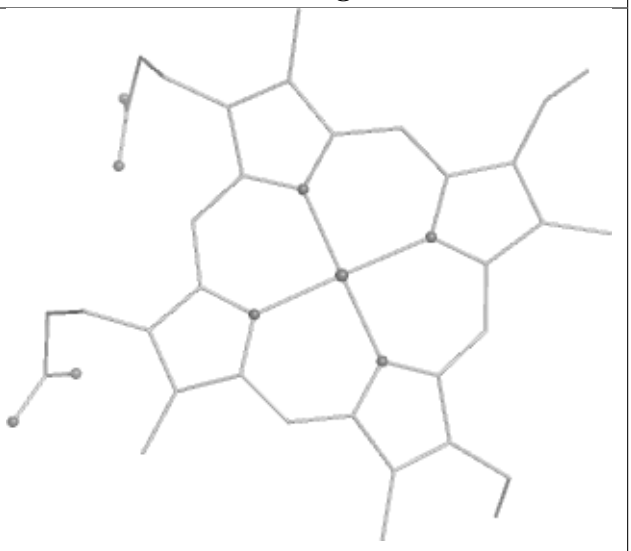
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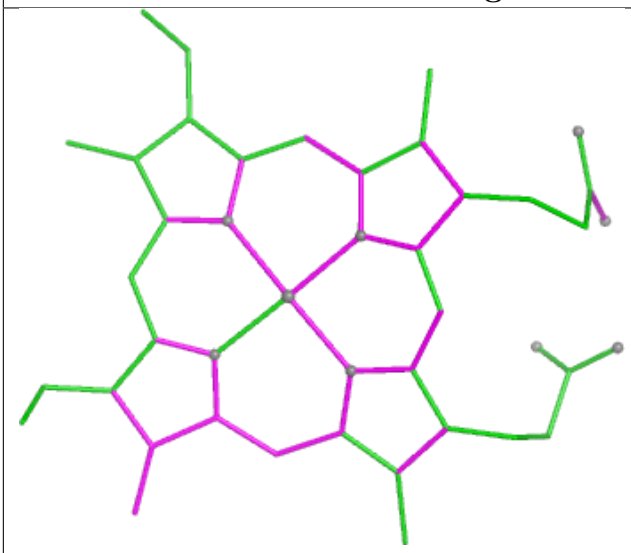


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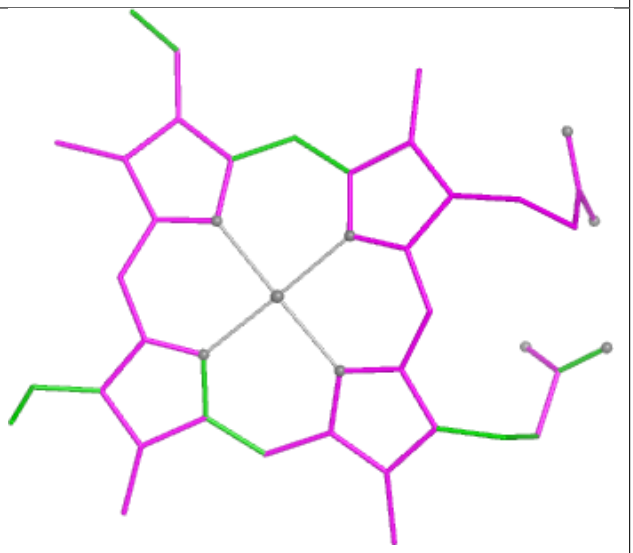


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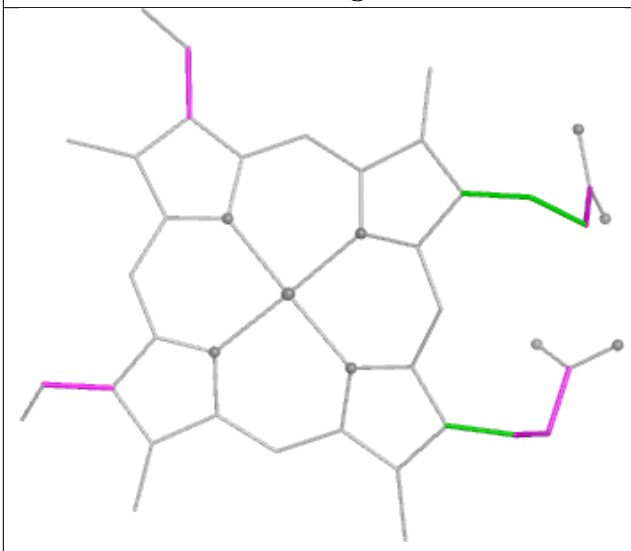
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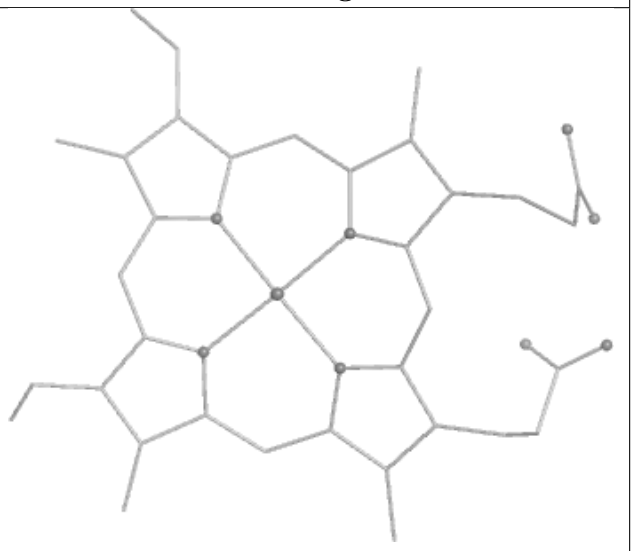
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Bond angles

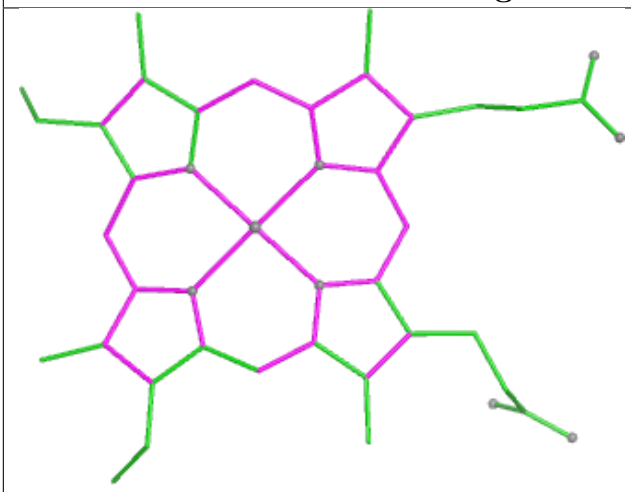


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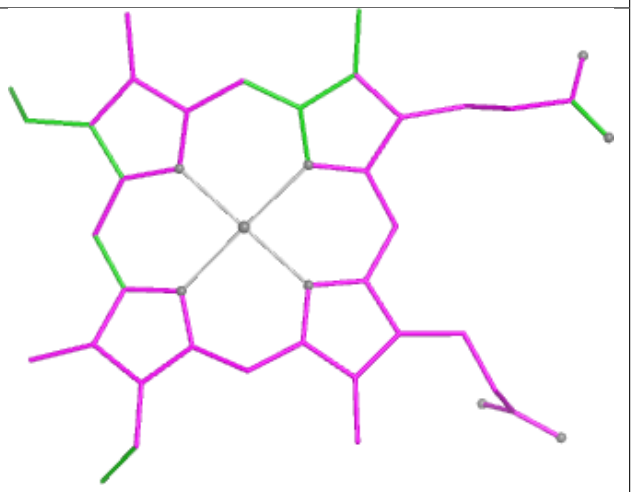


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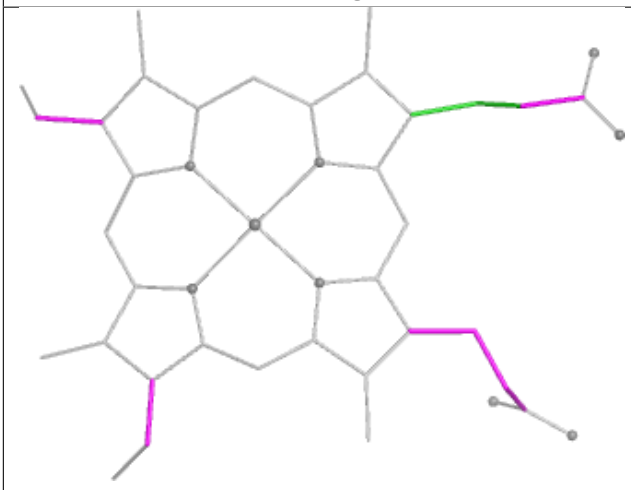
Ligand HEC YYY 601



