wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 01:07 PM EDT

PDB ID	:	4RKN / pdb_00004rkn
Title	:	Wolinella succinogenes octaheme sulfite reductase MccA, form II
Authors	:	Hermann, B.; Kern, M.; La Pietra, L.; Simon, J.; Einsle, O.
Deposited on	:	2014-10-13
Resolution	:	2.10 Å(reported)

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

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

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

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

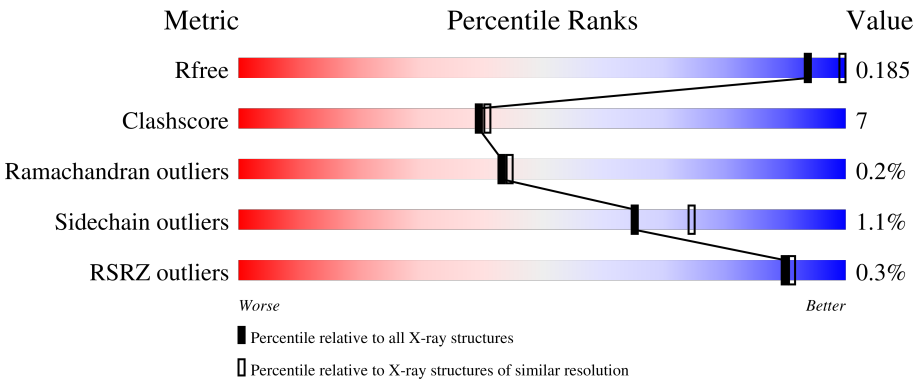
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	732	83% 7% 10%
1	B	732	85% 5% 10%
1	C	732	84% 6% 10%
1	D	732	82% 7% • 10%

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
5	SO3	D	912	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 23997 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 MccA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	660	5250	3299	923	991	37	0	3	0
1	B	660	5246	3295	923	991	37	0	3	0
1	C	659	5240	3292	922	989	37	0	3	0
1	D	660	5240	3291	922	990	37	0	2	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	691	SER	-	expression tag	UNP Q7MSJ8
A	692	ALA	-	expression tag	UNP Q7MSJ8
A	693	TRP	-	expression tag	UNP Q7MSJ8
A	694	SER	-	expression tag	UNP Q7MSJ8
A	695	HIS	-	expression tag	UNP Q7MSJ8
A	696	PRO	-	expression tag	UNP Q7MSJ8
A	697	GLN	-	expression tag	UNP Q7MSJ8
A	698	PHE	-	expression tag	UNP Q7MSJ8
A	699	GLU	-	expression tag	UNP Q7MSJ8
A	700	LYS	-	expression tag	UNP Q7MSJ8
A	701	GLY	-	expression tag	UNP Q7MSJ8
A	702	GLY	-	expression tag	UNP Q7MSJ8
A	703	GLY	-	expression tag	UNP Q7MSJ8
A	704	SER	-	expression tag	UNP Q7MSJ8
A	705	GLY	-	expression tag	UNP Q7MSJ8
A	706	GLY	-	expression tag	UNP Q7MSJ8
A	707	GLY	-	expression tag	UNP Q7MSJ8
A	708	SER	-	expression tag	UNP Q7MSJ8
A	709	GLY	-	expression tag	UNP Q7MSJ8
A	710	GLY	-	expression tag	UNP Q7MSJ8
A	711	SER	-	expression tag	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	712	ALA	-	expression tag	UNP Q7MSJ8
A	713	TRP	-	expression tag	UNP Q7MSJ8
A	714	SER	-	expression tag	UNP Q7MSJ8
A	715	HIS	-	expression tag	UNP Q7MSJ8
A	716	PRO	-	expression tag	UNP Q7MSJ8
A	717	GLN	-	expression tag	UNP Q7MSJ8
A	718	PHE	-	expression tag	UNP Q7MSJ8
A	719	GLU	-	expression tag	UNP Q7MSJ8
A	720	LYS	-	expression tag	UNP Q7MSJ8
B	691	SER	-	expression tag	UNP Q7MSJ8
B	692	ALA	-	expression tag	UNP Q7MSJ8
B	693	TRP	-	expression tag	UNP Q7MSJ8
B	694	SER	-	expression tag	UNP Q7MSJ8
B	695	HIS	-	expression tag	UNP Q7MSJ8
B	696	PRO	-	expression tag	UNP Q7MSJ8
B	697	GLN	-	expression tag	UNP Q7MSJ8
B	698	PHE	-	expression tag	UNP Q7MSJ8
B	699	GLU	-	expression tag	UNP Q7MSJ8
B	700	LYS	-	expression tag	UNP Q7MSJ8
B	701	GLY	-	expression tag	UNP Q7MSJ8
B	702	GLY	-	expression tag	UNP Q7MSJ8
B	703	GLY	-	expression tag	UNP Q7MSJ8
B	704	SER	-	expression tag	UNP Q7MSJ8
B	705	GLY	-	expression tag	UNP Q7MSJ8
B	706	GLY	-	expression tag	UNP Q7MSJ8
B	707	GLY	-	expression tag	UNP Q7MSJ8
B	708	SER	-	expression tag	UNP Q7MSJ8
B	709	GLY	-	expression tag	UNP Q7MSJ8
B	710	GLY	-	expression tag	UNP Q7MSJ8
B	711	SER	-	expression tag	UNP Q7MSJ8
B	712	ALA	-	expression tag	UNP Q7MSJ8
B	713	TRP	-	expression tag	UNP Q7MSJ8
B	714	SER	-	expression tag	UNP Q7MSJ8
B	715	HIS	-	expression tag	UNP Q7MSJ8
B	716	PRO	-	expression tag	UNP Q7MSJ8
B	717	GLN	-	expression tag	UNP Q7MSJ8
B	718	PHE	-	expression tag	UNP Q7MSJ8
B	719	GLU	-	expression tag	UNP Q7MSJ8
B	720	LYS	-	expression tag	UNP Q7MSJ8
C	691	SER	-	expression tag	UNP Q7MSJ8
C	692	ALA	-	expression tag	UNP Q7MSJ8
C	693	TRP	-	expression tag	UNP Q7MSJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	694	SER	-	expression tag	UNP Q7MSJ8
C	695	HIS	-	expression tag	UNP Q7MSJ8
C	696	PRO	-	expression tag	UNP Q7MSJ8
C	697	GLN	-	expression tag	UNP Q7MSJ8
C	698	PHE	-	expression tag	UNP Q7MSJ8
C	699	GLU	-	expression tag	UNP Q7MSJ8
C	700	LYS	-	expression tag	UNP Q7MSJ8
C	701	GLY	-	expression tag	UNP Q7MSJ8
C	702	GLY	-	expression tag	UNP Q7MSJ8
C	703	GLY	-	expression tag	UNP Q7MSJ8
C	704	SER	-	expression tag	UNP Q7MSJ8
C	705	GLY	-	expression tag	UNP Q7MSJ8
C	706	GLY	-	expression tag	UNP Q7MSJ8
C	707	GLY	-	expression tag	UNP Q7MSJ8
C	708	SER	-	expression tag	UNP Q7MSJ8
C	709	GLY	-	expression tag	UNP Q7MSJ8
C	710	GLY	-	expression tag	UNP Q7MSJ8
C	711	SER	-	expression tag	UNP Q7MSJ8
C	712	ALA	-	expression tag	UNP Q7MSJ8
C	713	TRP	-	expression tag	UNP Q7MSJ8
C	714	SER	-	expression tag	UNP Q7MSJ8
C	715	HIS	-	expression tag	UNP Q7MSJ8
C	716	PRO	-	expression tag	UNP Q7MSJ8
C	717	GLN	-	expression tag	UNP Q7MSJ8
C	718	PHE	-	expression tag	UNP Q7MSJ8
C	719	GLU	-	expression tag	UNP Q7MSJ8
C	720	LYS	-	expression tag	UNP Q7MSJ8
D	691	SER	-	expression tag	UNP Q7MSJ8
D	692	ALA	-	expression tag	UNP Q7MSJ8
D	693	TRP	-	expression tag	UNP Q7MSJ8
D	694	SER	-	expression tag	UNP Q7MSJ8
D	695	HIS	-	expression tag	UNP Q7MSJ8
D	696	PRO	-	expression tag	UNP Q7MSJ8
D	697	GLN	-	expression tag	UNP Q7MSJ8
D	698	PHE	-	expression tag	UNP Q7MSJ8
D	699	GLU	-	expression tag	UNP Q7MSJ8
D	700	LYS	-	expression tag	UNP Q7MSJ8
D	701	GLY	-	expression tag	UNP Q7MSJ8
D	702	GLY	-	expression tag	UNP Q7MSJ8
D	703	GLY	-	expression tag	UNP Q7MSJ8
D	704	SER	-	expression tag	UNP Q7MSJ8
D	705	GLY	-	expression tag	UNP Q7MSJ8

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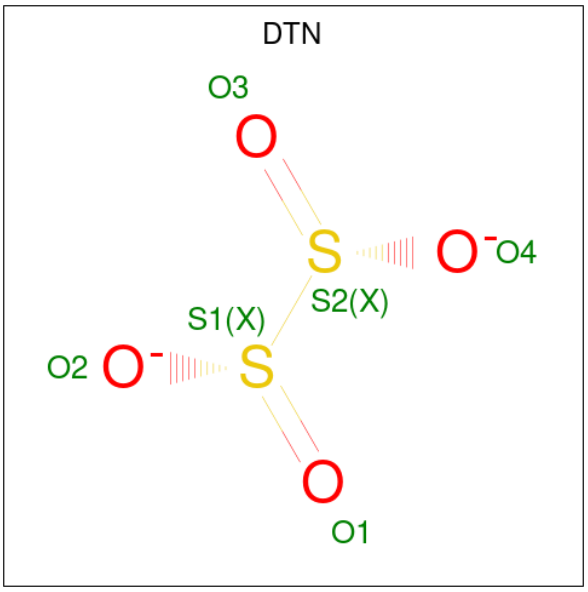
Chain	Residue	Modelled	Actual	Comment	Reference
D	706	GLY	-	expression tag	UNP Q7MSJ8
D	707	GLY	-	expression tag	UNP Q7MSJ8
D	708	SER	-	expression tag	UNP Q7MSJ8
D	709	GLY	-	expression tag	UNP Q7MSJ8
D	710	GLY	-	expression tag	UNP Q7MSJ8
D	711	SER	-	expression tag	UNP Q7MSJ8
D	712	ALA	-	expression tag	UNP Q7MSJ8
D	713	TRP	-	expression tag	UNP Q7MSJ8
D	714	SER	-	expression tag	UNP Q7MSJ8
D	715	HIS	-	expression tag	UNP Q7MSJ8
D	716	PRO	-	expression tag	UNP Q7MSJ8
D	717	GLN	-	expression tag	UNP Q7MSJ8
D	718	PHE	-	expression tag	UNP Q7MSJ8
D	719	GLU	-	expression tag	UNP Q7MSJ8
D	720	LYS	-	expression tag	UNP Q7MSJ8

- Molecule 2 is DITHIONITE (CCD ID: DTN) (formula: O_4S_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	O	S		0	0
			6	4	2			
2	A	1	Total	O	S		0	0
			6	4	2			
2	B	1	Total	O	S		0	0
			6	4	2			
2	C	1	Total	O	S		0	0
			6	4	2			

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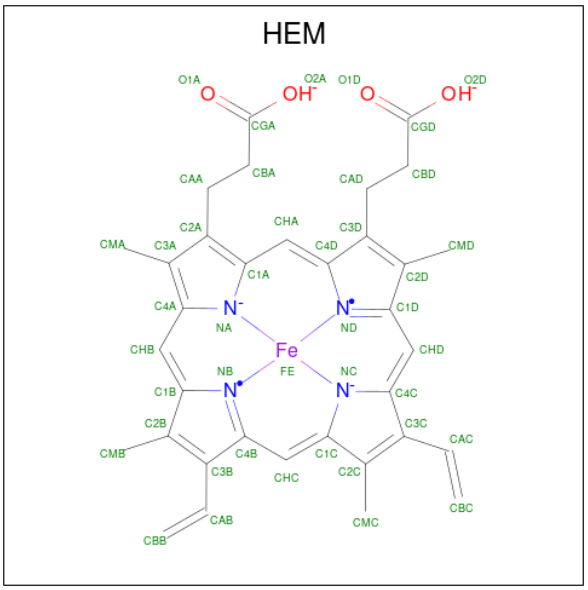
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	D	1	6	4	2	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	86	68	2	8	8	0	1
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	B	1	86	68	2	8	8	0	1
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	86	68	2	8	8	0	1
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	86	68	2	8	8	0	1
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0

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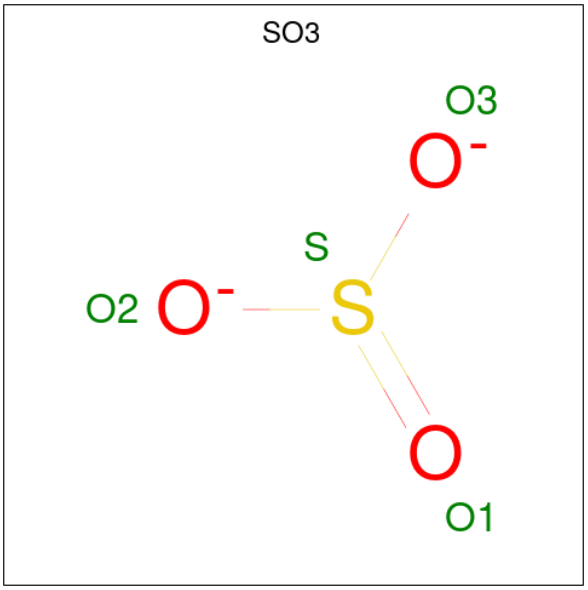
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
3	D	1	43	34	1	4	4	0	0

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is SULFITE ION (CCD ID: SO3) (formula: O_3S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	4	3	1	0	0
5	B	1	4	3	1	0	0
5	C	1	4	3	1	0	0
5	D	1	4	3	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	D	1	4	3	1	0	0

- Molecule 6 is water.

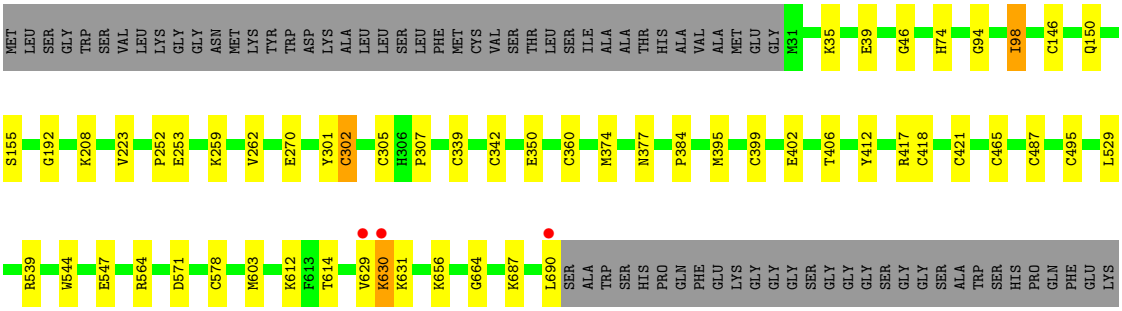
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	335	335	335	0	0
			Total	O		
6	B	355	355	355	0	0
			Total	O		
6	C	312	312	312	0	0
			Total	O		
6	D	417	417	417	0	0

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.

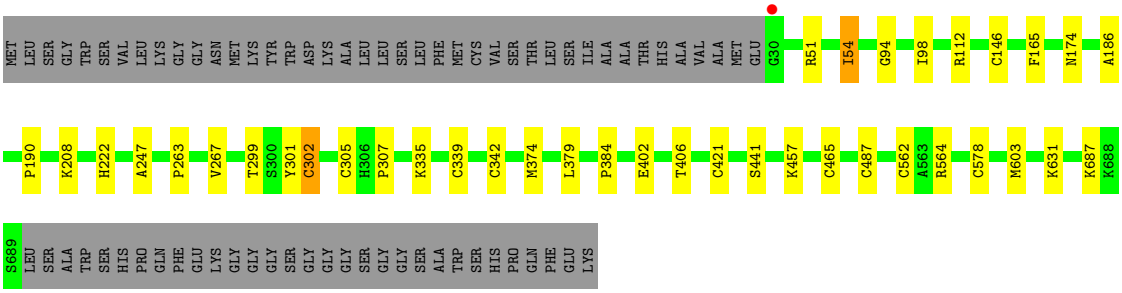
- Molecule 1: MccA

Chain A:



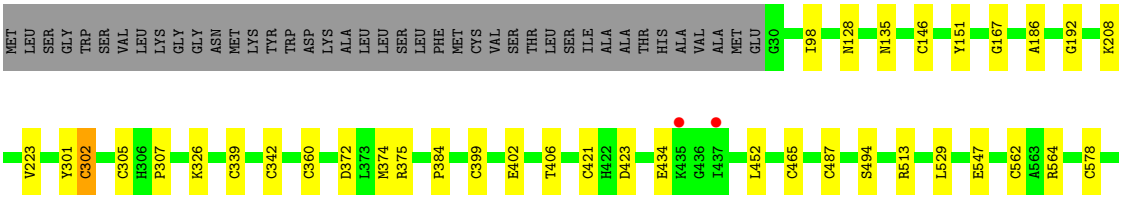
- Molecule 1: MccA

Chain B:



- Molecule 1: MccA

Chain C:



K593 L626 S635 R639 I644 G664 M686 K687 K688 SER LEU SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

- Molecule 1: MccA

Chain D: 82% 7% • 10%

MET LEU SER GLY TRP SER VAL LEU LYS GLY GLY ASN MET LYS TYR TRP ASP LYS ALA LEU LEU SER LEU PHE MET CYS VAL SER THR LEU SER ILE ALA ALA THR HIS ALA VAL ALA MET GLU G30 G94 I98 K108 E116 S119 Y123 C146 A186 Q191

G192 I193 T194 K208 V223 Q243 A247 L250 K259 V267 L282 T299 S300 Y301 C302 C305 H306 P307 C342 H343 C360 C363 S368 D372 R375 N376 N377 P378 L379 C399 E402 T406 C421 K438 C465 N482

C487 R513 V556 R564 C578 V602 M603 T607 I620 V629 R639 V640 Y641 E642 L643 I644 K656 G664 T668 D673 V676 R684 I685 M686 S689 LEU SER ALA TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY SER GLY GLY GLY SER

GLY GLY SER ALA TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	186.47Å 186.47Å 232.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.26 – 2.10 47.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.26-2.10) 99.8 (47.26-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.135 , 0.175 0.150 , 0.185	Depositor DCC
R_{free} test set	8789 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -2/3*h-1/3*k+2/3*l,-1/3*h-2/3*k-2/3*l,2/3*h-2/3*k+1/3*l 0.009 for -h,1/3*h-1/3*k+2/3*l,2/3*h+4/3*k+1/3*l 0.009 for -1/3*h+1/3*k-2/3*l,-k,-4/3*h-2/3*k+1/3*l 0.011 for -h,2/3*h+1/3*k-2/3*l,-2/3*h-4/3*k-1/3*l 0.011 for 1/3*h+2/3*k+2/3*l,-k,4/3*h+2/3*k-1/3*l 0.015 for -1/3*h-2/3*k-2/3*l,-2/3*h-1/3*k+2/3*l,-2/3*h+2/3*k-1/3*l 0.019 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	23997	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CU, DTN, SO3

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	1.14	6/5383 (0.1%)	1.05	5/7251 (0.1%)
1	B	1.15	1/5379 (0.0%)	1.06	4/7245 (0.1%)
1	C	1.15	2/5373 (0.0%)	1.06	6/7237 (0.1%)
1	D	1.25	12/5370 (0.2%)	1.09	7/7233 (0.1%)
All	All	1.18	21/21505 (0.1%)	1.06	22/28966 (0.1%)

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	635	SER	CA-C	6.50	1.61	1.52
1	A	614	THR	C-O	-6.15	1.17	1.24
1	D	607	THR	C-O	-6.00	1.18	1.24
1	D	641	TYR	CA-C	-5.97	1.45	1.52
1	D	267	VAL	C-O	-5.74	1.16	1.24

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	644	ILE	CB-CA-C	-6.96	102.62	112.22
1	A	74	HIS	CA-C-N	6.66	127.19	119.47
1	A	74	HIS	C-N-CA	6.66	127.19	119.47
1	C	186	ALA	N-CA-C	6.50	120.09	110.48
1	C	98	ILE	CB-CA-C	-5.94	105.76	111.05

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	5250	0	5072	74	0
1	B	5246	0	5063	69	0
1	C	5240	0	5059	65	0
1	D	5240	0	5054	74	0
2	A	12	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
2	D	6	0	0	0	0
3	A	387	0	270	54	0
3	B	387	0	270	55	0
3	C	387	0	270	58	0
3	D	387	0	270	57	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	A	4	0	0	1	0
5	B	4	0	0	1	0
5	C	4	0	0	1	0
5	D	8	0	0	3	0
6	A	335	0	0	5	0
6	B	355	0	0	4	0
6	C	312	0	0	3	0
6	D	417	0	0	5	0
All	All	23997	0	21328	296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 296 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:B:562:CYS:SG	3:B:909:HEM:CAB	2.01	1.48
1:D:578:CYS:SG	3:D:909:HEM:CAC	2.03	1.47
1:B:339:CYS:SG	3:B:904[A]:HEM:CAB	2.03	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:562:CYS:SG	3:C:909:HEM:CAB	2.02	1.47
1:D:305:CYS:SG	3:D:903:HEM:CAC	2.03	1.47

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	661/732 (90%)	631 (96%)	28 (4%)	2 (0%)	36	36
1	B	661/732 (90%)	635 (96%)	26 (4%)	0	100	100
1	C	660/732 (90%)	629 (95%)	30 (4%)	1 (0%)	43	44
1	D	660/732 (90%)	633 (96%)	25 (4%)	2 (0%)	36	36
All	All	2642/2928 (90%)	2528 (96%)	109 (4%)	5 (0%)	43	44

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	630	LYS
1	D	301	TYR
1	A	664	GLY
1	C	664	GLY
1	D	664	GLY

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	563/613 (92%)	557 (99%)	6 (1%)	65	74
1	B	562/613 (92%)	555 (99%)	7 (1%)	63	72
1	C	561/613 (92%)	556 (99%)	5 (1%)	70	78
1	D	561/613 (92%)	555 (99%)	6 (1%)	65	74
All	All	2247/2452 (92%)	2223 (99%)	24 (1%)	65	74

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	326	LYS
1	C	564	ARG
1	C	547	GLU
1	D	250	LEU
1	B	54	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	621	GLN
1	D	377	ASN
1	D	446	GLN
1	A	377	ASN
1	A	497	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 50 ligands modelled in this entry, 4 are monoatomic - leaving 46 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	HEM	A	903	5,1	50,50,50	1.64	11 (22%)	67,82,82	1.73	15 (22%)
3	HEM	B	902	1	50,50,50	1.51	10 (20%)	67,82,82	1.68	13 (19%)
3	HEM	B	904[A]	1	50,50,50	1.51	9 (18%)	67,82,82	1.78	17 (25%)
3	HEM	C	908	1	50,50,50	1.36	8 (16%)	67,82,82	1.67	12 (17%)
3	HEM	B	907	1	50,50,50	1.61	10 (20%)	67,82,82	1.75	16 (23%)
3	HEM	D	906	1	50,50,50	1.36	4 (8%)	67,82,82	1.67	12 (17%)
3	HEM	C	904[A]	1	50,50,50	1.49	10 (20%)	67,82,82	1.79	16 (23%)
3	HEM	B	904[B]	1	50,50,50	1.53	9 (18%)	67,82,82	1.75	15 (22%)
3	HEM	B	903	5,1	50,50,50	1.65	9 (18%)	67,82,82	1.65	16 (23%)
3	HEM	C	907	1	50,50,50	1.46	8 (16%)	67,82,82	1.78	19 (28%)
3	HEM	C	904[B]	1	50,50,50	1.47	8 (16%)	67,82,82	1.70	15 (22%)
3	HEM	D	903	5,1	50,50,50	1.83	12 (24%)	67,82,82	1.57	15 (22%)
3	HEM	B	906	1	50,50,50	1.51	9 (18%)	67,82,82	1.86	15 (22%)
2	DTN	A	901	-	0,5,5	-	-	0,6,6	-	-
5	SO3	D	912	3	1,3,3	6.54	1 (100%)	0,3,3	-	-
3	HEM	A	908	1	50,50,50	1.55	6 (12%)	67,82,82	1.62	15 (22%)
3	HEM	C	909	1	50,50,50	1.55	9 (18%)	67,82,82	1.78	17 (25%)
3	HEM	B	905	1	50,50,50	1.46	7 (14%)	67,82,82	1.56	9 (13%)
2	DTN	D	901	-	0,5,5	-	-	0,6,6	-	-
2	DTN	A	911	-	0,5,5	-	-	0,6,6	-	-
3	HEM	C	905	1	50,50,50	1.70	9 (18%)	67,82,82	1.49	9 (13%)
3	HEM	A	902	1	50,50,50	1.57	9 (18%)	67,82,82	1.81	16 (23%)
3	HEM	D	905	1	50,50,50	1.59	9 (18%)	67,82,82	1.38	9 (13%)
3	HEM	D	907	1	50,50,50	1.56	5 (10%)	67,82,82	1.97	19 (28%)
3	HEM	A	909	1	50,50,50	1.48	8 (16%)	67,82,82	1.96	19 (28%)
3	HEM	D	908	1	50,50,50	1.48	6 (12%)	67,82,82	1.81	17 (25%)
2	DTN	B	901	-	0,5,5	-	-	0,6,6	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO3	B	911	4,3	1,3,3	5.15	1 (100%)	0,3,3	-	-
3	HEM	A	904[A]	1	50,50,50	1.53	12 (24%)	67,82,82	1.79	17 (25%)
2	DTN	C	901	-	0,5,5	-	-	0,6,6	-	-
3	HEM	A	905	1	50,50,50	1.63	7 (14%)	67,82,82	1.57	14 (20%)
5	SO3	C	911	3	1,3,3	5.90	1 (100%)	0,3,3	-	-
5	SO3	A	912	4,3	1,3,3	7.78	1 (100%)	0,3,3	-	-
3	HEM	D	902	1	50,50,50	1.68	9 (18%)	67,82,82	1.72	13 (19%)
3	HEM	A	904[B]	1	50,50,50	1.56	12 (24%)	67,82,82	1.83	19 (28%)
3	HEM	D	909	1	50,50,50	1.49	10 (20%)	67,82,82	1.97	18 (26%)
3	HEM	C	903	5,1	50,50,50	1.69	9 (18%)	67,82,82	1.66	18 (26%)
3	HEM	B	909	1	50,50,50	1.55	7 (14%)	67,82,82	1.76	16 (23%)
3	HEM	C	906	1	50,50,50	1.64	9 (18%)	67,82,82	1.72	16 (23%)
3	HEM	C	902	1	50,50,50	1.64	11 (22%)	67,82,82	1.80	17 (25%)
3	HEM	A	907	1	50,50,50	1.60	9 (18%)	67,82,82	1.86	18 (26%)
3	HEM	D	904[A]	1	50,50,50	1.41	5 (10%)	67,82,82	1.72	17 (25%)
5	SO3	D	911	-	1,3,3	9.03	1 (100%)	0,3,3	-	-
3	HEM	A	906	1	50,50,50	1.62	11 (22%)	67,82,82	1.59	13 (19%)
3	HEM	D	904[B]	1	50,50,50	1.50	6 (12%)	67,82,82	1.70	15 (22%)
3	HEM	B	908	1	50,50,50	1.43	10 (20%)	67,82,82	1.70	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	HEM	A	903	5,1	-	2/14/54/54	-
3	HEM	B	902	1	-	3/14/54/54	-
3	HEM	B	904[A]	1	-	3/14/54/54	-
3	HEM	C	908	1	-	5/14/54/54	-
3	HEM	B	907	1	-	3/14/54/54	-
3	HEM	D	906	1	-	3/14/54/54	-
3	HEM	C	904[A]	1	-	4/14/54/54	-
3	HEM	B	904[B]	1	-	3/14/54/54	-
3	HEM	B	903	5,1	-	2/14/54/54	-
3	HEM	C	907	1	-	3/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	904[B]	1	-	3/14/54/54	-
3	HEM	D	903	5,1	-	3/14/54/54	-
3	HEM	B	906	1	-	3/14/54/54	-
2	DTN	A	901	-	-	0/0/4/4	-
3	HEM	A	908	1	-	5/14/54/54	-
3	HEM	C	909	1	-	5/14/54/54	-
3	HEM	B	905	1	-	2/14/54/54	-
2	DTN	D	901	-	-	0/0/4/4	-
2	DTN	A	911	-	-	0/0/4/4	-
3	HEM	C	905	1	-	2/14/54/54	-
3	HEM	A	902	1	-	2/14/54/54	-
3	HEM	D	905	1	-	2/14/54/54	-
3	HEM	D	907	1	-	3/14/54/54	-
3	HEM	A	909	1	-	5/14/54/54	-
3	HEM	D	908	1	-	7/14/54/54	-
2	DTN	B	901	-	-	0/0/4/4	-
3	HEM	A	904[A]	1	-	2/14/54/54	-
2	DTN	C	901	-	-	0/0/4/4	-
3	HEM	A	905	1	-	2/14/54/54	-
3	HEM	D	902	1	-	2/14/54/54	-
3	HEM	A	904[B]	1	-	2/14/54/54	-
3	HEM	D	909	1	-	7/14/54/54	-
3	HEM	C	903	5,1	-	2/14/54/54	-
3	HEM	B	909	1	-	7/14/54/54	-
3	HEM	C	906	1	-	4/14/54/54	-
3	HEM	C	902	1	-	2/14/54/54	-
3	HEM	A	907	1	-	3/14/54/54	-
3	HEM	D	904[A]	1	-	4/14/54/54	-
3	HEM	A	906	1	-	4/14/54/54	-
3	HEM	D	904[B]	1	-	2/14/54/54	-
3	HEM	B	908	1	-	6/14/54/54	-

The worst 5 of 317 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	911	SO3	O1-S	9.03	1.83	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	912	SO3	O1-S	7.78	1.77	1.44
5	D	912	SO3	O1-S	6.54	1.72	1.44
3	A	905	HEM	FE-NB	6.12	2.13	1.94
5	C	911	SO3	O1-S	5.90	1.69	1.44

The worst 5 of 550 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	907	HEM	CHC-C4B-NB	5.91	130.78	124.42
3	A	904[B]	HEM	CHC-C4B-NB	5.80	130.66	124.42
3	A	909	HEM	CHC-C4B-NB	5.79	130.65	124.42
3	B	909	HEM	CHC-C4B-NB	5.74	130.60	124.42
3	B	907	HEM	C1B-NB-C4B	5.71	111.97	105.21

There are no chirality outliers.

