wwPDB X-ray Structure Validation Summary Report (i)

May 14, 2020 – 02:23 pm BST

PDB ID	:	1FGJ
Title	:	X-RAY STRUCTURE OF HYDROXYLAMINE OXIDOREDUCTASE
Authors	:	Tanaka, N.; Igarashi, N.; Moriyama, H.
Deposited on	:	1997-03-03
Resolution	:	2.80 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

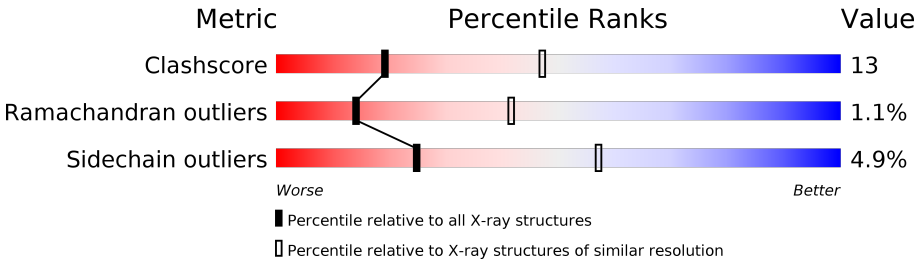
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	546	64% 26% • 9%
1	B	546	64% 24% • 9%

2 Entry composition (i)

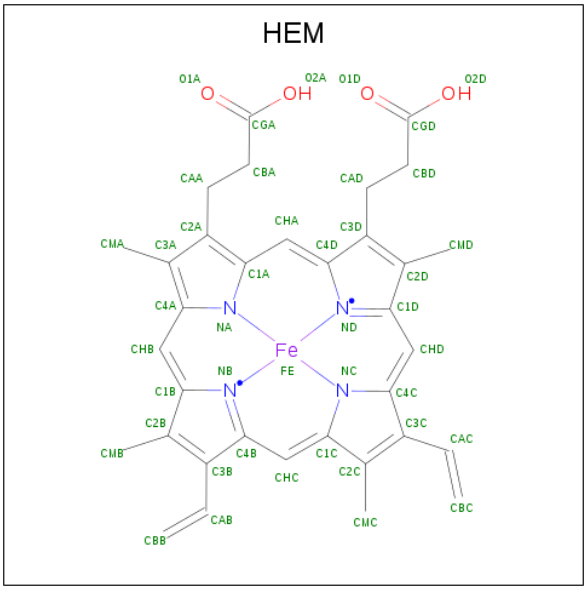
There are 3 unique types of molecules in this entry. The entry contains 8648 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HYDROXYLAMINE OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3980	2474	706	768	32			
1	B	499	Total	C	N	O	S	0	0	0
			3980	2474	706	768	32			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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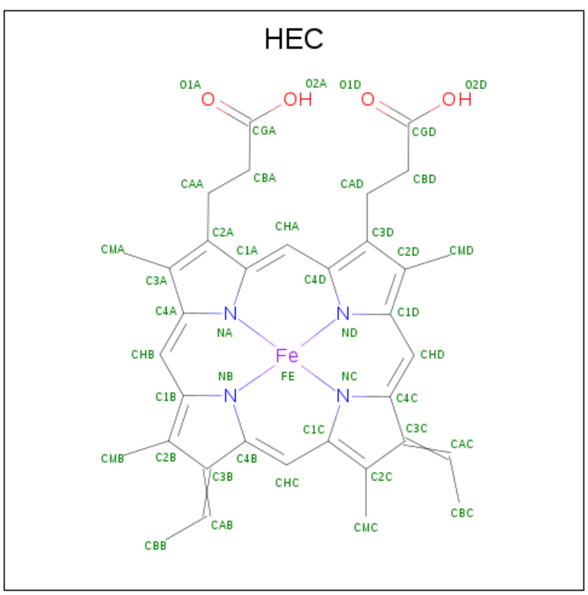
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	A	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2	B	1	Total C Fe N O 43 34 1 4 4	0	0
2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

- Molecule 3 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

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

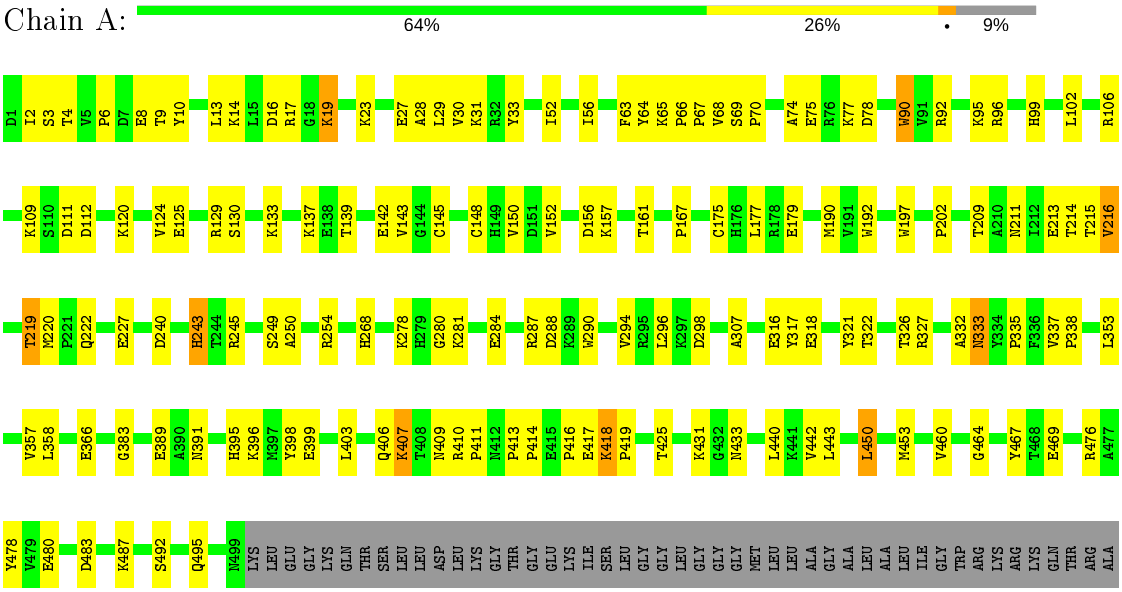
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

Note EDS was not executed.

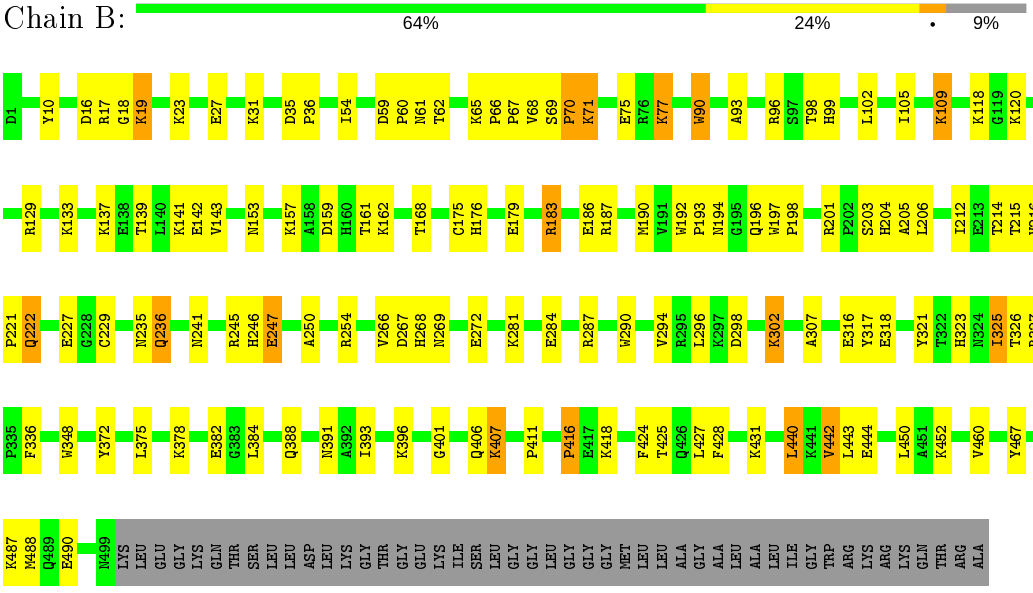
- Molecule 1: HYDROXYLAMINE OXIDOREDUCTASE

Chain A:



- Molecule 1: HYDROXYLAMINE OXIDOREDUCTASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	96.20Å 96.20Å 265.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	99.2 (8.00-2.80)	Depositor
R_{merge}	0.79	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8648	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/4083	0.63	0/5534
1	B	0.38	0/4083	0.61	0/5534
All	All	0.38	0/8166	0.62	0/11068

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3980	0	3779	99	3
1	B	3980	0	3779	114	2
2	A	301	0	210	5	0
2	B	301	0	210	6	0
3	A	43	0	30	5	3
3	B	43	0	30	6	2
All	All	8648	0	8038	215	5

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 13.