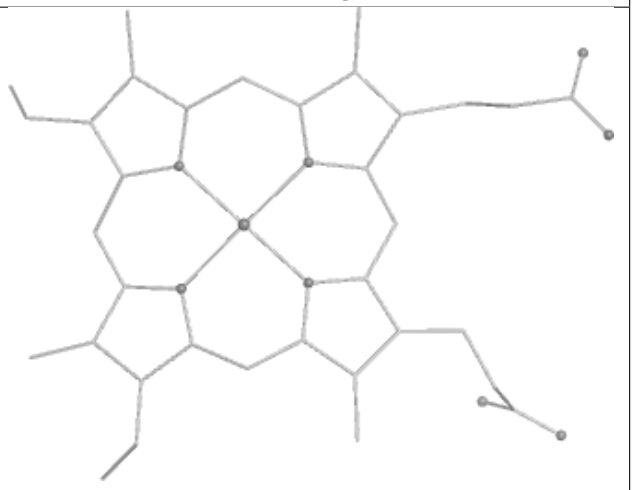
Bond lengths



Bond angles

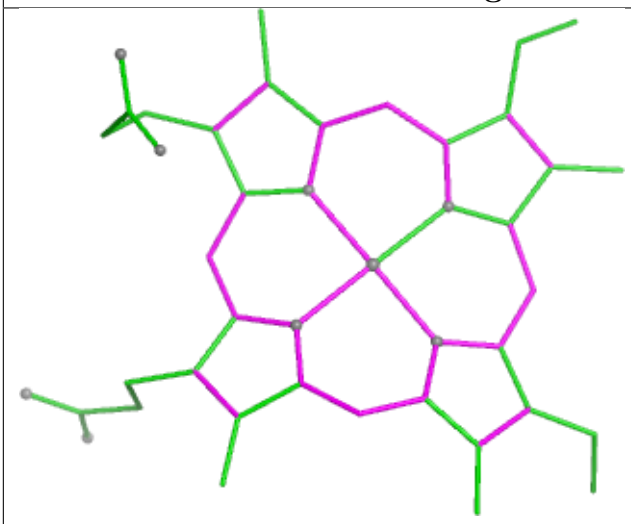


Torsions

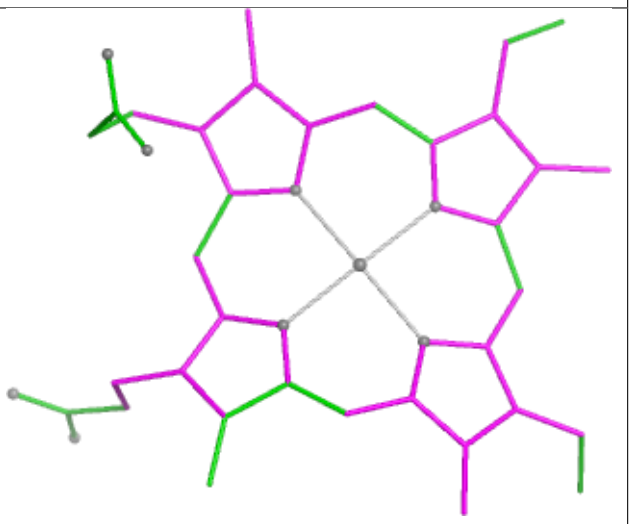


Rings

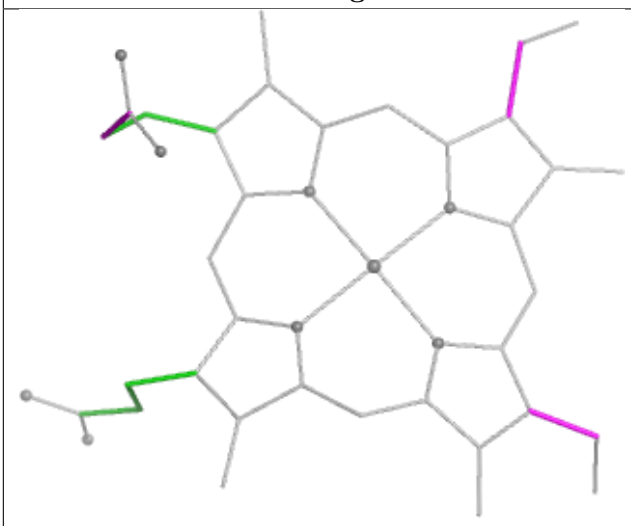
Ligand HEC MMM 608



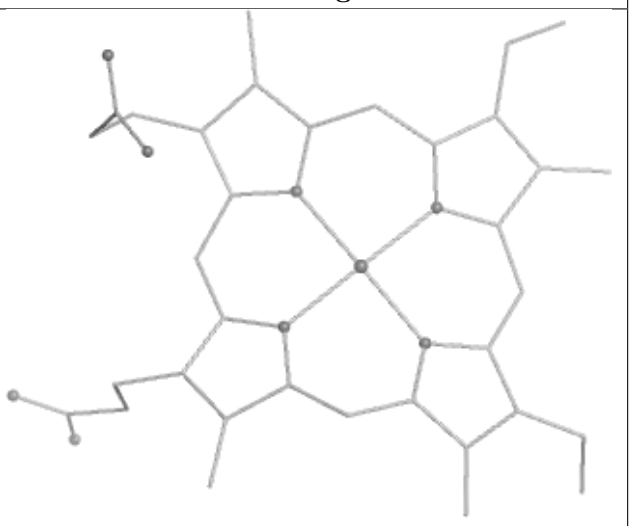
Bond lengths



Bond angles

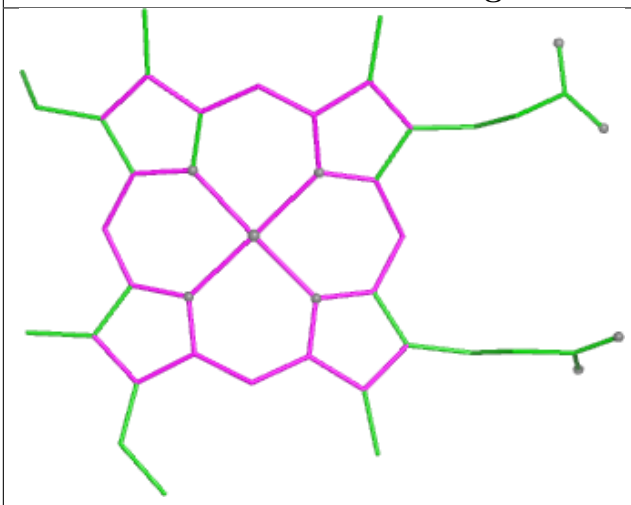


Torsions

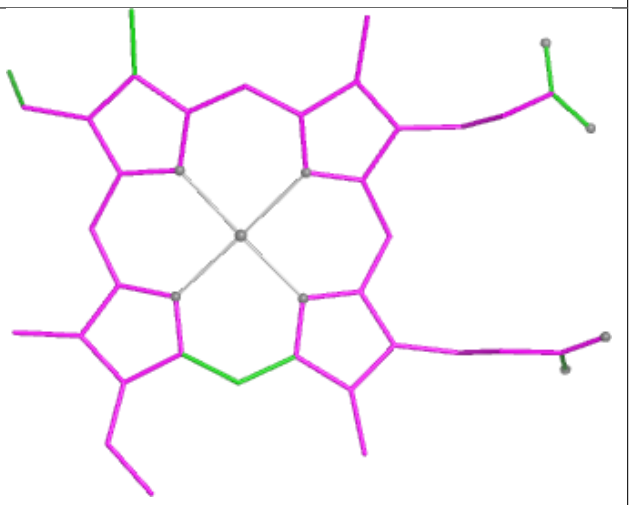


Rings

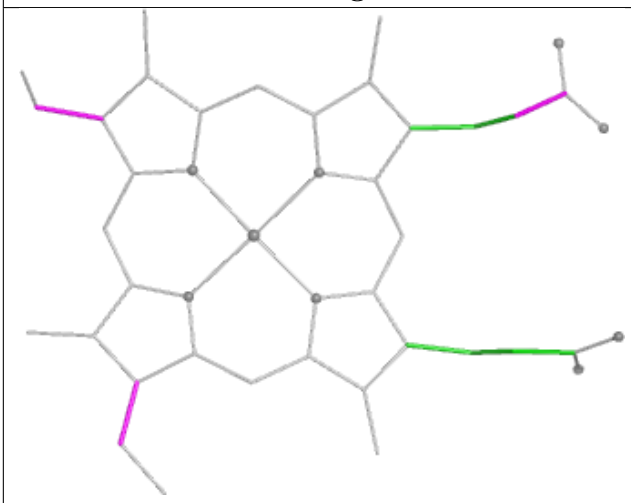
Ligand HEC MMM 601



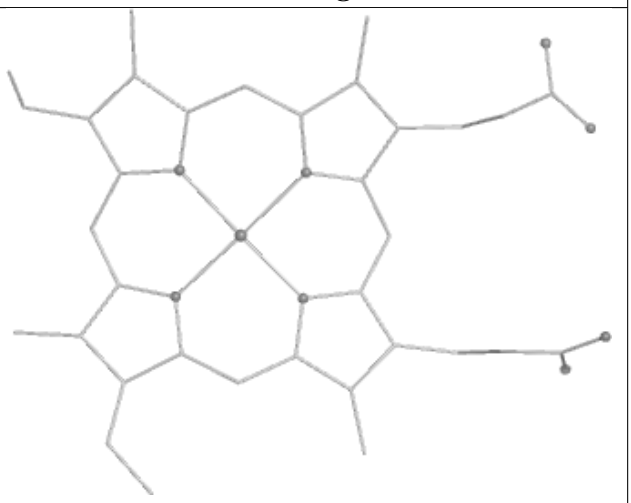
Bond lengths



Bond angles

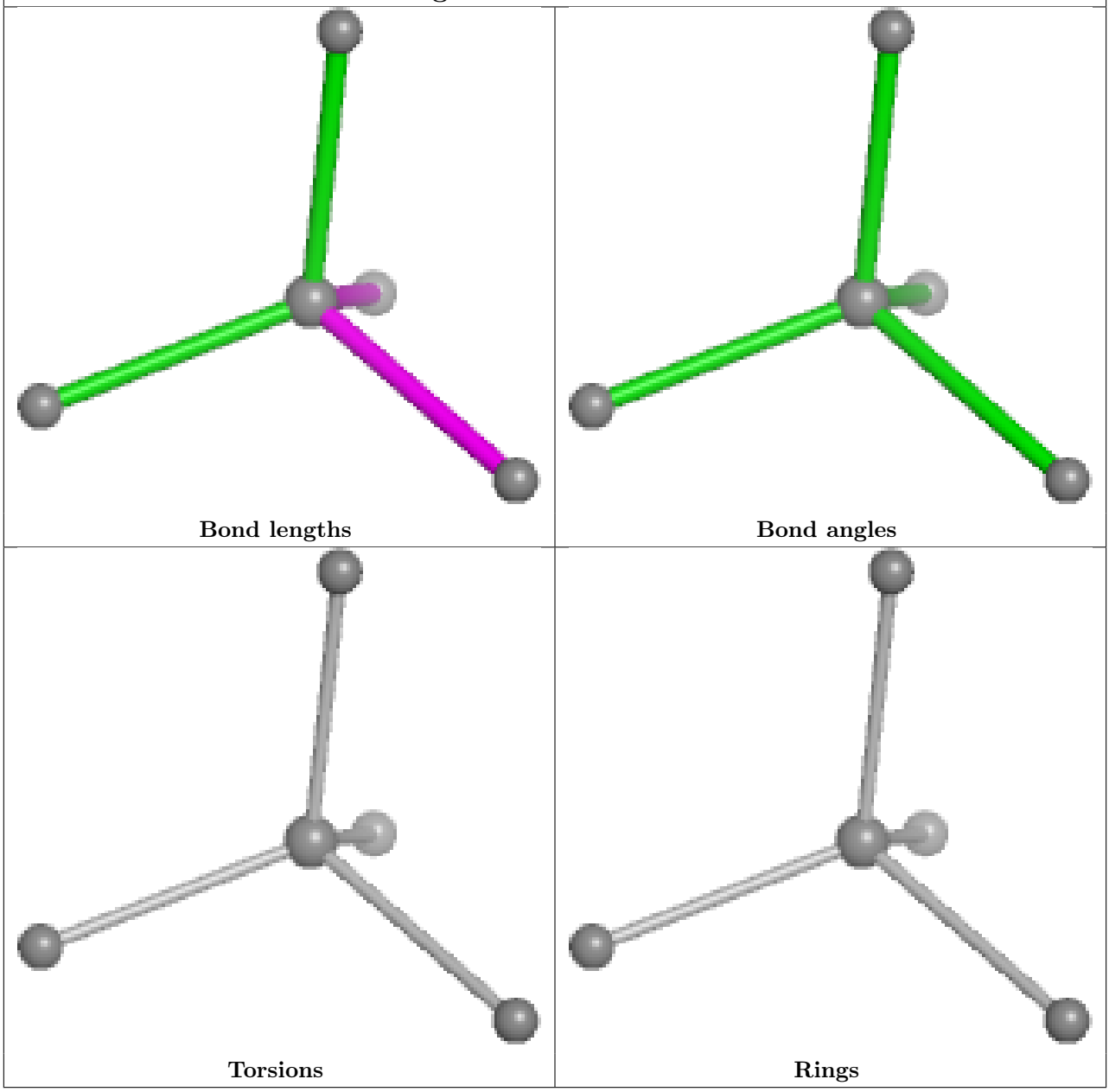


Torsions



Rings

Ligand PO4 AAA 610



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AAA	495/495 (100%)	-1.07	0	100	100	12, 22, 36, 55	2 (0%)
1	MMM	495/495 (100%)	-1.06	0	100	100	10, 21, 37, 69	3 (0%)
1	YYY	495/495 (100%)	-1.06	0	100	100	9, 22, 38, 53	2 (0%)
All	All	1485/1485 (100%)	-1.07	0	100	100	9, 22, 38, 69	7 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	AAA	601	43/43	0.99	0.04	16,23,32,38	0
2	HEC	AAA	602	43/43	0.99	0.04	19,22,25,32	0
2	HEC	AAA	603	43/43	0.99	0.04	22,28,32,33	0
2	HEC	AAA	604	43/43	0.99	0.03	10,15,18,19	0
2	HEC	AAA	605	43/43	0.99	0.04	17,22,25,27	0

Continued on next page...

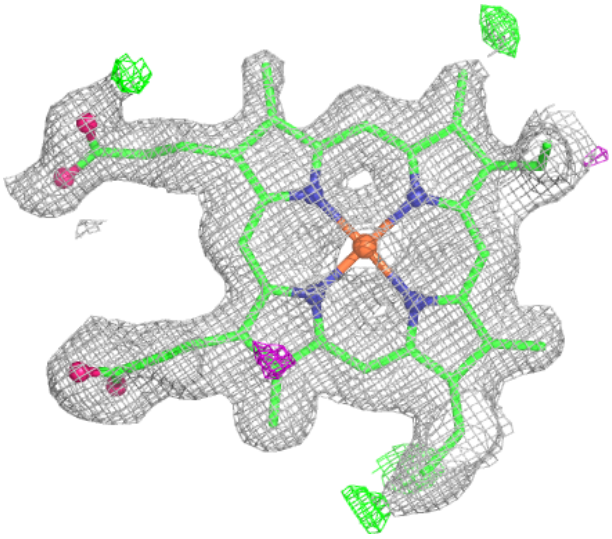
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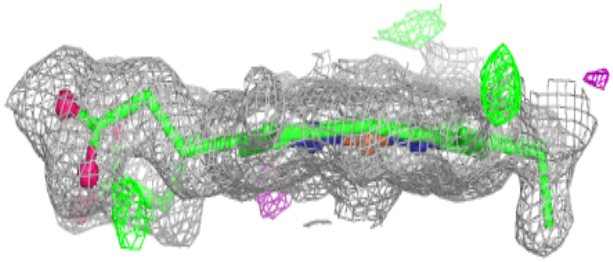
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEC	AAA	606	43/43	0.99	0.03	12,15,18,21	0
2	HEC	AAA	607[A]	43/43	0.99	0.03	11,14,18,18	3
2	HEC	AAA	607[B]	43/43	0.99	0.03	11,14,18,18	3
2	HEC	AAA	608	43/43	0.99	0.03	13,18,27,34	0
2	HEC	MMM	601	43/43	0.99	0.04	22,26,30,39	0
2	HEC	MMM	602	43/43	0.99	0.04	16,21,23,26	0
2	HEC	MMM	603	43/43	0.99	0.04	24,26,35,42	0
2	HEC	MMM	604	43/43	0.99	0.03	11,15,17,22	0
2	HEC	MMM	605	43/43	0.99	0.04	14,21,29,30	0
2	HEC	MMM	606	43/43	0.99	0.03	11,14,16,21	0
2	HEC	MMM	607	43/43	0.99	0.03	12,15,20,23	0
2	HEC	MMM	608	43/43	0.99	0.03	13,17,27,35	0
2	HEC	YYY	601	43/43	0.99	0.04	20,25,31,40	0
2	HEC	YYY	602	43/43	0.99	0.04	17,24,27,29	0
2	HEC	YYY	603	43/43	0.99	0.04	20,27,29,31	0
2	HEC	YYY	604	43/43	0.99	0.03	12,16,20,23	0
2	HEC	YYY	605	43/43	0.99	0.03	14,22,27,36	0
2	HEC	YYY	606	43/43	0.99	0.03	13,16,18,20	0
2	HEC	YYY	608	43/43	0.99	0.03	14,22,28,31	0
3	CA	MMM	609	1/1	0.99	0.02	21,21,21,21	0
4	PO4	AAA	610	5/5	0.99	0.03	17,18,20,21	0
4	PO4	MMM	610	5/5	0.99	0.03	19,21,23,24	0
4	PO4	YYY	610	5/5	0.99	0.04	16,20,23,23	0
3	CA	AAA	609	1/1	1.00	0.01	21,21,21,21	0
2	HEC	YYY	607	43/43	1.00	0.03	13,16,20,22	0
3	CA	YYY	609	1/1	1.00	0.02	18,18,18,18	0