5 of 122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	903	HEM	C4D-C3D-CAD-CBD
3	C	903	HEM	C4D-C3D-CAD-CBD
3	C	904[A]	HEM	C1A-C2A-CAA-CBA
3	D	903	HEM	C4D-C3D-CAD-CBD
3	A	903	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

39 monomers are involved in 230 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	HEM	11	0
3	B	902	HEM	5	0
3	B	904[A]	HEM	8	0
3	C	908	HEM	4	0
3	B	907	HEM	4	0
3	D	906	HEM	5	0
3	C	904[A]	HEM	9	0
3	B	904[B]	HEM	7	0
3	B	903	HEM	13	0
3	C	907	HEM	4	0
3	C	904[B]	HEM	4	0
3	D	903	HEM	16	0
3	B	906	HEM	4	0

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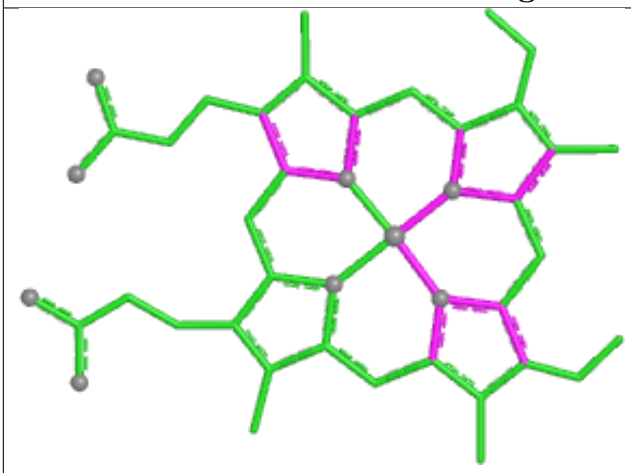
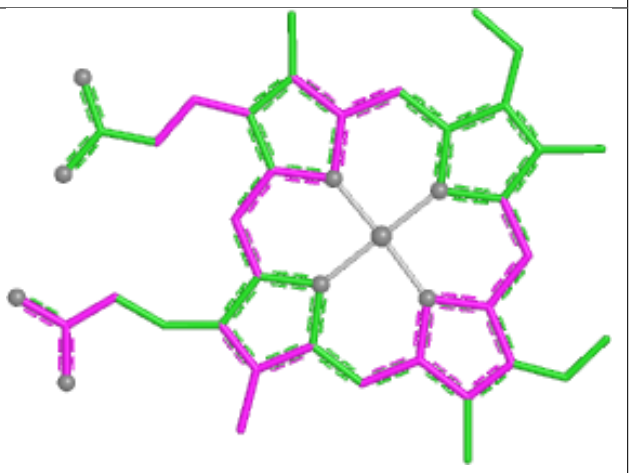
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	912	SO3	3	0
3	A	908	HEM	4	0
3	C	909	HEM	9	0
3	C	905	HEM	7	0
3	A	902	HEM	5	0
3	D	905	HEM	9	0
3	D	907	HEM	4	0
3	A	909	HEM	4	0
3	D	908	HEM	4	0
5	B	911	SO3	1	0
3	A	904[A]	HEM	8	0
3	A	905	HEM	5	0
5	C	911	SO3	1	0
5	A	912	SO3	1	0
3	D	902	HEM	5	0
3	A	904[B]	HEM	7	0
3	D	909	HEM	4	0
3	C	903	HEM	14	0
3	B	909	HEM	10	0
3	C	906	HEM	4	0
3	C	902	HEM	5	0
3	A	907	HEM	5	0
3	D	904[A]	HEM	5	0
3	A	906	HEM	5	0
3	D	904[B]	HEM	5	0
3	B	908	HEM	4	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.

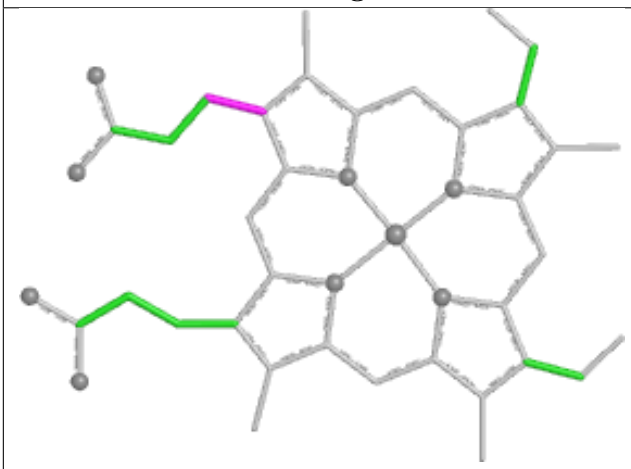
Ligand HEM A 903



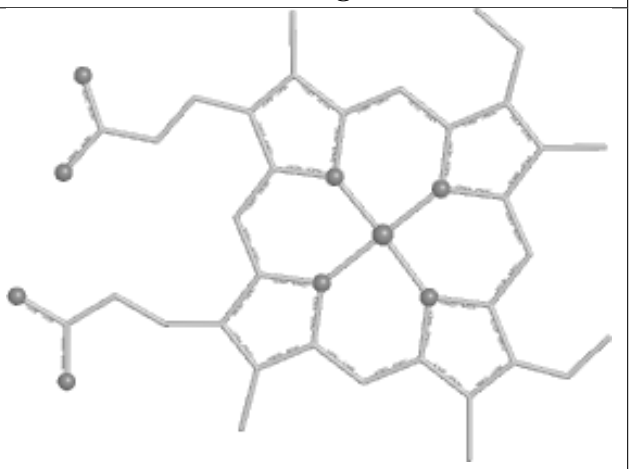
Bond lengths



Bond angles

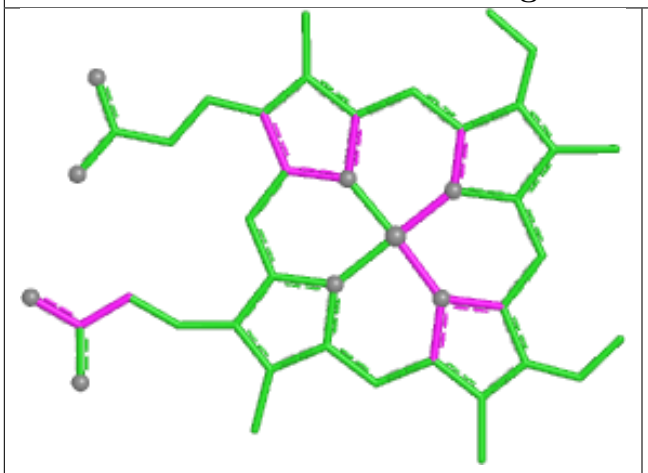


Torsions

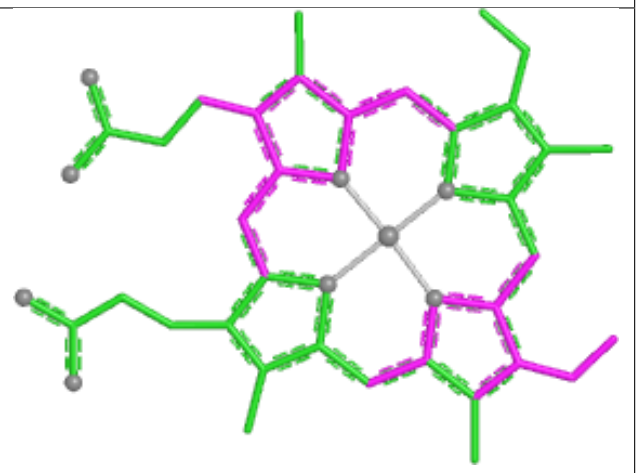


Rings

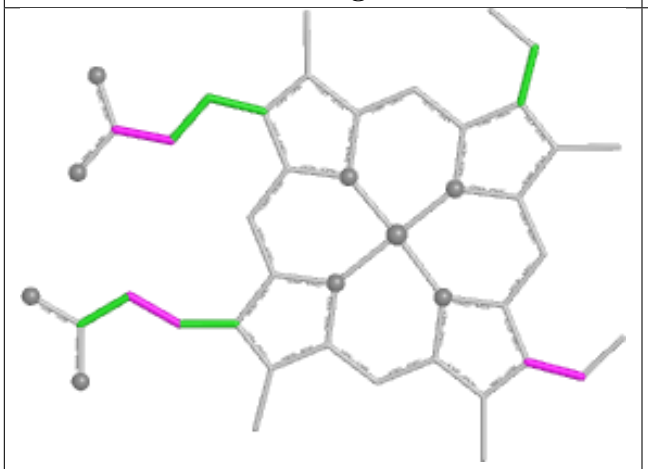
Ligand HEM B 902



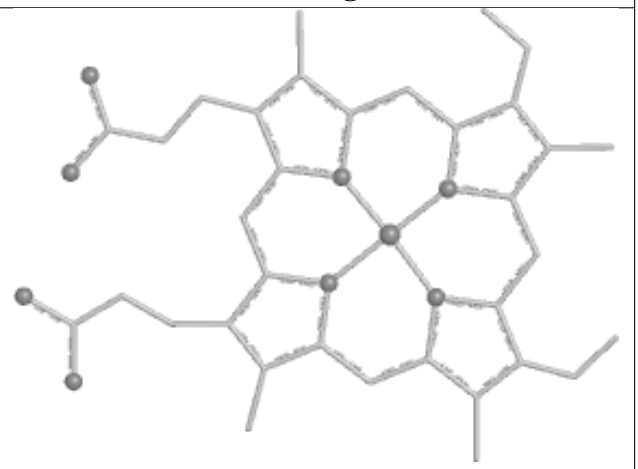
Bond lengths



Bond angles

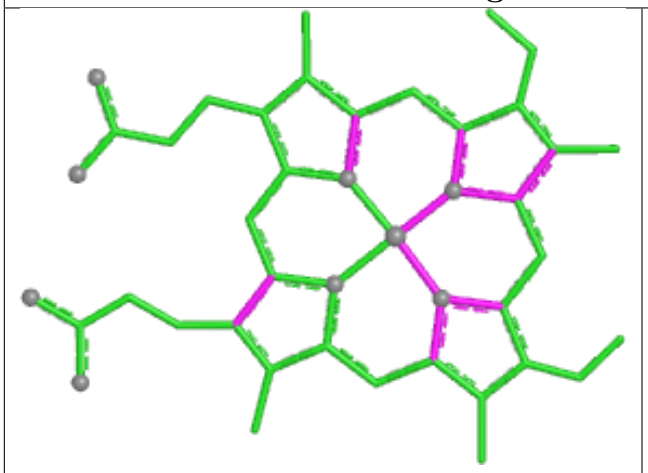


Torsions

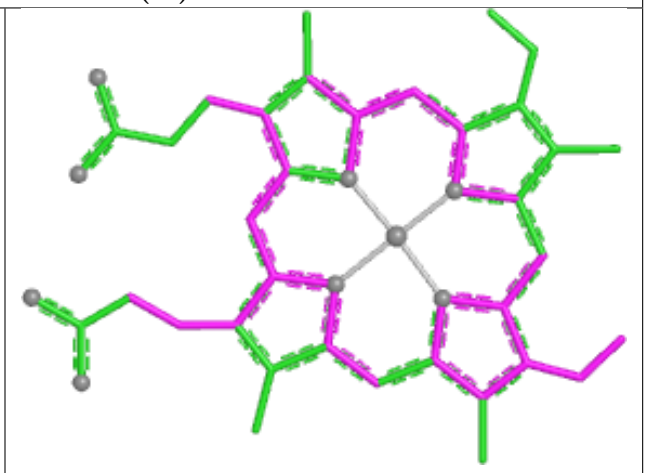


Rings

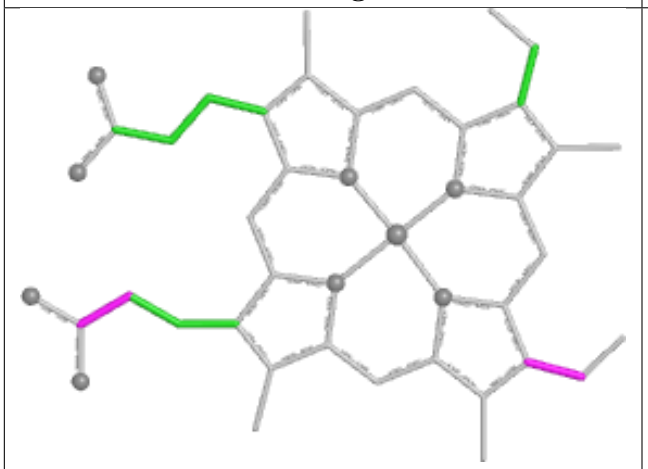
Ligand HEM B 904 (A)



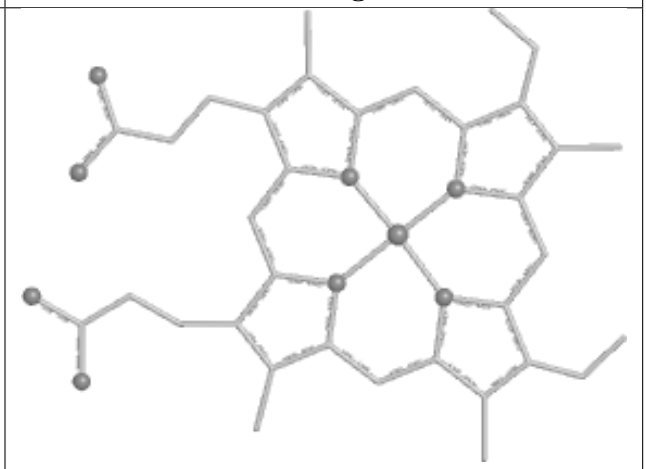
Bond lengths



Bond angles

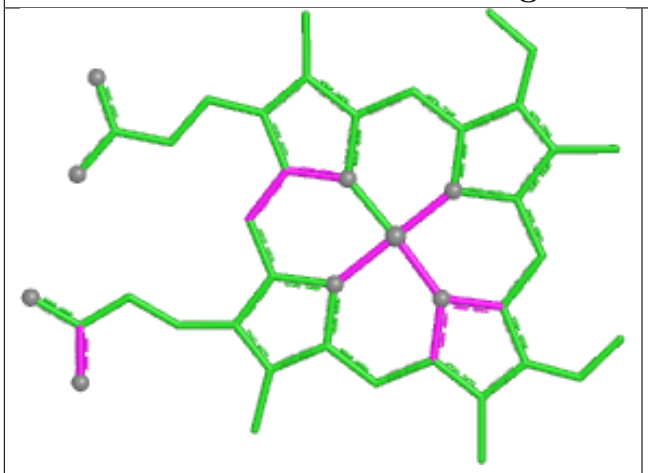


Torsions

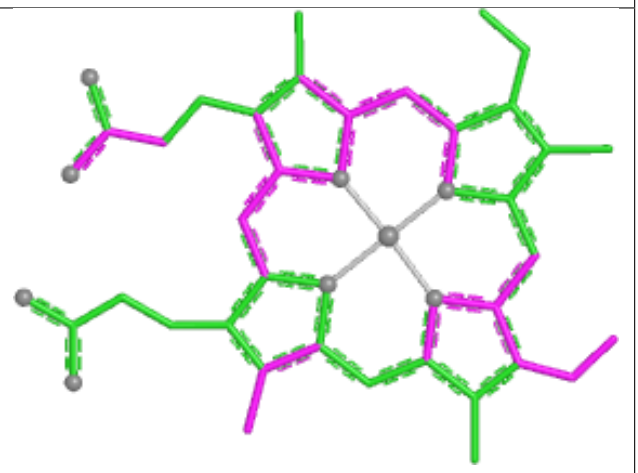


Rings

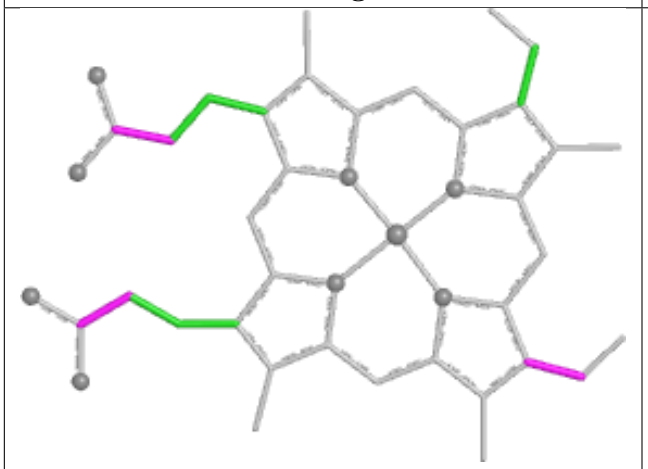
Ligand HEM C 908



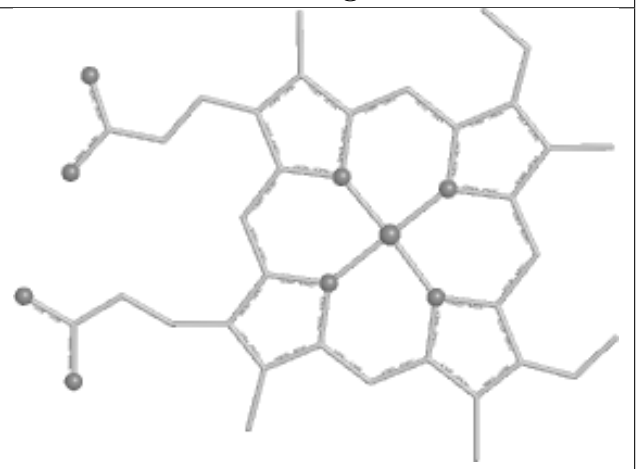
Bond lengths



Bond angles

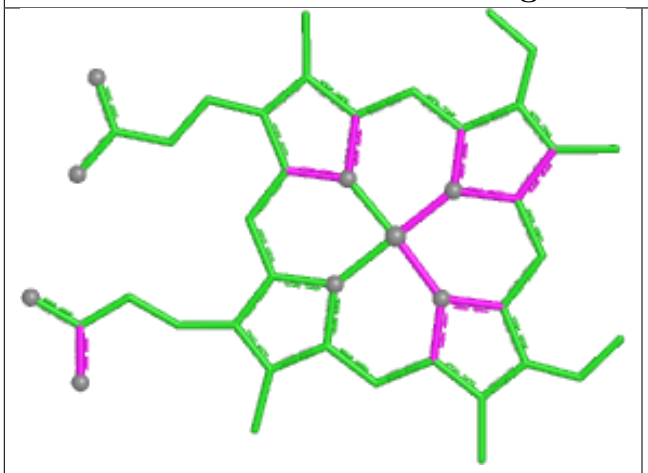


Torsions



Rings

Ligand HEM B 907



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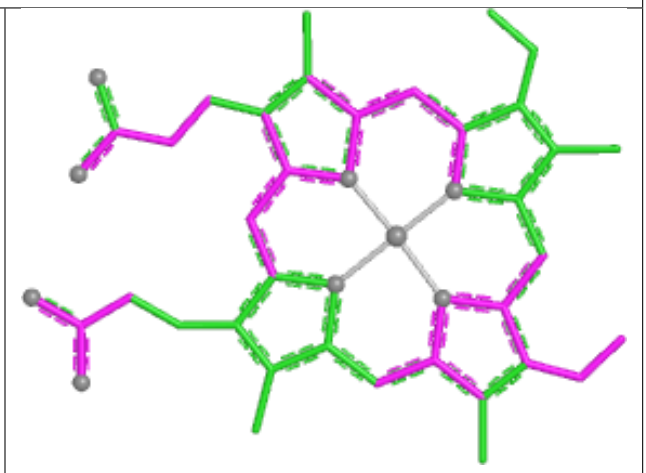
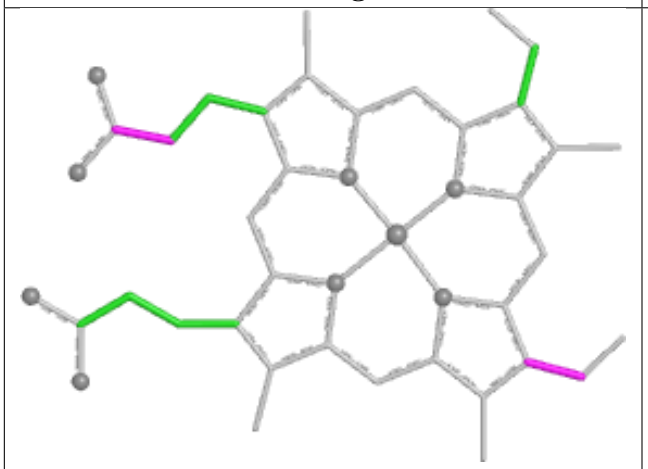


Bond angles



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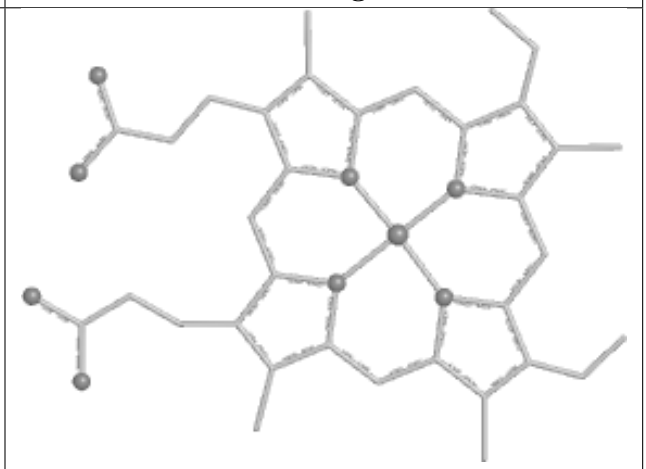
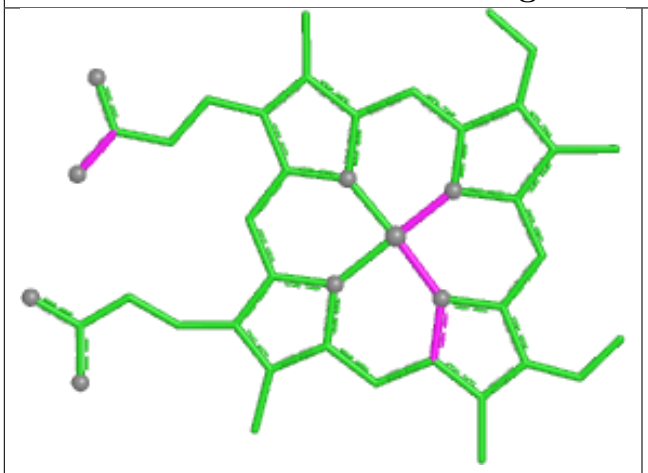


Rings

Ligand HEM D 906



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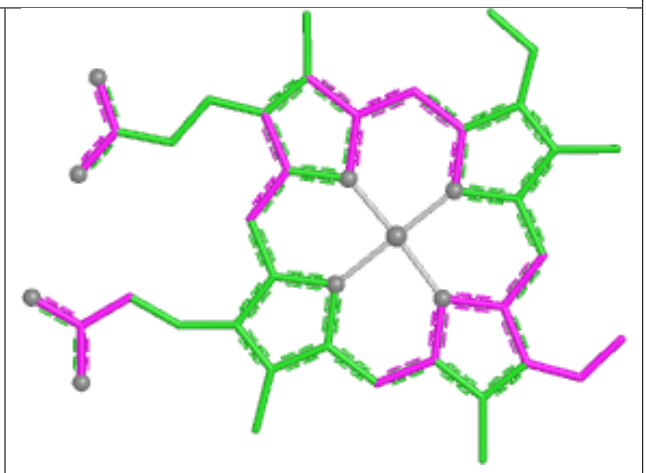
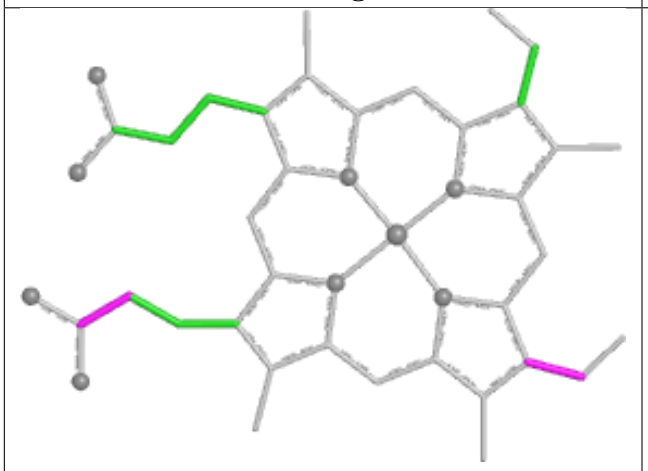
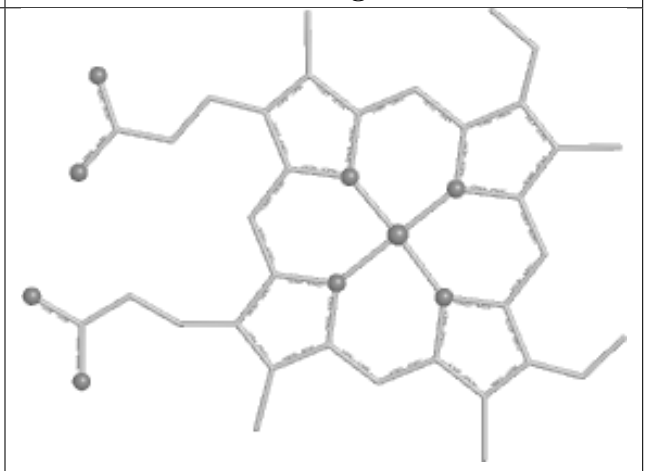


Bond angles

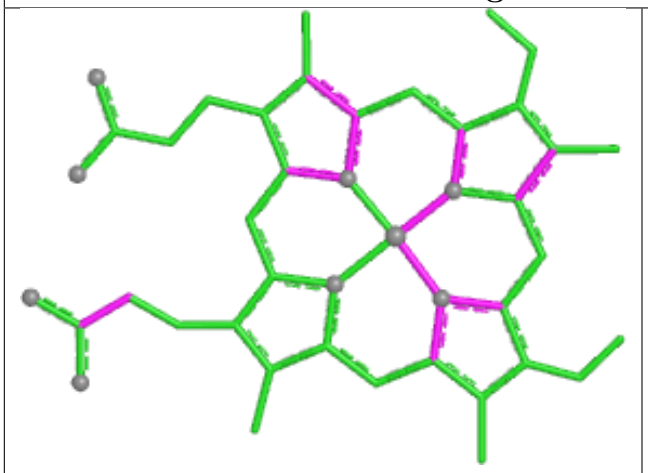


Torsions



Rings

Ligand HEM C 904 (A)



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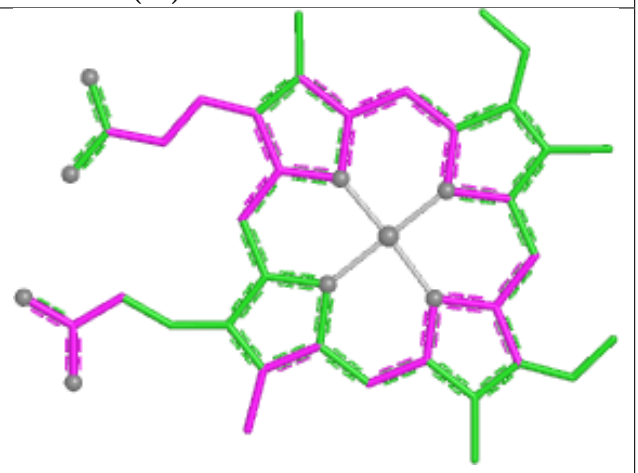
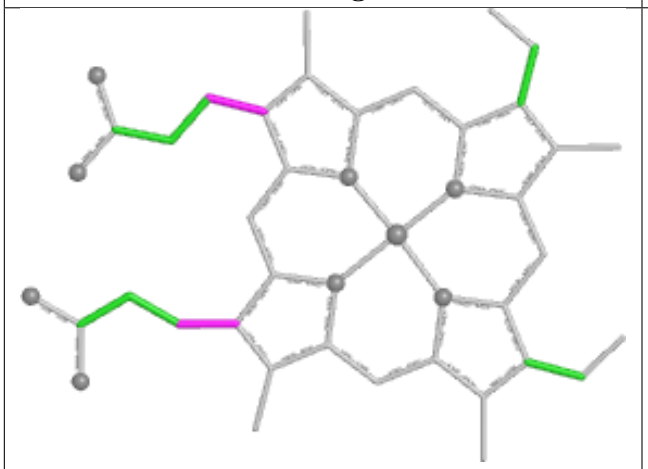


Bond angles



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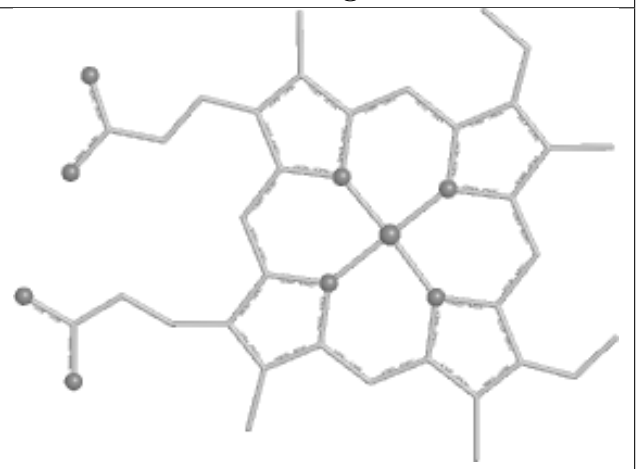
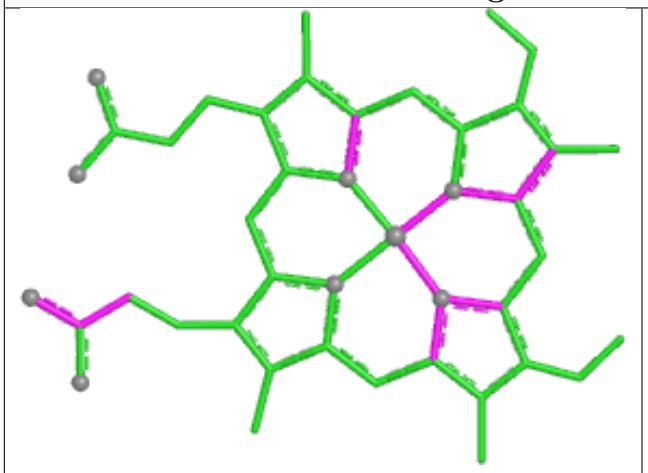


Rings

Ligand HEM B 904 (B)



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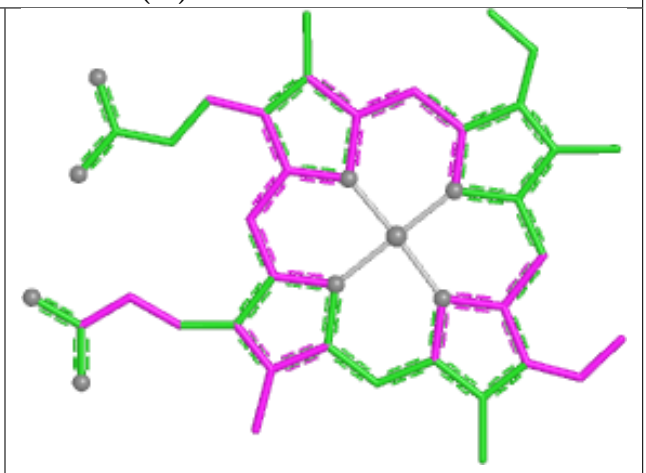
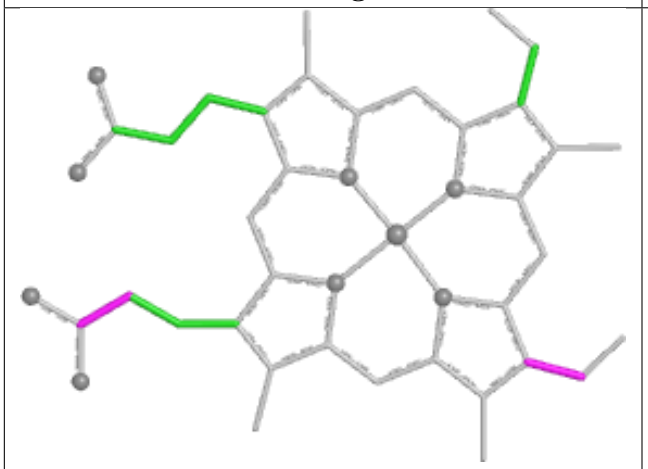
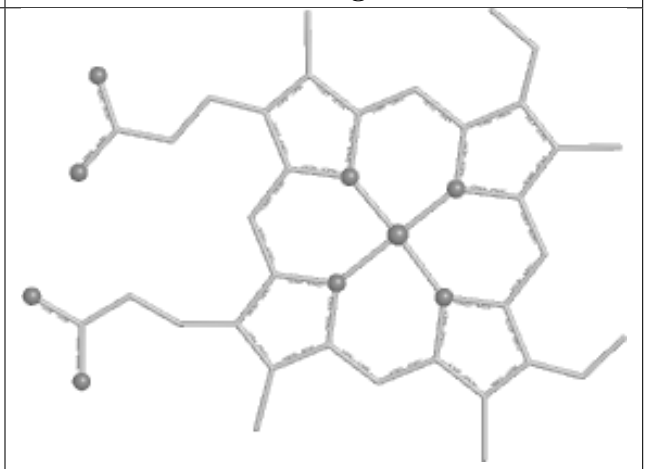