The worst 5 of 215 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:THR:HG22	1:A:416:PRO:HD2	1.51	0.92
1:B:69:SER:HB2	1:B:70:PRO:HD3	1.51	0.91
1:A:202:PRO:HB2	2:A:552:HEM:HBA1	1.54	0.89
1:B:219:THR:HG22	1:B:416:PRO:HD2	1.66	0.78
1:A:69:SER:HB2	1:A:70:PRO:HD3	1.68	0.76

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:TYR:OH	3:A:550:HEC:C4B[2_655]	1.48	0.72
1:A:467:TYR:CE1	3:A:550:HEC:CHC[2_655]	1.79	0.41
1:B:467:TYR:CE1	3:B:550:HEC:CHC[3_665]	1.95	0.25
1:A:467:TYR:OH	3:A:550:HEC:C3B[2_655]	2.00	0.20
1:B:467:TYR:OH	3:B:550:HEC:C4B[3_665]	2.11	0.09

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	497/546 (91%)	455 (92%)	35 (7%)	7 (1%)	11	34
1	B	497/546 (91%)	450 (90%)	43 (9%)	4 (1%)	19	49
All	All	994/1092 (91%)	905 (91%)	78 (8%)	11 (1%)	14	41

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	327	ARG
1	B	247	GLU

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Mol	Chain	Res	Type
1	B	268	HIS
1	A	150	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/460 (93%)	407 (95%)	20 (5%)	26	59
1	B	427/460 (93%)	405 (95%)	22 (5%)	23	55
All	All	854/920 (93%)	812 (95%)	42 (5%)	25	57

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	443	LEU
1	B	90	TRP
1	B	443	LEU
1	A	450	LEU
1	B	71	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	482	GLN
1	B	153	ASN
1	B	482	GLN
1	B	38	HIS
1	B	127	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	549	1	27,50,50	1.67	6 (22%)	17,82,82	1.49	4 (23%)
2	HEM	B	552	1	27,50,50	1.69	8 (29%)	17,82,82	2.15	5 (29%)
2	HEM	A	554	1	27,50,50	1.82	8 (29%)	17,82,82	1.50	2 (11%)
2	HEM	B	551	1	27,50,50	1.87	7 (25%)	17,82,82	1.21	1 (5%)
2	HEM	B	549	1	27,50,50	1.86	8 (29%)	17,82,82	1.78	4 (23%)
2	HEM	A	551	1	27,50,50	1.81	8 (29%)	17,82,82	1.29	1 (5%)
2	HEM	B	548	1	27,50,50	1.70	7 (25%)	17,82,82	1.76	3 (17%)
2	HEM	A	548	1	27,50,50	1.85	9 (33%)	17,82,82	1.75	4 (23%)
2	HEM	A	552	1	27,50,50	1.91	5 (18%)	17,82,82	2.59	5 (29%)
2	HEM	B	553	1	27,50,50	1.75	7 (25%)	17,82,82	1.02	1 (5%)
2	HEM	B	554	1	27,50,50	1.75	7 (25%)	17,82,82	1.32	3 (17%)
2	HEM	B	547	1	27,50,50	1.62	5 (18%)	17,82,82	1.20	1 (5%)
2	HEM	A	547	1	27,50,50	1.53	5 (18%)	17,82,82	1.42	2 (11%)
2	HEM	A	553	1	27,50,50	1.75	6 (22%)	17,82,82	1.83	2 (11%)
3	HEC	A	550	1	26,50,50	1.61	6 (23%)	18,82,82	2.05	5 (27%)
3	HEC	B	550	1	26,50,50	2.03	6 (23%)	18,82,82	1.55	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	549	1	-	0/6/54/54	-
2	HEM	B	552	1	-	3/6/54/54	-
2	HEM	A	554	1	-	0/6/54/54	-
2	HEM	B	551	1	-	0/6/54/54	-
2	HEM	B	549	1	-	0/6/54/54	-
2	HEM	A	551	1	-	0/6/54/54	-
2	HEM	B	548	1	-	2/6/54/54	-
2	HEM	A	548	1	-	1/6/54/54	-
2	HEM	A	552	1	-	4/6/54/54	-
2	HEM	B	553	1	-	0/6/54/54	-
2	HEM	B	554	1	-	1/6/54/54	-
2	HEM	B	547	1	-	0/6/54/54	-
2	HEM	A	547	1	-	1/6/54/54	-
2	HEM	A	553	1	-	0/6/54/54	-
3	HEC	A	550	1	-	0/6/54/54	-
3	HEC	B	550	1	-	0/6/54/54	-

The worst 5 of 108 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	550	HEC	C3B-C2B	-6.67	1.33	1.40
2	A	552	HEM	C3B-CAB	4.94	1.58	1.47
2	A	552	HEM	C3C-CAC	4.53	1.57	1.47
3	A	550	HEC	C3C-C2C	-4.46	1.36	1.40
3	B	550	HEC	C3C-C2C	-4.45	1.36	1.40

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	552	HEM	CBD-CAD-C3D	7.22	125.78	112.48
3	A	550	HEC	CBA-CAA-C2A	6.18	123.86	112.48
2	A	553	HEM	CBA-CAA-C2A	5.93	123.42	112.49
2	B	552	HEM	CBA-CAA-C2A	5.67	122.95	112.49
2	A	552	HEM	C4C-C3C-C2C	-4.62	103.67	106.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	552	HEM	C1A-C2A-CAA-CBA
2	B	552	HEM	C3A-C2A-CAA-CBA
2	B	552	HEM	C2D-C3D-CAD-CBD
2	B	548	HEM	C3A-C2A-CAA-CBA
2	A	548	HEM	C3A-C2A-CAA-CBA

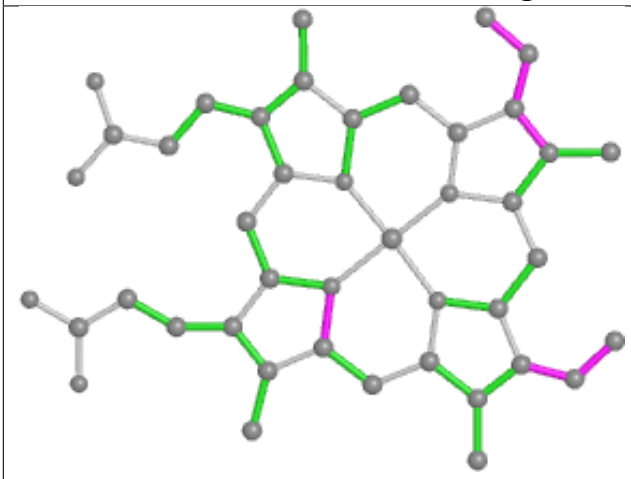
There are no ring outliers.

9 monomers are involved in 26 short contacts:

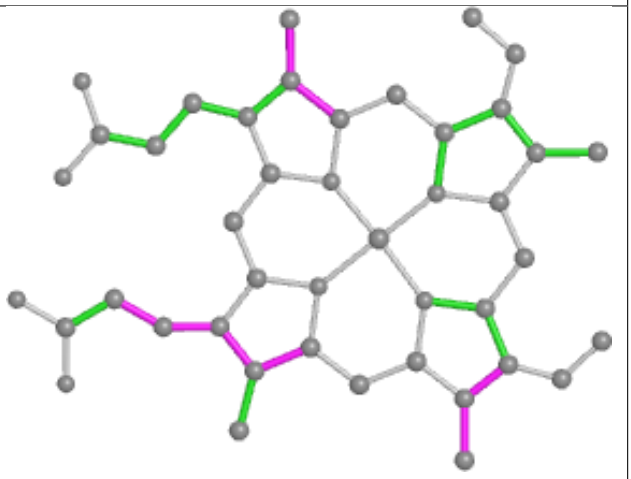
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	552	HEM	3	0
2	B	551	HEM	2	0
2	B	549	HEM	1	0
2	A	551	HEM	1	0
2	A	548	HEM	1	0
2	A	552	HEM	2	0
2	A	547	HEM	1	0
3	A	550	HEC	5	3
3	B	550	HEC	6	2

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.