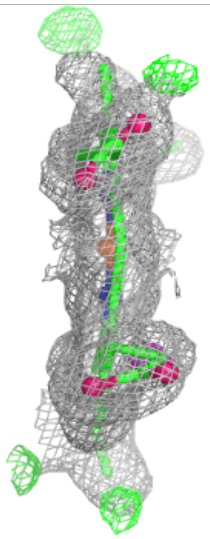
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC AAA 601:

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

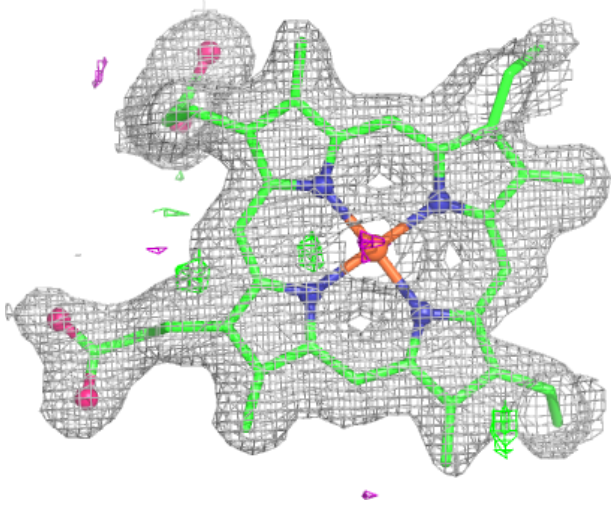


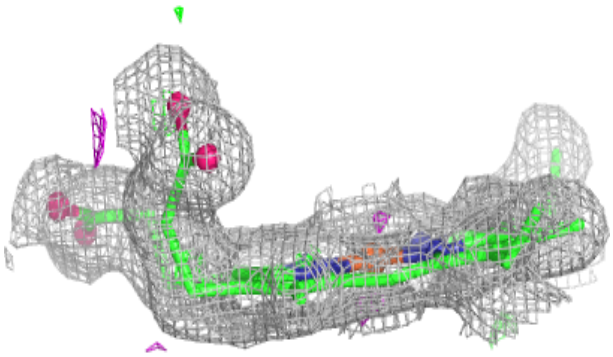


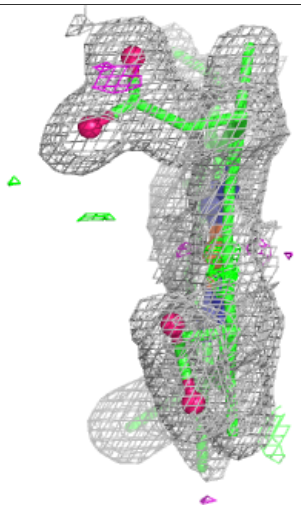


Electron density around HEC AAA 602:

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

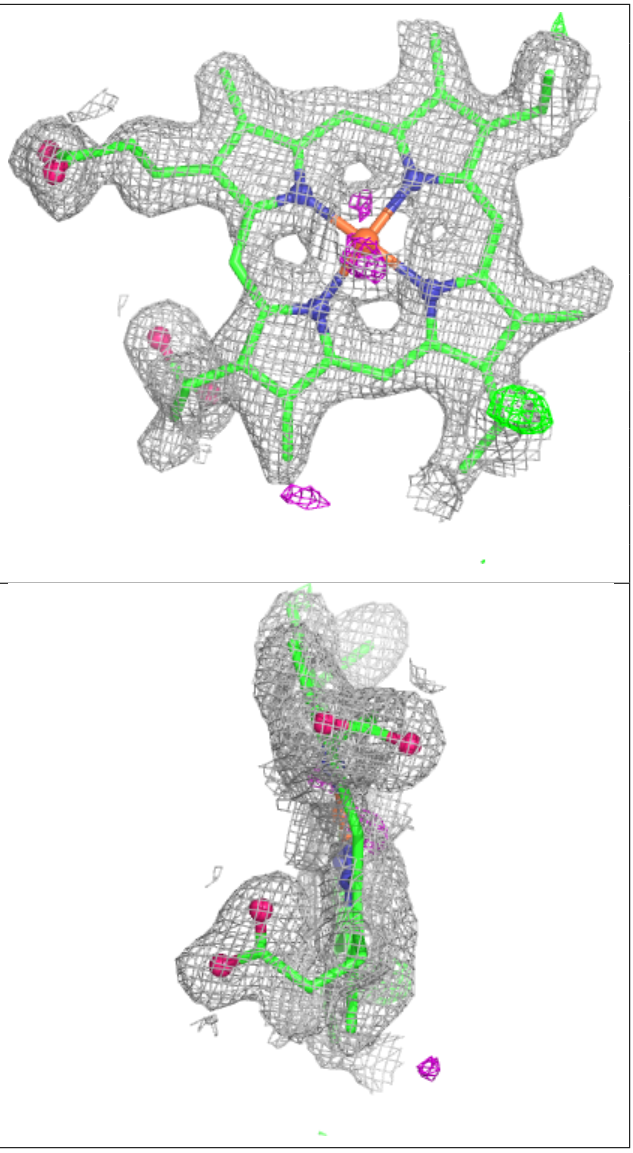






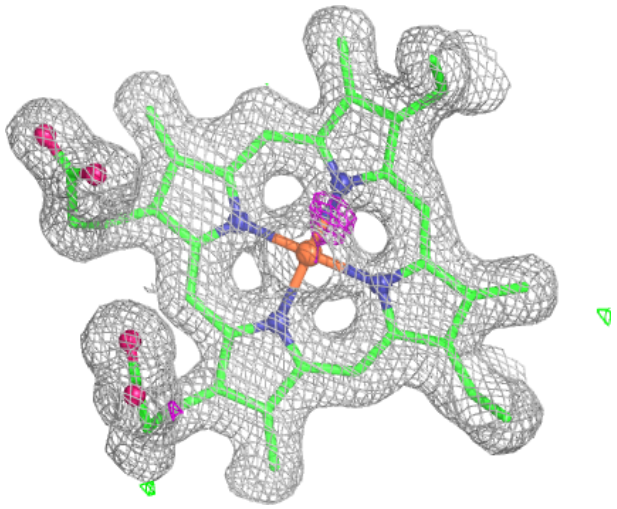
Electron density around HEC AAA 603:

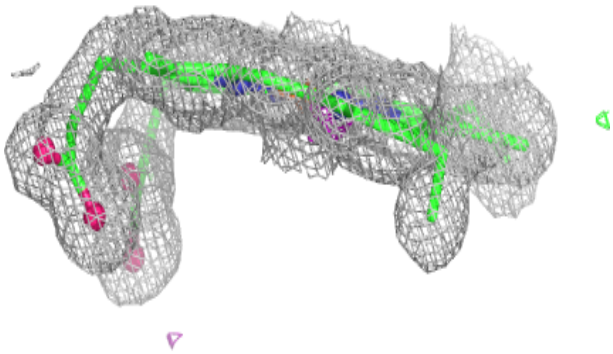
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

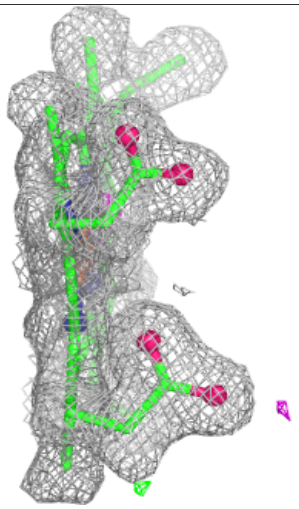


Electron density around HEC AAA 604:

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

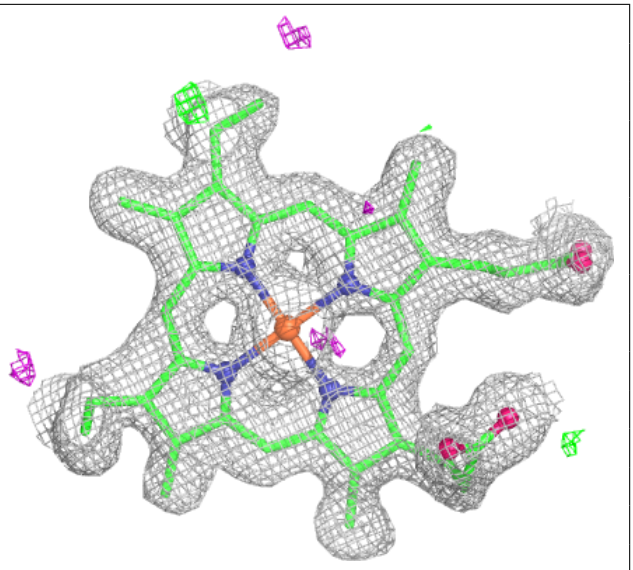


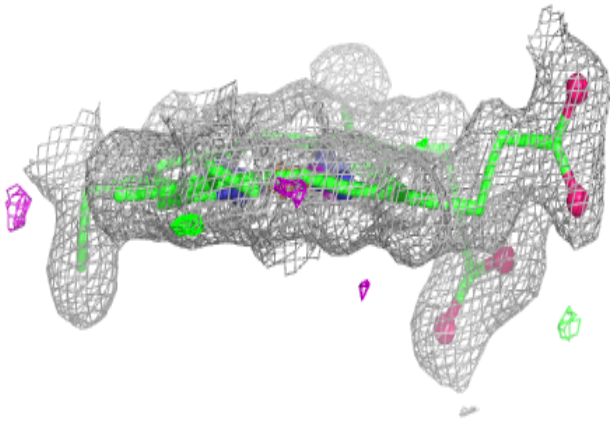


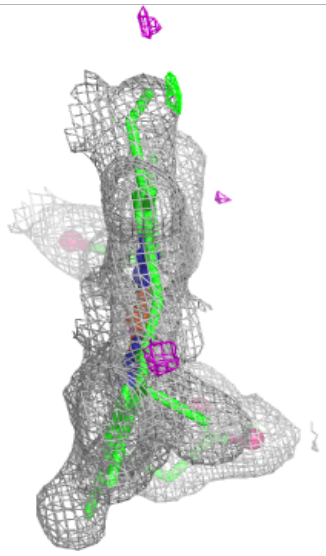


Electron density around HEC AAA 605:

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

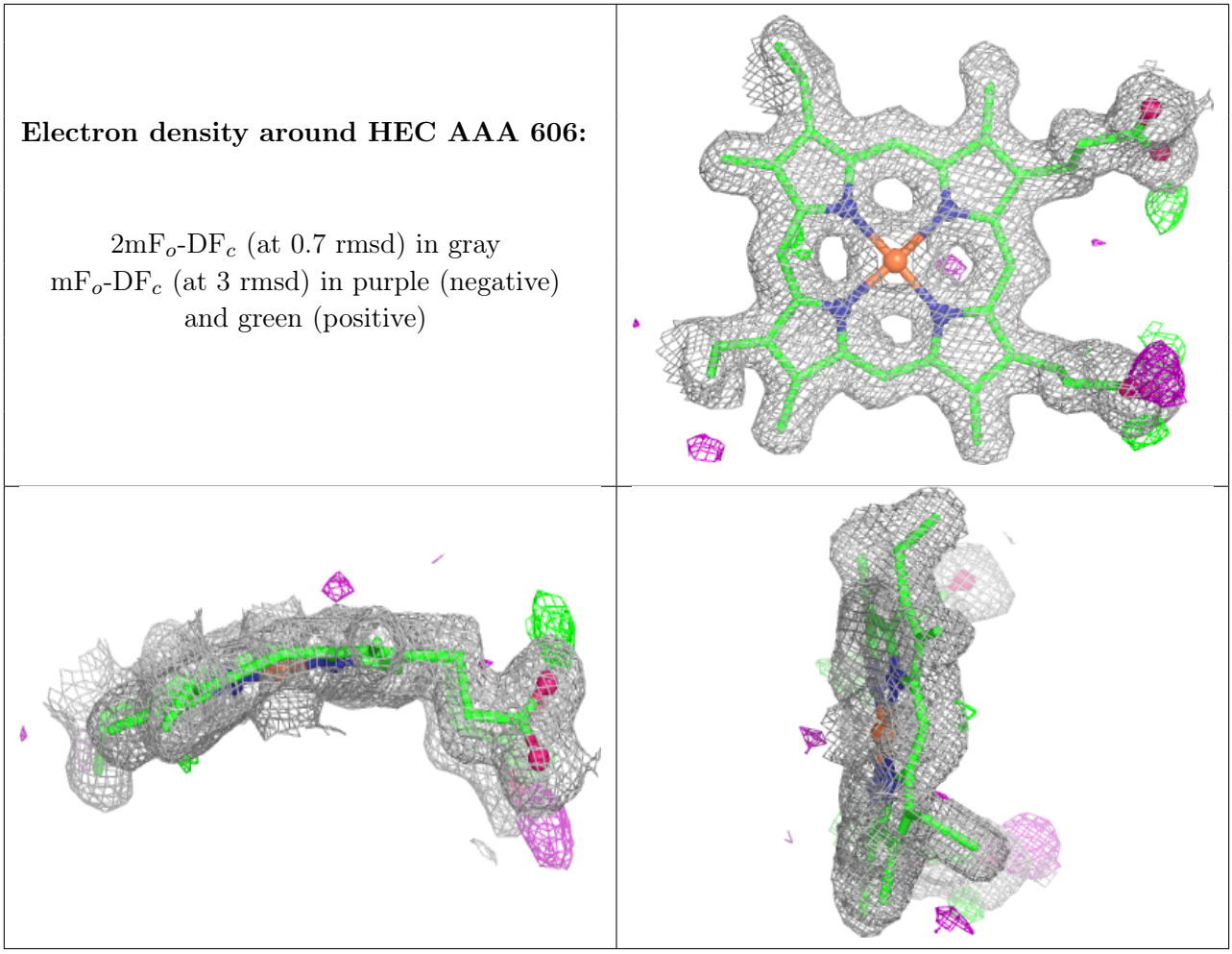






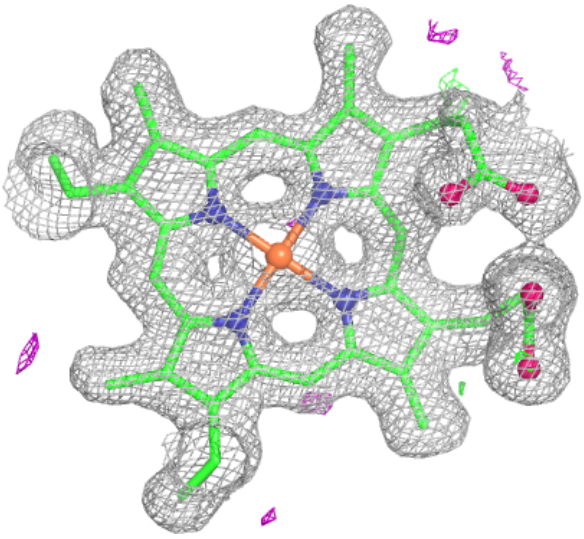
Electron density around HEC AAA 606:

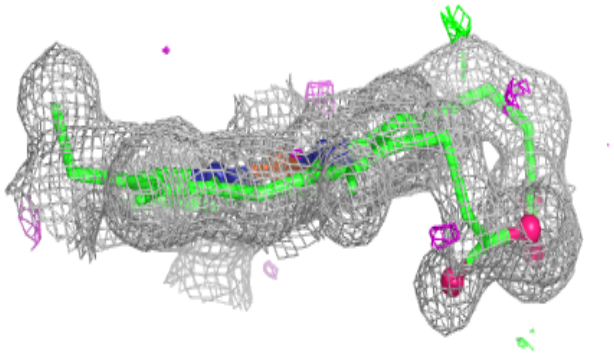
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

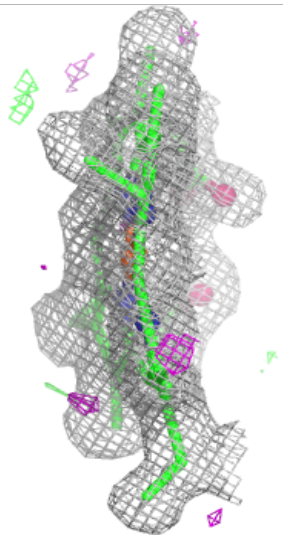


Electron density around HEC AAA 607 (A):

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

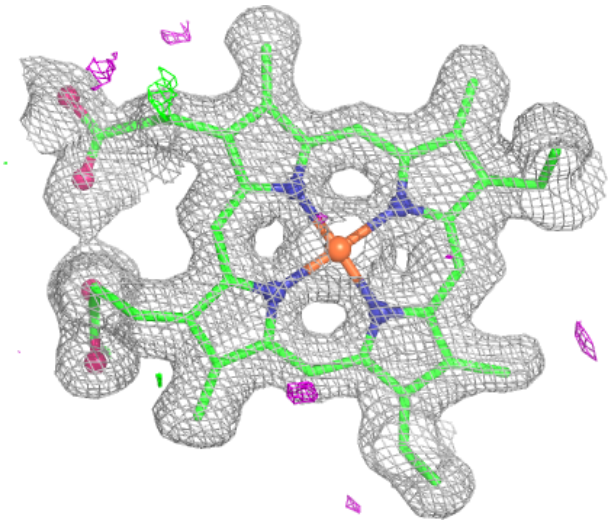


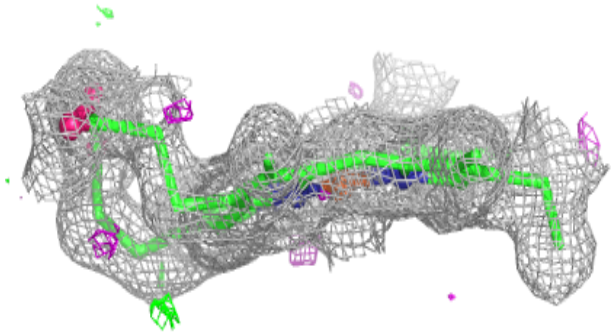


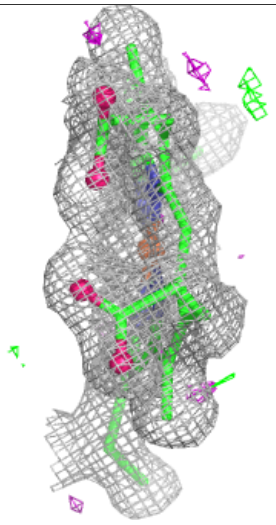


Electron density around HEC AAA 607 (B):

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

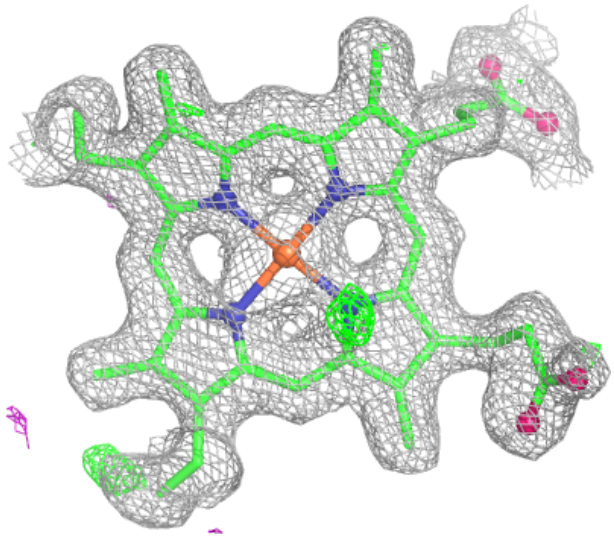


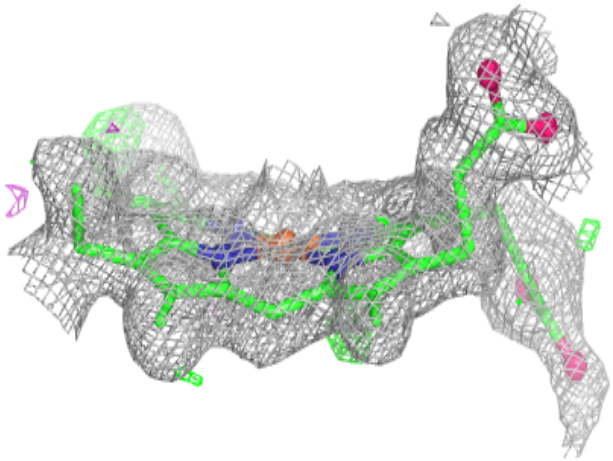


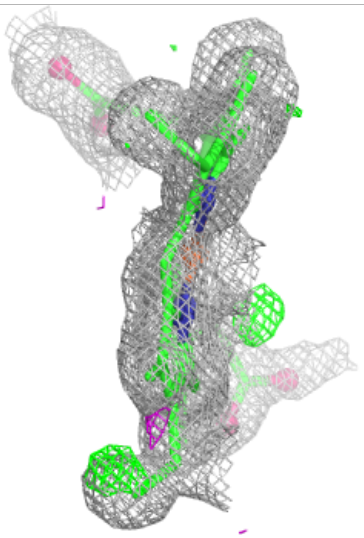


Electron density around HEC AAA 608:

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

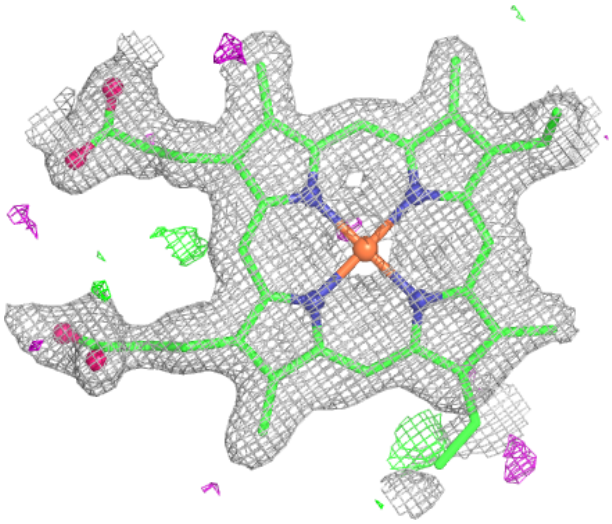


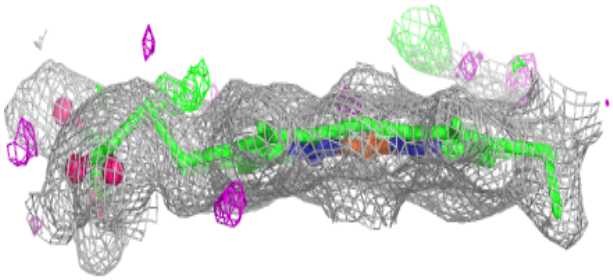


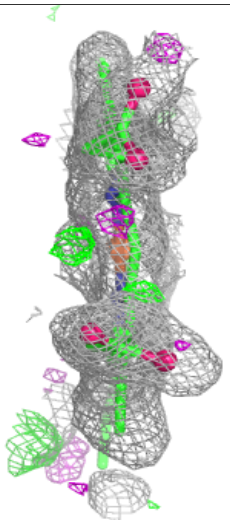


Electron density around HEC MMM 601:

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

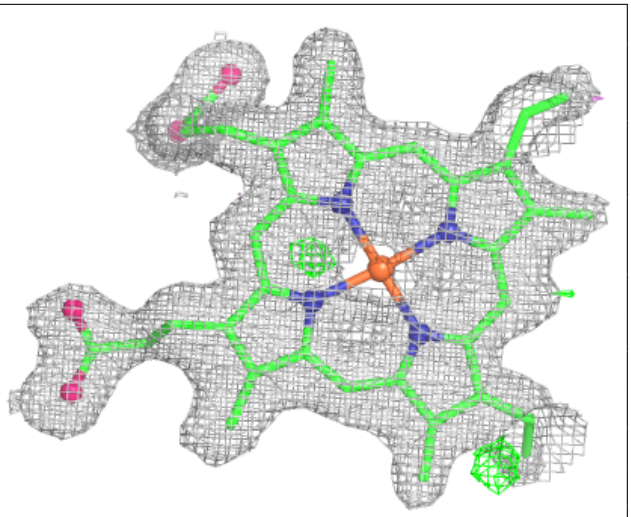


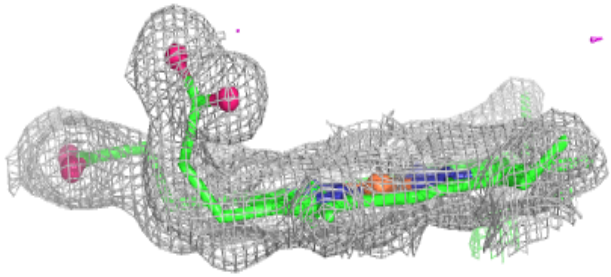


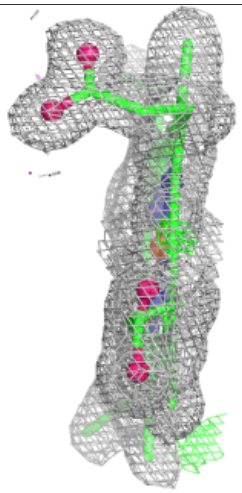


Electron density around HEC MMM 602:

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

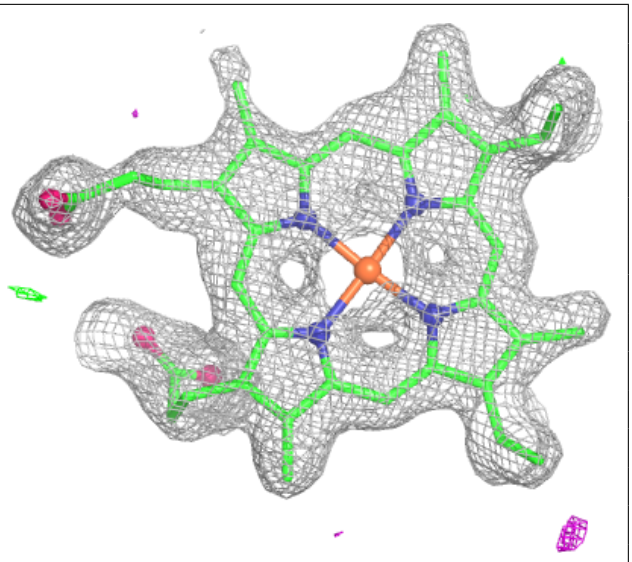


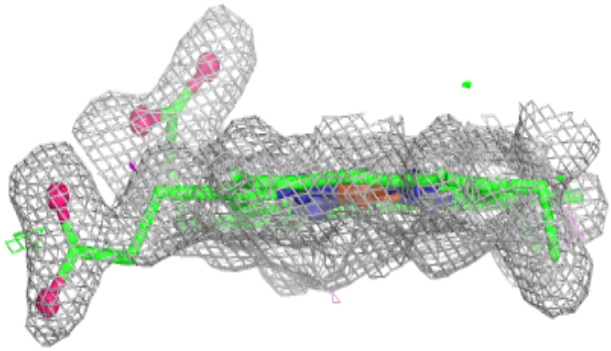


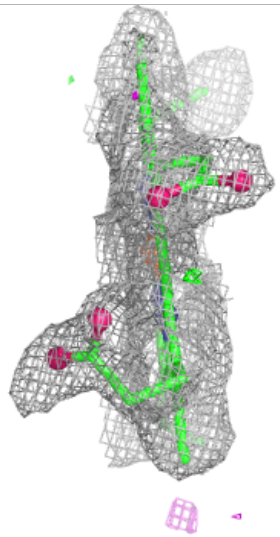


Electron density around HEC MMM 603:

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

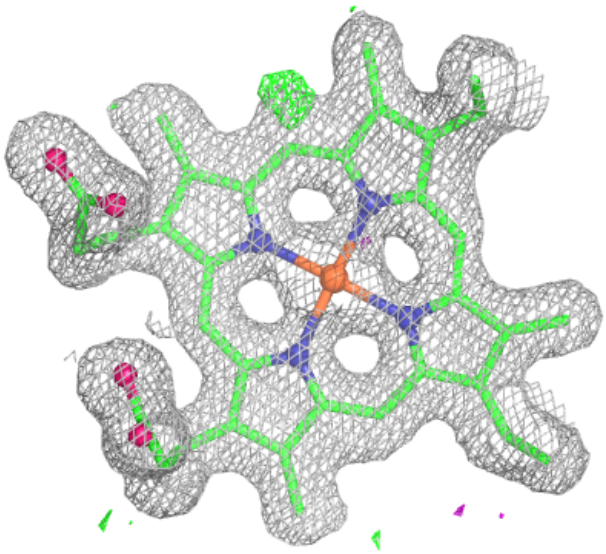


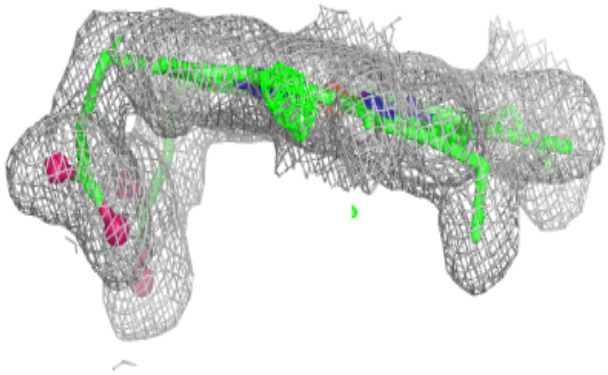


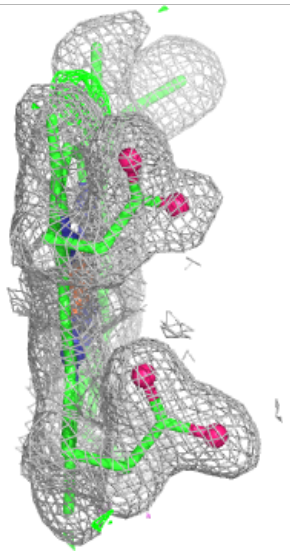


Electron density around HEC MMM 604:

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

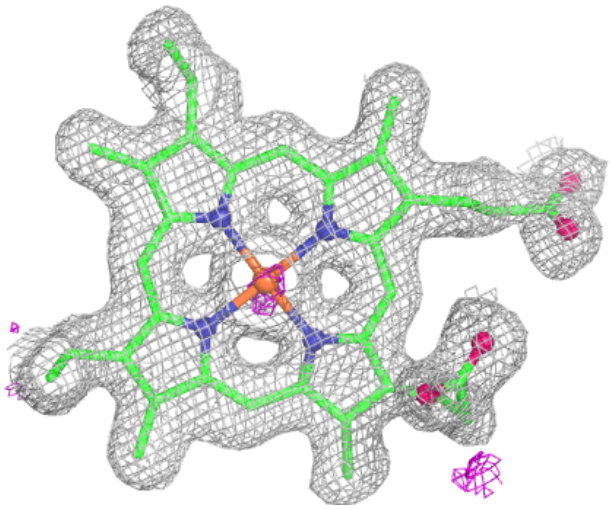


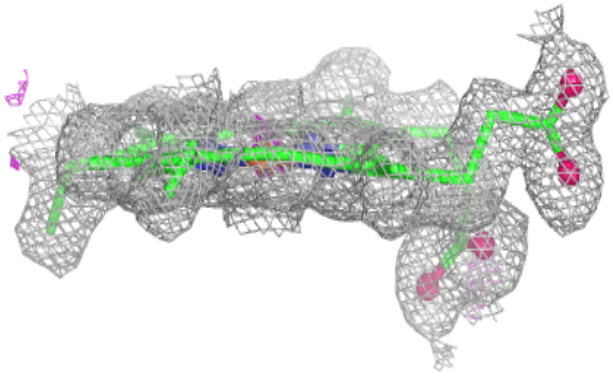


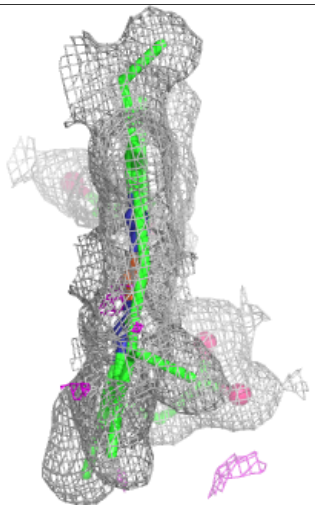


Electron density around HEC MMM 605:

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

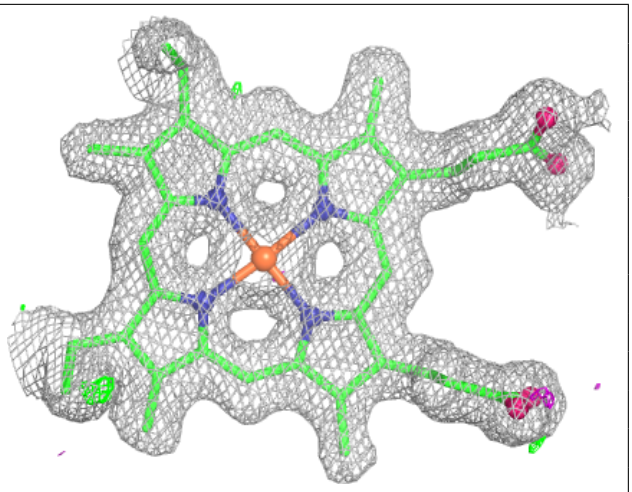


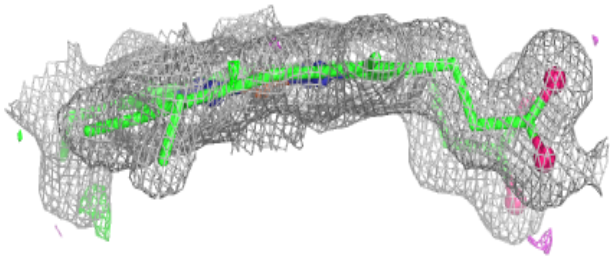


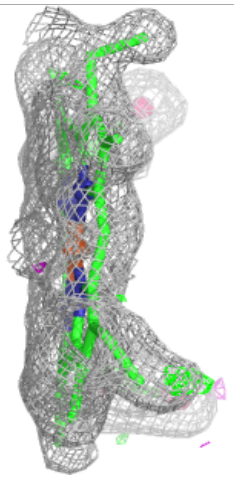


Electron density around HEC MMM 606:

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

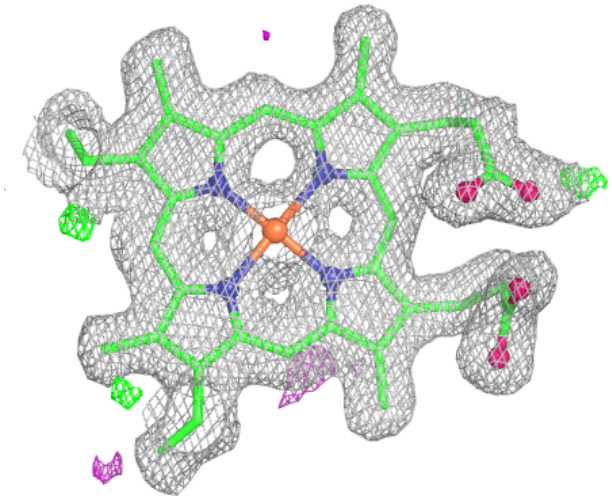


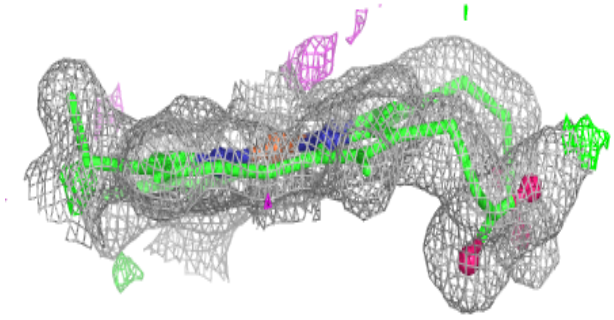


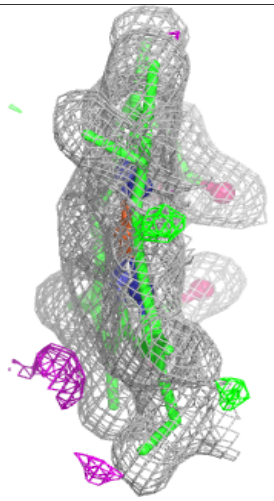


Electron density around HEC MMM 607:

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

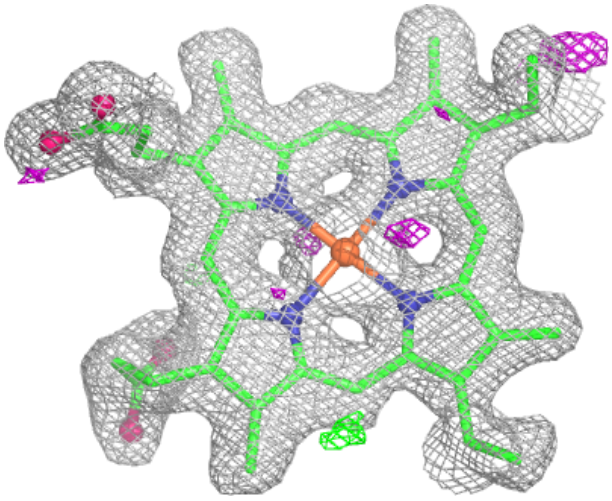


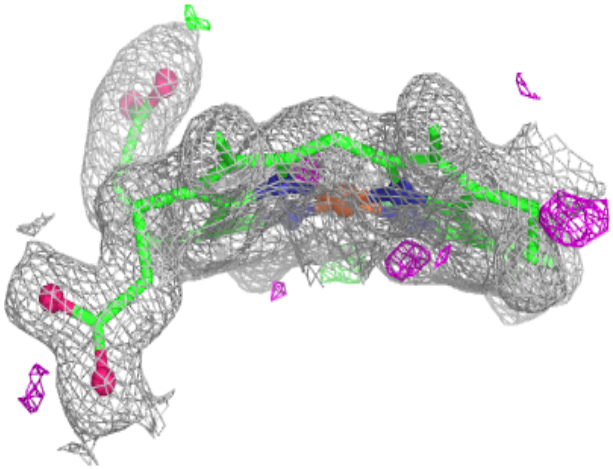


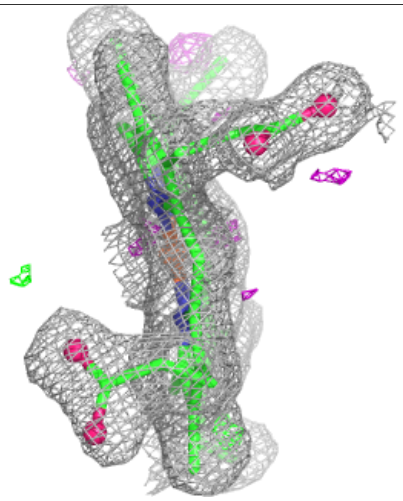


Electron density around HEC MMM 608:

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

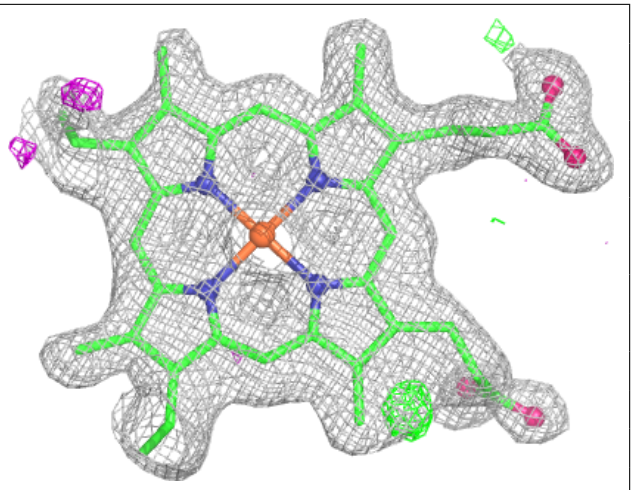


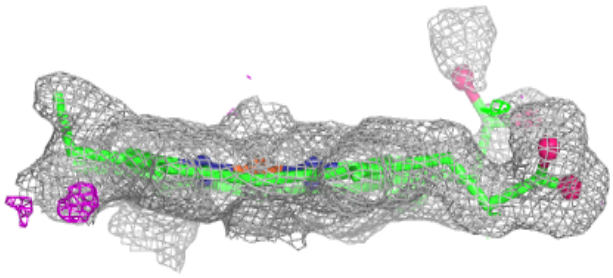


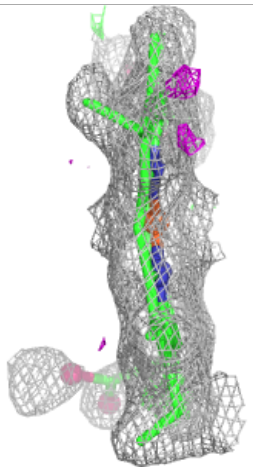


Electron density around HEC YYY 601:

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

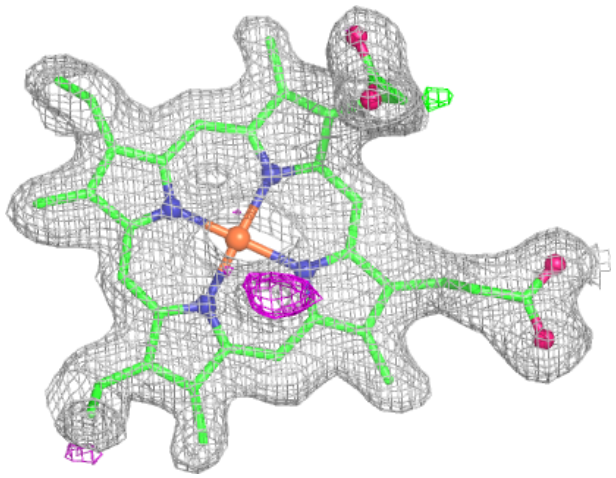


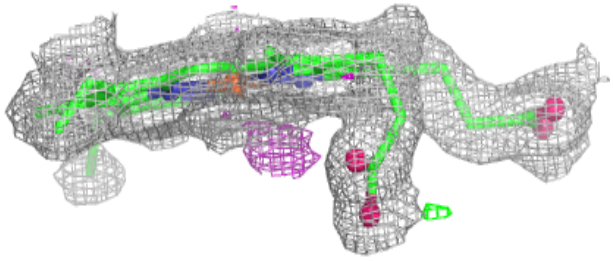


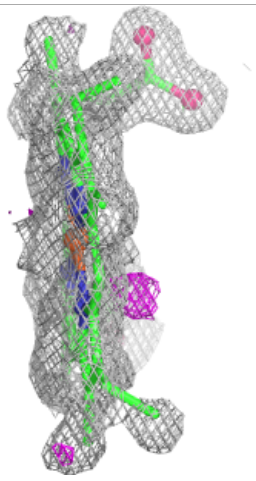


Electron density around HEC YYY 602:

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

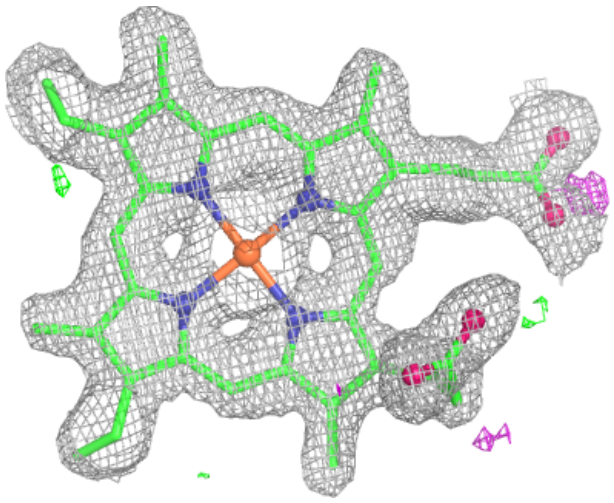


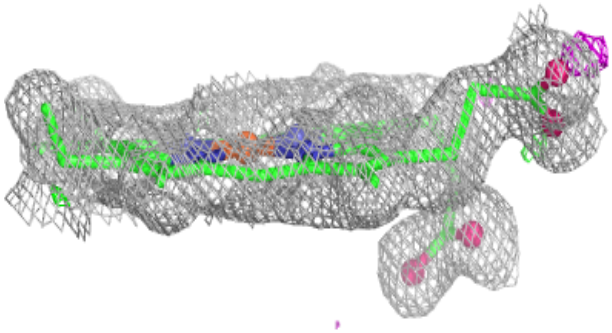




Electron density around HEC YYY 603:

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

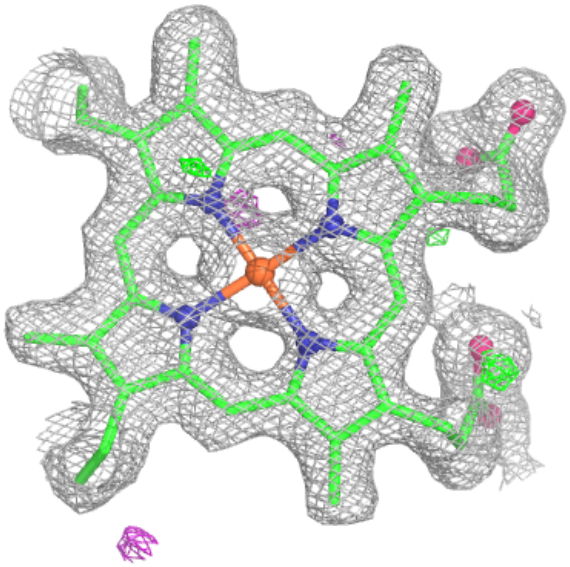


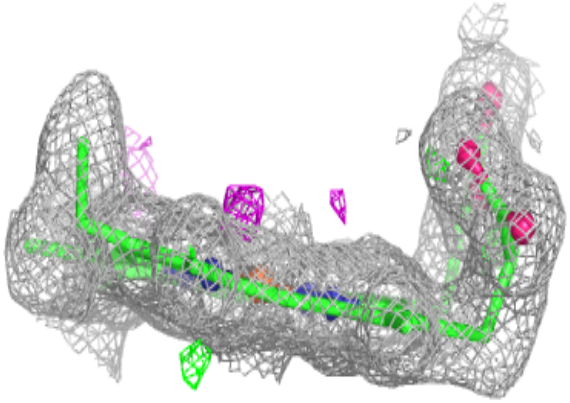


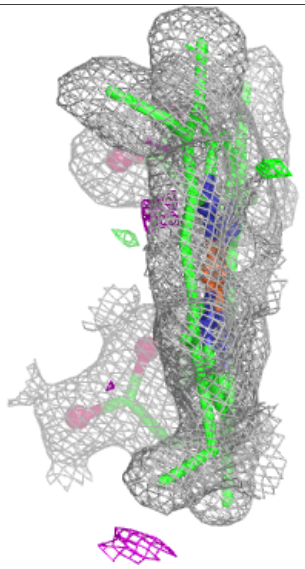


Electron density around HEC YYY 604:

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

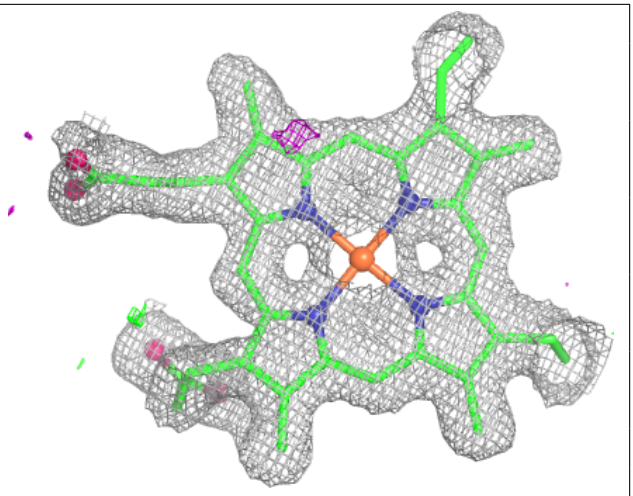


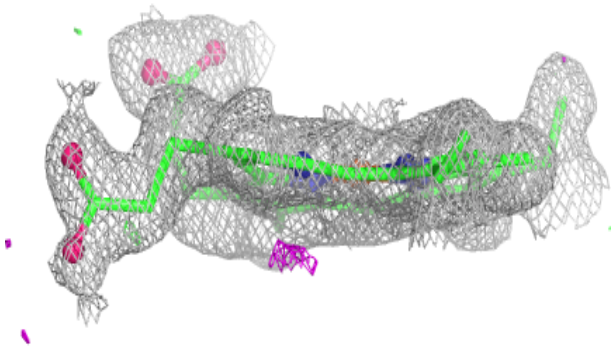


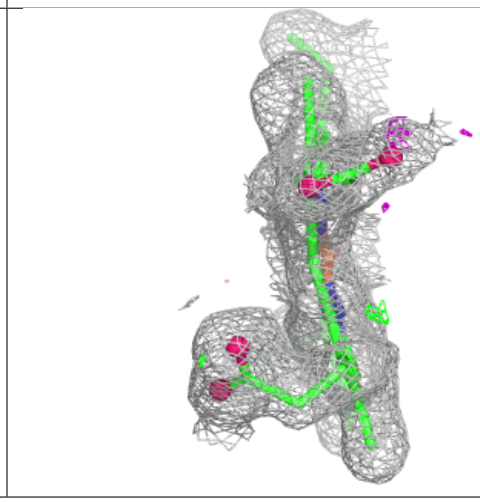


Electron density around HEC YYY 605:

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

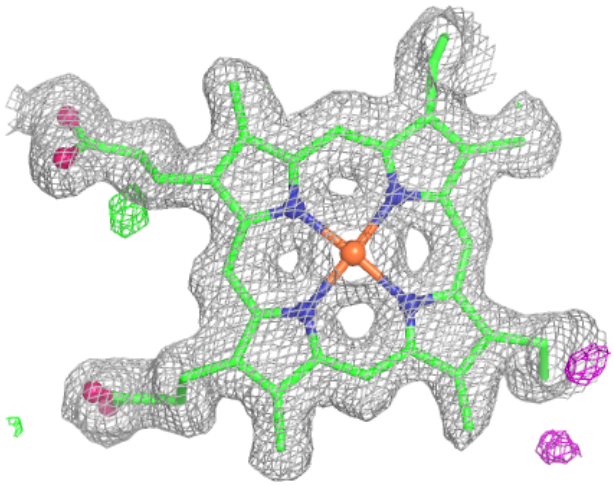


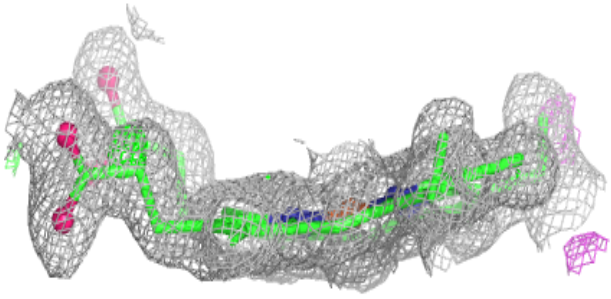


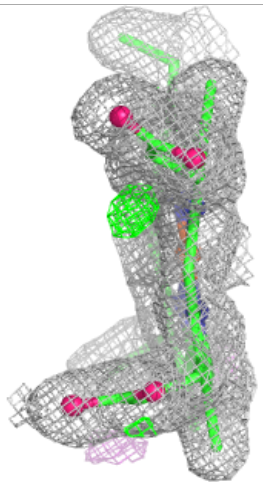


Electron density around HEC YYY 606:

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

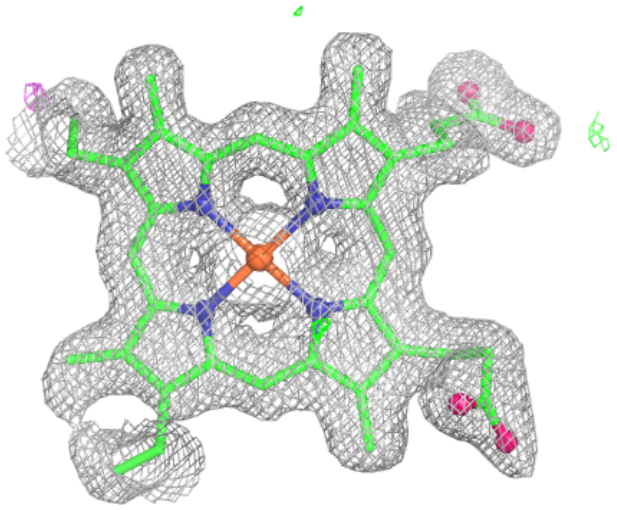


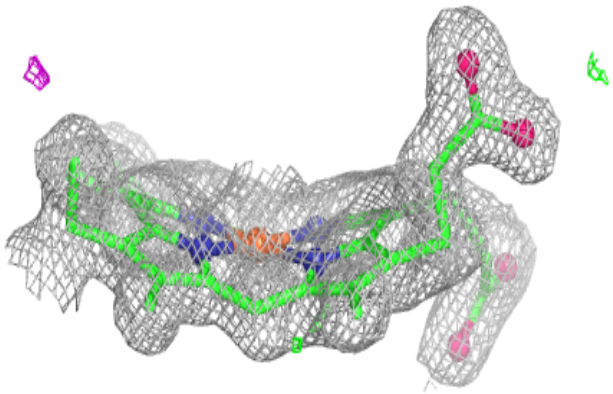


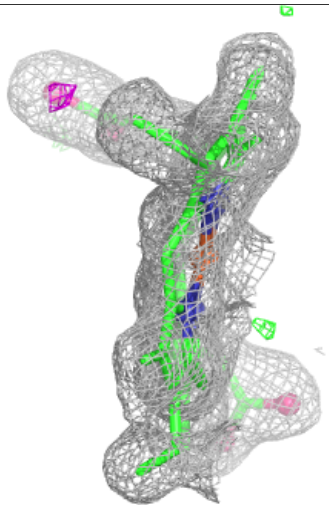


Electron density around HEC YYY 608:

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

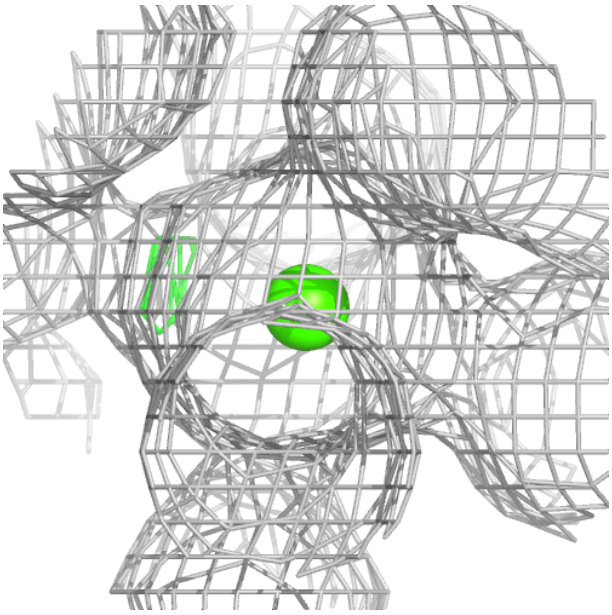


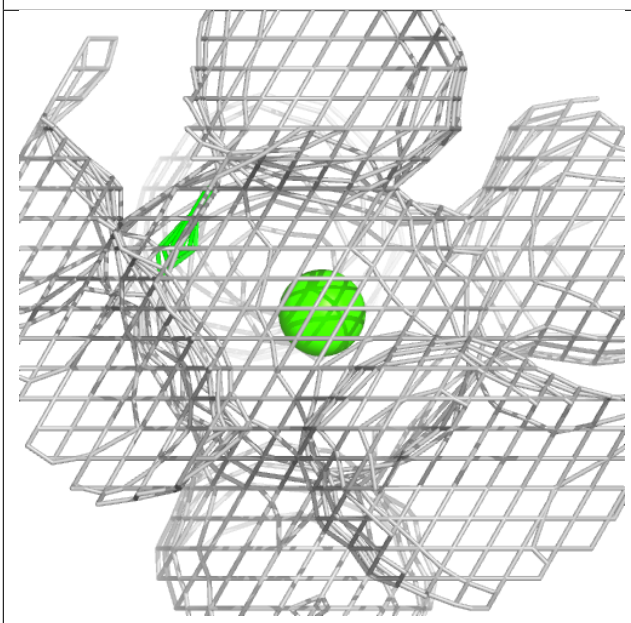


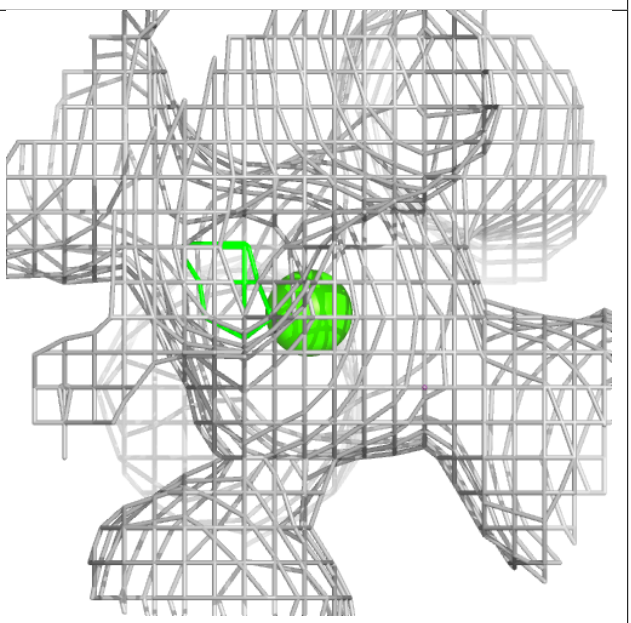


Electron density around CA MMM 609:

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

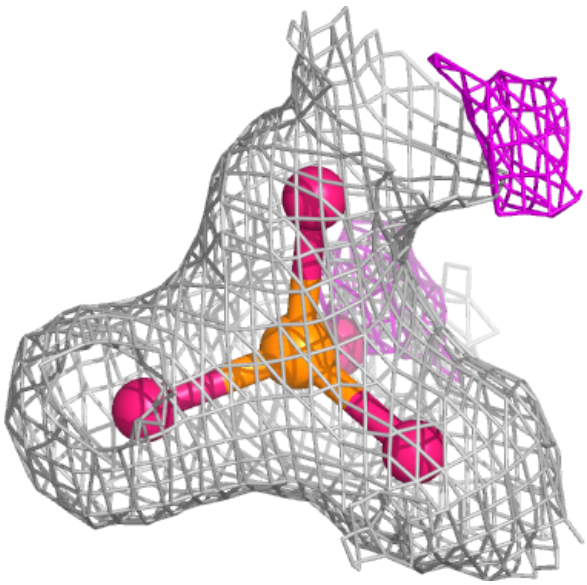


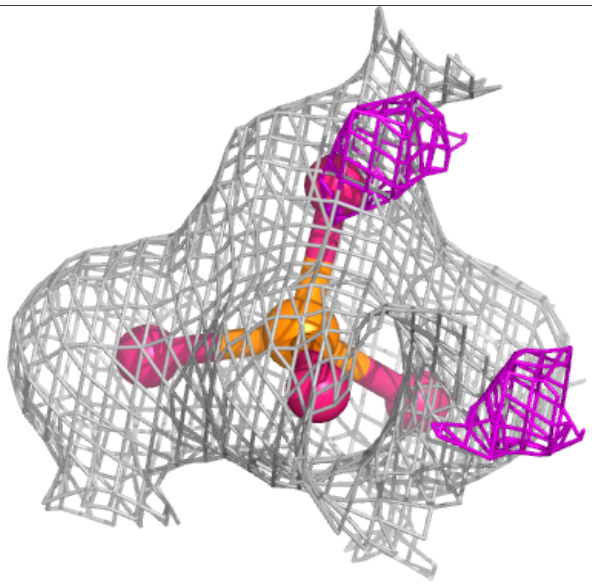


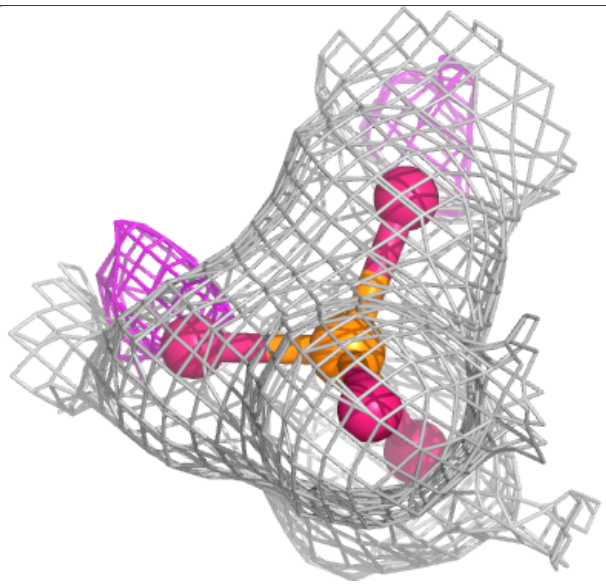


Electron density around PO4 AAA 610:

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

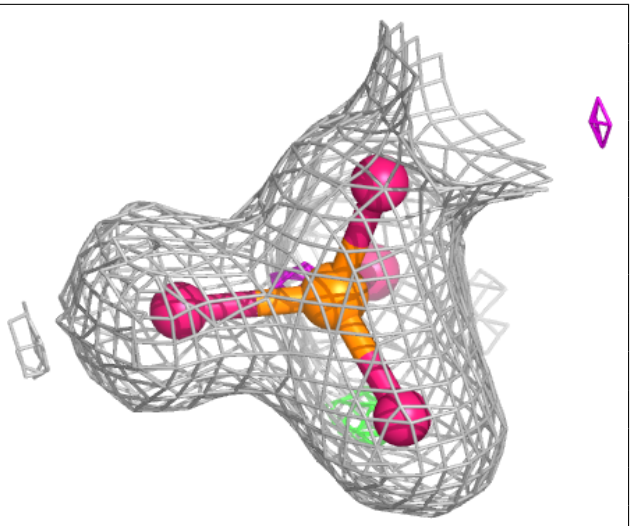


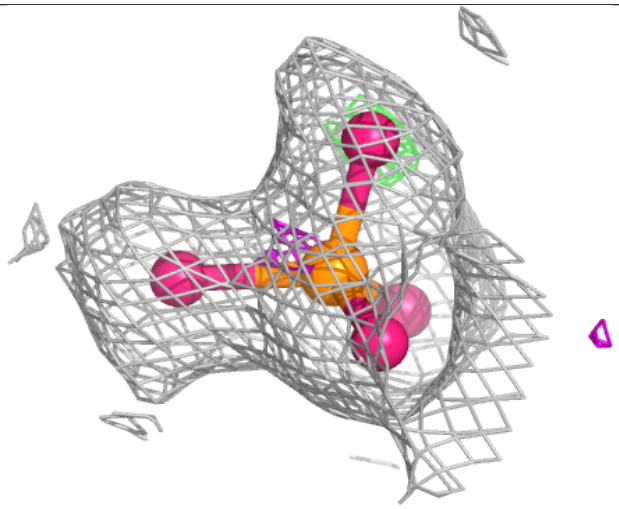


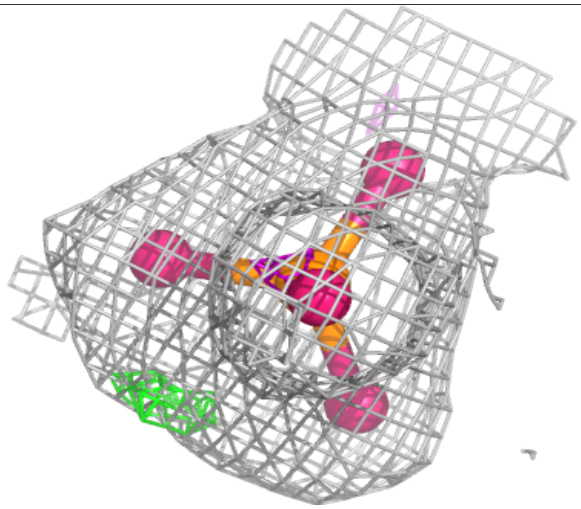


Electron density around PO4 MMM 610:

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

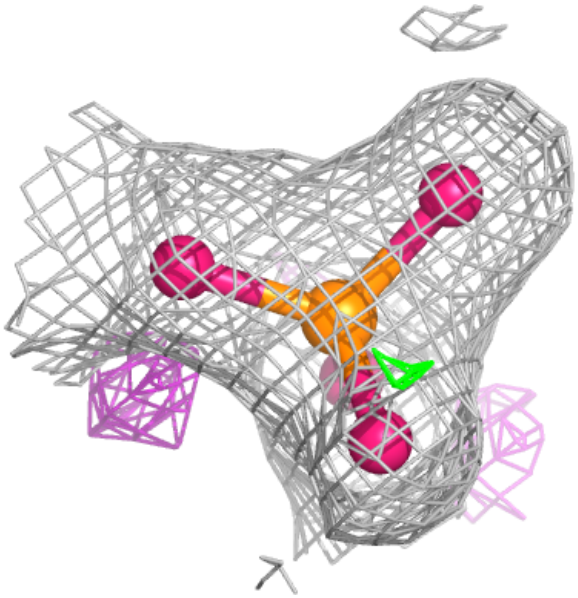


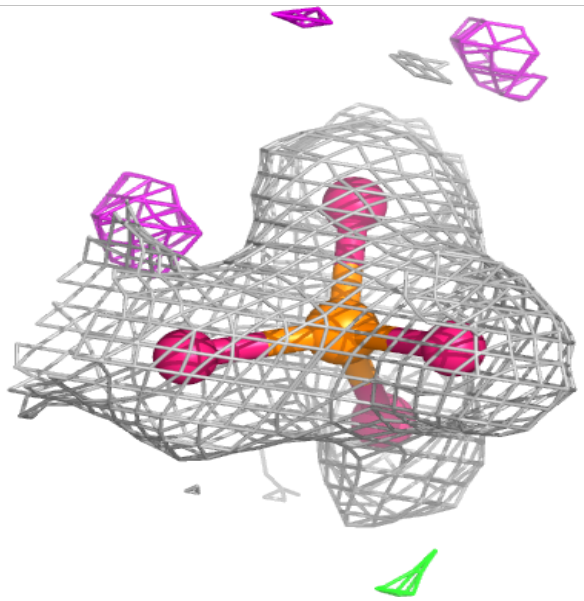


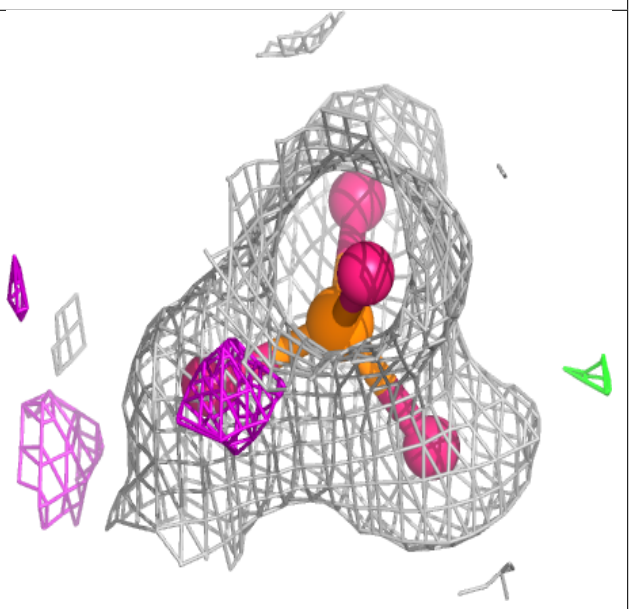


Electron density around PO4 YYY 610:

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

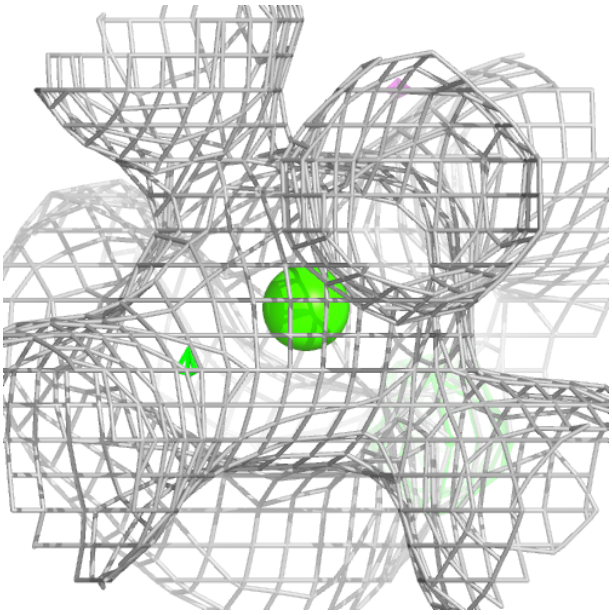


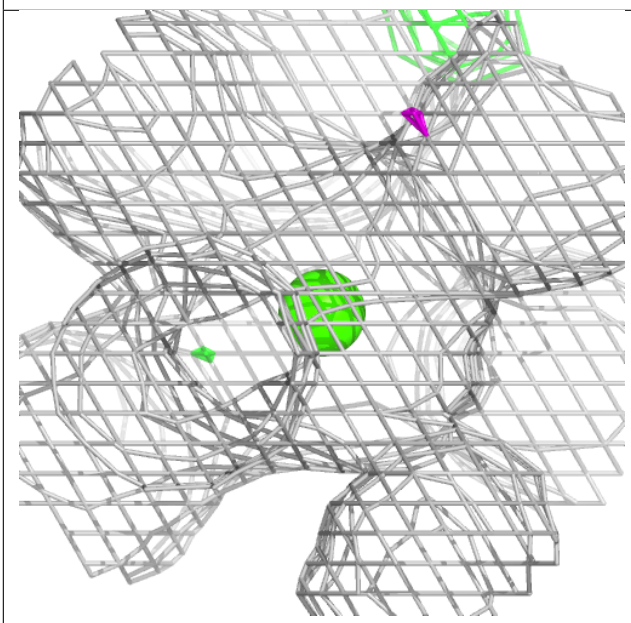


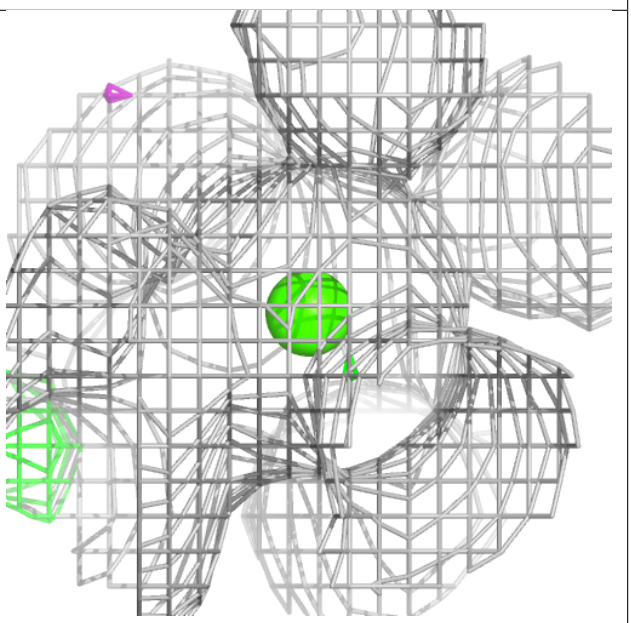


Electron density around CA AAA 609:

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

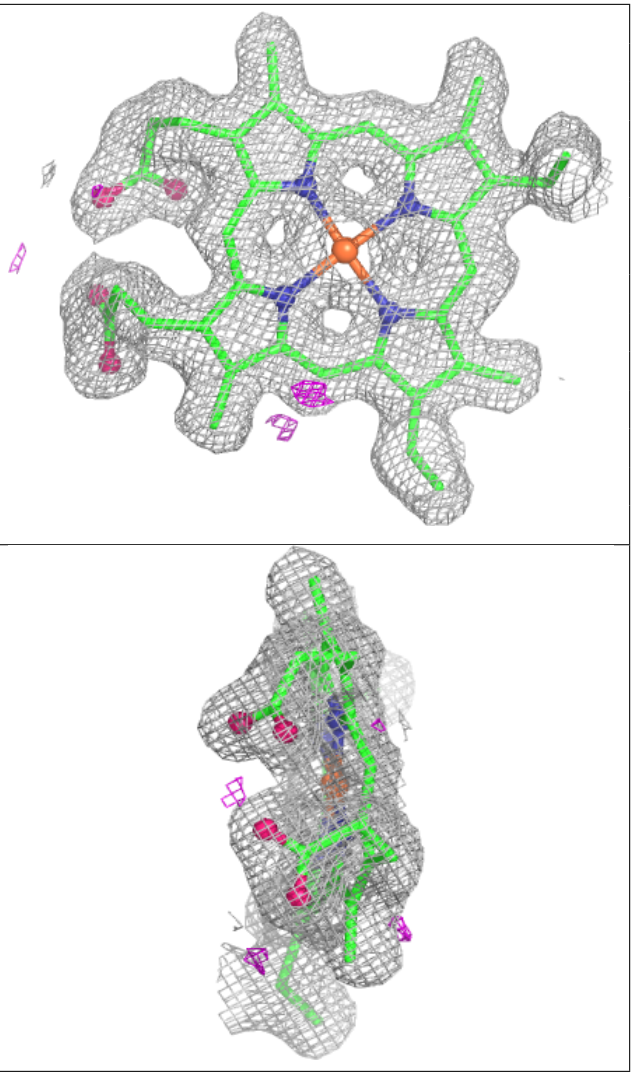






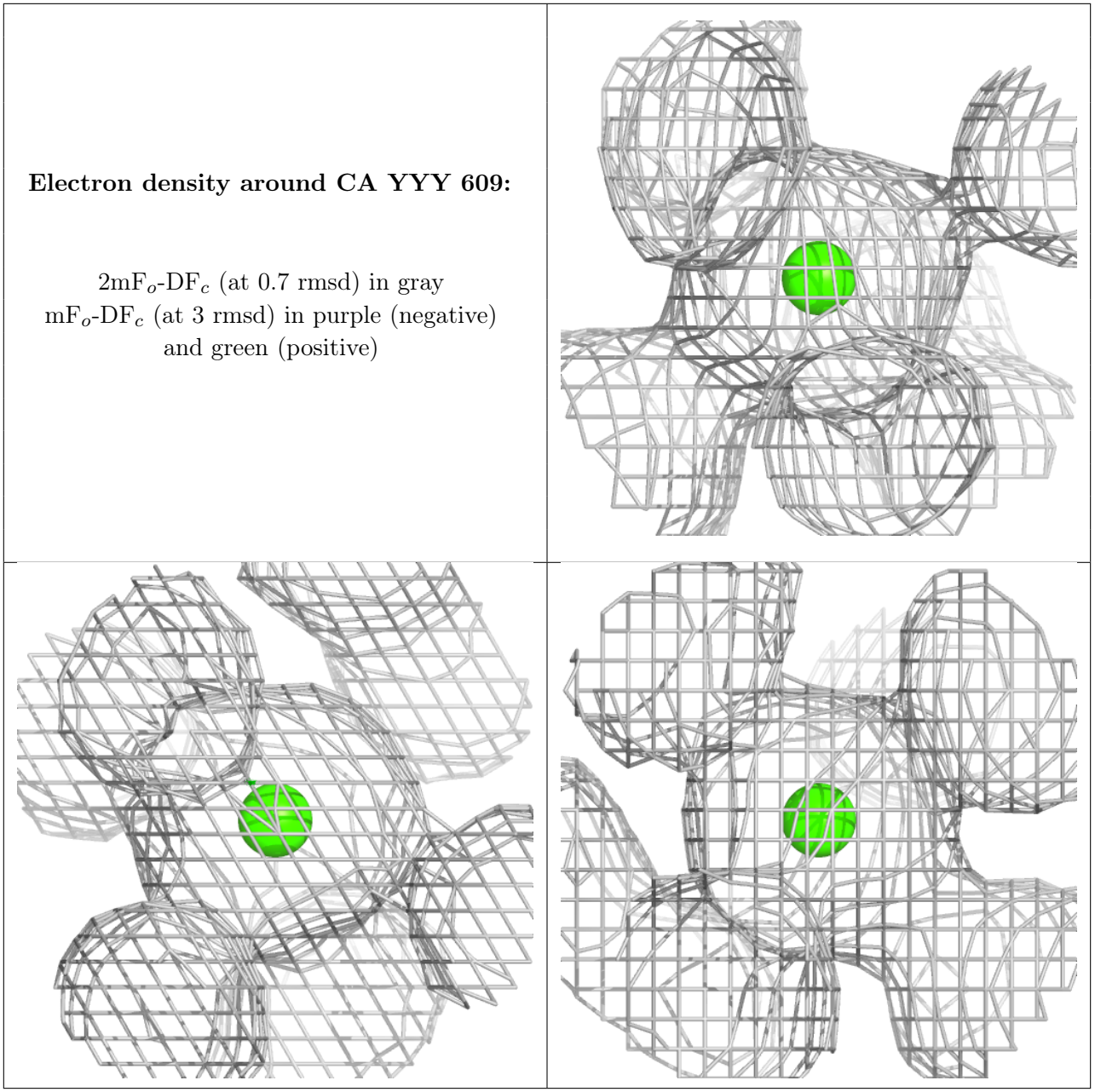
Electron density around HEC YYY 607:

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



Electron density around CA YYY 609:

$2mF_o$-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.