Bond angles

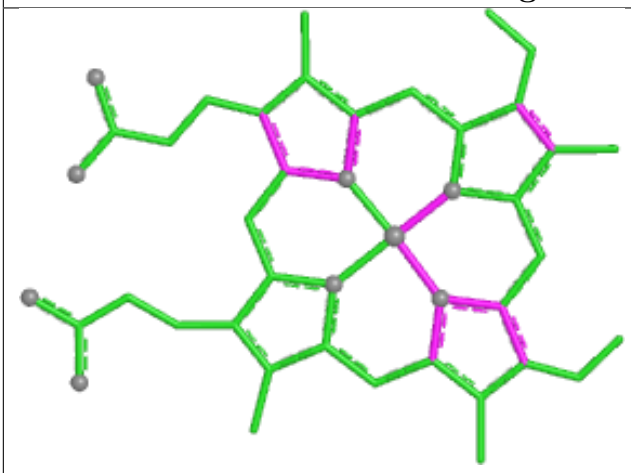


Torsions

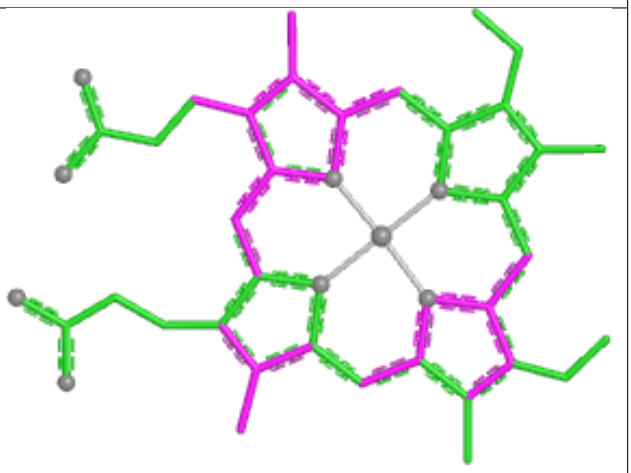


Rings

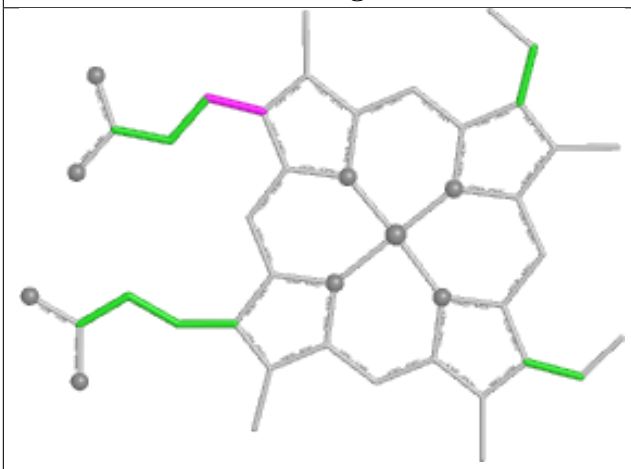
Ligand HEM B 903



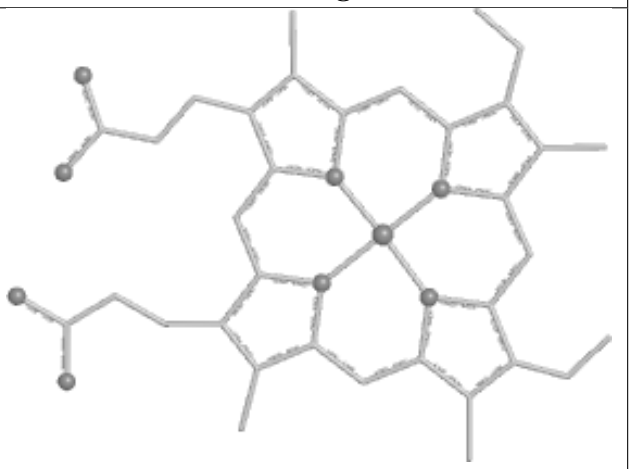
Bond lengths



Bond angles

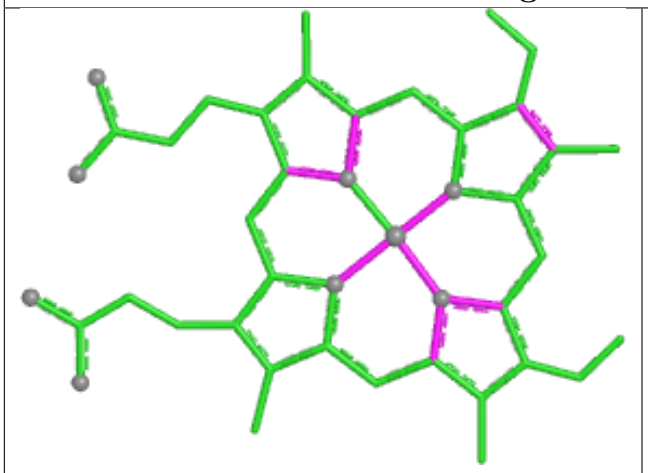


Torsions

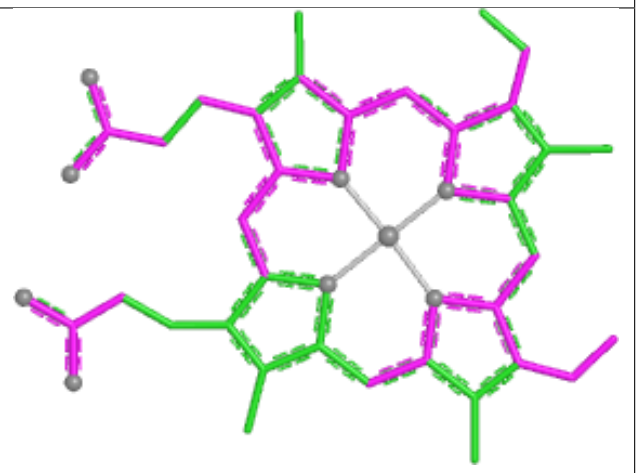


Rings

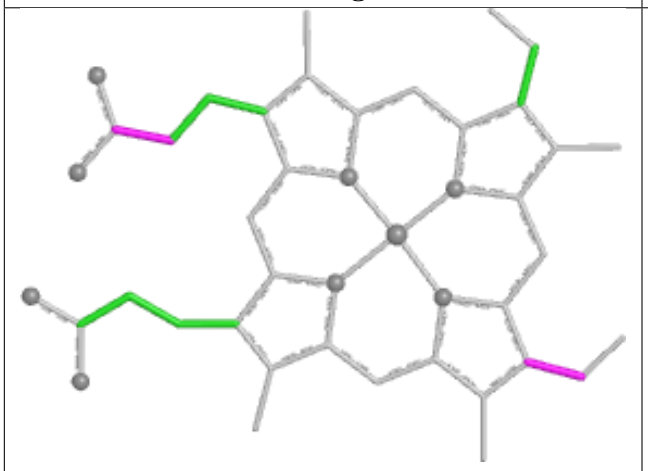
Ligand HEM C 907



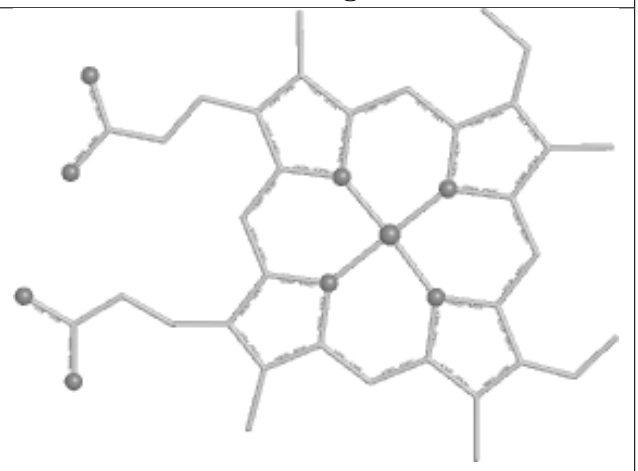
Bond lengths



Bond angles

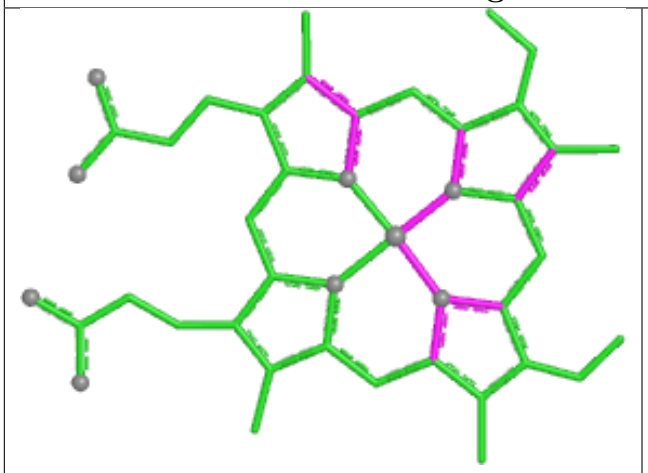


Torsions

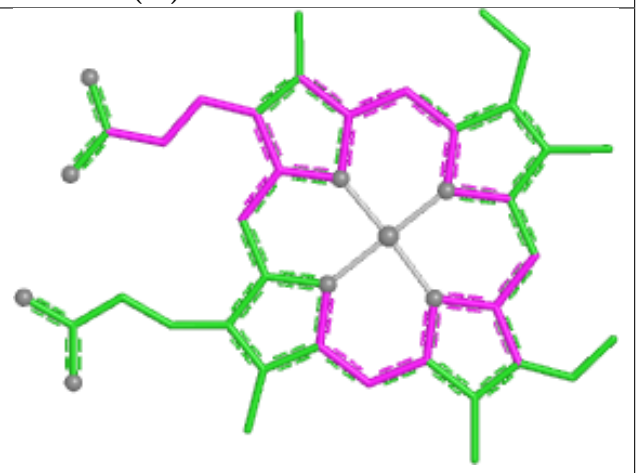


Rings

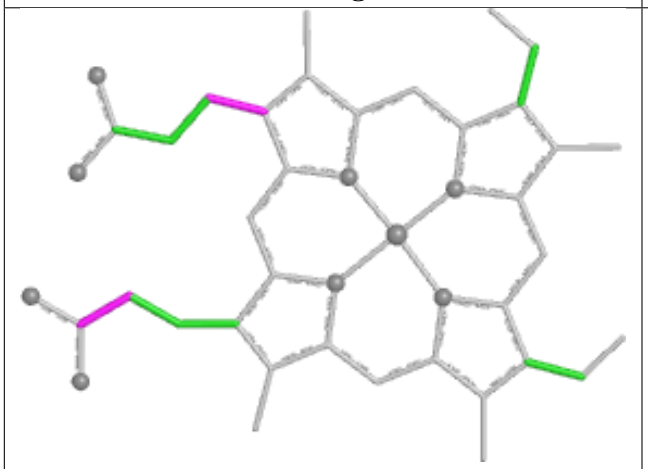
Ligand HEM C 904 (B)



Bond lengths



Bond angles



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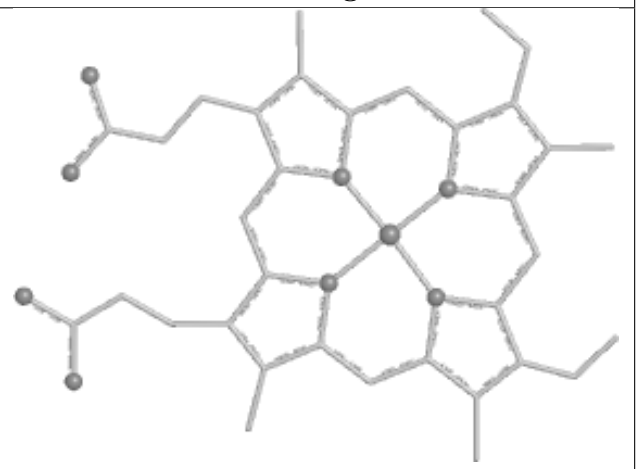
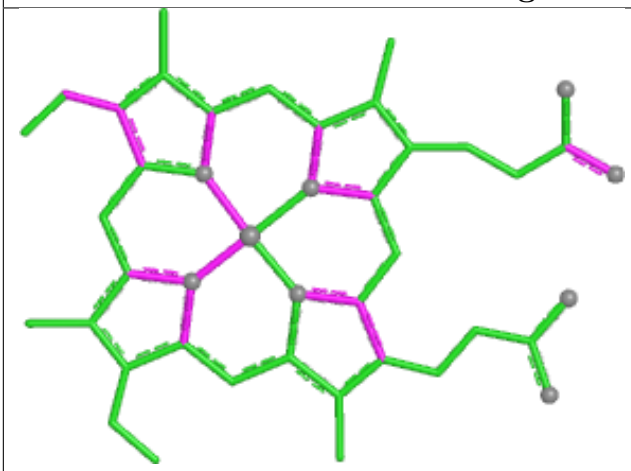
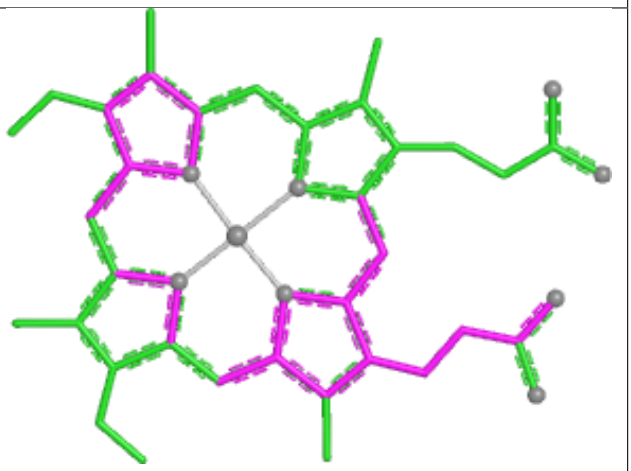