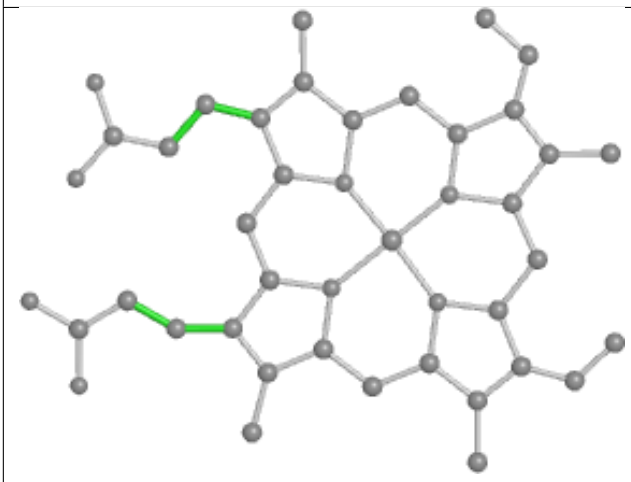
Ligand HEM A 549



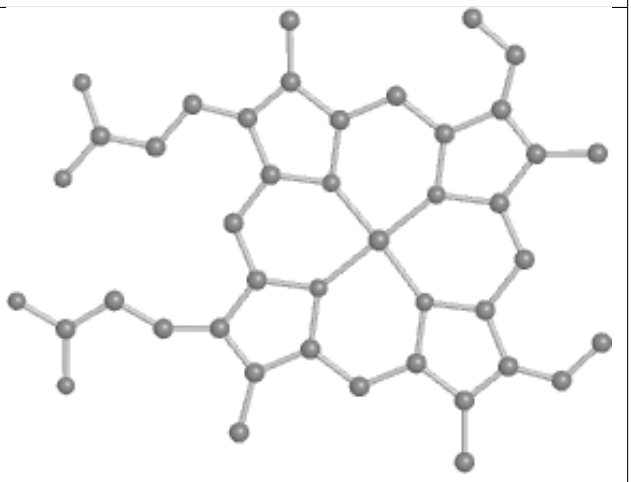
Bond lengths



Bond angles

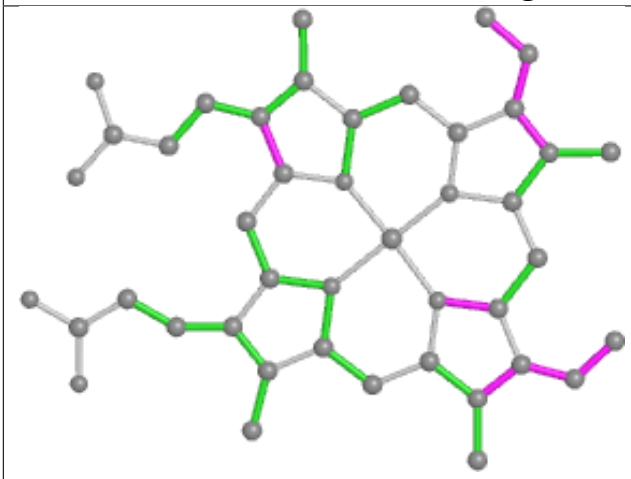


Torsions

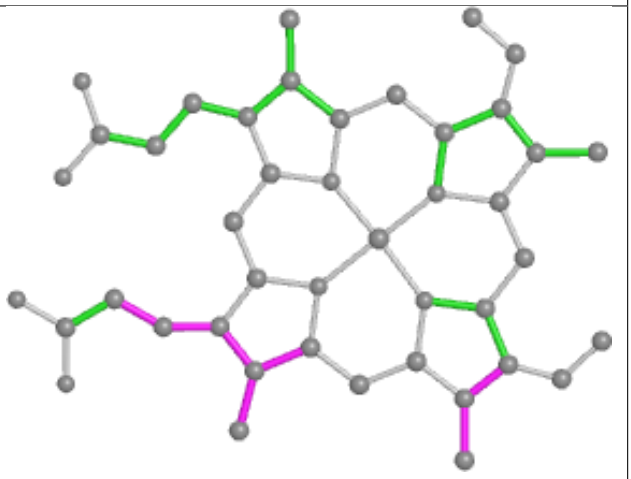


Rings

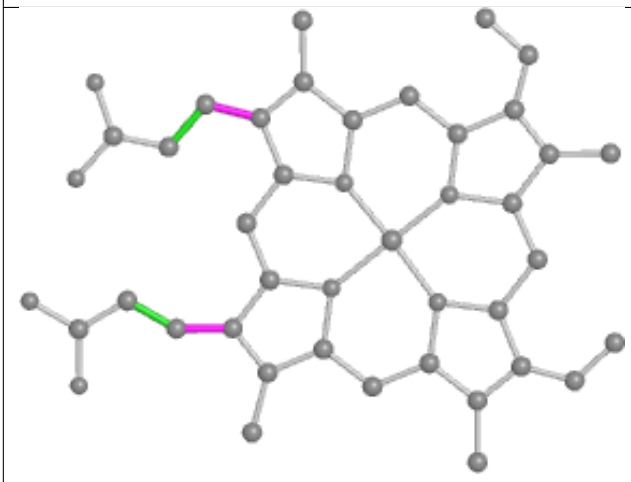
Ligand HEM B 552



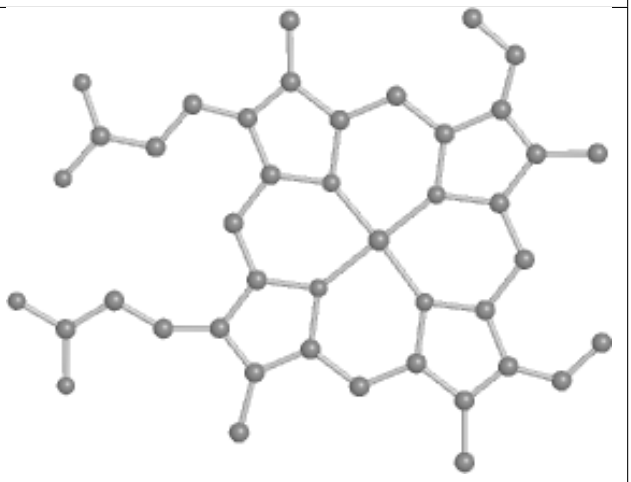
Bond lengths



Bond angles

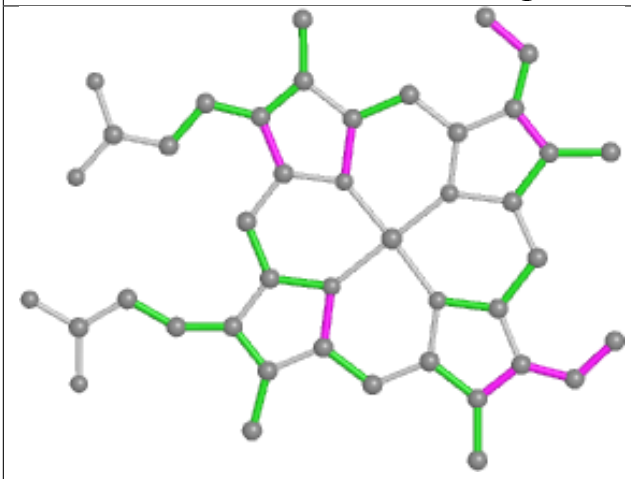


Torsions

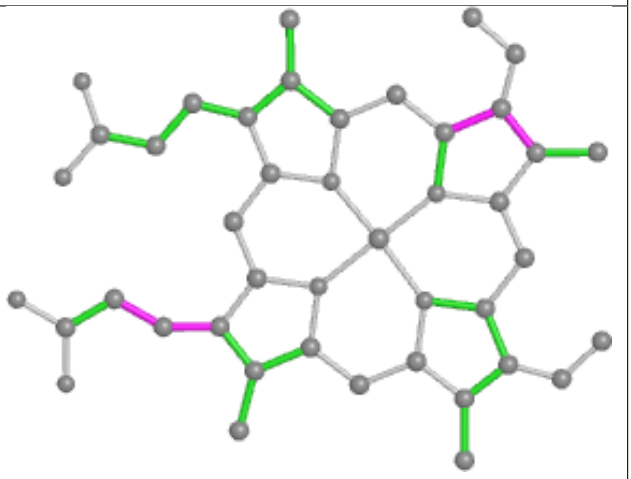


Rings

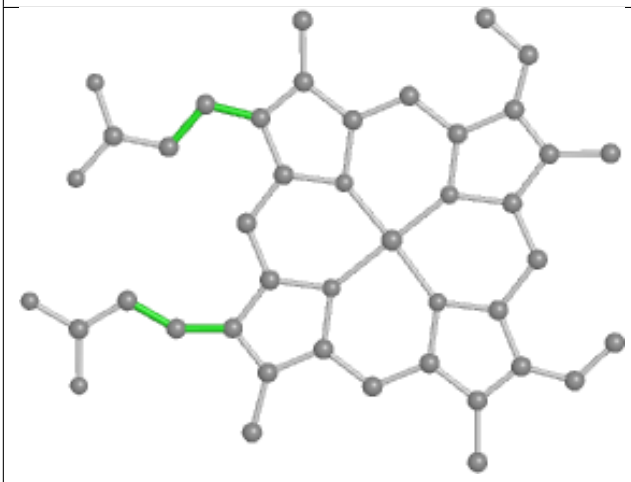
Ligand HEM A 554



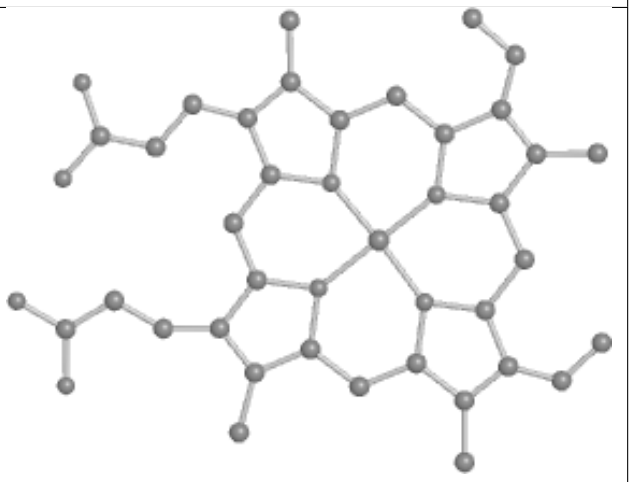
Bond lengths



Bond angles

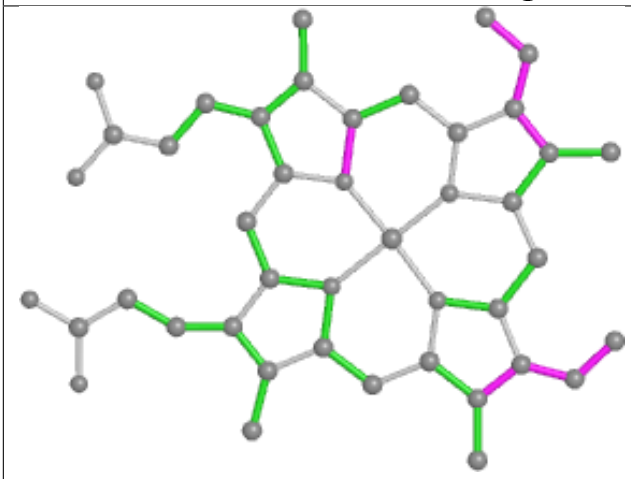


Torsions

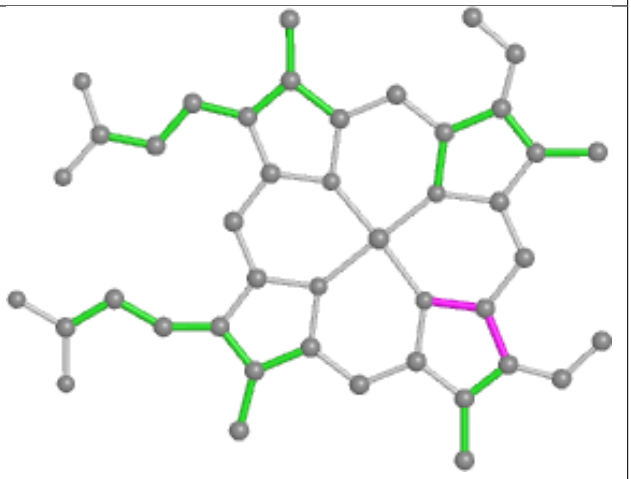


Rings

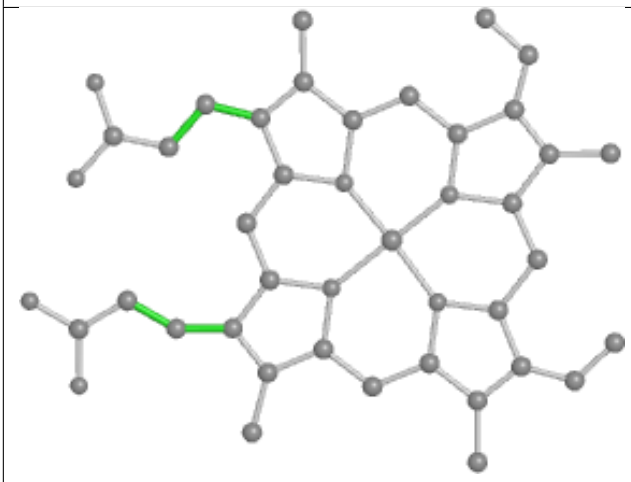
Ligand HEM B 551



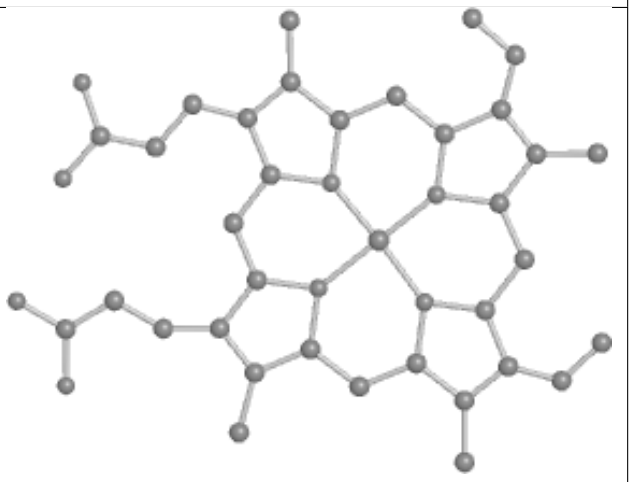
Bond lengths



Bond angles

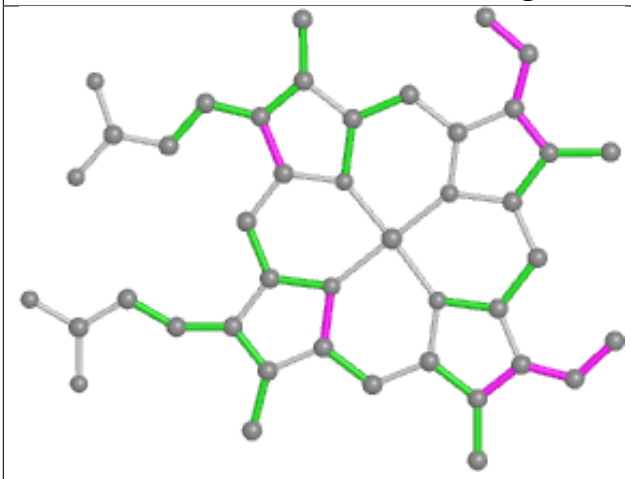


Torsions



Rings

Ligand HEM B 549



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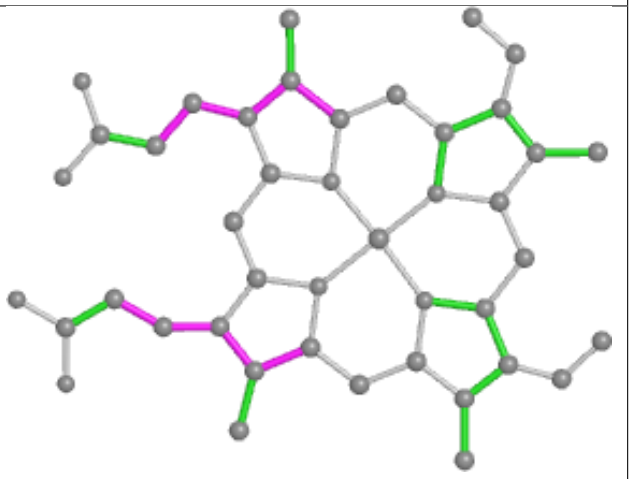
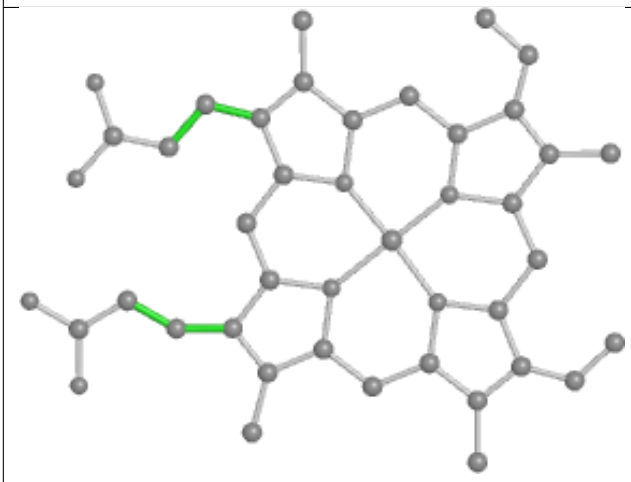
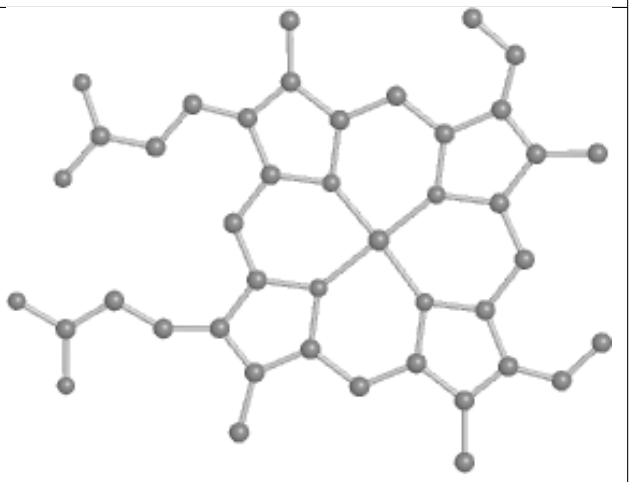


Bond angles

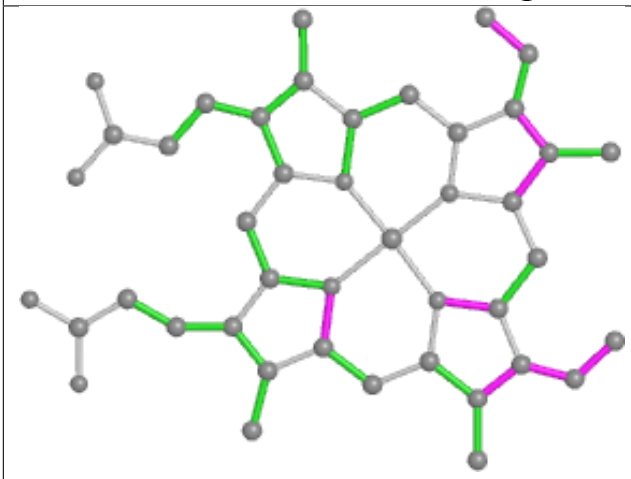


Torsions



Rings

Ligand HEM A 551



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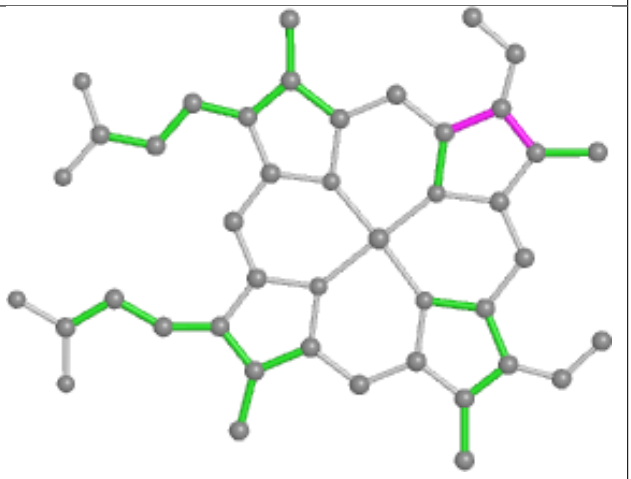
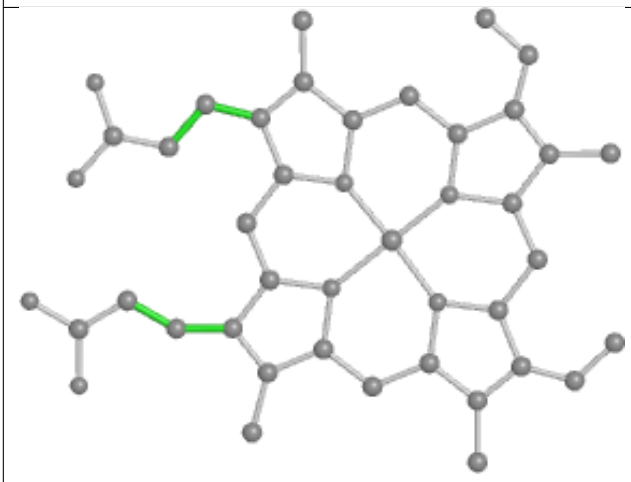
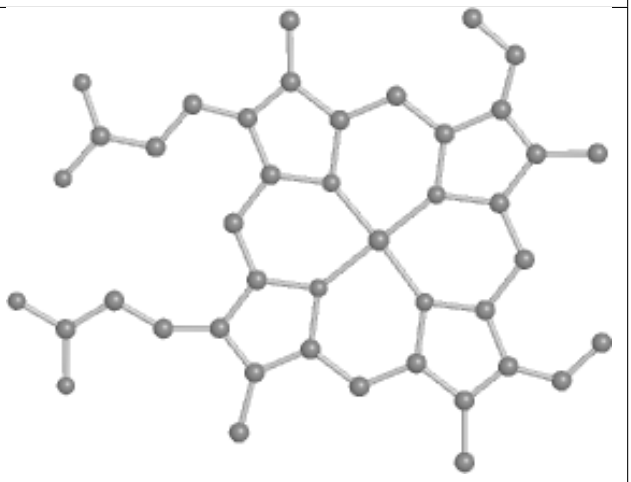