Rings

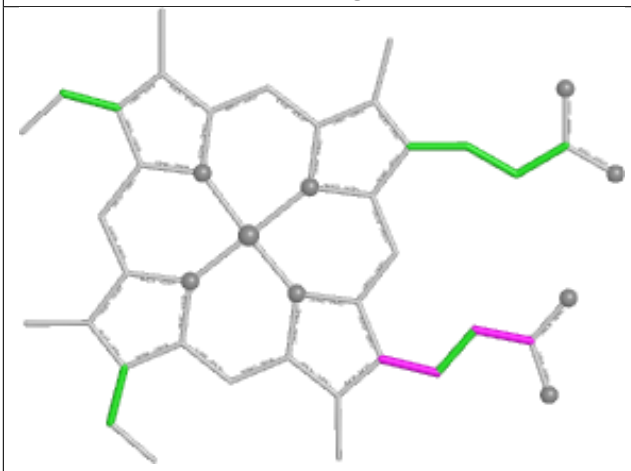
Ligand HEM D 903



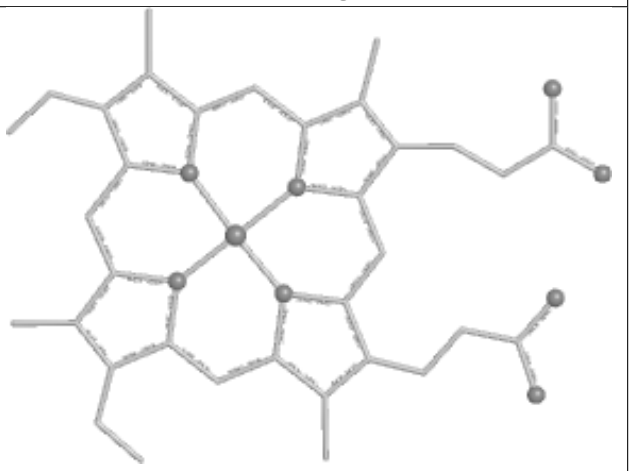
Bond lengths



Bond angles

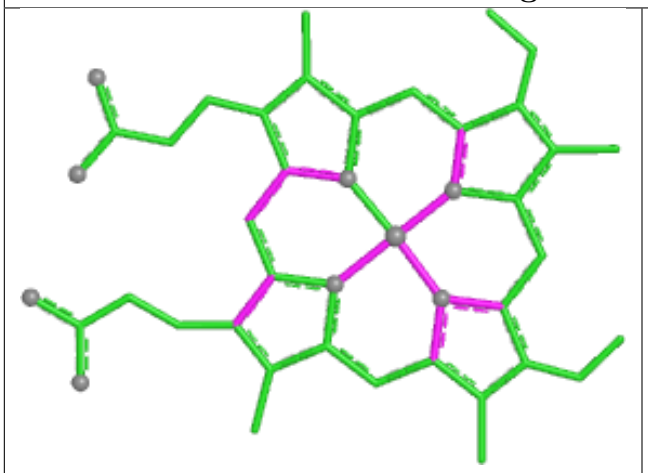


Torsions

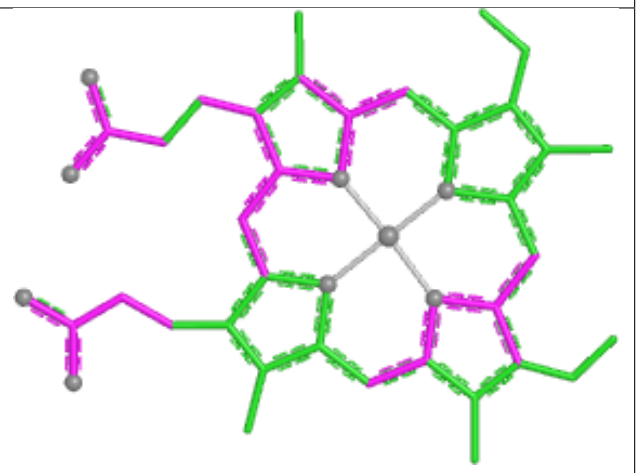


Rings

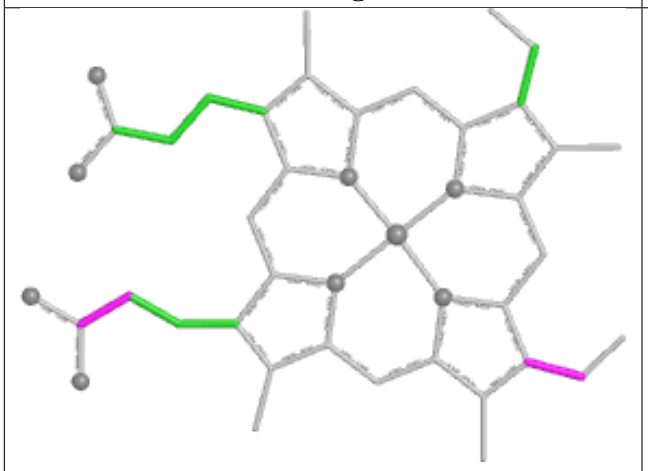
Ligand HEM B 906



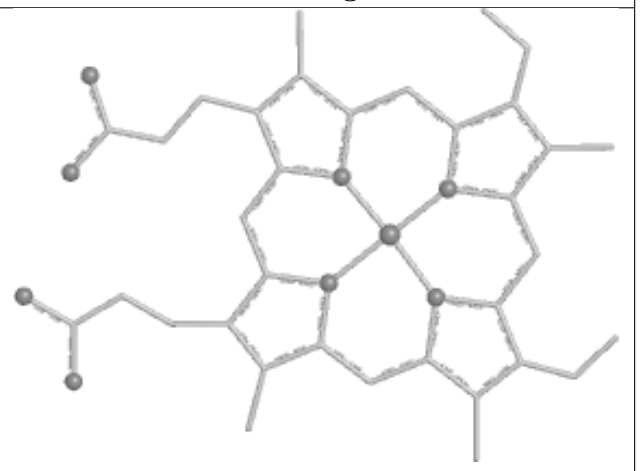
Bond lengths



Bond angles

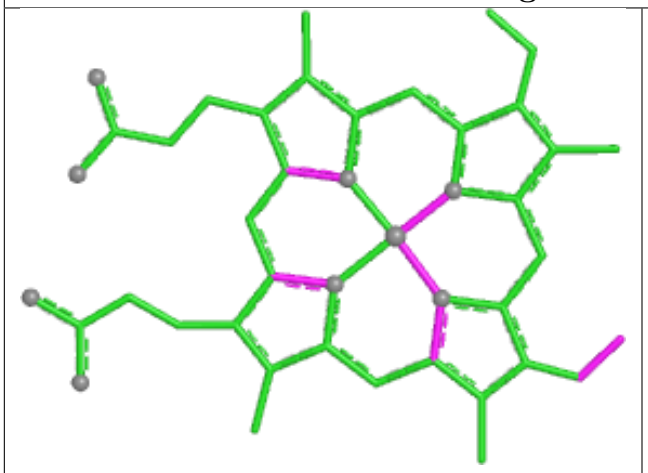


Torsions

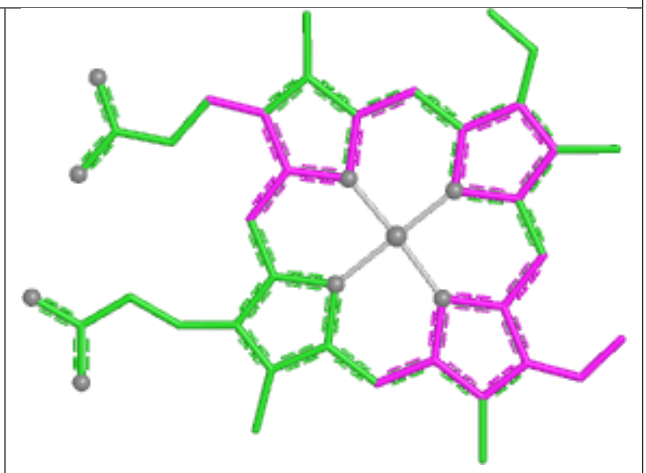


Rings

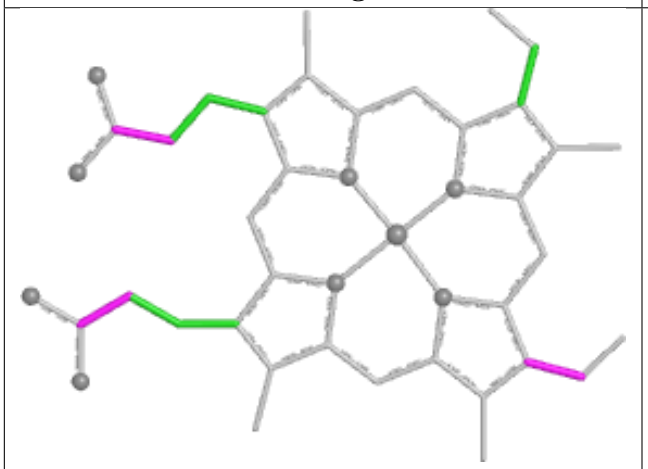
Ligand HEM A 908



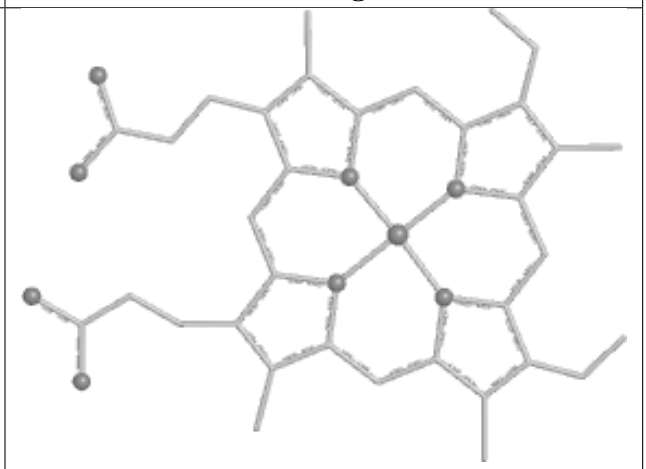
Bond lengths



Bond angles

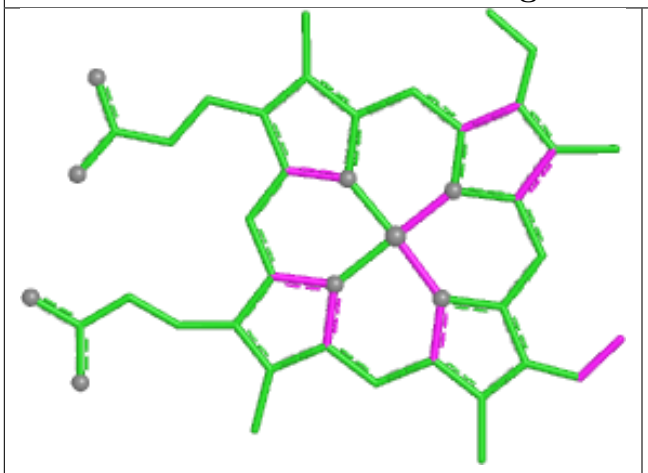


Torsions

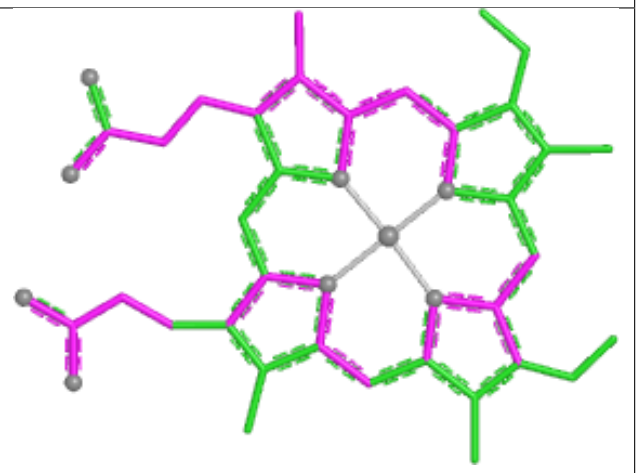


Rings

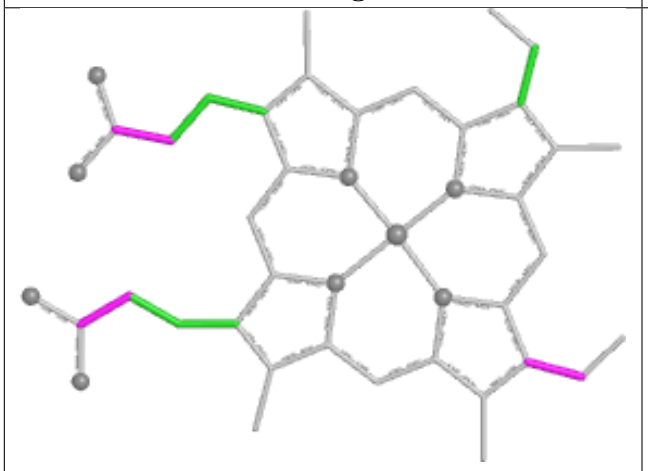
Ligand HEM C 909



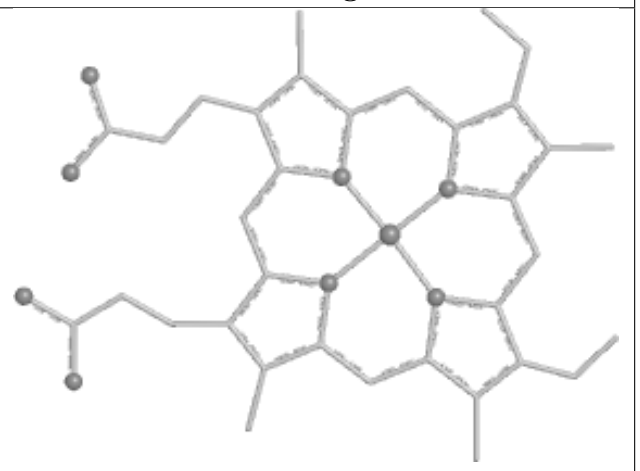
Bond lengths



Bond angles

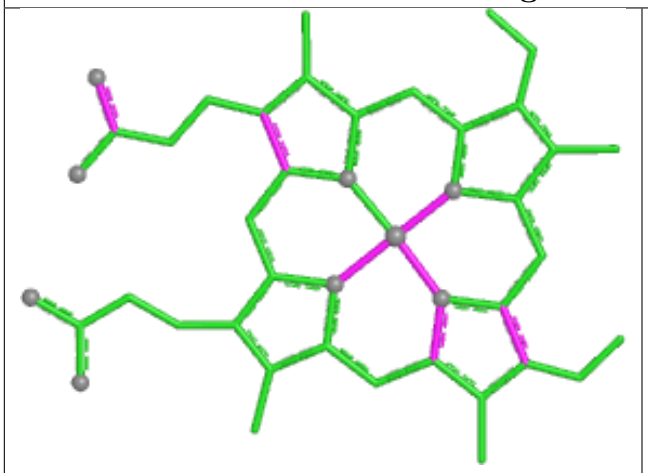


Torsions

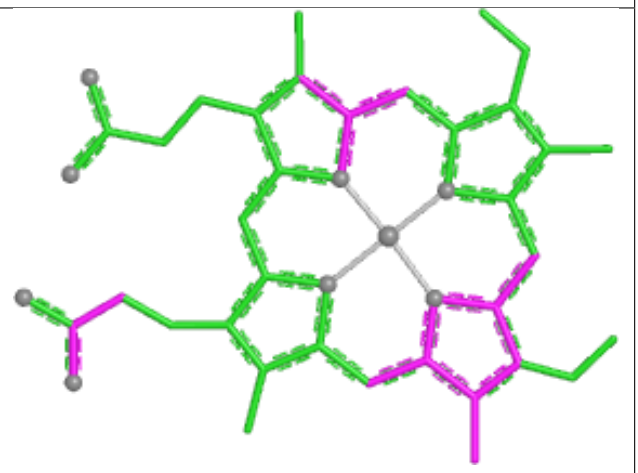


Rings

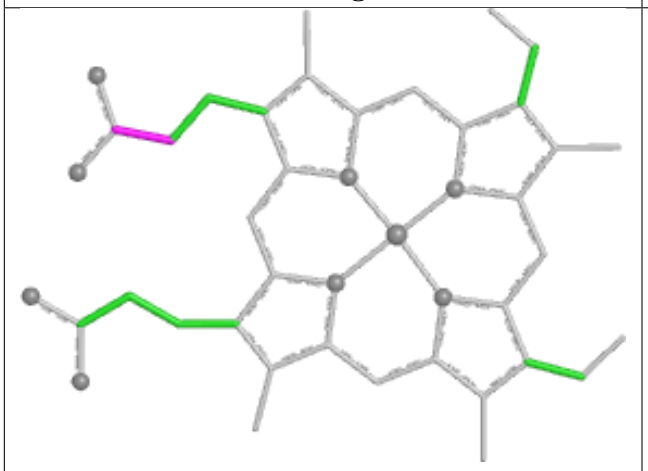
Ligand HEM B 905



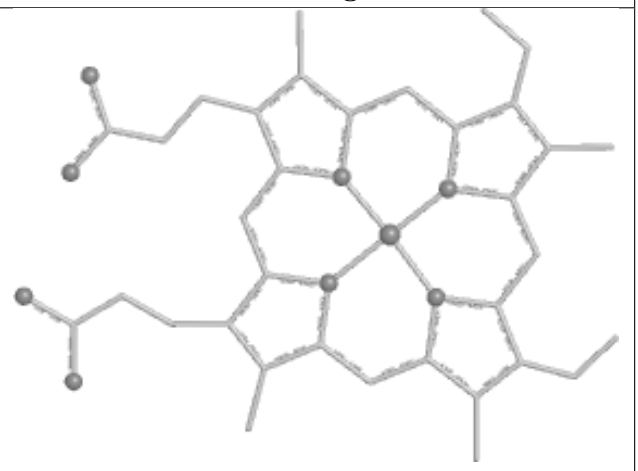
Bond lengths



Bond angles

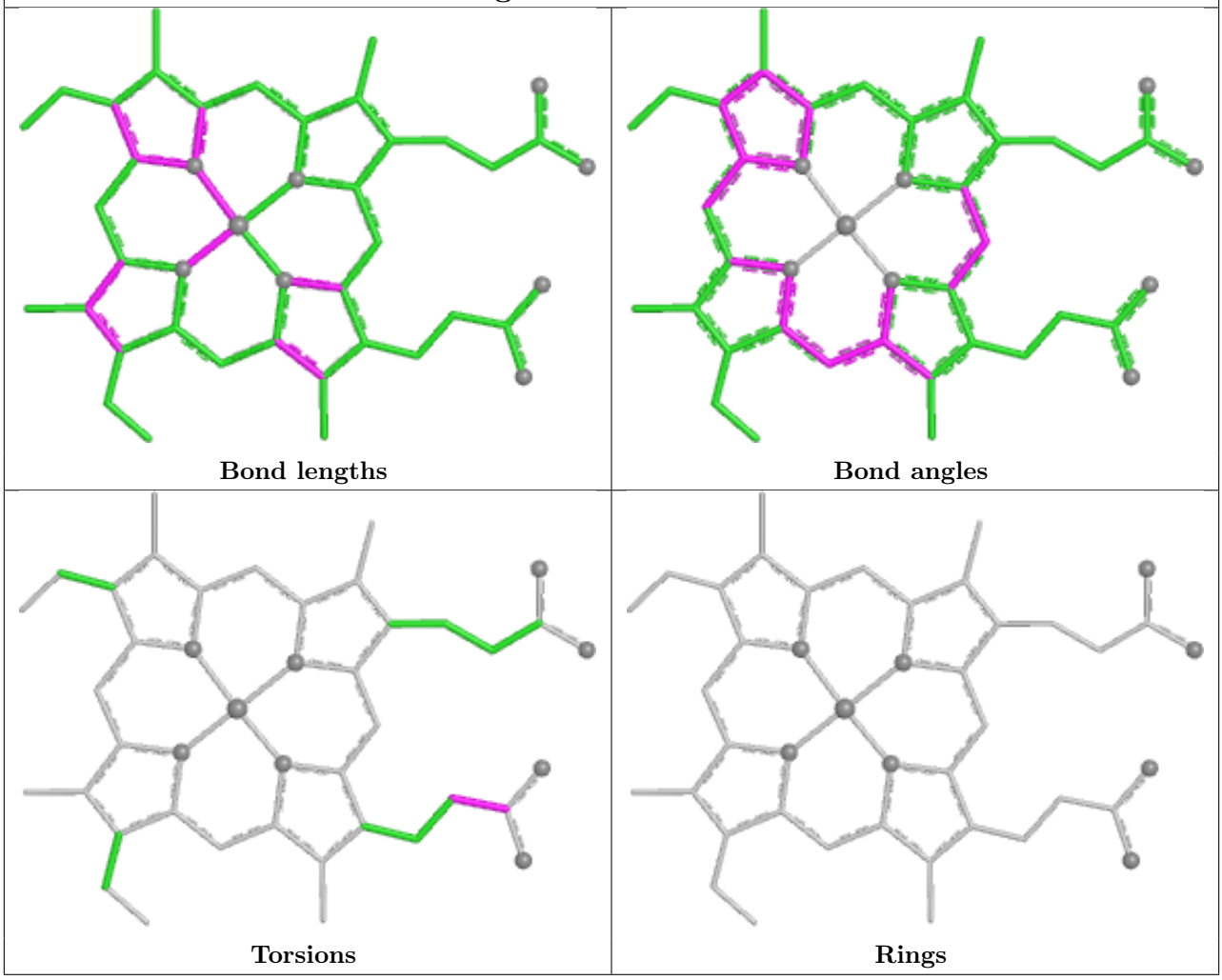


Torsions

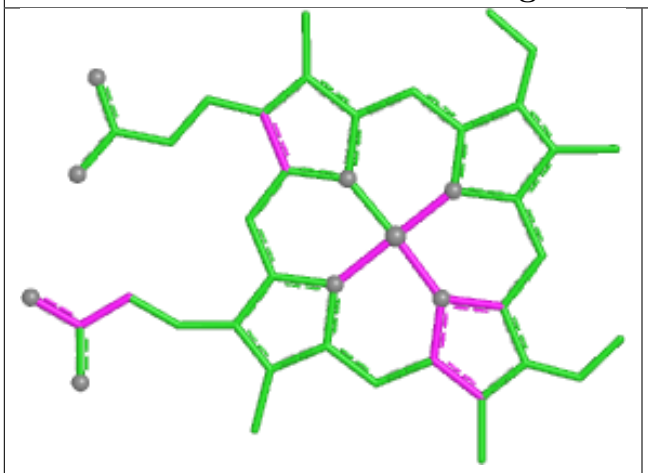


Rings

Ligand HEM C 905



Ligand HEM A 902



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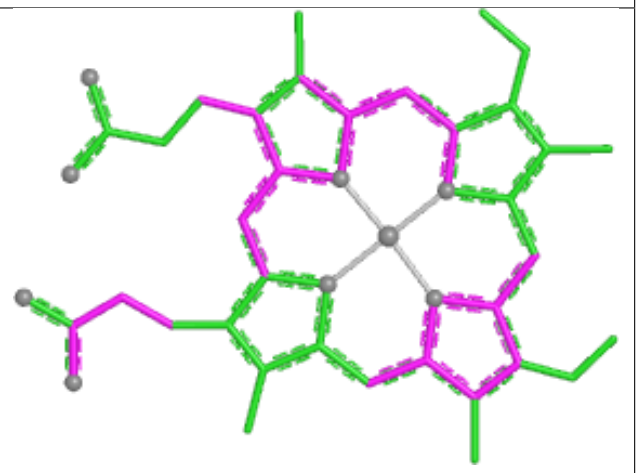
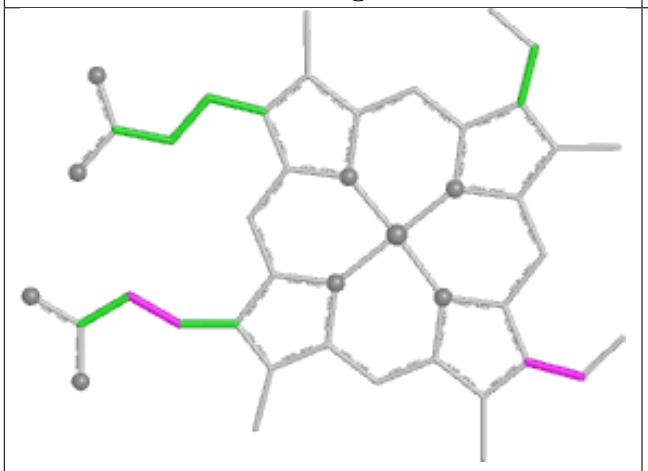
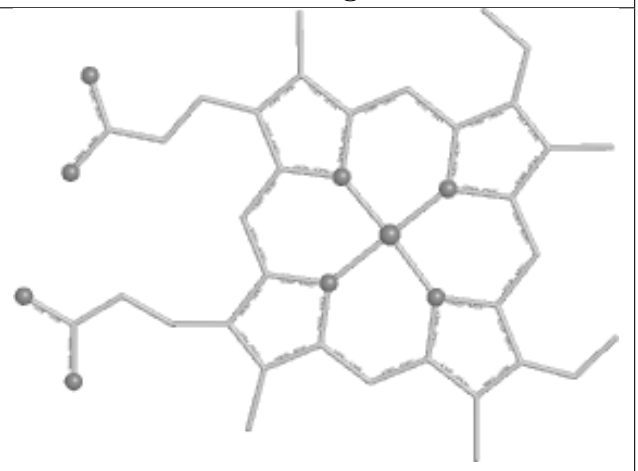


Bond angles

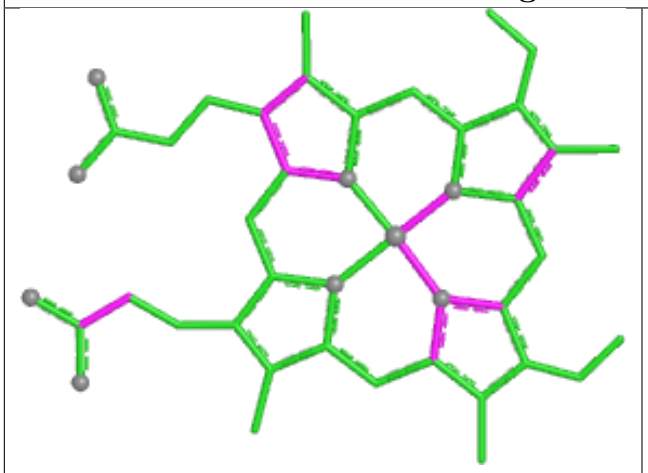


Torsions



Rings

Ligand HEM D 905



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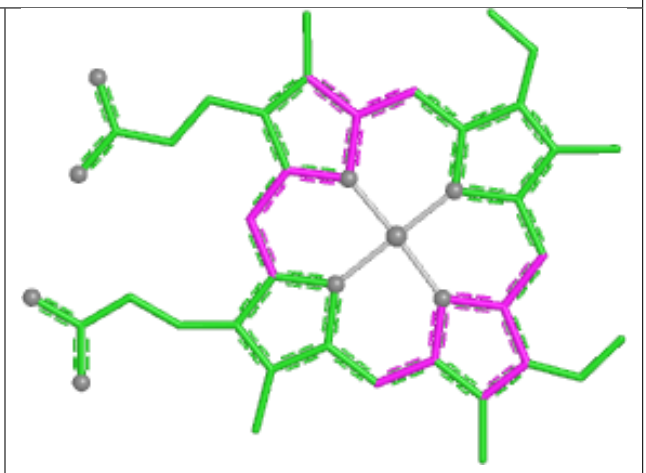
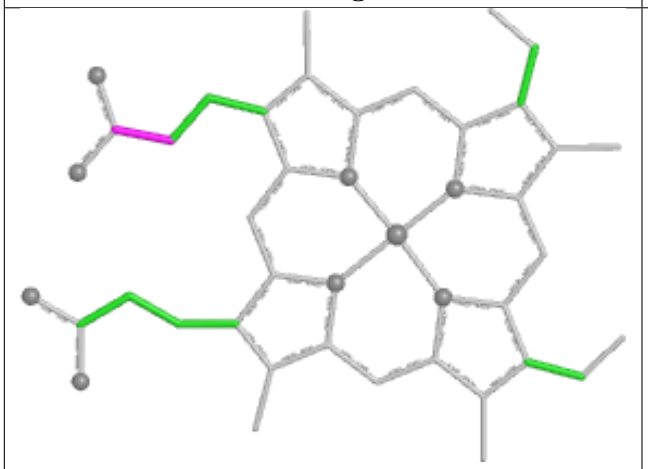


Bond angles



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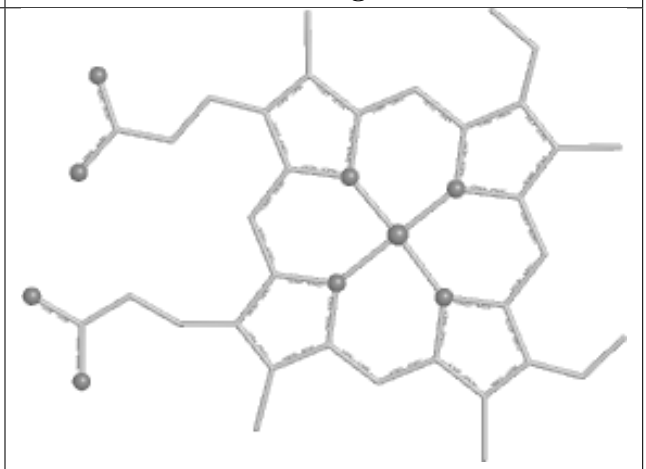
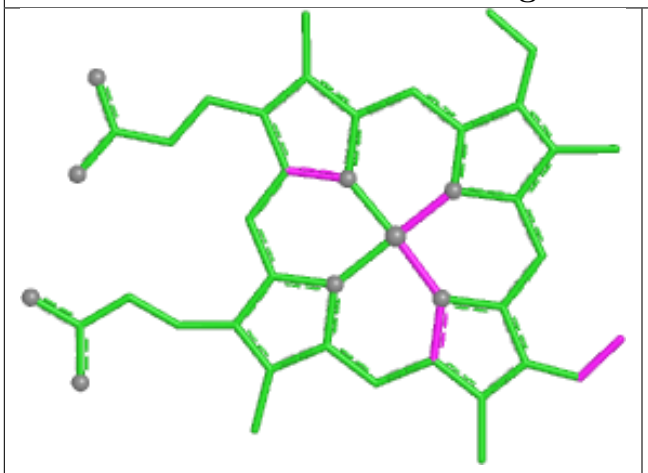


Rings

Ligand HEM D 907



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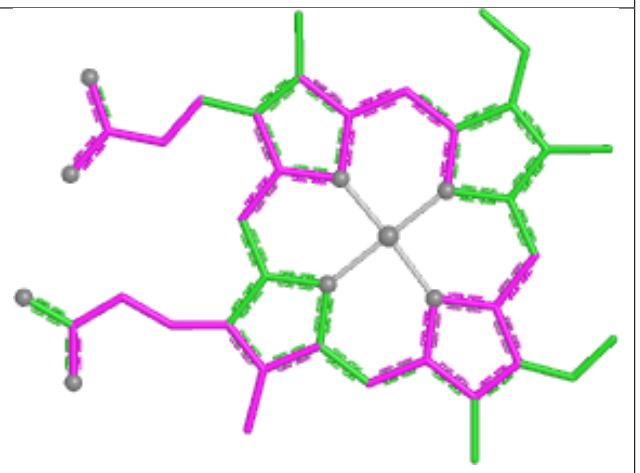
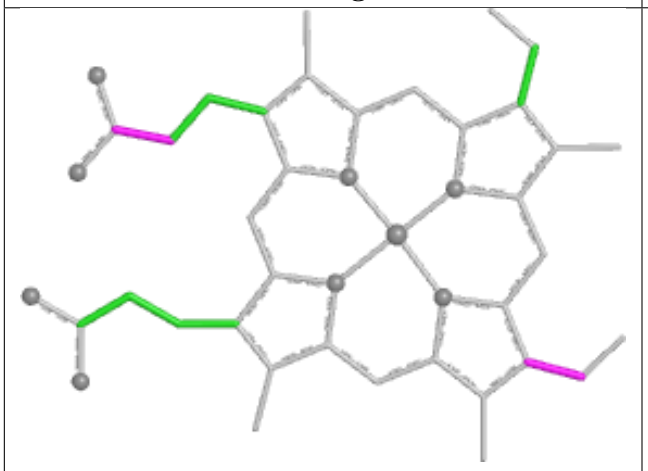


Bond angles



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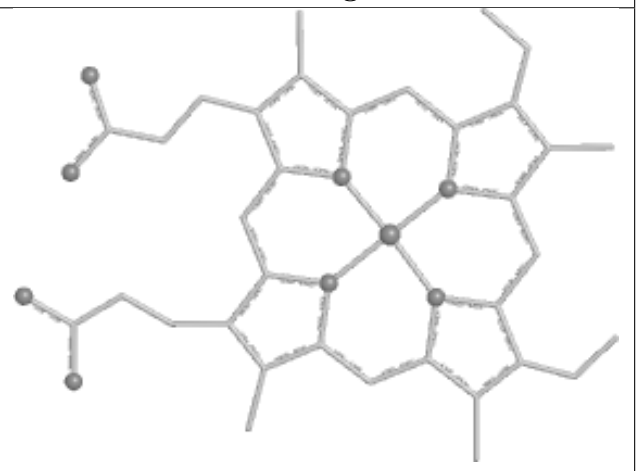
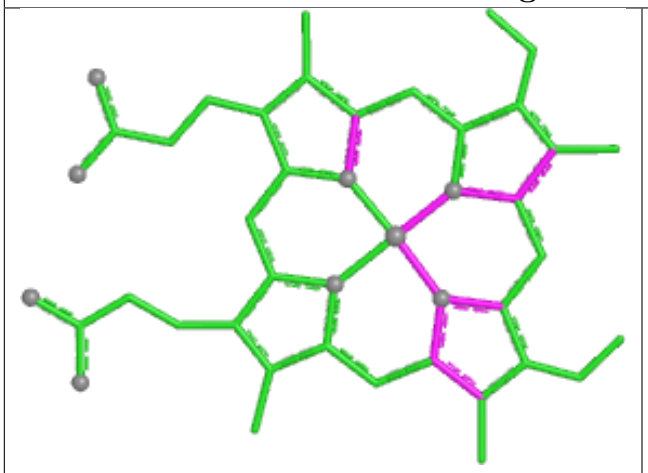


Rings

Ligand HEM A 909



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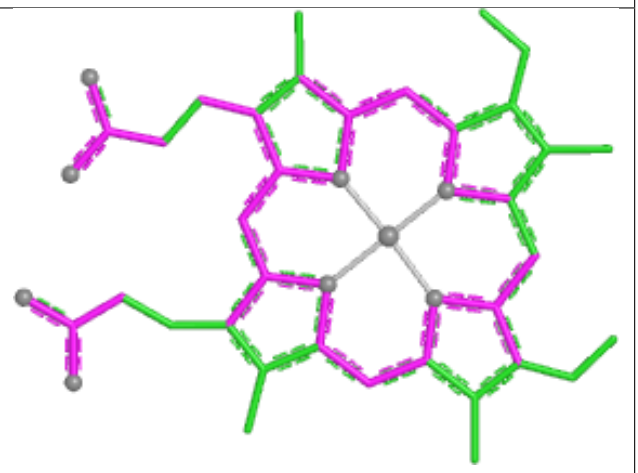

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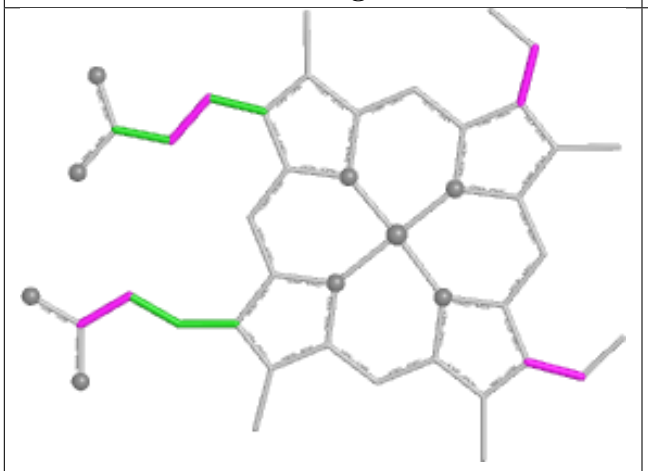

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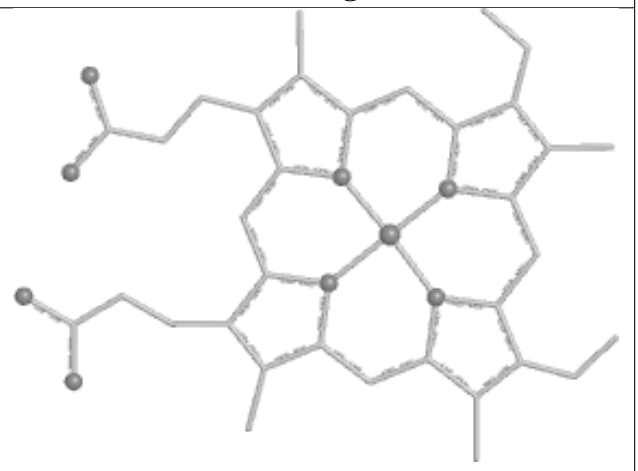
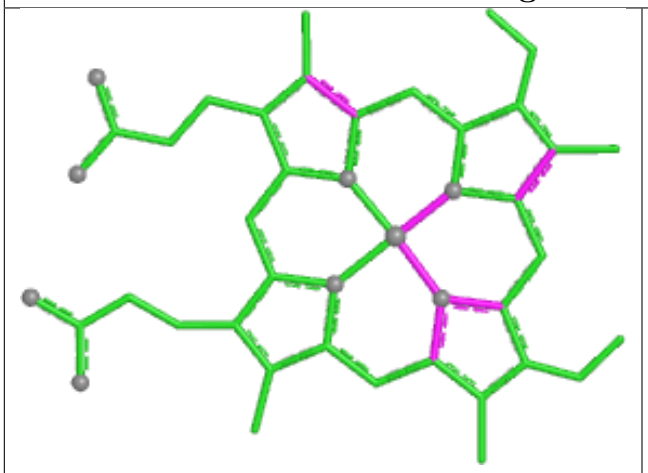


Rings

Ligand HEM D 908



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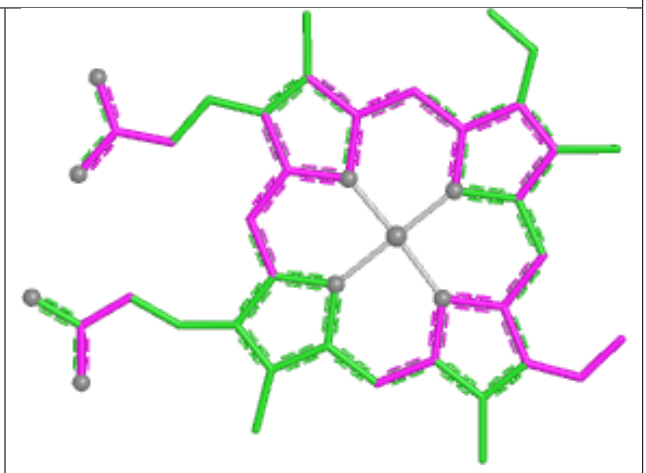

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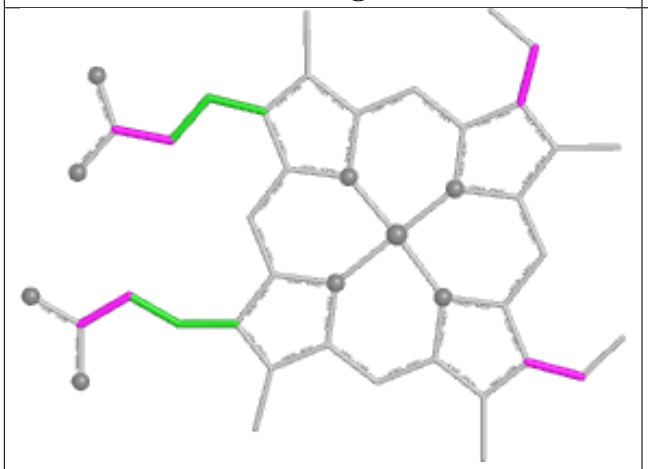

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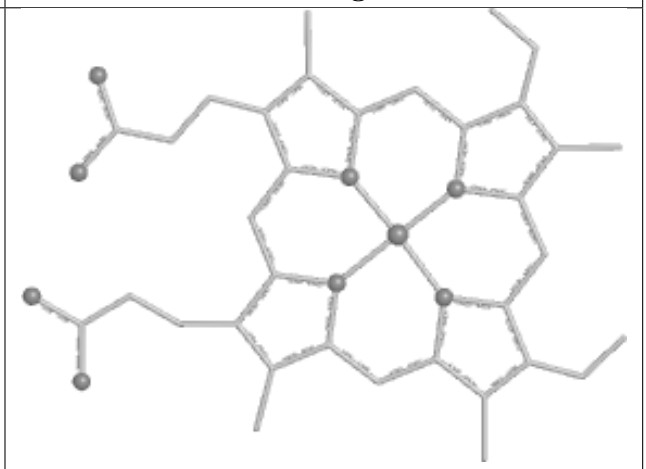
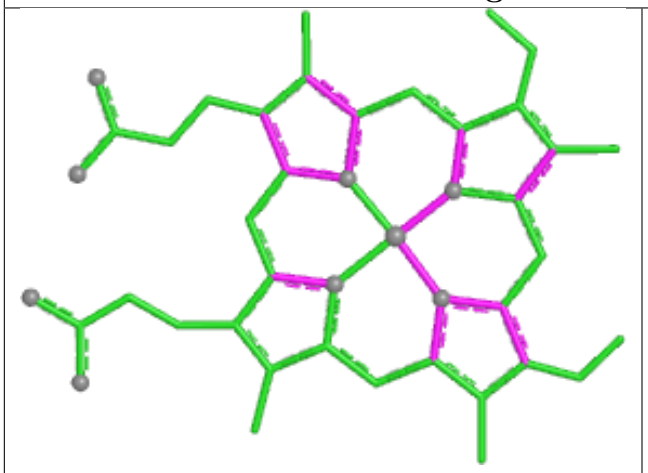


Rings

Ligand HEM A 904 (A)



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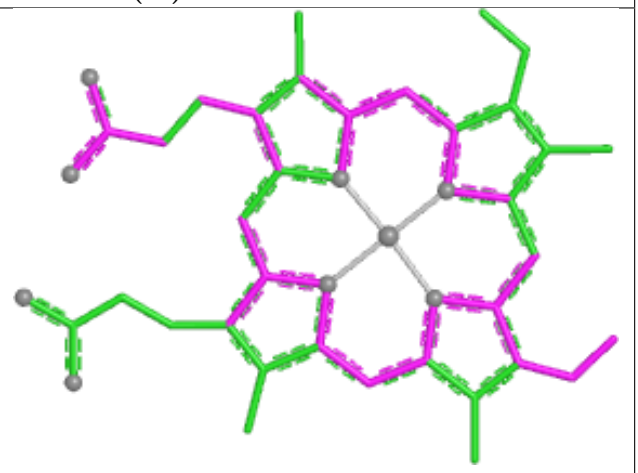
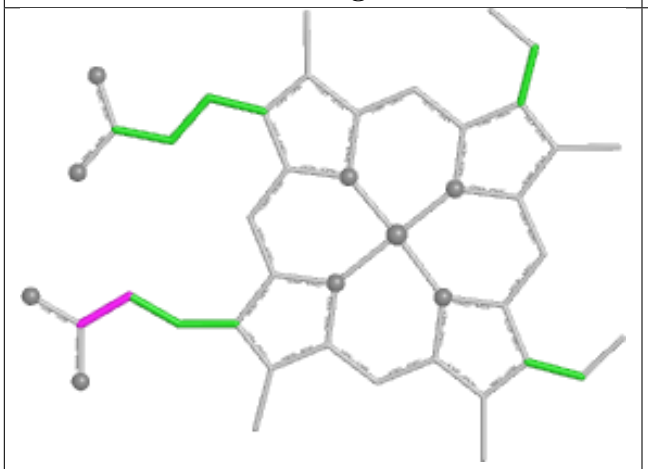


Bond angles



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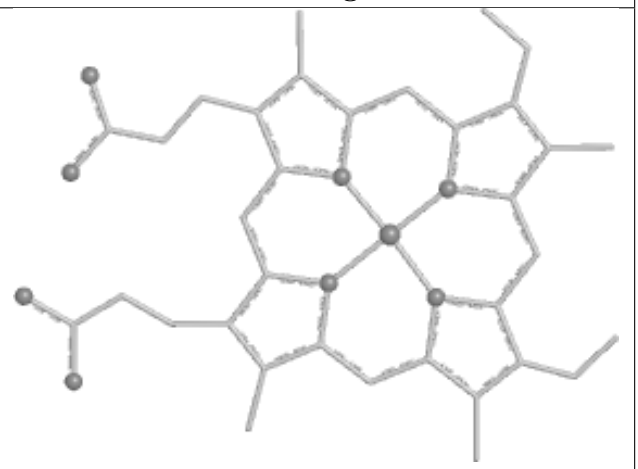
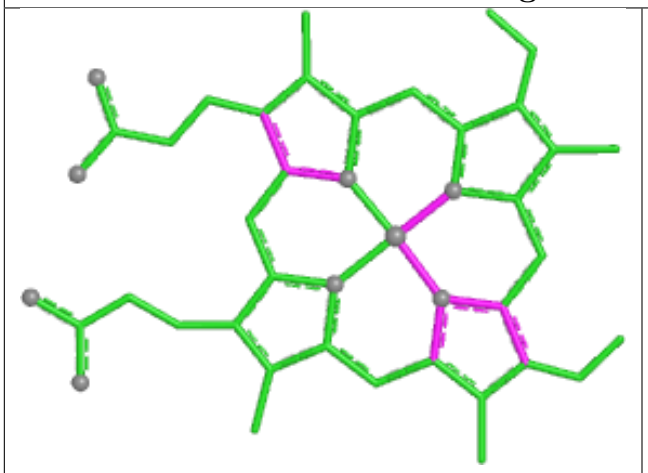


Rings

Ligand HEM A 905



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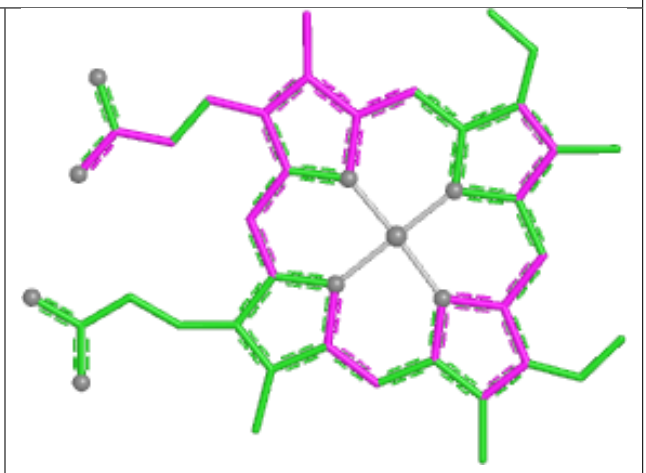
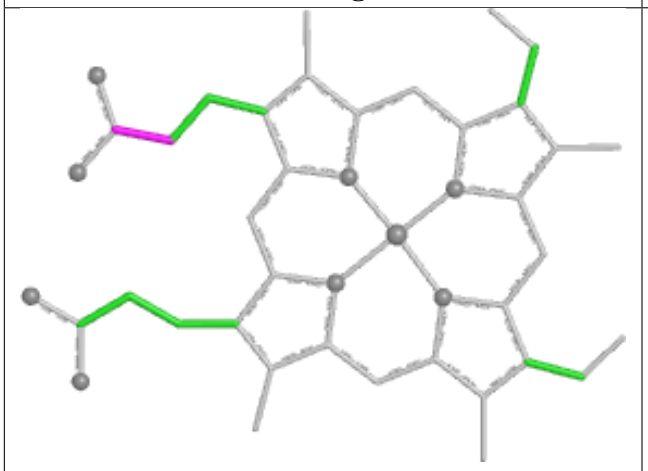
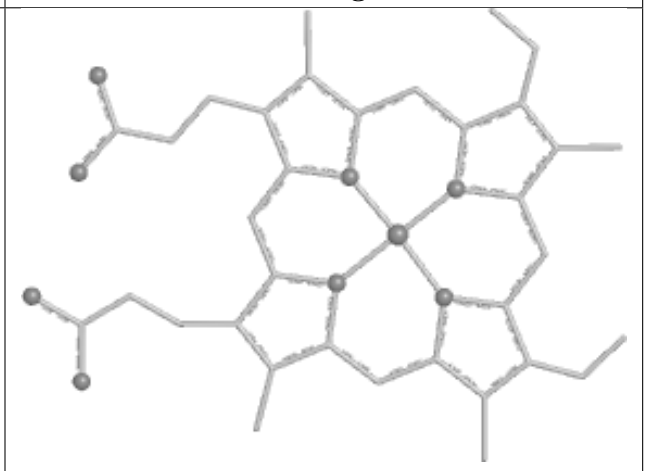


Bond angles

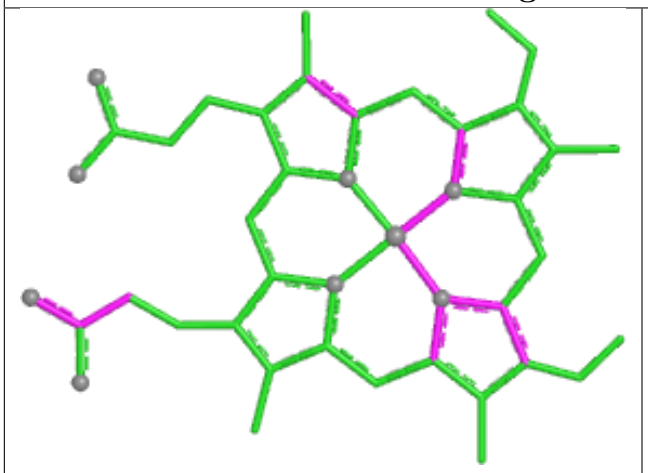


Torsions



Rings

Ligand HEM D 902



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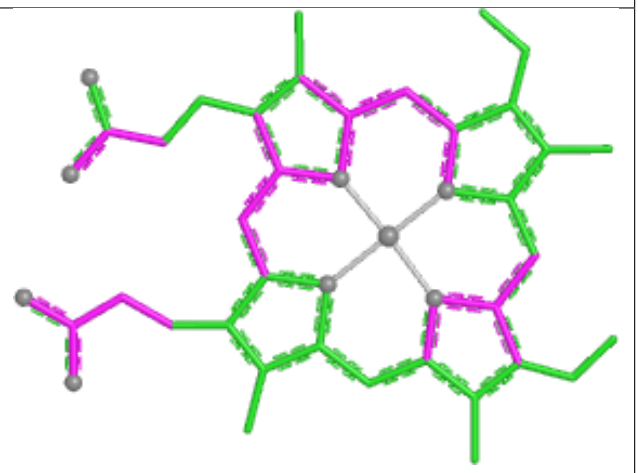
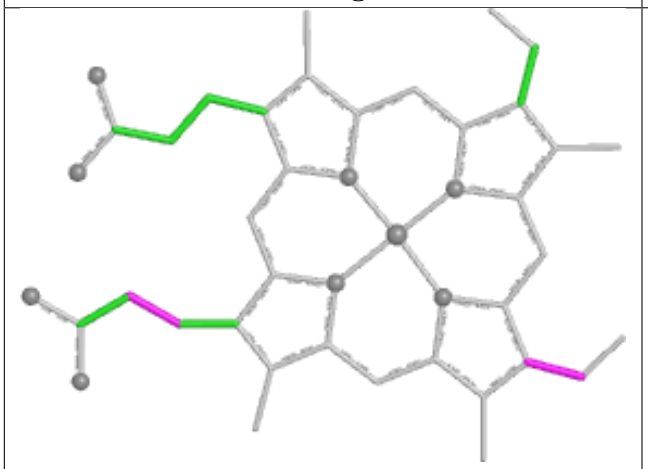


Bond angles



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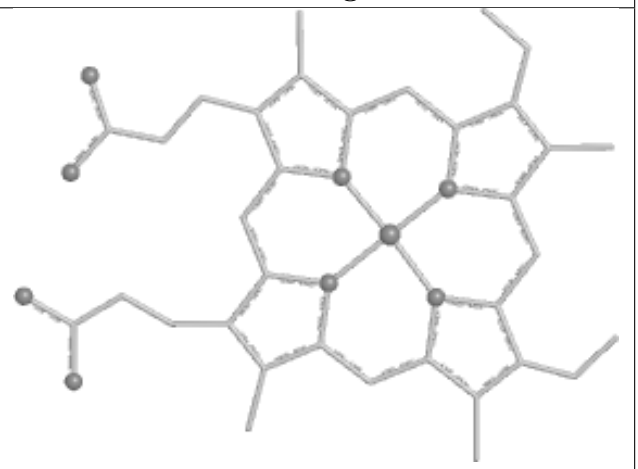
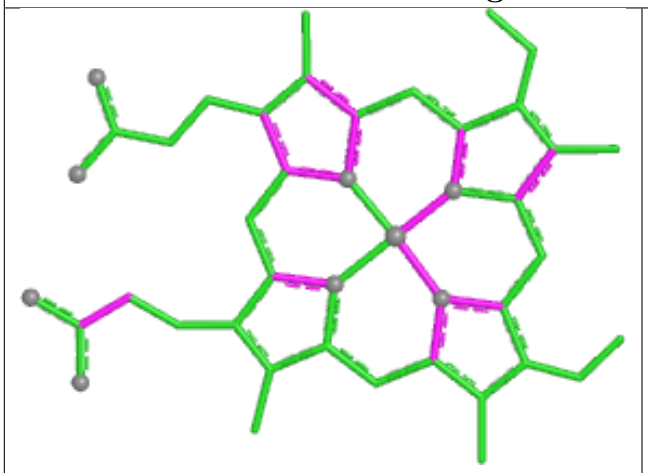


Rings

Ligand HEM A 904 (B)



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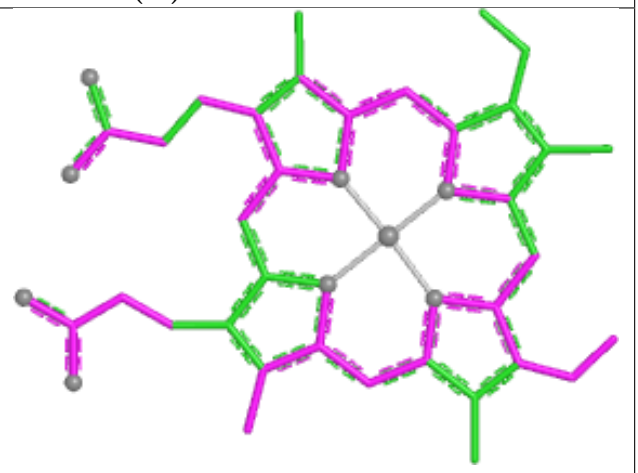
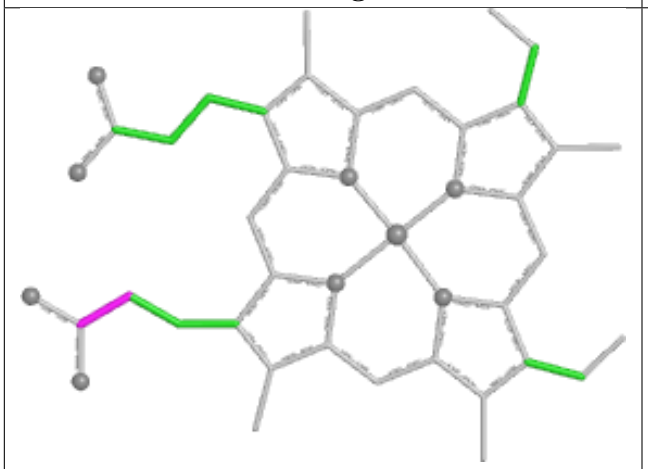
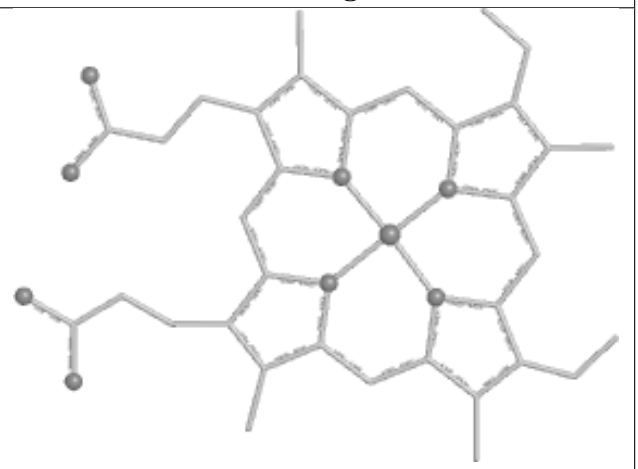


Bond angles

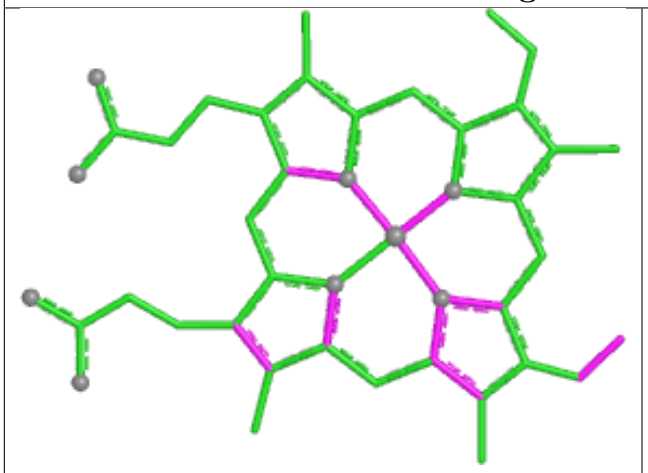


Torsions



Rings

Ligand HEM D 909



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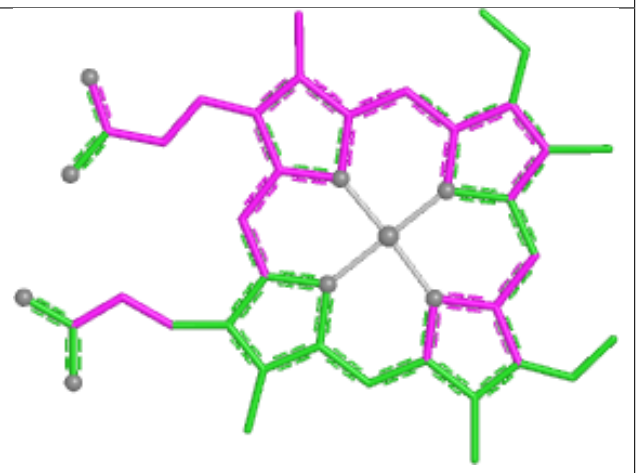
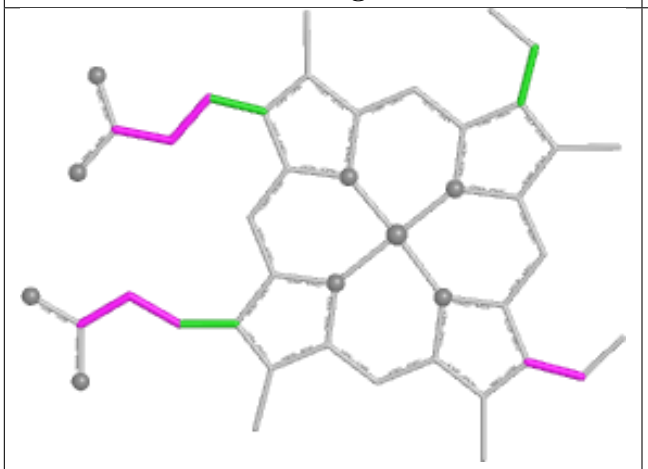
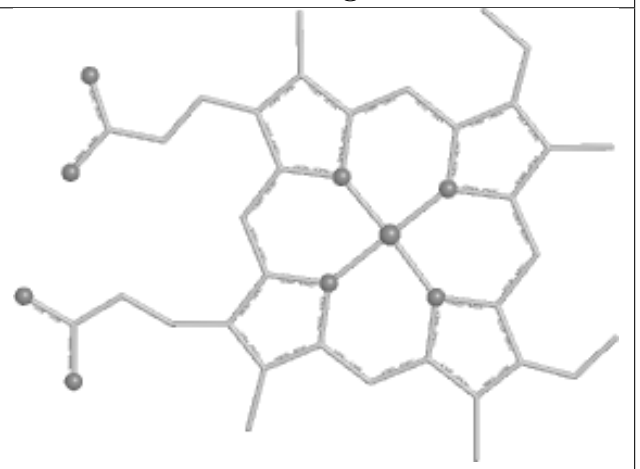


Bond angles

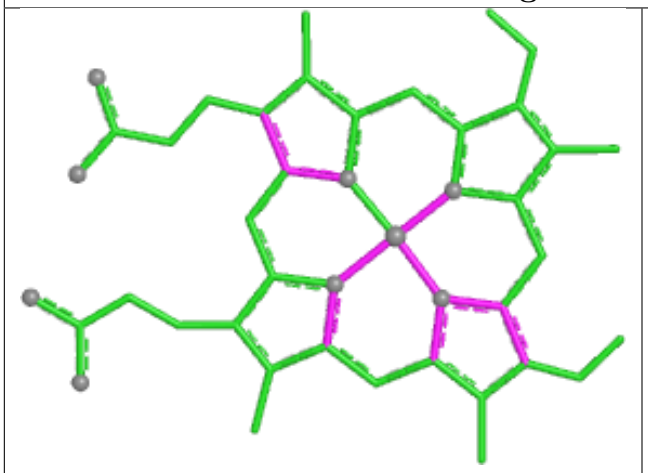


Torsions

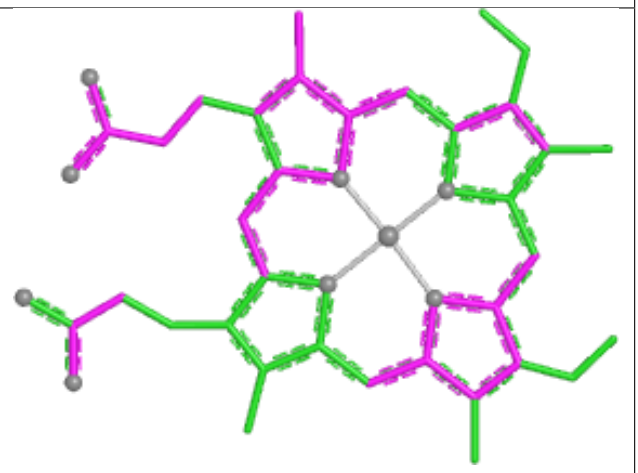


Rings

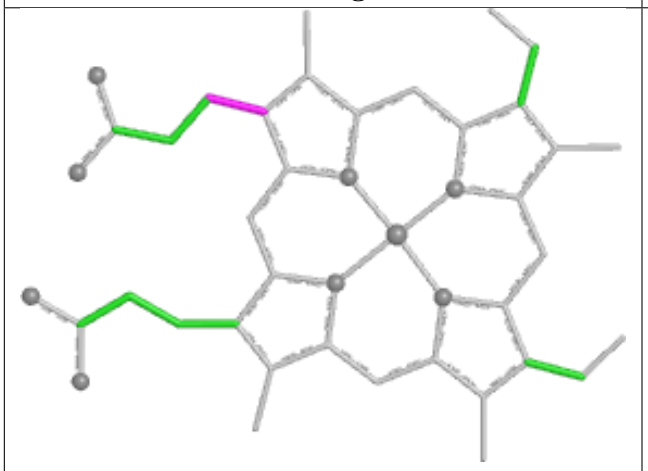
Ligand HEM C 903



Bond lengths



Bond angles



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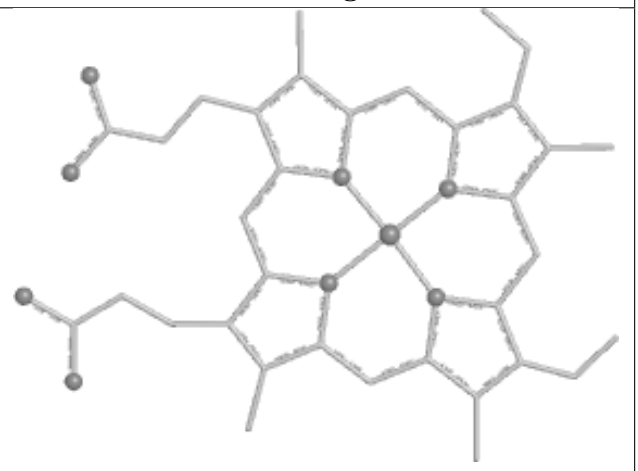
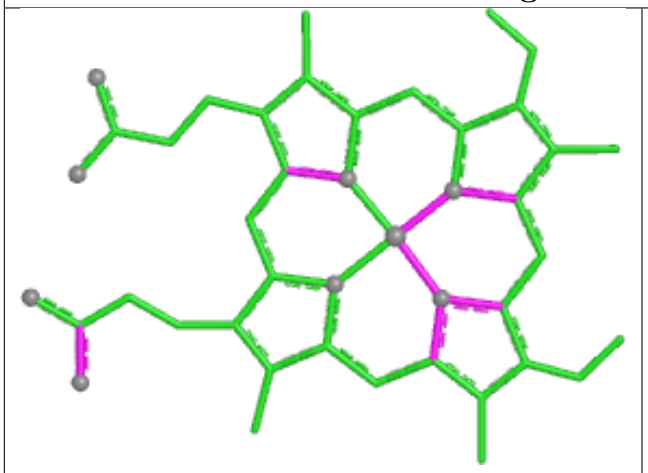


Rings

Ligand HEM B 909



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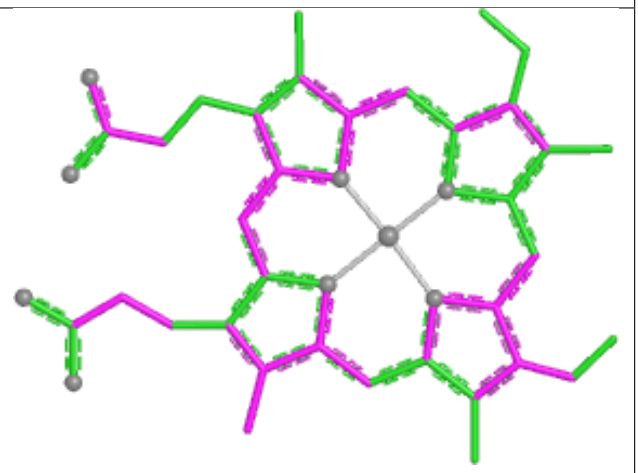
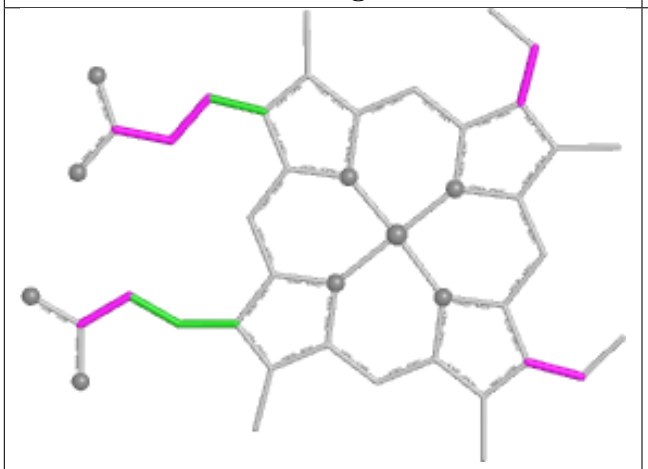


Bond angles



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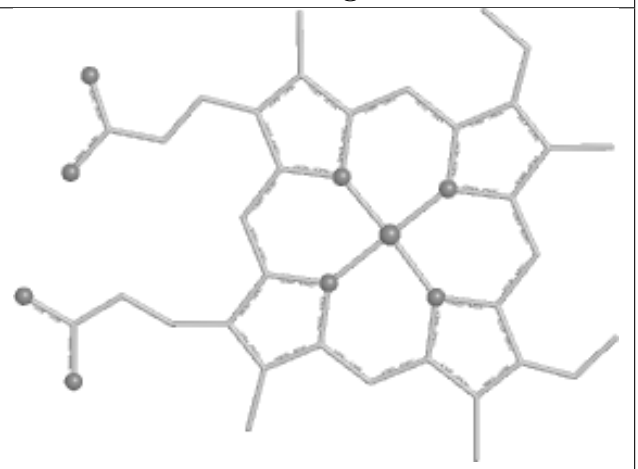
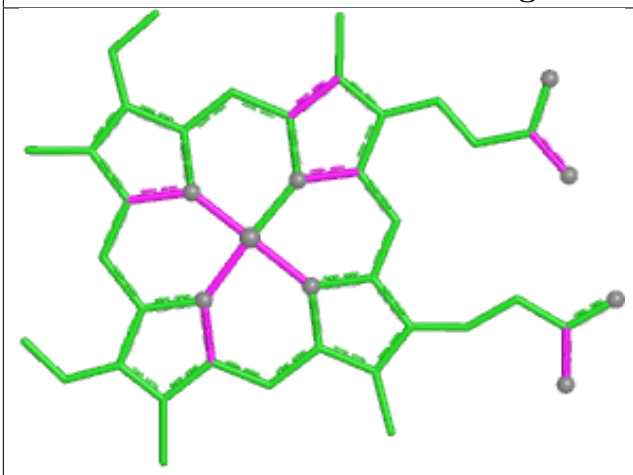
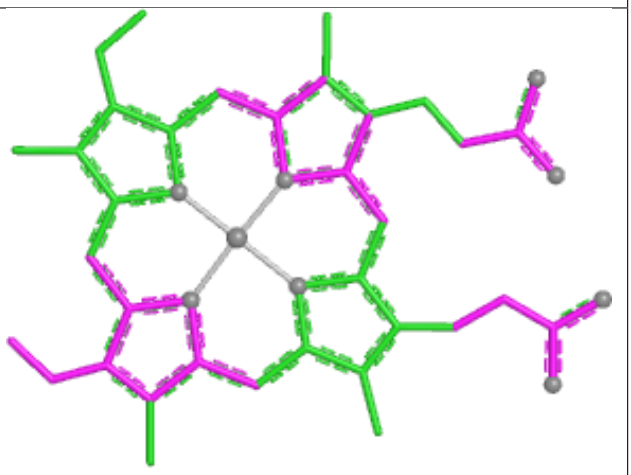


Rings

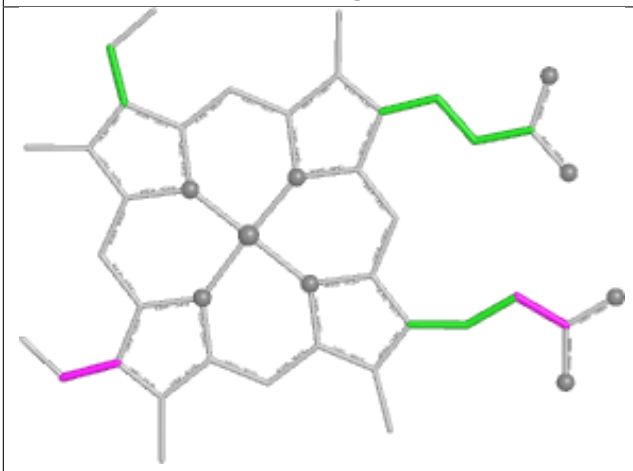
Ligand HEM C 906



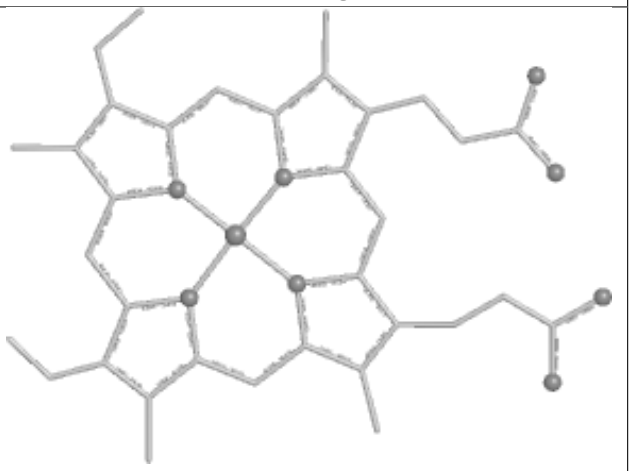
Bond lengths



Bond angles

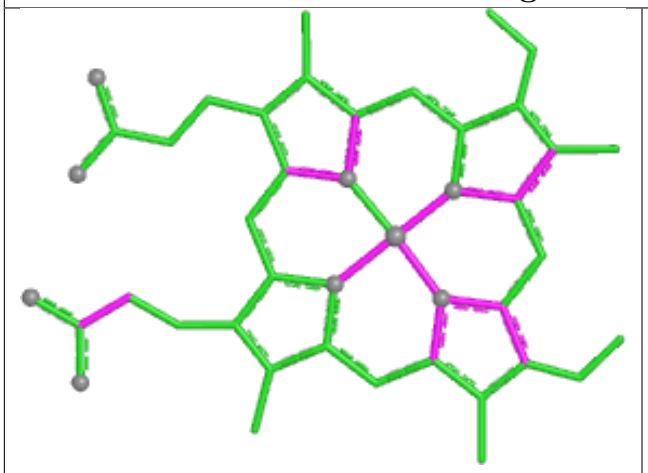


Torsions

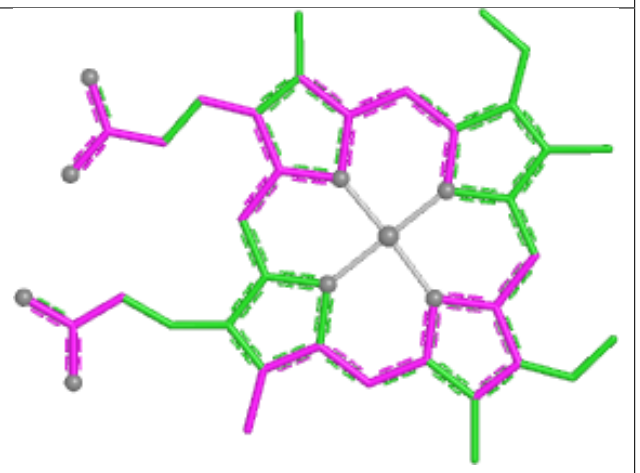


Rings

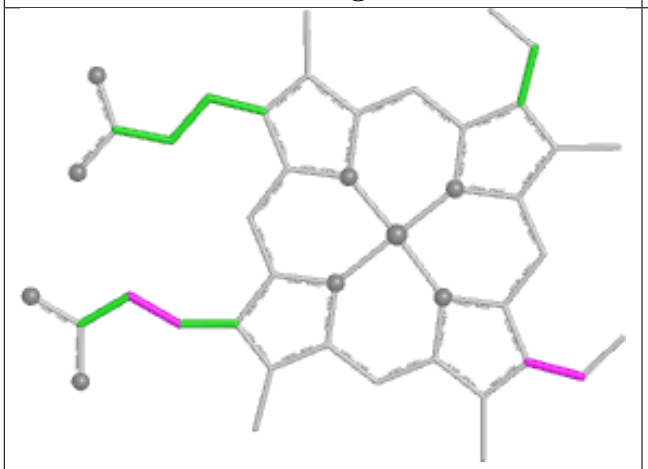
Ligand HEM C 902



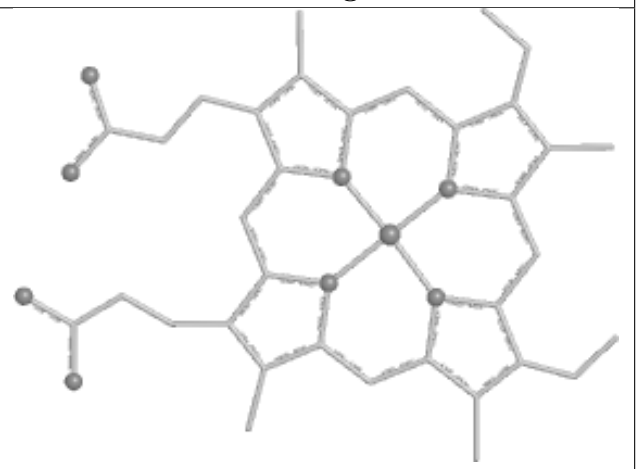
Bond lengths



Bond angles

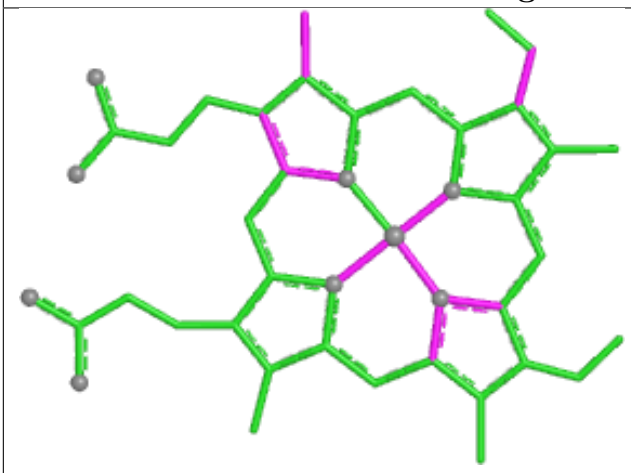


Torsions

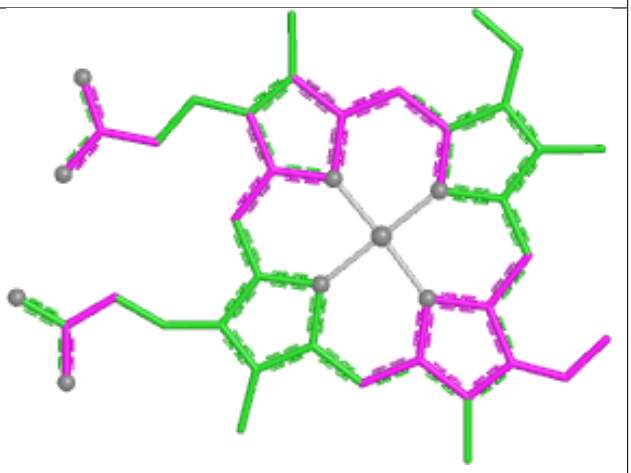


Rings

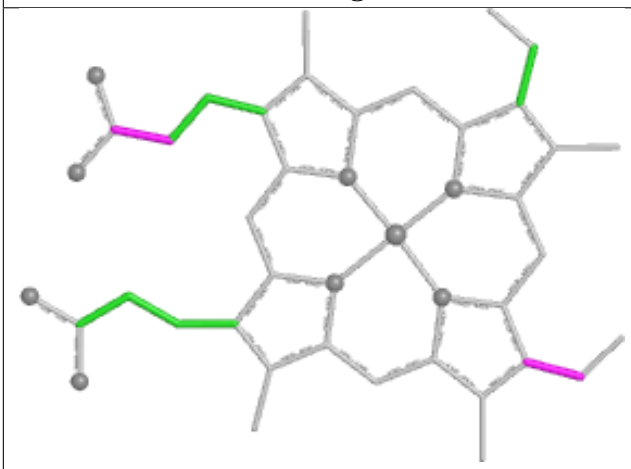
Ligand HEM A 907



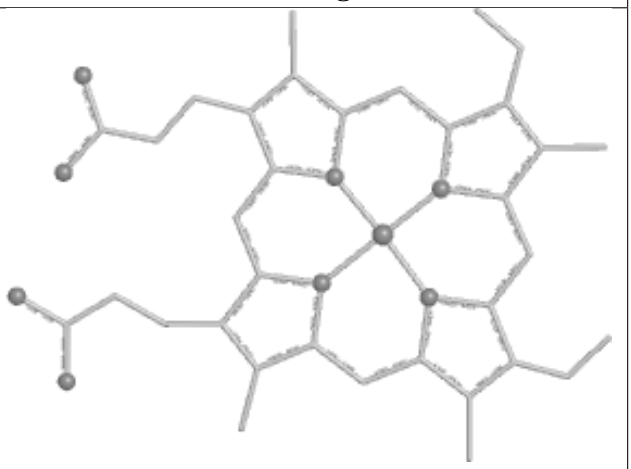
Bond lengths



Bond angles

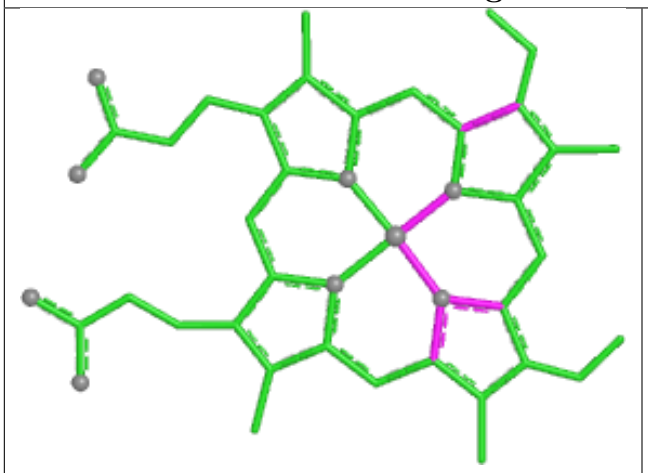


Torsions



Rings

Ligand HEM D 904 (A)