Bond angles

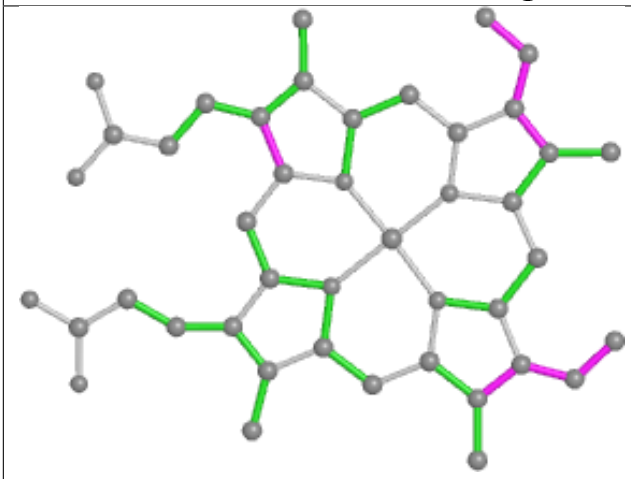


Torsions

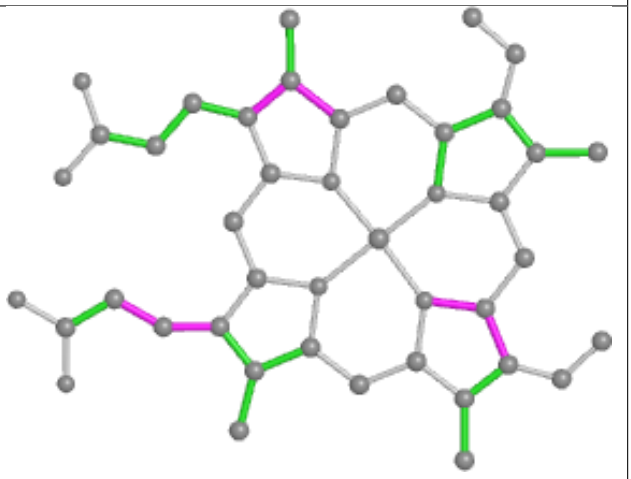


Rings

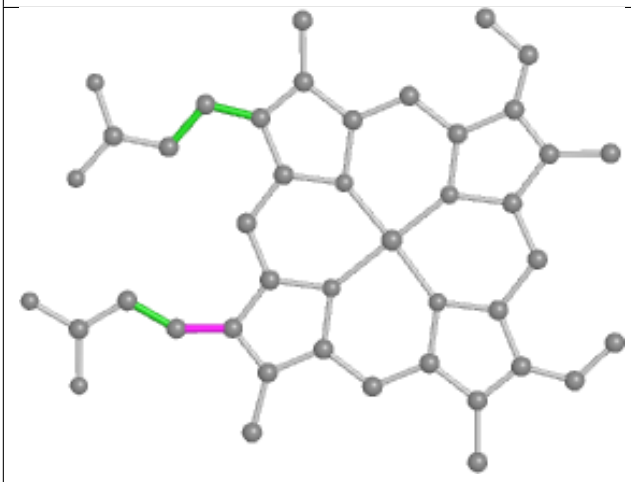
Ligand HEM B 548



Bond lengths



Bond angles



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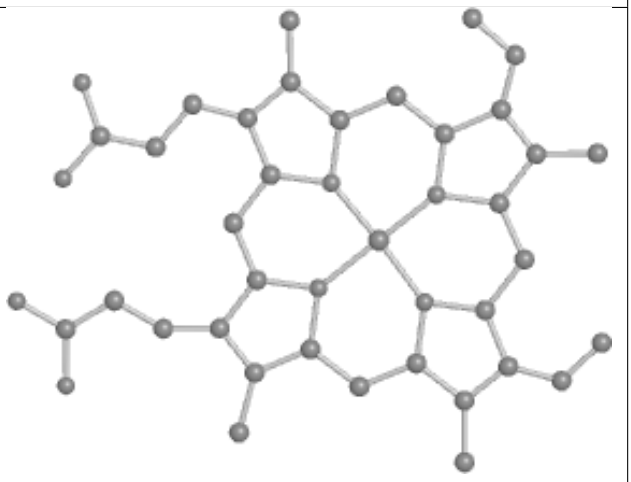
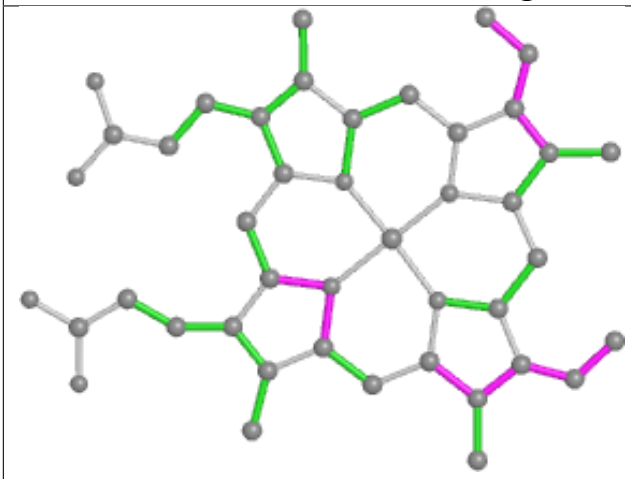


Rings

Ligand HEM A 548



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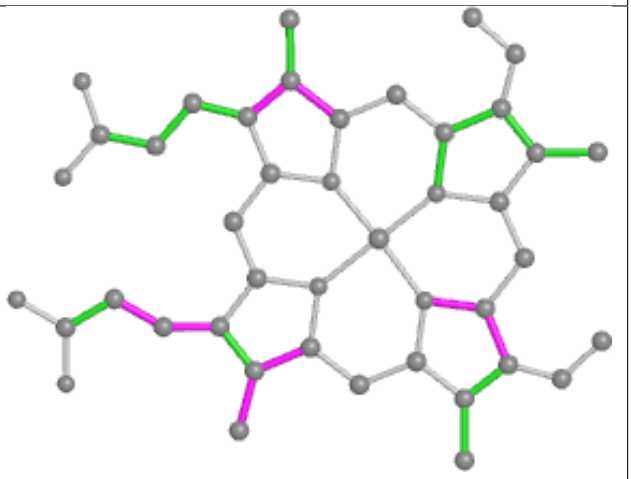
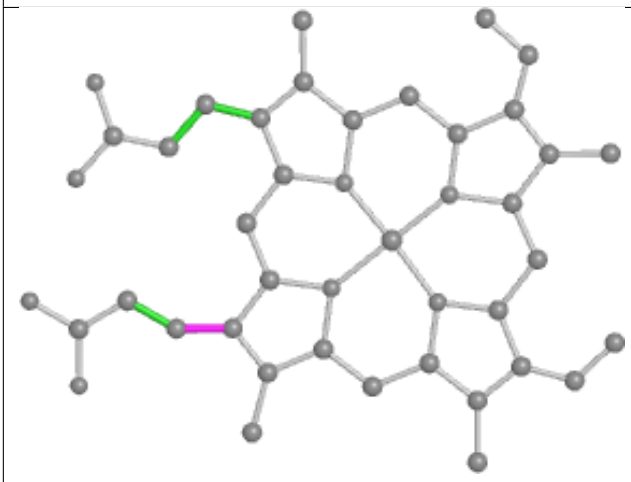
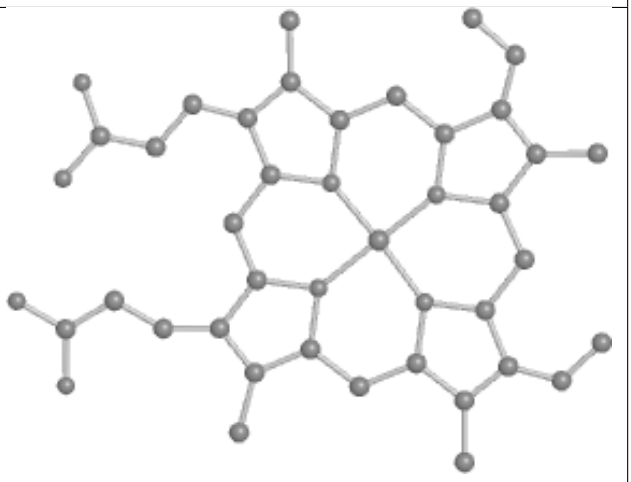


Bond angles

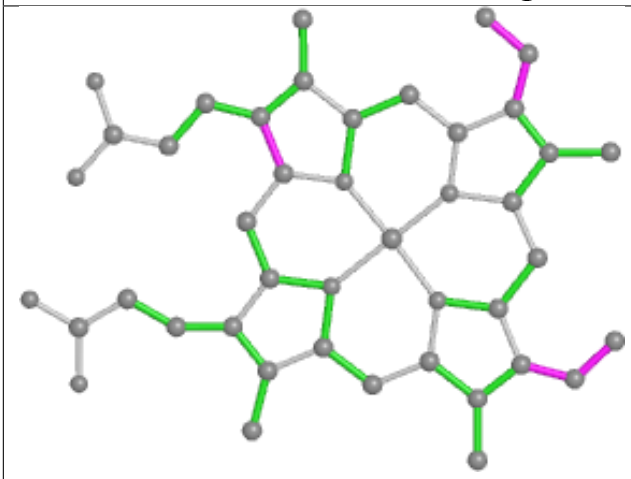


Torsions

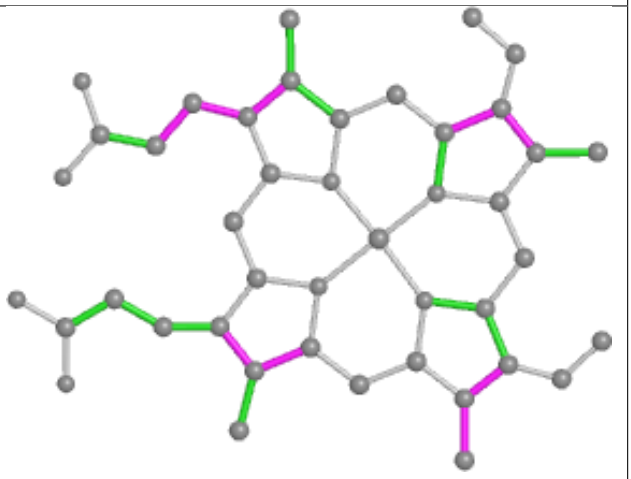


Rings

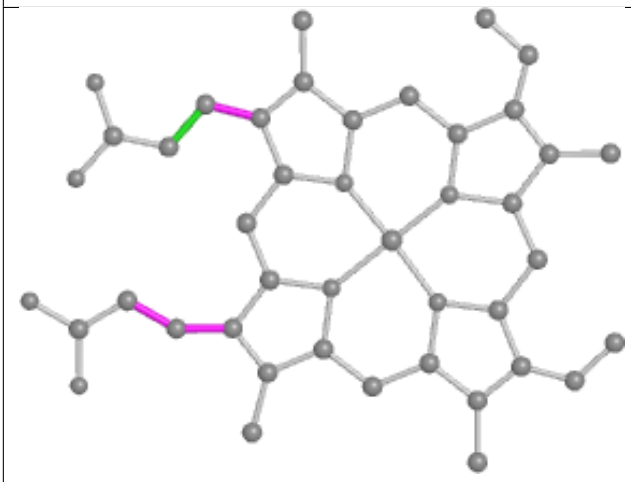
Ligand HEM A 552



Bond lengths



Bond angles



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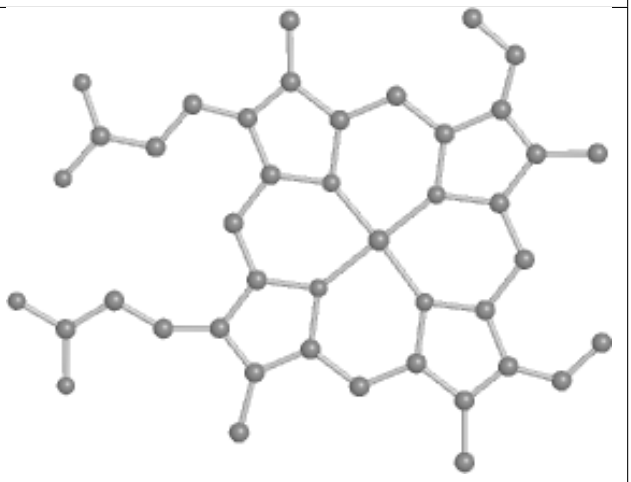
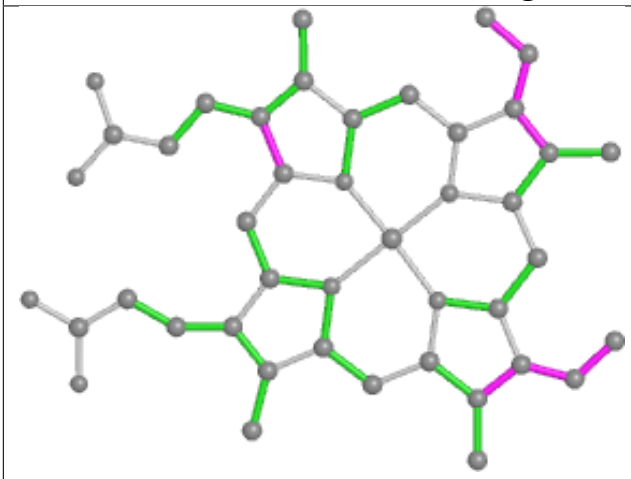
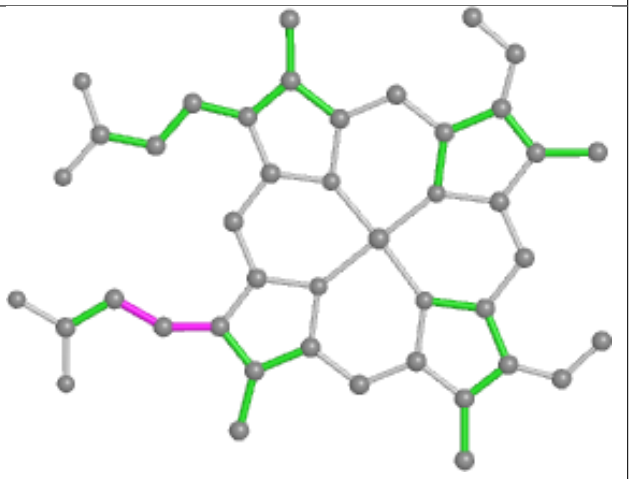