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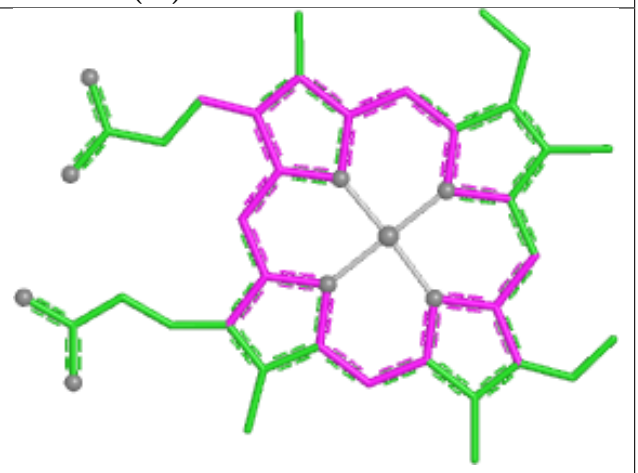
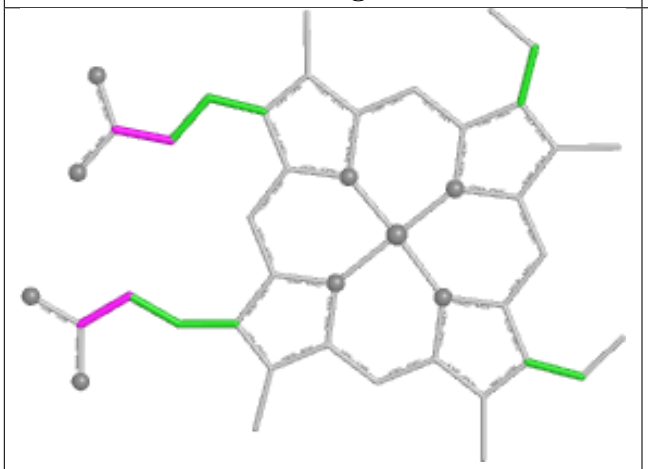
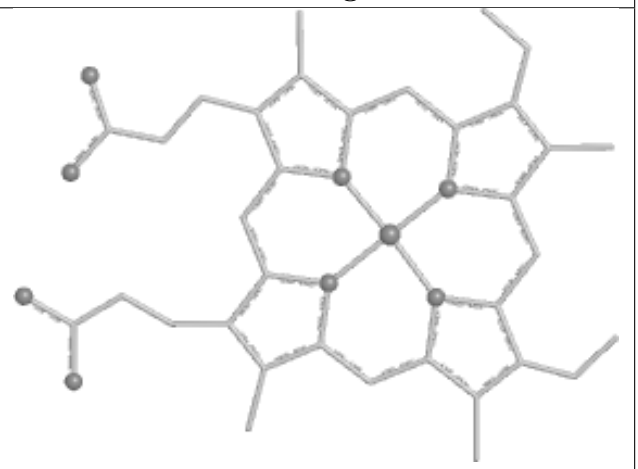


Bond angles

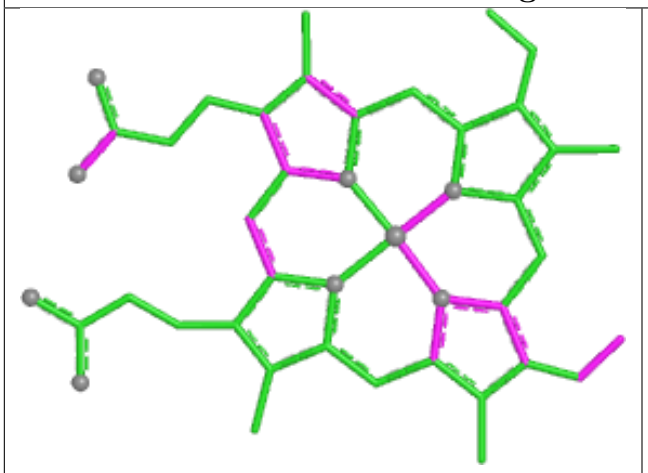


Torsions

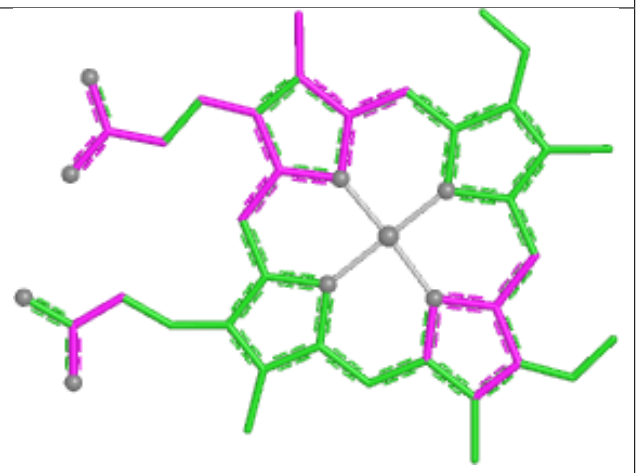


Rings

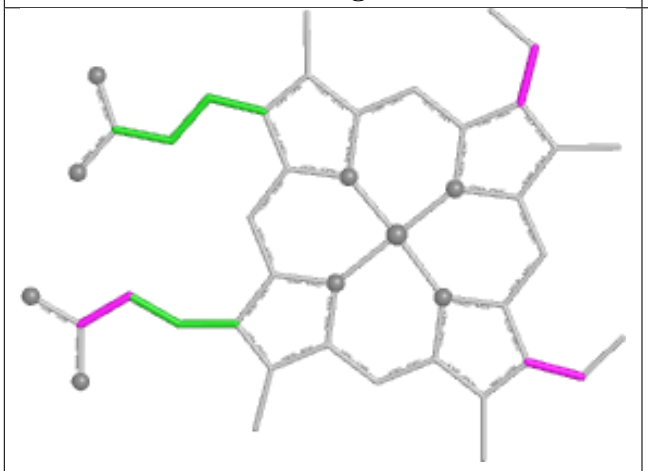
Ligand HEM A 906



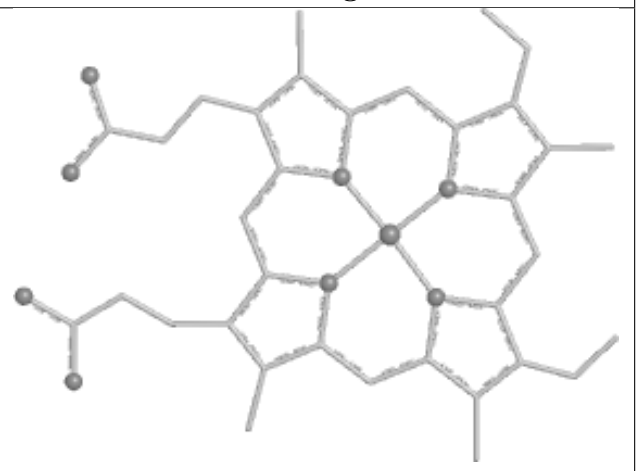
Bond lengths



Bond angles

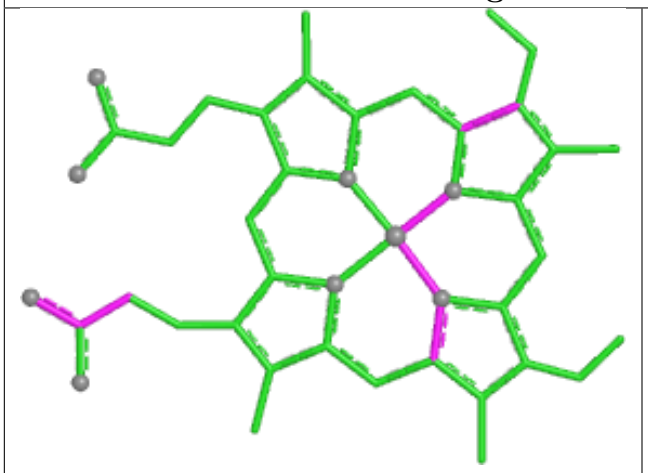


Torsions

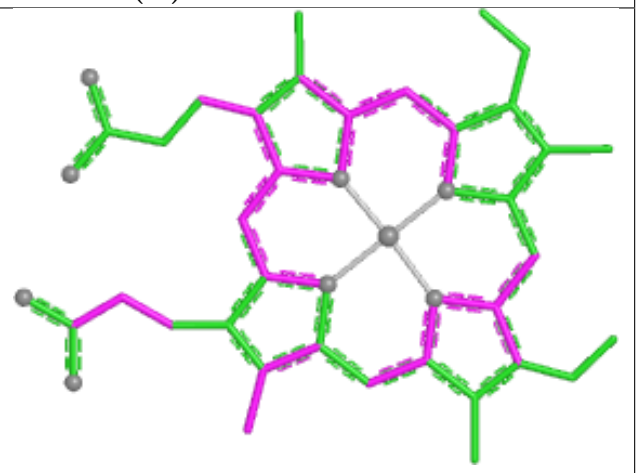


Rings

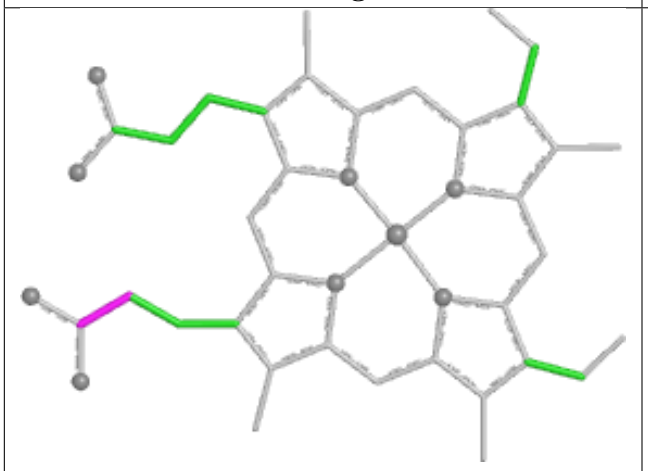
Ligand HEM D 904 (B)



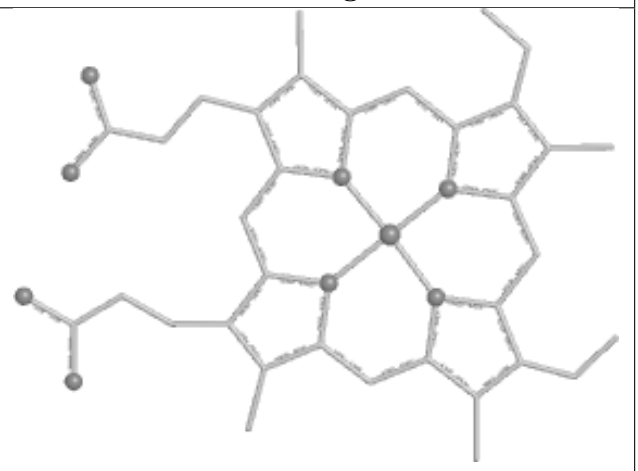
Bond lengths



Bond angles

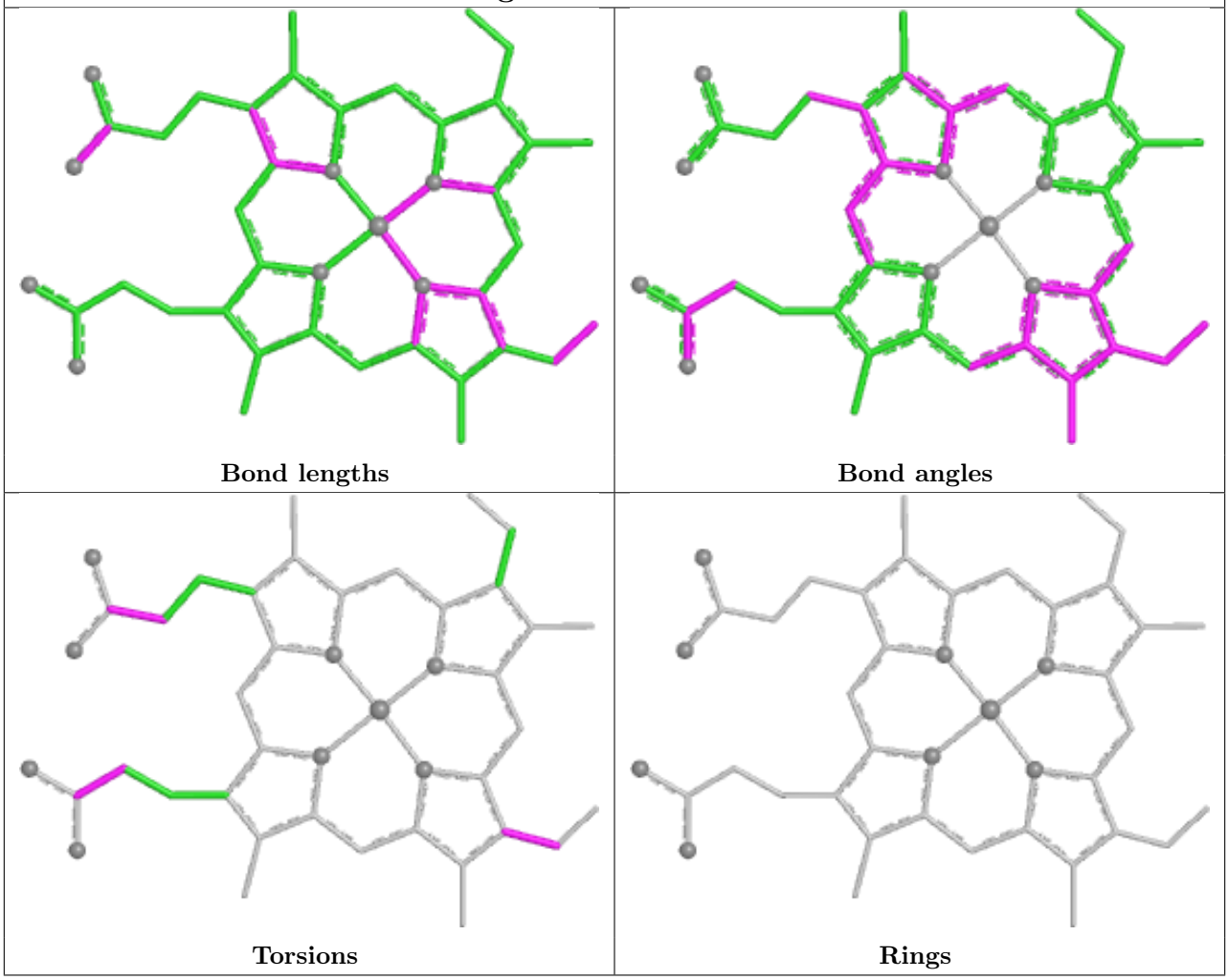


Torsions



Rings

Ligand HEM B 908



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	660/732 (90%)	-0.52	3 (0%)	87	88	11, 26, 43, 82	3 (0%)
1	B	660/732 (90%)	-0.57	1 (0%)	91	92	11, 24, 43, 67	3 (0%)
1	C	659/732 (90%)	-0.45	2 (0%)	90	91	13, 27, 46, 71	3 (0%)
1	D	660/732 (90%)	-0.66	3 (0%)	87	88	8, 21, 40, 76	2 (0%)
All	All	2639/2928 (90%)	-0.55	9 (0%)	90	91	8, 25, 44, 82	11 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	629	VAL	2.8
1	B	30	GLY	2.4
1	D	379	LEU	2.4
1	C	437	ILE	2.2
1	D	629	VAL	2.2

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
2	DTN	A	901	6/6	0.84	0.16	25,33,40,42	6
2	DTN	C	901	6/6	0.89	0.11	56,57,64,67	6
2	DTN	B	901	6/6	0.90	0.13	27,36,37,40	6
2	DTN	D	901	6/6	0.90	0.14	33,38,51,51	6
2	DTN	A	911	6/6	0.93	0.09	23,28,36,37	6
5	SO3	D	911	4/4	0.93	0.09	40,48,50,62	0
3	HEM	A	909	43/43	0.97	0.07	19,23,45,72	0
3	HEM	B	907	43/43	0.97	0.06	15,16,29,54	0
3	HEM	B	909	43/43	0.97	0.06	17,20,40,71	0
3	HEM	C	902	43/43	0.97	0.06	15,19,22,25	0
3	HEM	C	903	43/43	0.97	0.06	18,21,26,29	0
3	HEM	C	904[A]	43/43	0.97	0.06	14,17,19,21	43
3	HEM	C	904[B]	43/43	0.97	0.06	15,17,19,21	43
3	HEM	C	907	43/43	0.97	0.06	16,18,29,45	0
3	HEM	C	909	43/43	0.97	0.06	20,23,41,61	0
4	CU	C	910	1/1	0.97	0.04	17,17,17,17	1
3	HEM	A	903	43/43	0.97	0.06	16,19,22,24	0
3	HEM	B	906	43/43	0.98	0.05	13,16,25,34	0
3	HEM	A	904[A]	43/43	0.98	0.05	14,17,18,20	43
3	HEM	B	908	43/43	0.98	0.05	14,17,21,22	0
3	HEM	A	904[B]	43/43	0.98	0.05	12,18,19,20	43
3	HEM	A	906	43/43	0.98	0.05	13,16,24,31	0
3	HEM	A	907	43/43	0.98	0.06	14,16,25,47	0
3	HEM	A	908	43/43	0.98	0.04	15,17,20,23	0
3	HEM	A	902	43/43	0.98	0.06	17,19,24,28	0
3	HEM	C	905	43/43	0.98	0.05	16,18,20,21	0
3	HEM	C	906	43/43	0.98	0.05	15,18,24,34	0
3	HEM	B	902	43/43	0.98	0.05	16,18,22,25	0
3	HEM	C	908	43/43	0.98	0.05	17,19,24,26	0
3	HEM	B	903	43/43	0.98	0.05	15,18,20,22	0
3	HEM	D	902	43/43	0.98	0.04	12,13,19,22	0
3	HEM	D	903	43/43	0.98	0.04	11,13,14,15	0
3	HEM	D	904[A]	43/43	0.98	0.05	10,11,13,15	43
3	HEM	D	904[B]	43/43	0.98	0.05	9,12,14,15	43
3	HEM	D	906	43/43	0.98	0.05	9,12,17,30	0
3	HEM	D	907	43/43	0.98	0.06	12,14,23,54	0
3	HEM	D	908	43/43	0.98	0.04	12,14,21,22	0
3	HEM	D	909	43/43	0.98	0.07	14,19,54,66	0
3	HEM	B	904[A]	43/43	0.98	0.05	15,16,18,20	43
5	SO3	A	912	4/4	0.98	0.07	21,22,25,35	0
5	SO3	C	911	4/4	0.98	0.07	23,25,30,38	0
3	HEM	B	904[B]	43/43	0.98	0.05	11,16,19,21	43
5	SO3	D	912	4/4	0.98	0.06	15,17,21,24	0

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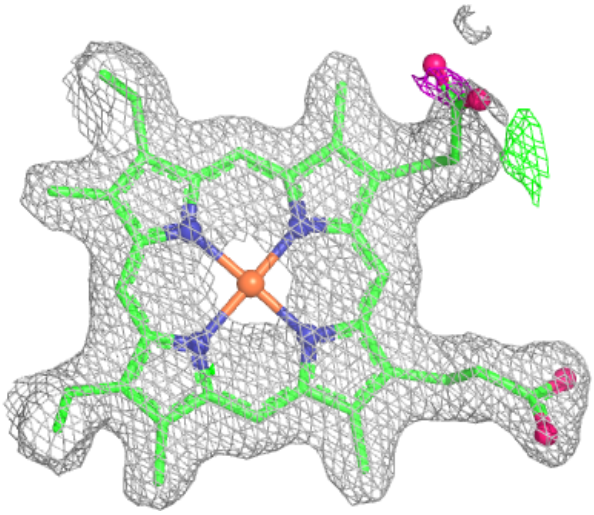
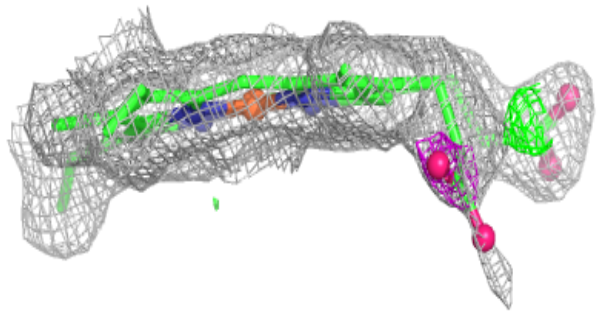
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	D	905	43/43	0.99	0.04	10,11,13,14	0
5	SO3	B	911	4/4	0.99	0.07	23,23,31,34	0
3	HEM	B	905	43/43	0.99	0.04	14,15,18,18	0
4	CU	A	910	1/1	0.99	0.04	15,15,15,15	1
3	HEM	A	905	43/43	0.99	0.04	13,17,19,21	0
4	CU	D	910	1/1	1.00	0.01	9,9,9,9	1
4	CU	B	910	1/1	1.00	0.04	11,11,11,11	1

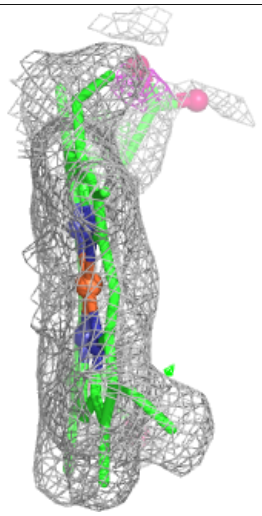
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM A 909:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

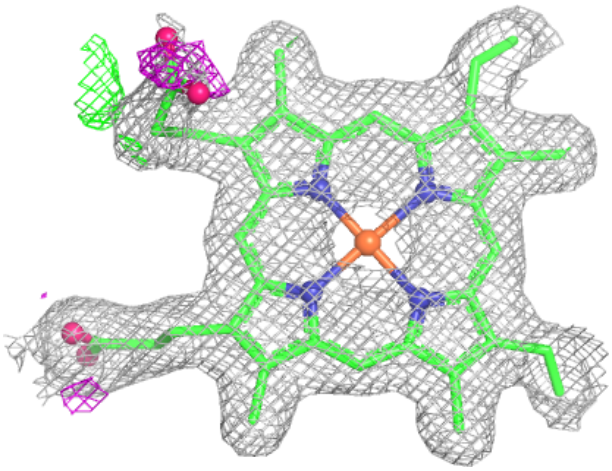


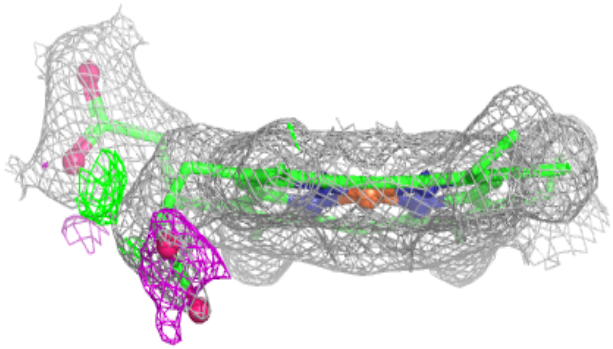


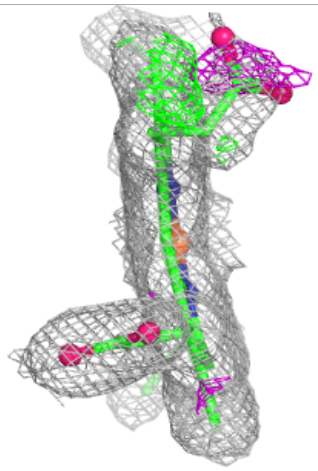


Electron density around HEM B 907:

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

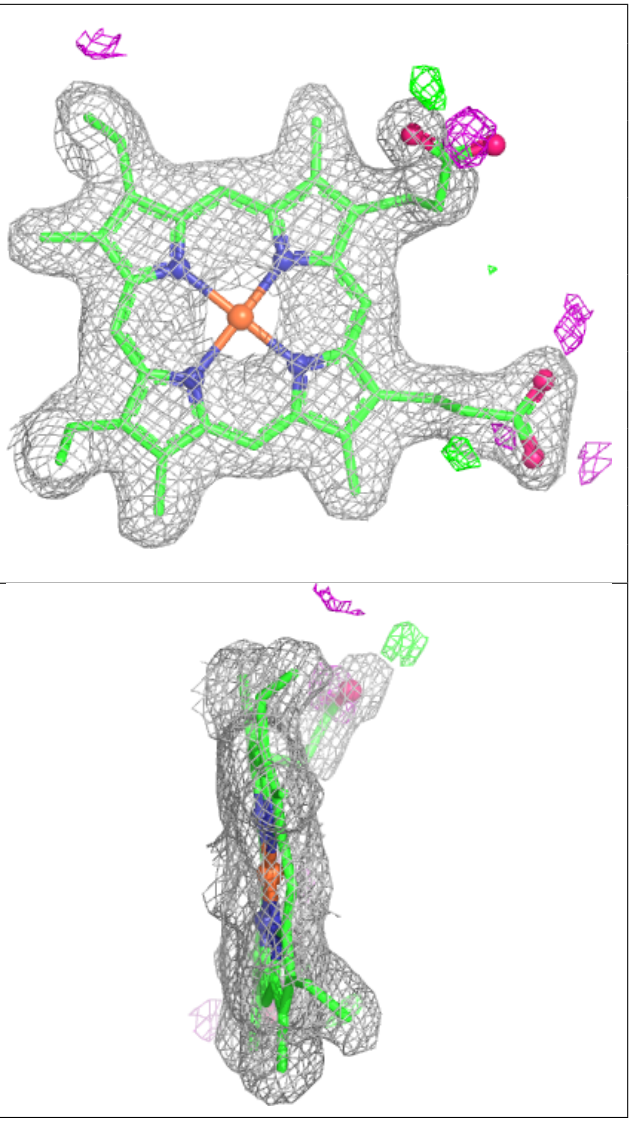






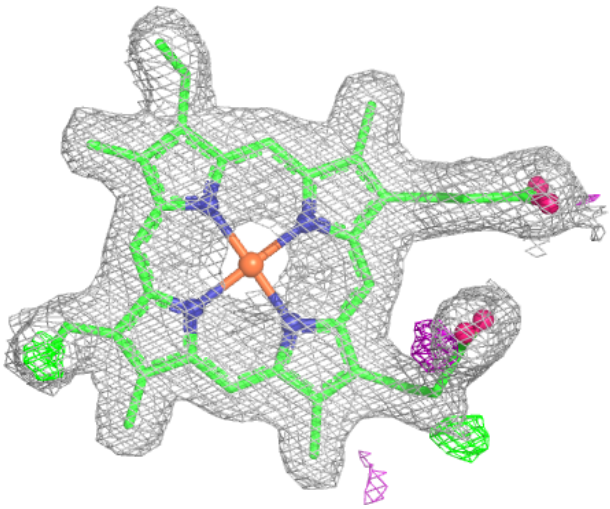
Electron density around HEM B 909:

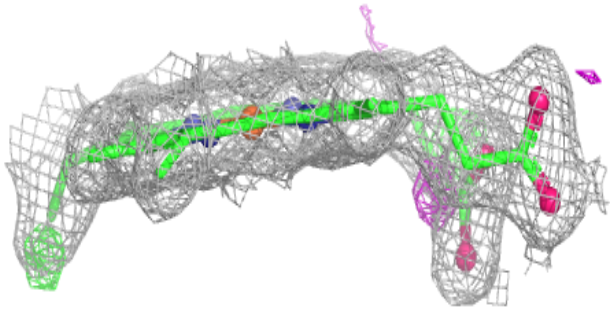
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

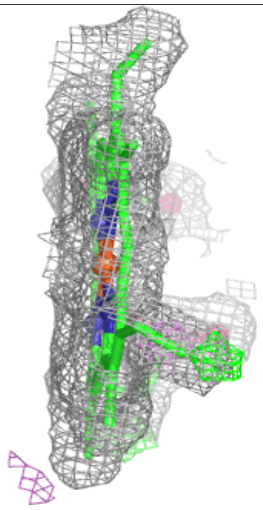


Electron density around HEM C 902:

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

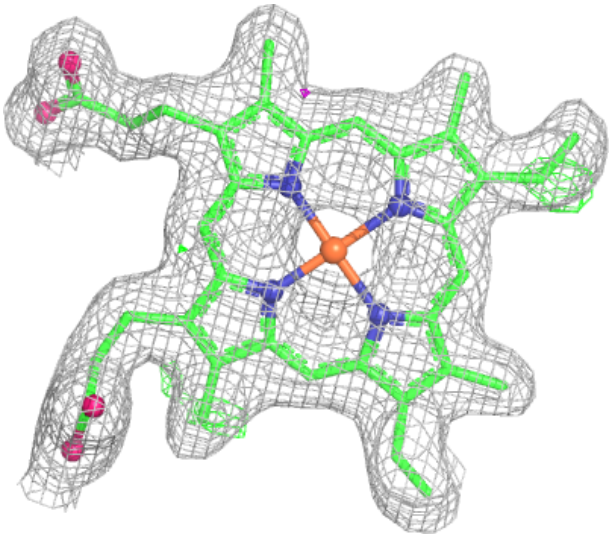


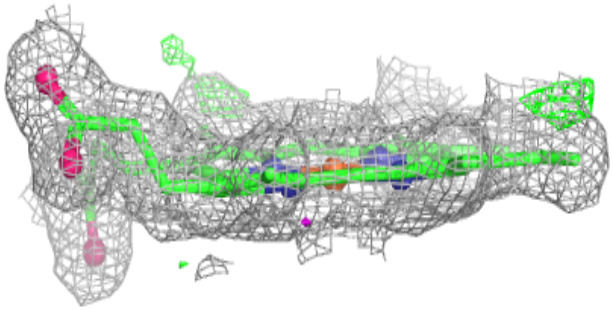


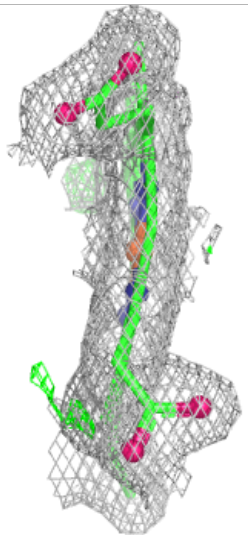


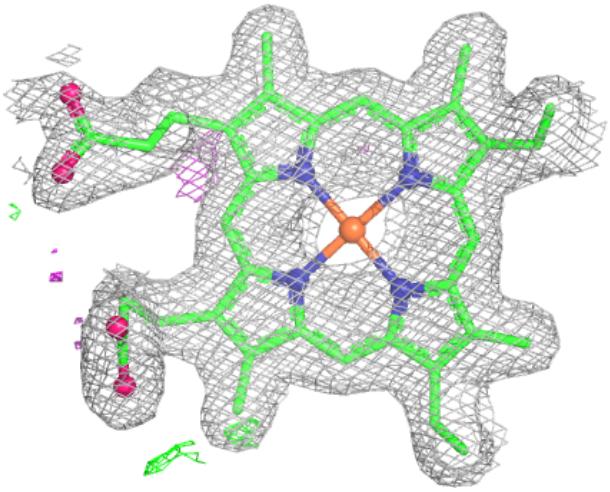
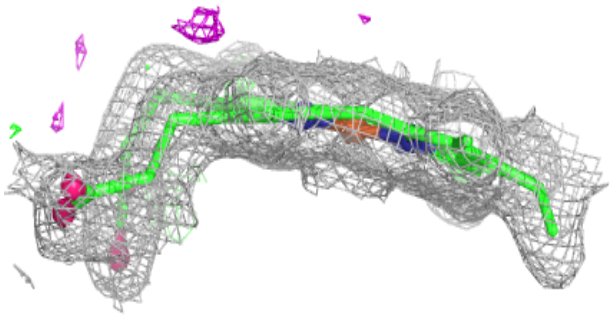
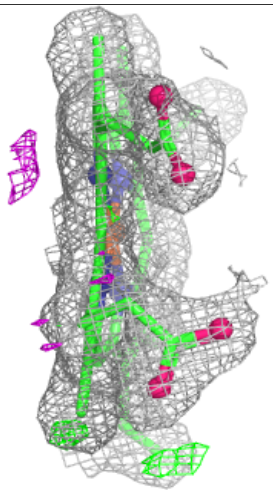
Electron density around HEM C 903:

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



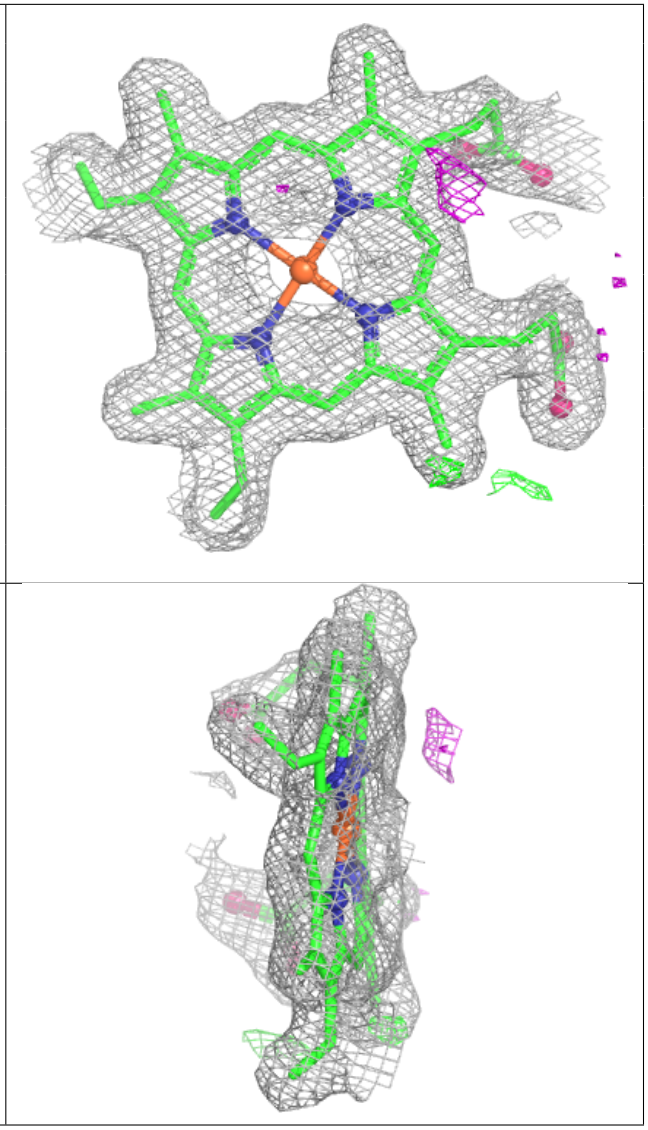




Electron density around HEM C 904 (A): 2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)	
	

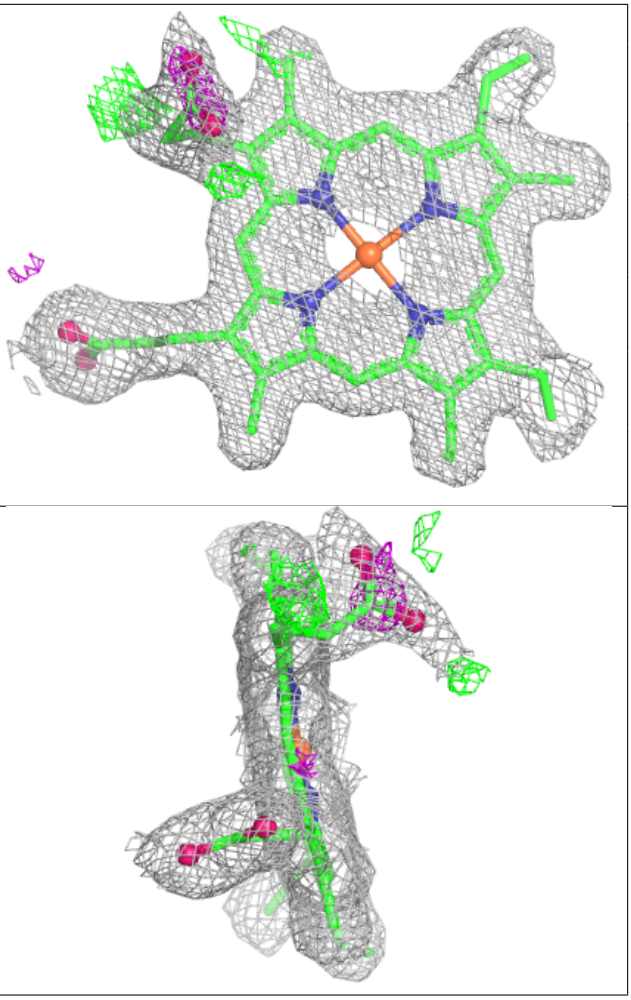
Electron density around HEM C 904 (B):

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



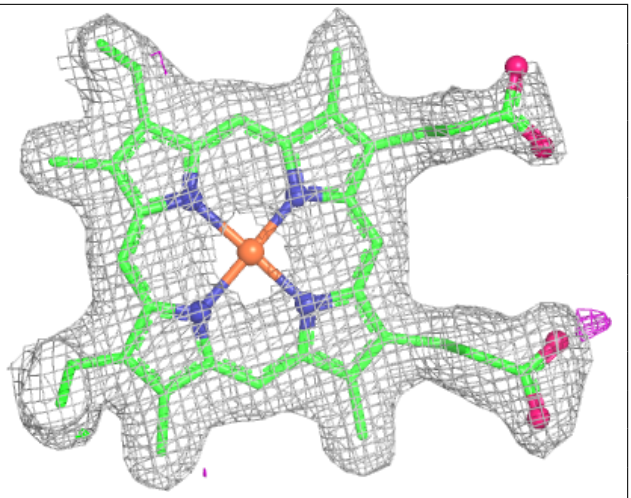
Electron density around HEM C 907:

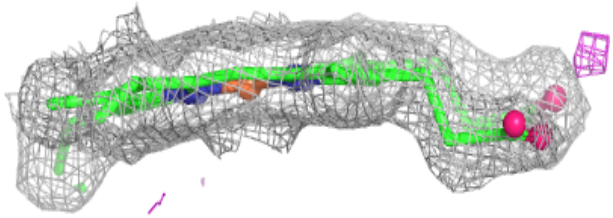
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

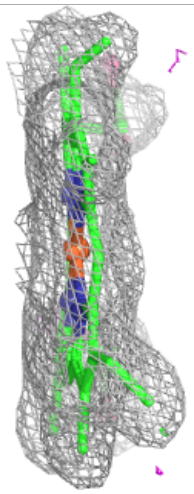


Electron density around HEM C 909:

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

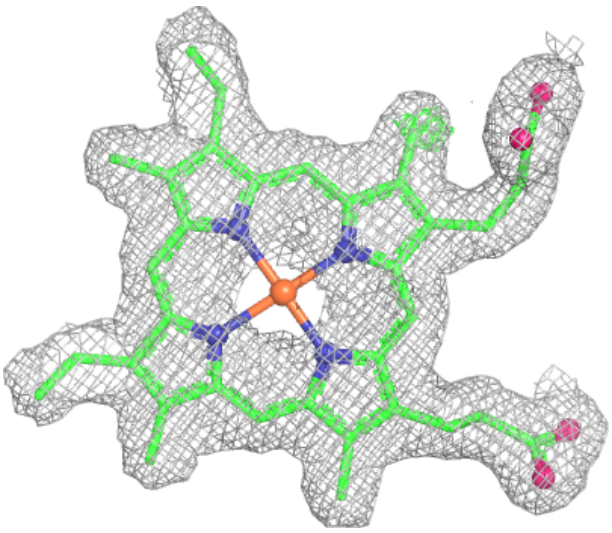


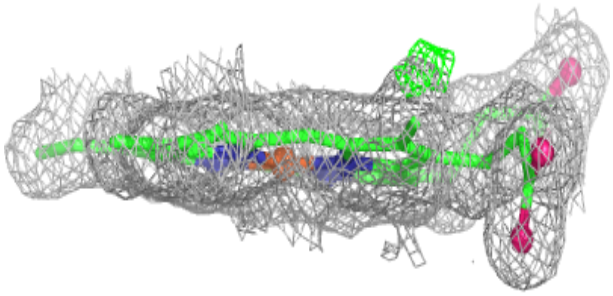


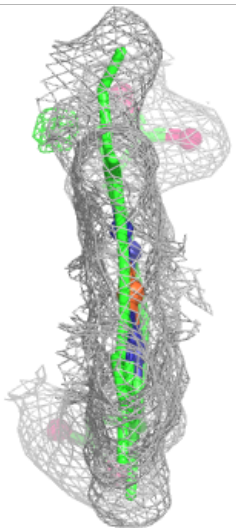


Electron density around HEM A 903:

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

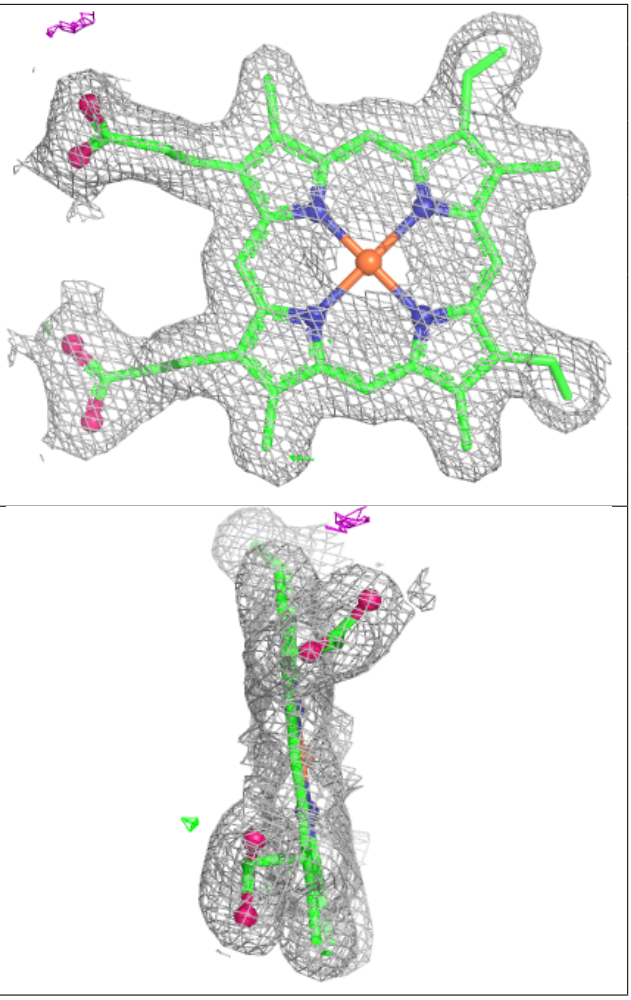






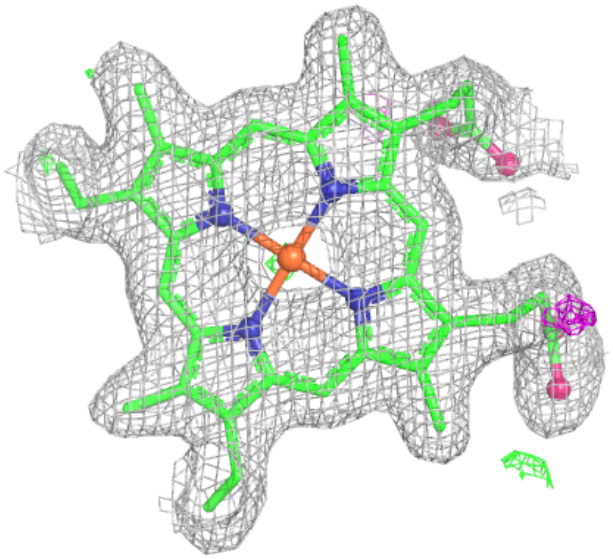
Electron density around HEM B 906:

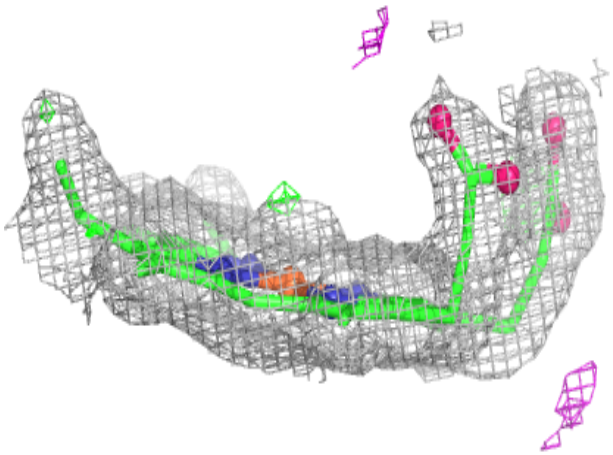
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

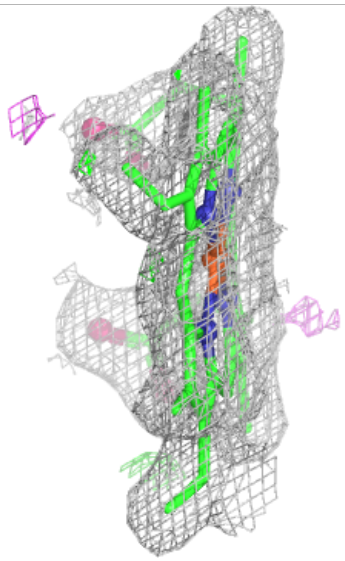


Electron density around HEM A 904 (A):

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

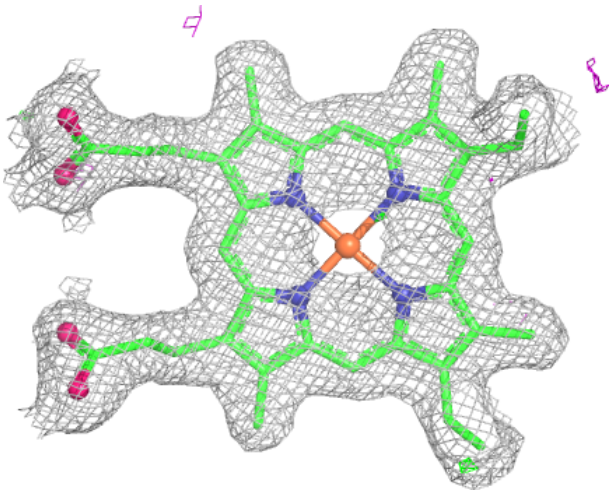


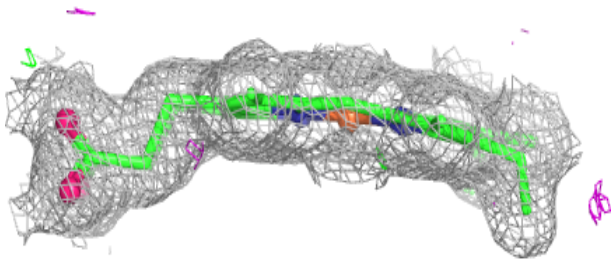


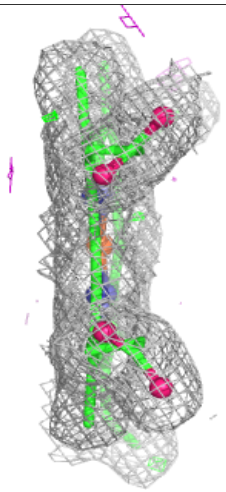


Electron density around HEM B 908:

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

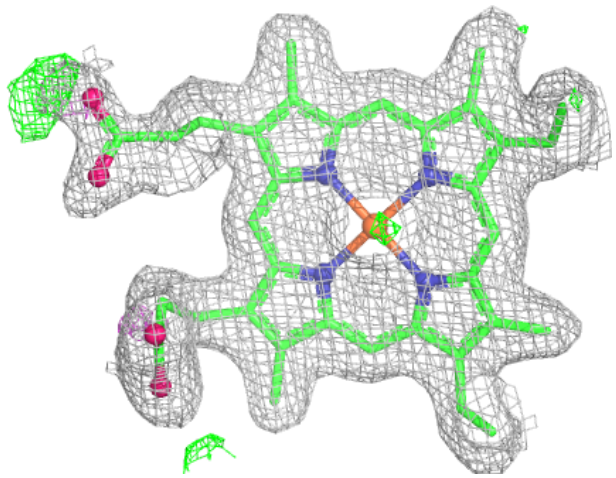


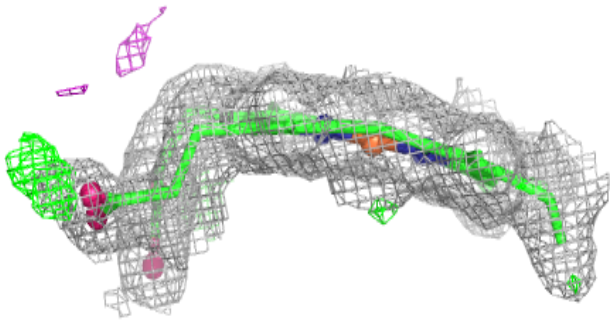


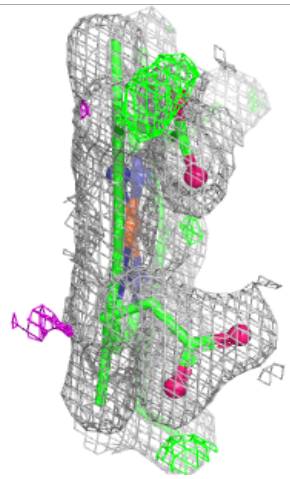


Electron density around HEM A 904 (B):

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

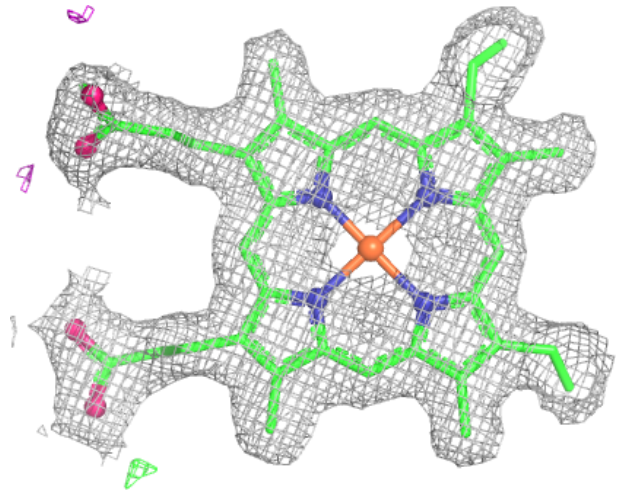


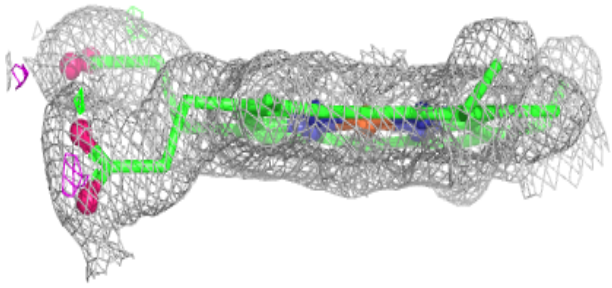


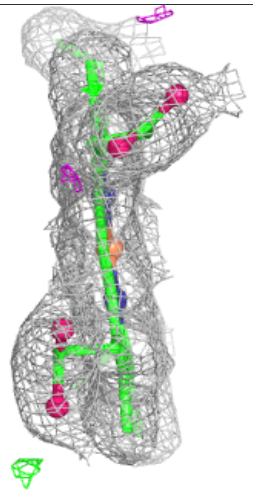


Electron density around HEM A 906:

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

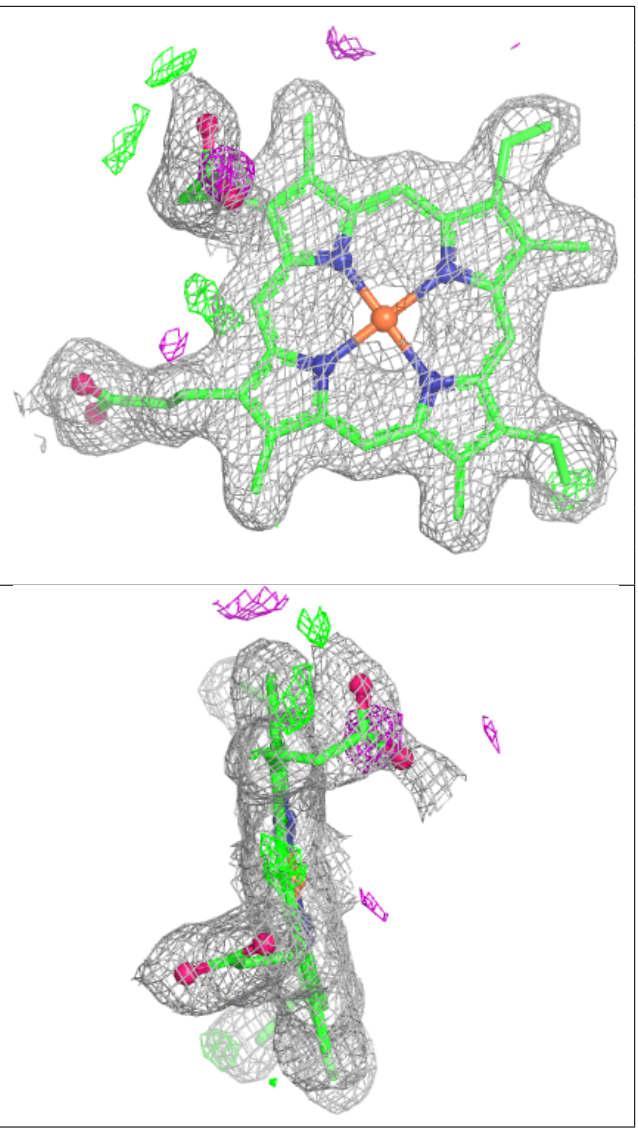






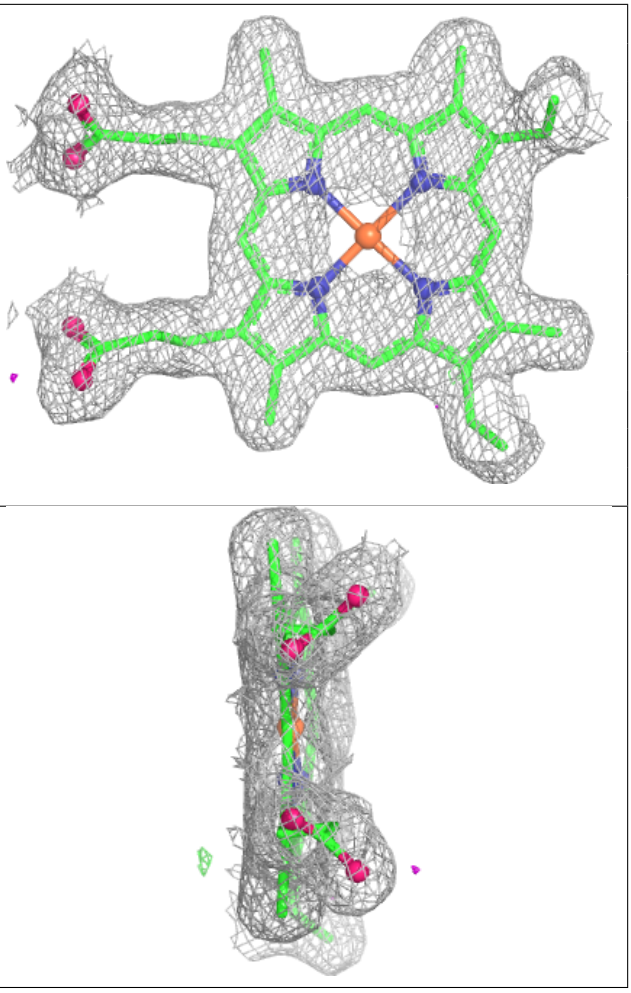
Electron density around HEM A 907:

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



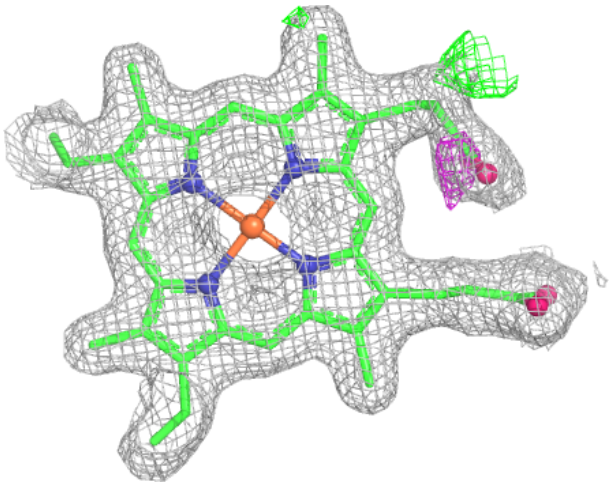
Electron density around HEM A 908:

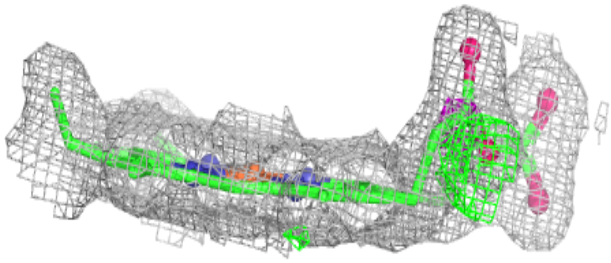
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

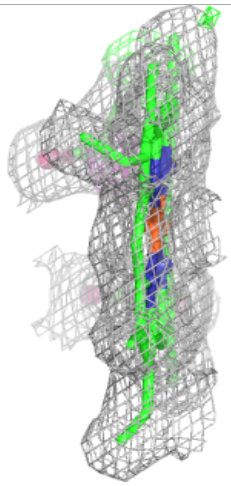


Electron density around HEM A 902:

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

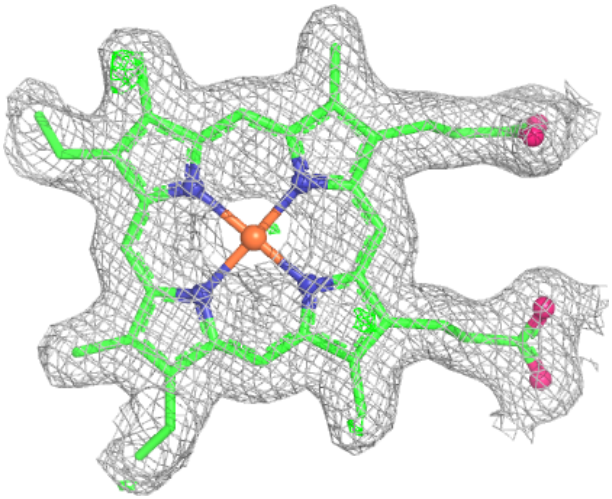


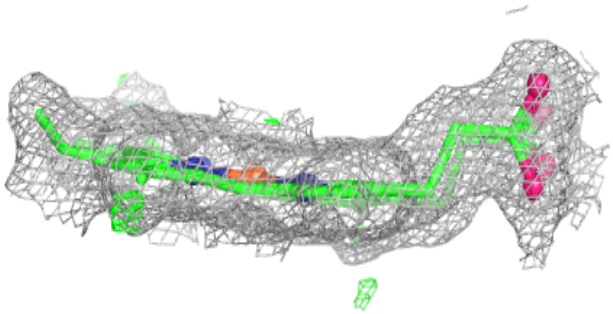


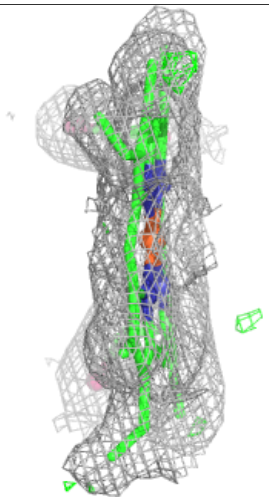


Electron density around HEM C 905:

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

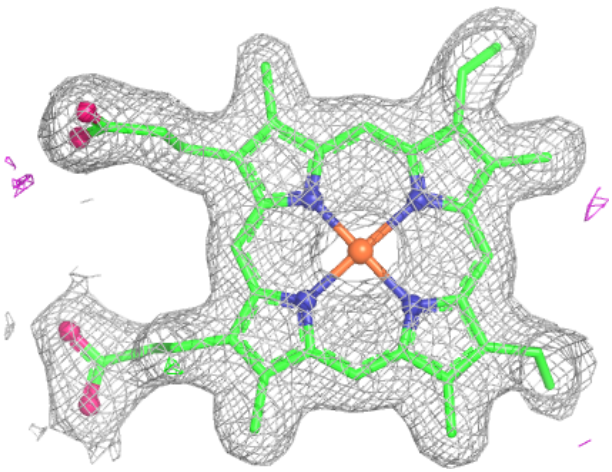


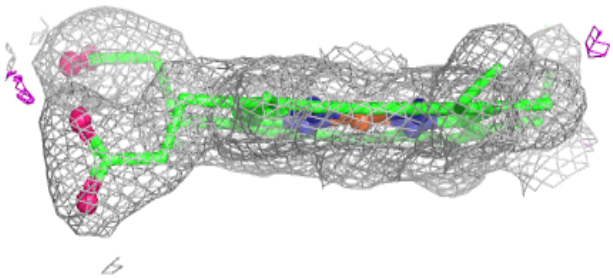


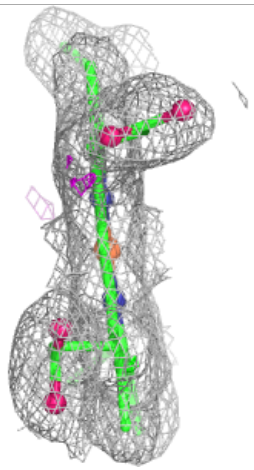


Electron density around HEM C 906:

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

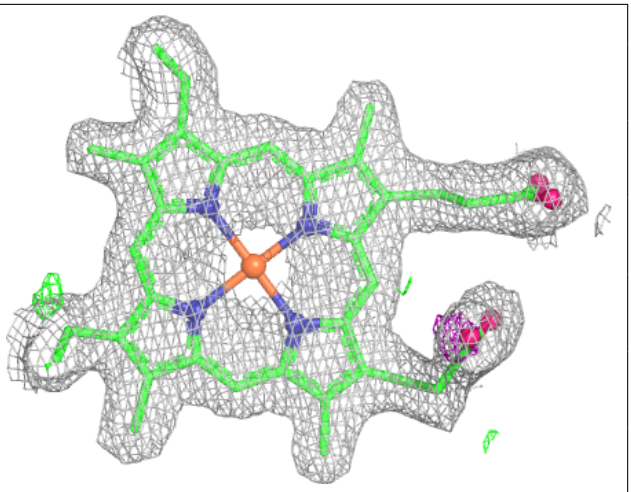


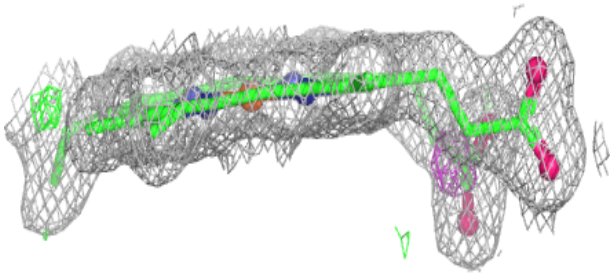


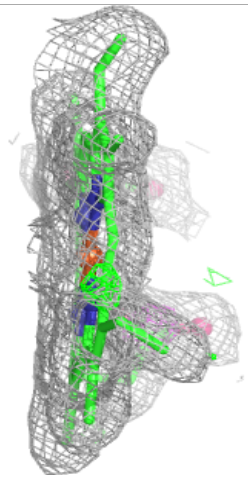


Electron density around HEM B 902:

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

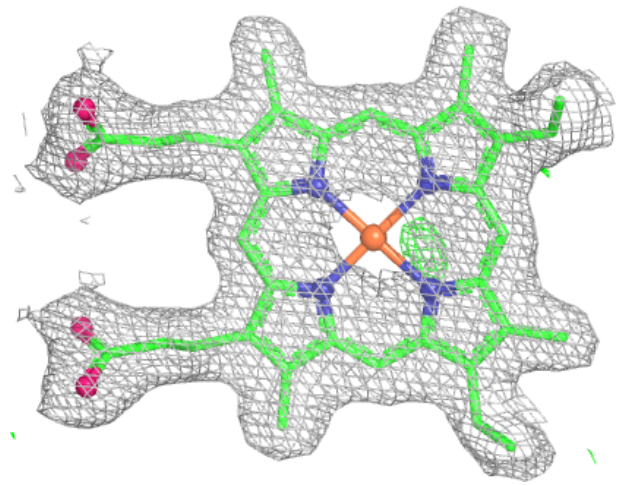


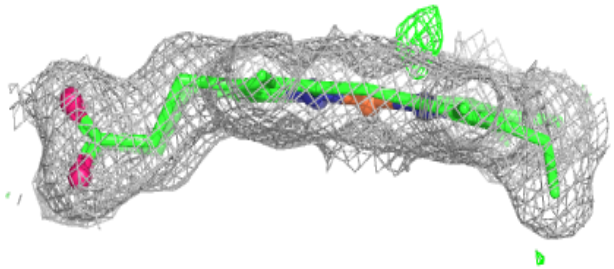


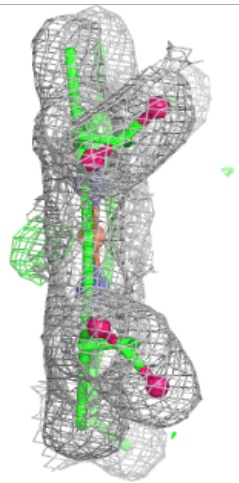


Electron density around HEM C 908:

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

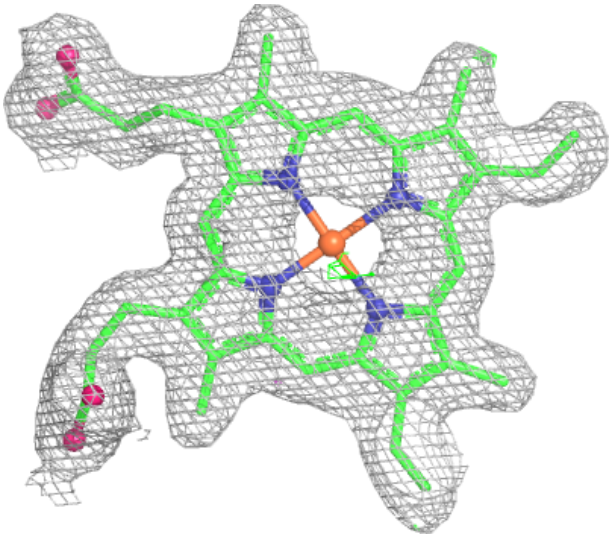


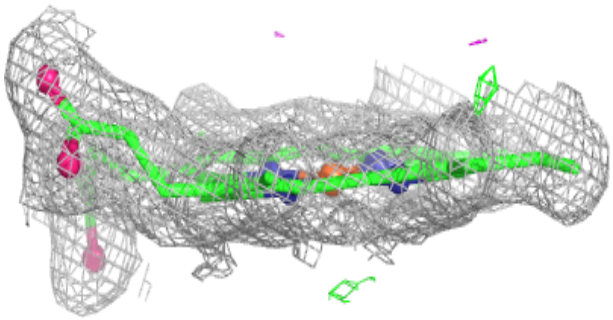


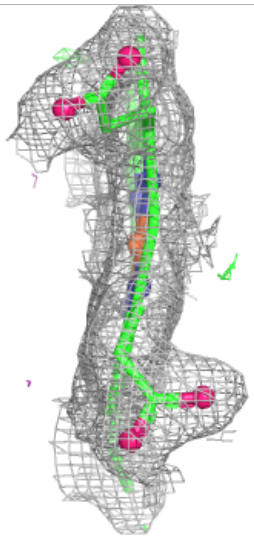


Electron density around HEM B 903:

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

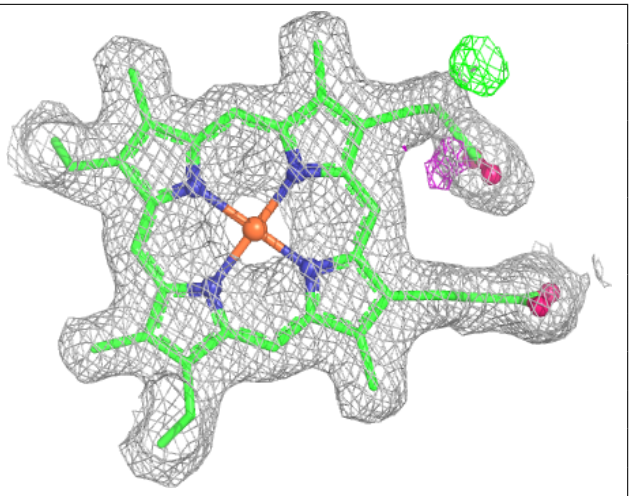


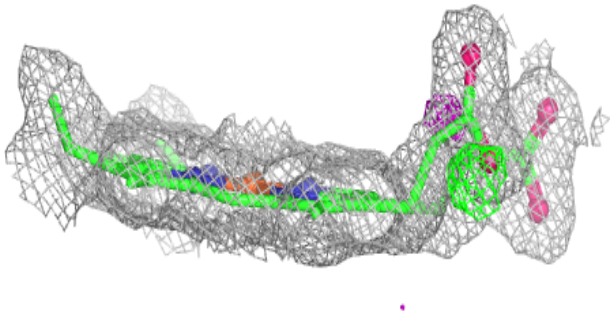


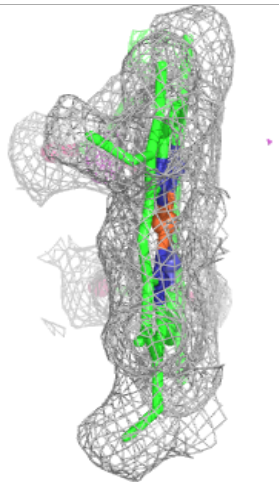


Electron density around HEM D 902:

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

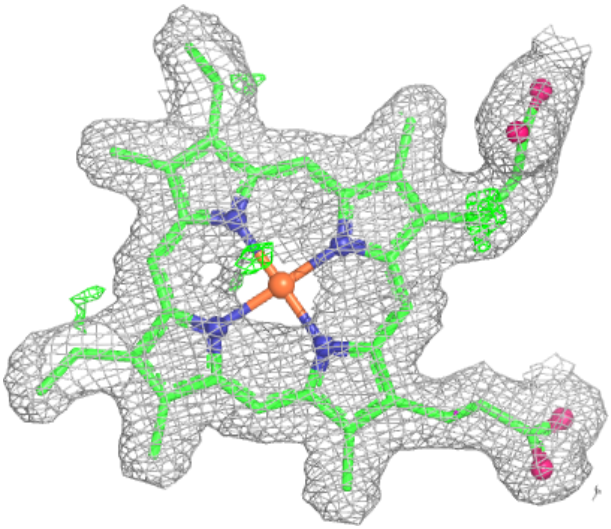


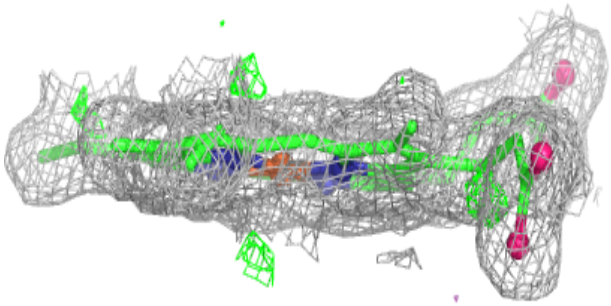


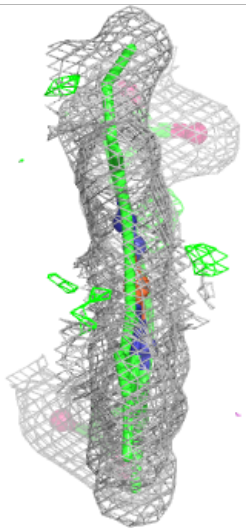


Electron density around HEM D 903:

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

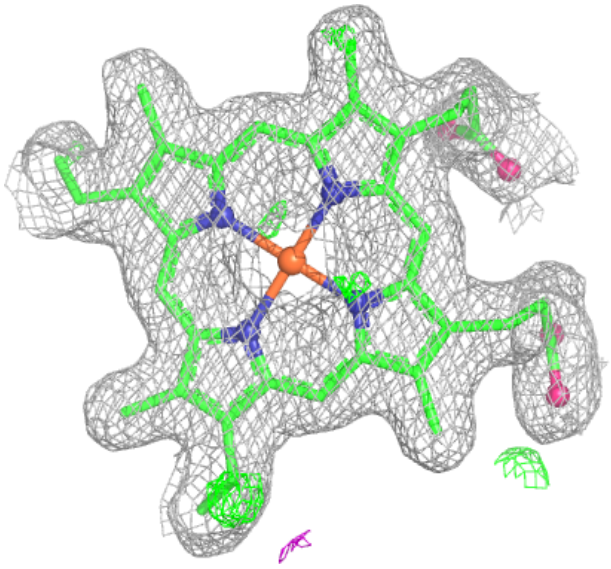


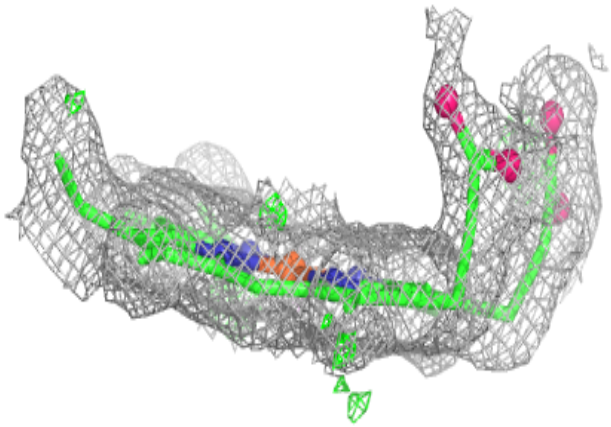


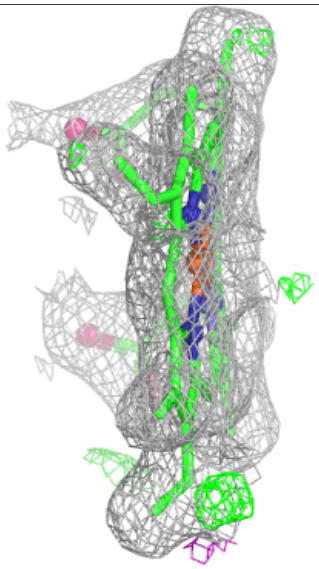


Electron density around HEM D 904 (A):

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

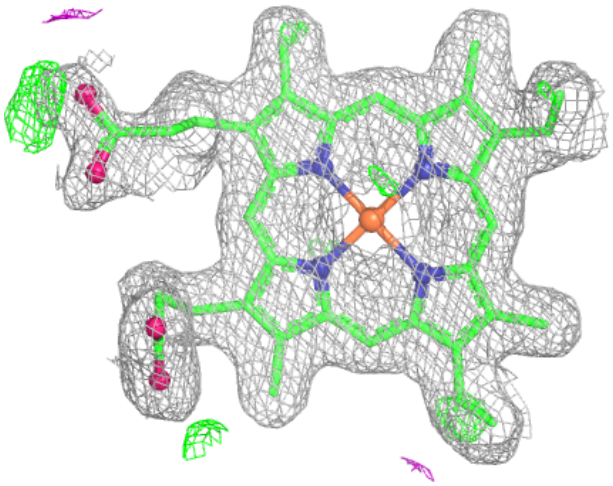


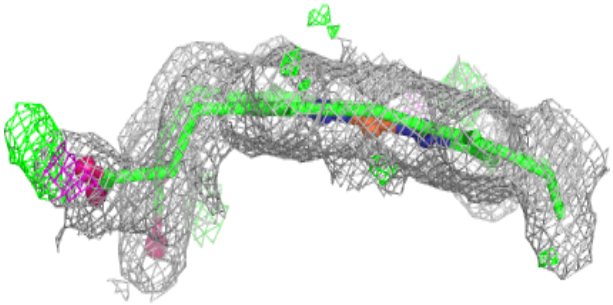


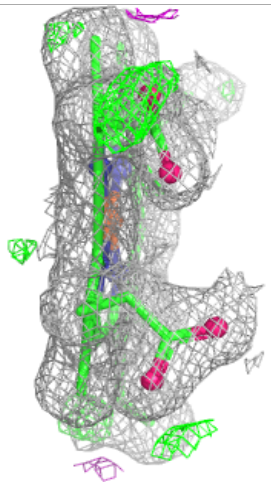


Electron density around HEM D 904 (B):

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

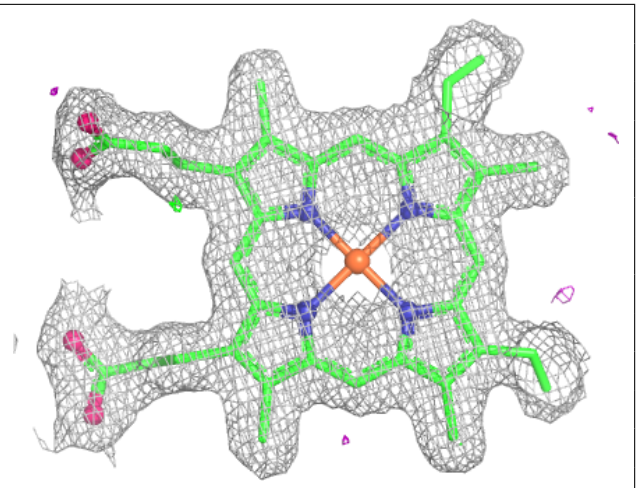


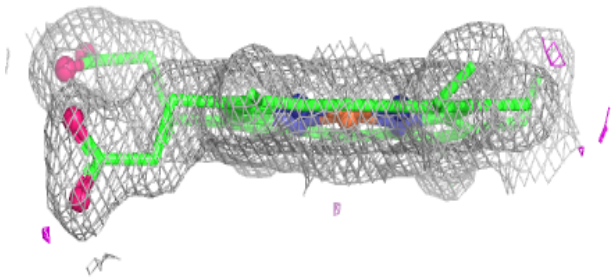


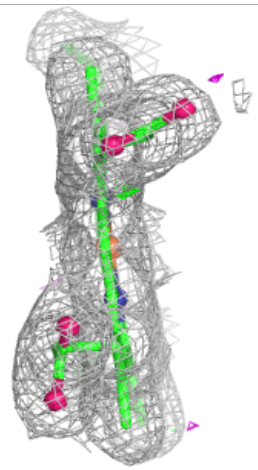


Electron density around HEM D 906:

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

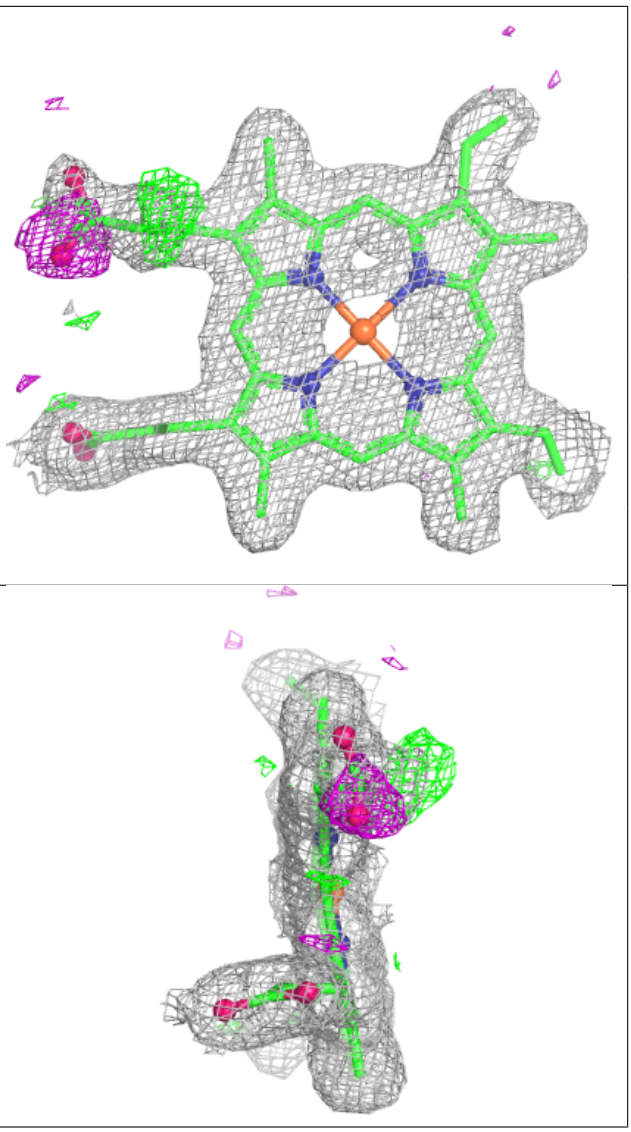






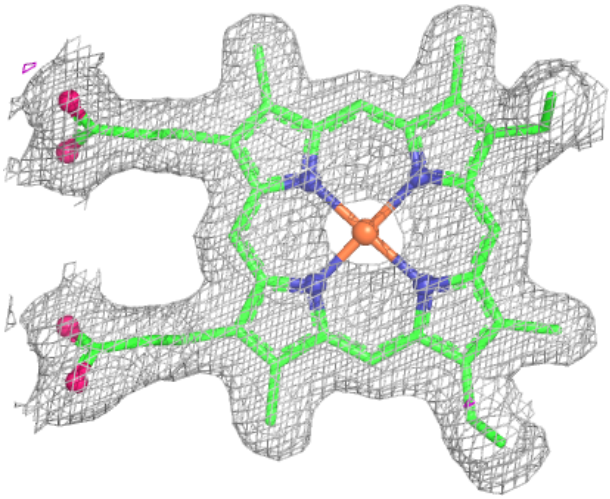
Electron density around HEM D 907:

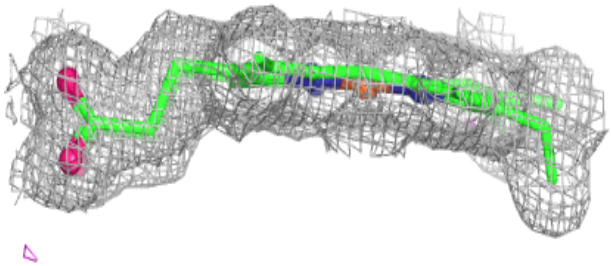
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

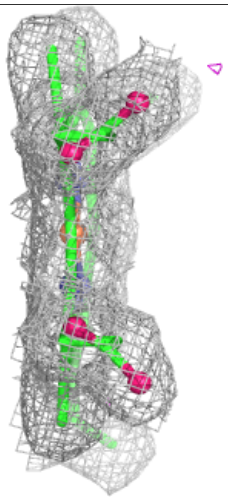


Electron density around HEM D 908:

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

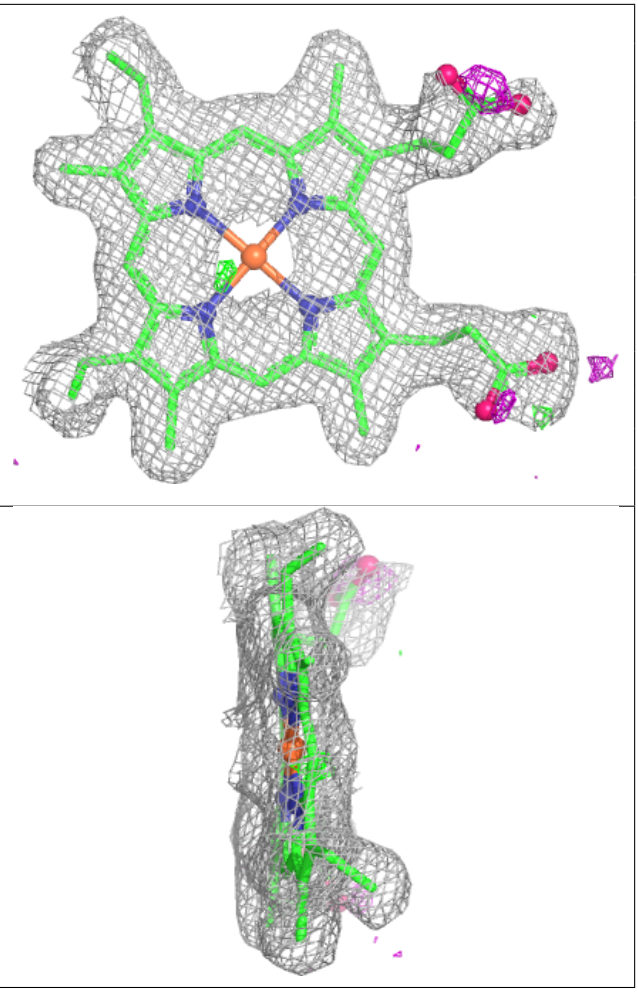






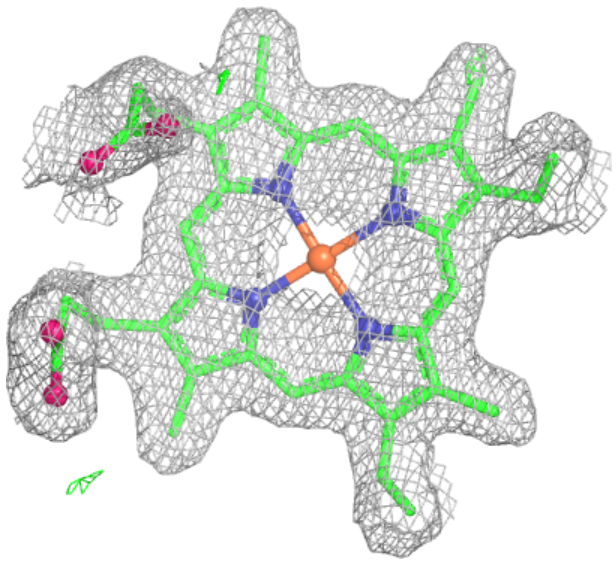
Electron density around HEM D 909:

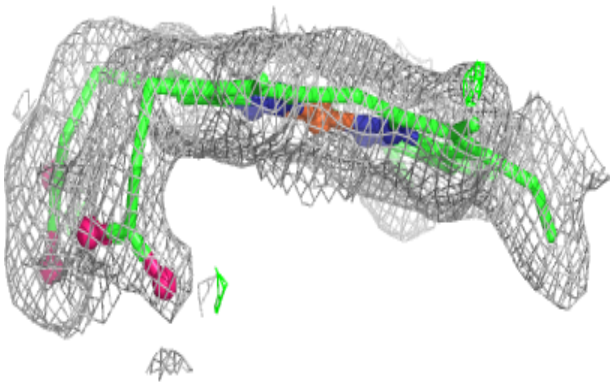
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

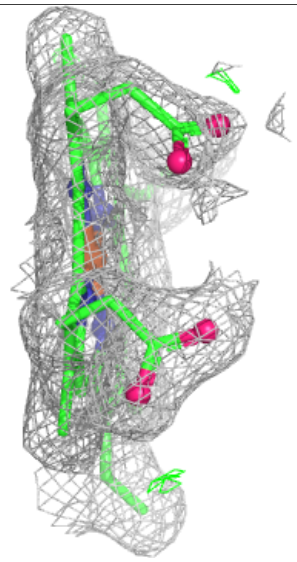


Electron density around HEM B 904 (A):

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

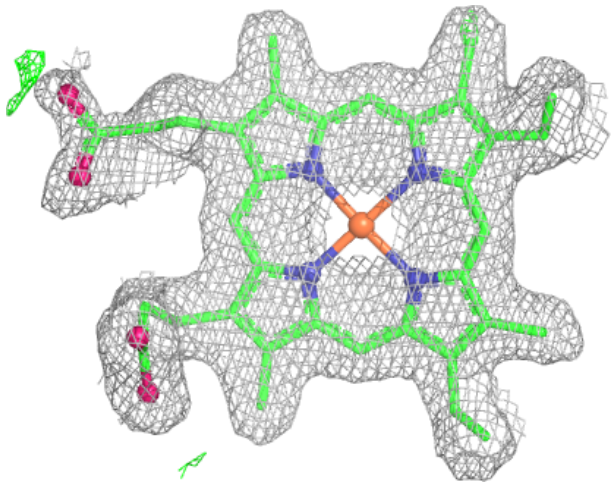


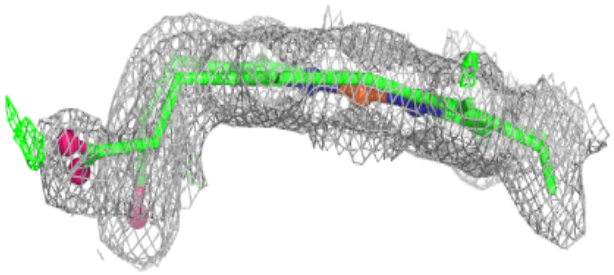


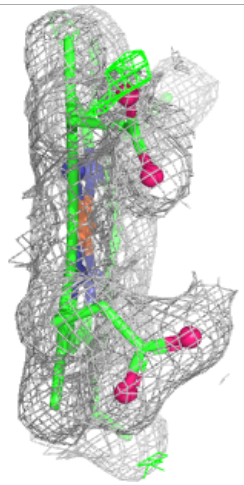


Electron density around HEM B 904 (B):

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

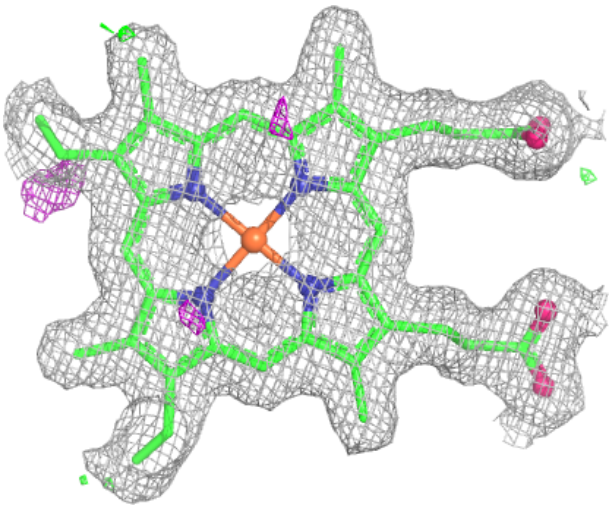


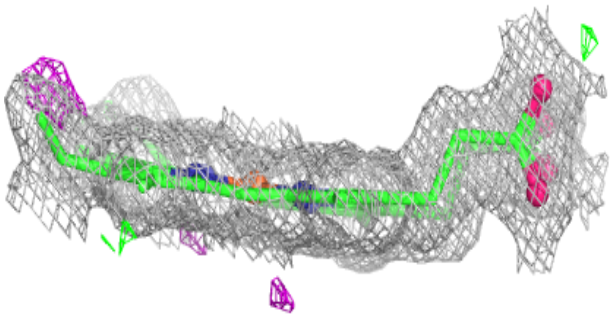


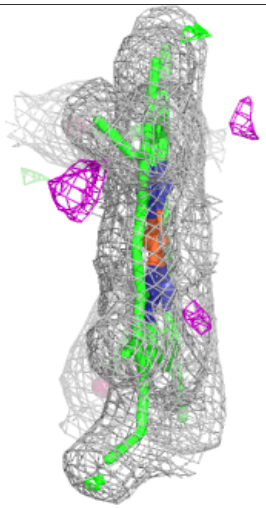


Electron density around HEM D 905:

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

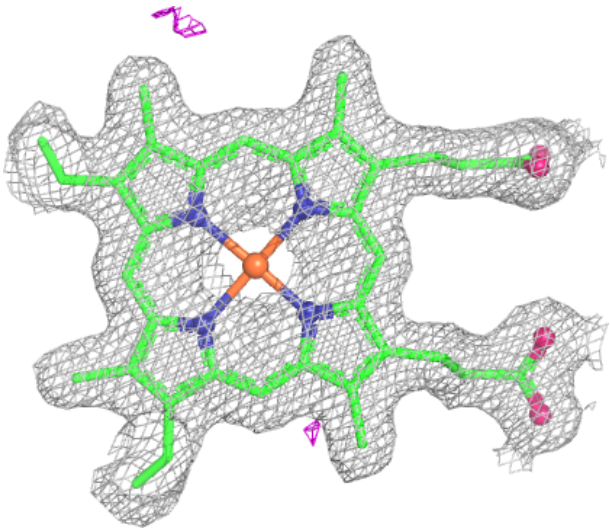


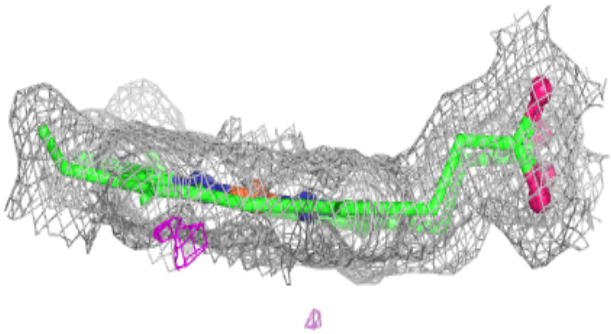


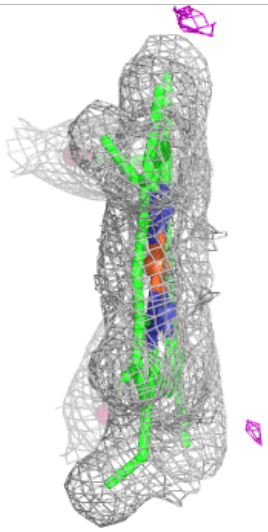


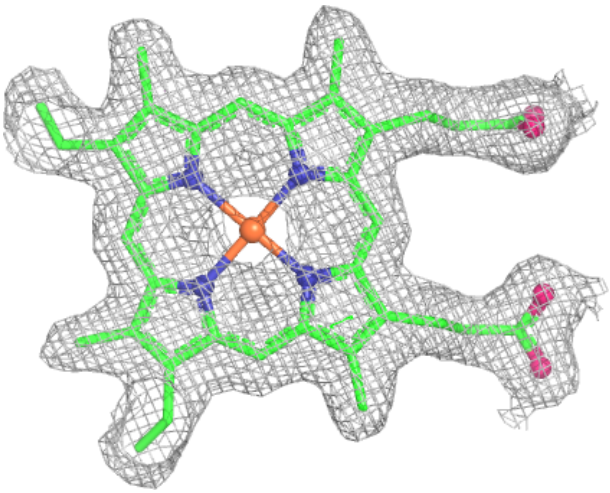
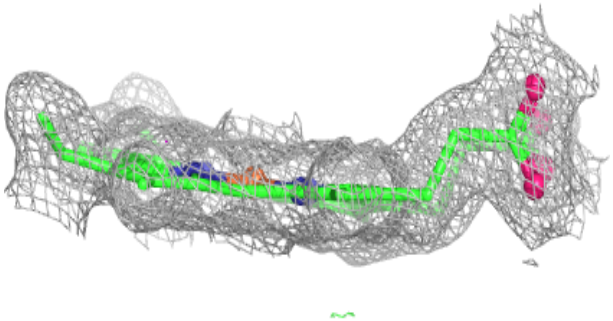
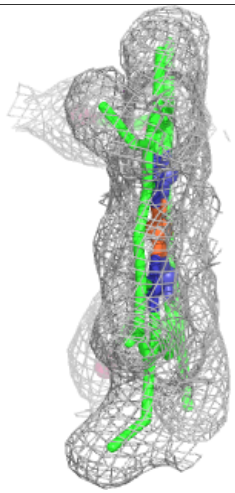
Electron density around HEM B 905:

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







Electron density around HEM A 905: 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 (i)

There are no such residues in this entry.