Rings

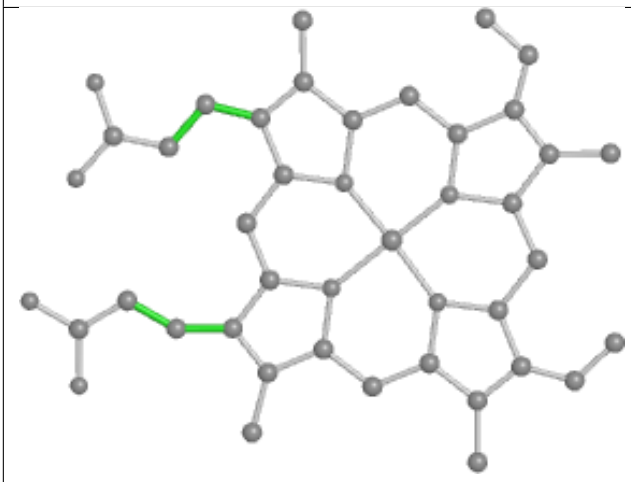
Ligand HEM B 553



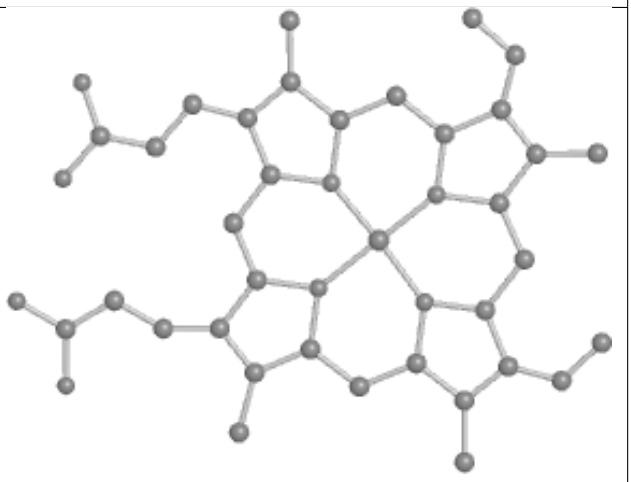
Bond lengths



Bond angles

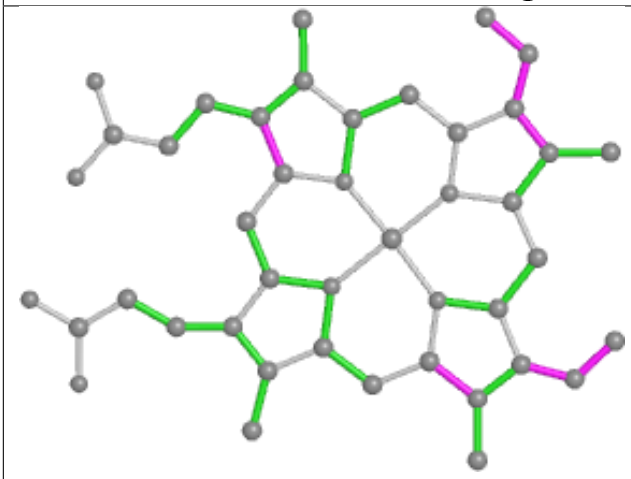


Torsions



Rings

Ligand HEM B 554



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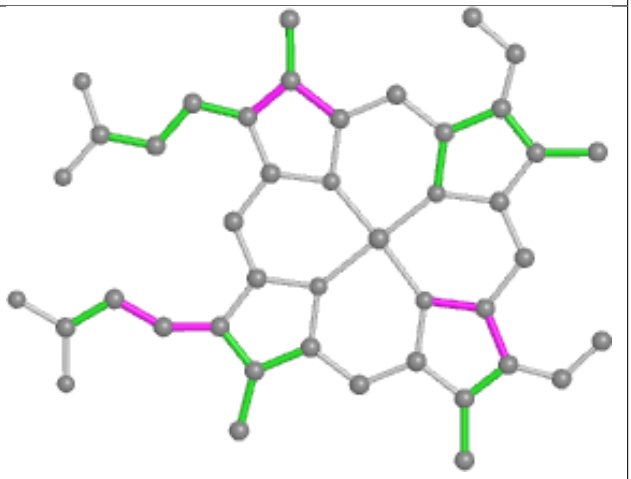
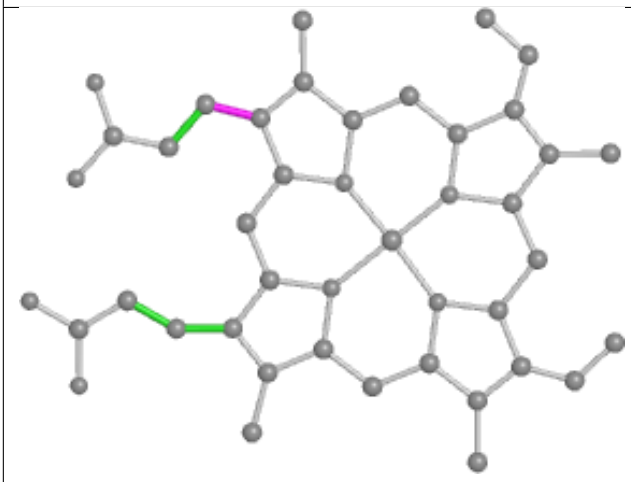
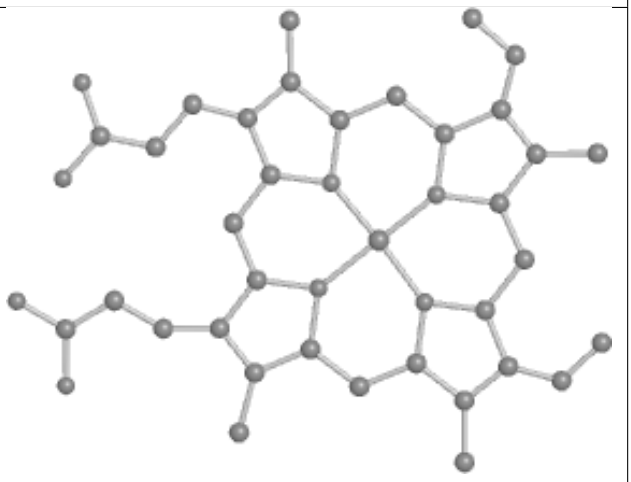


Bond angles

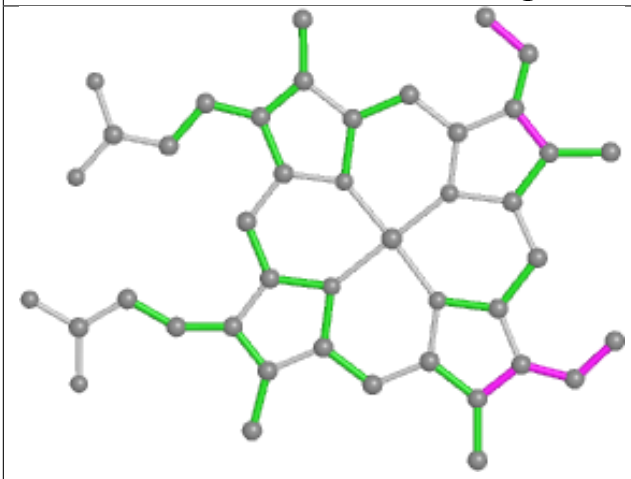


Torsions

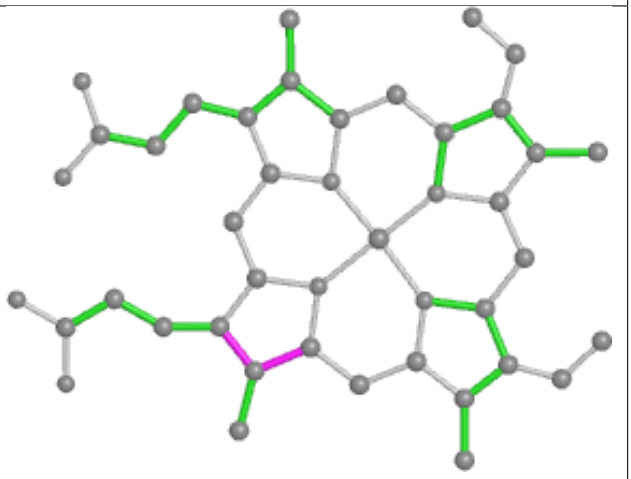


Rings

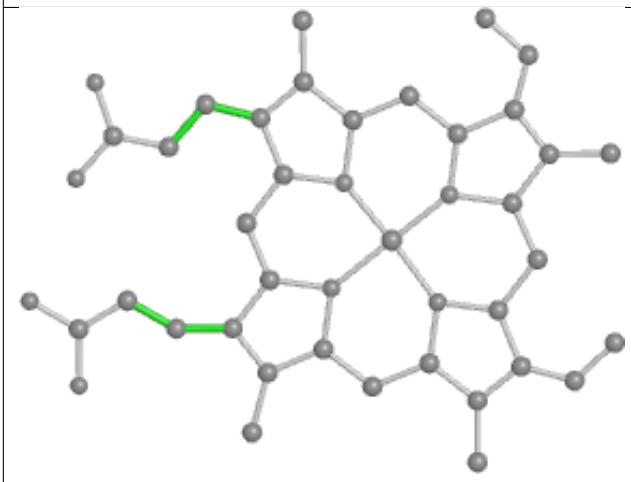
Ligand HEM B 547



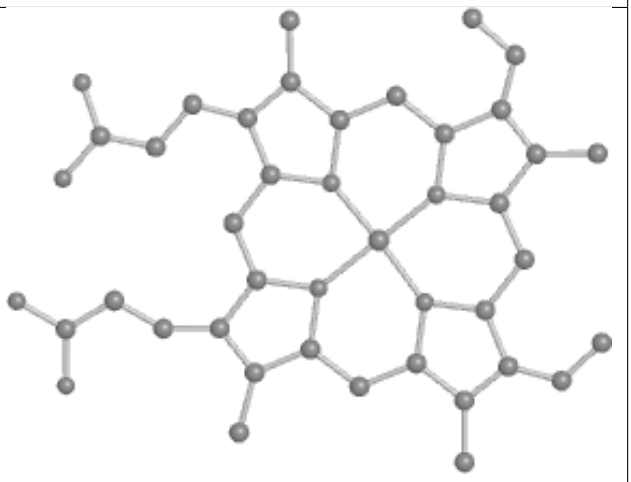
Bond lengths



Bond angles

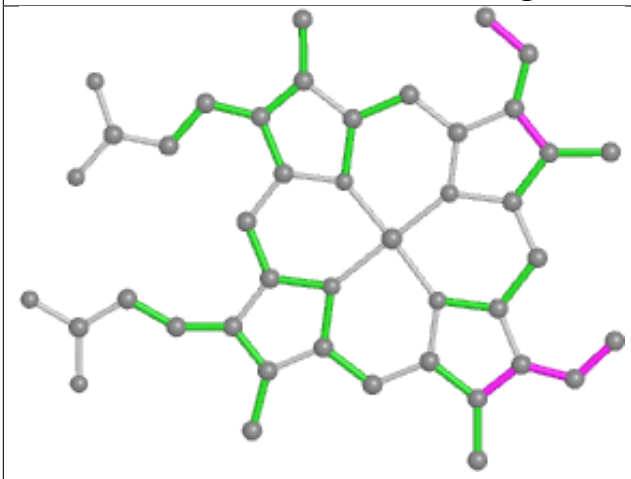


Torsions

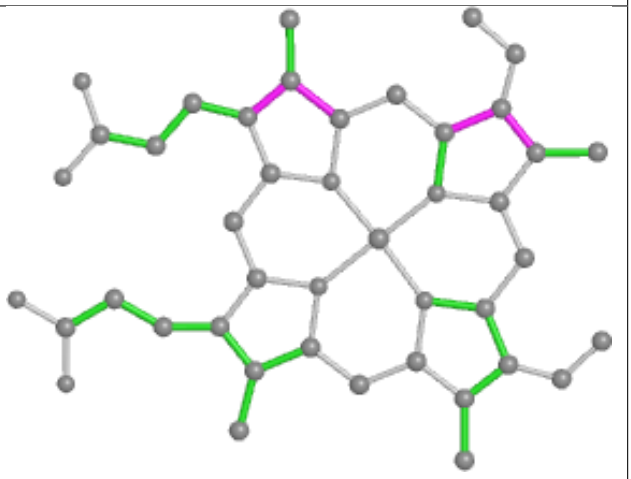


Rings

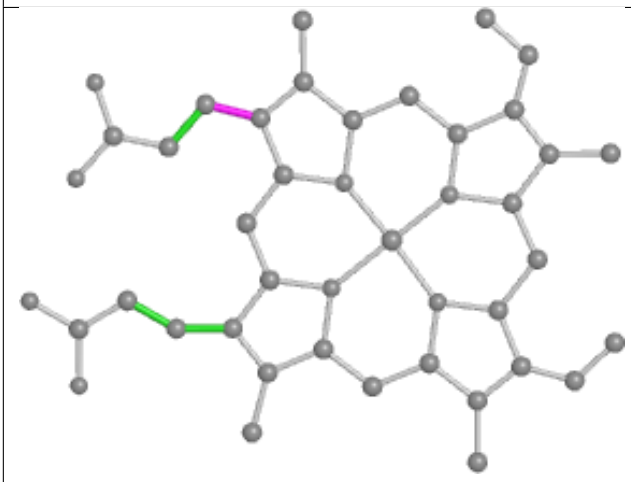
Ligand HEM A 547



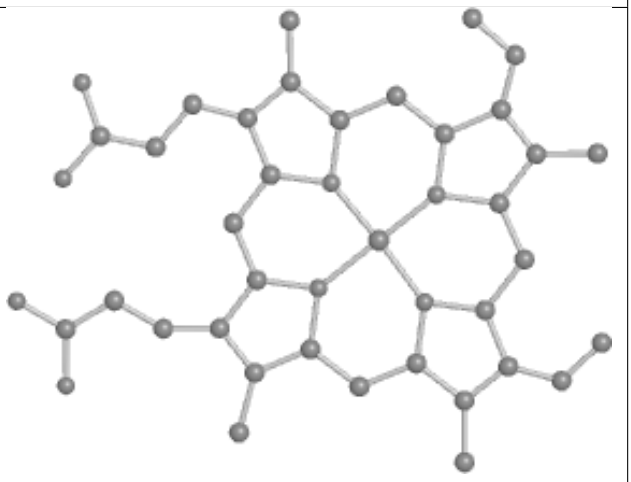
Bond lengths



Bond angles

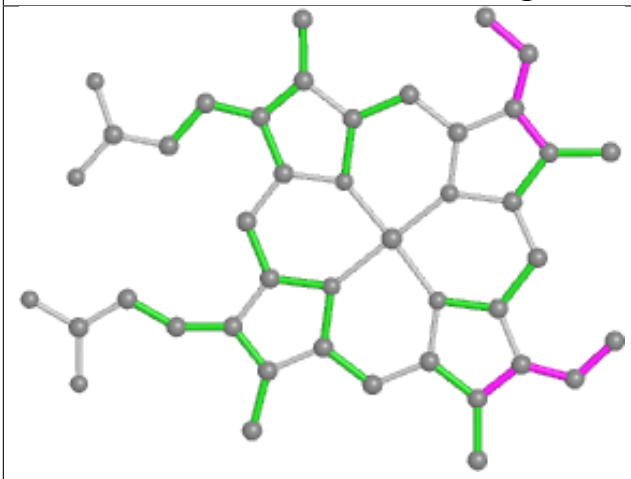


Torsions

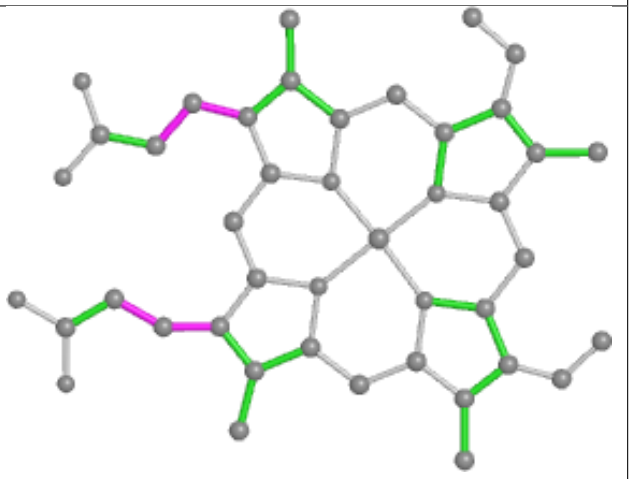


Rings

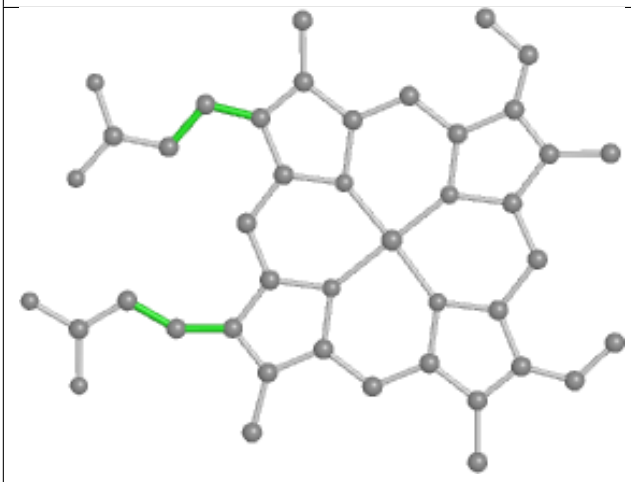
Ligand HEM A 553



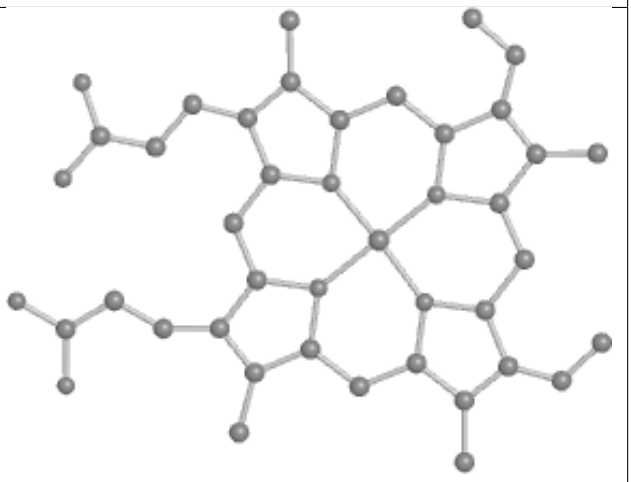
Bond lengths



Bond angles

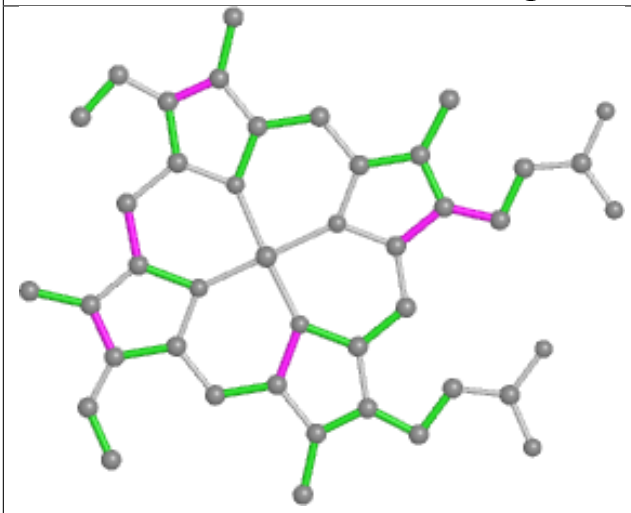


Torsions

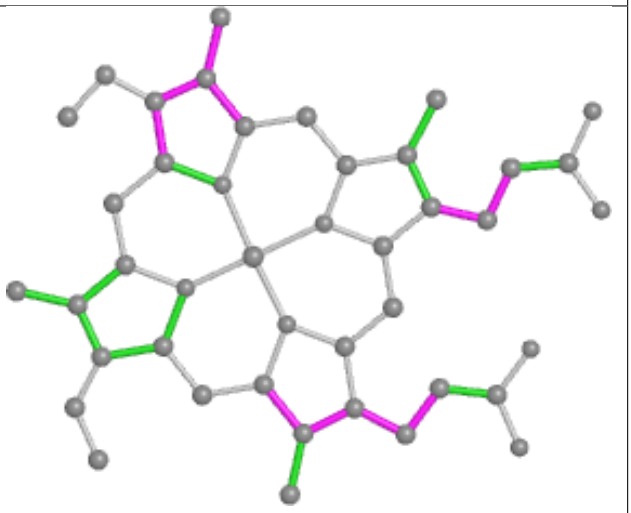


Rings

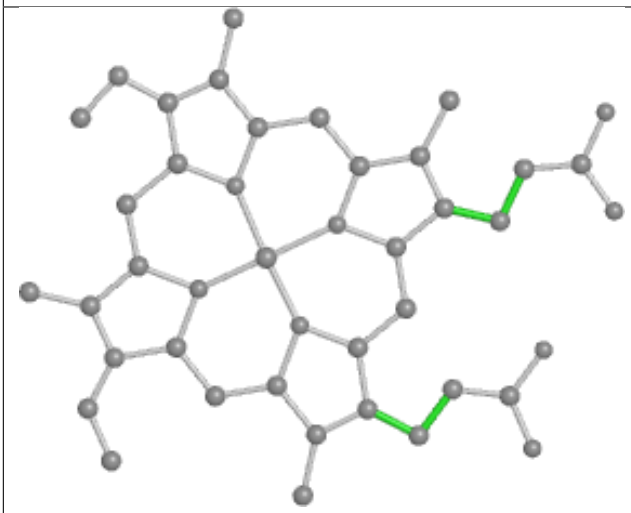
Ligand HEC A 550



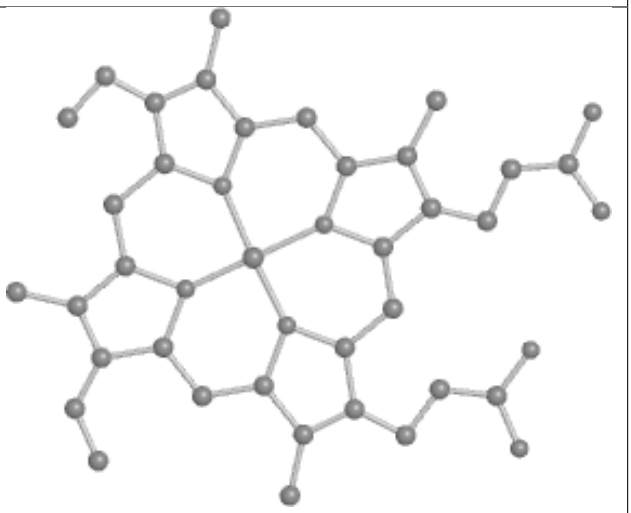
Bond lengths



Bond angles

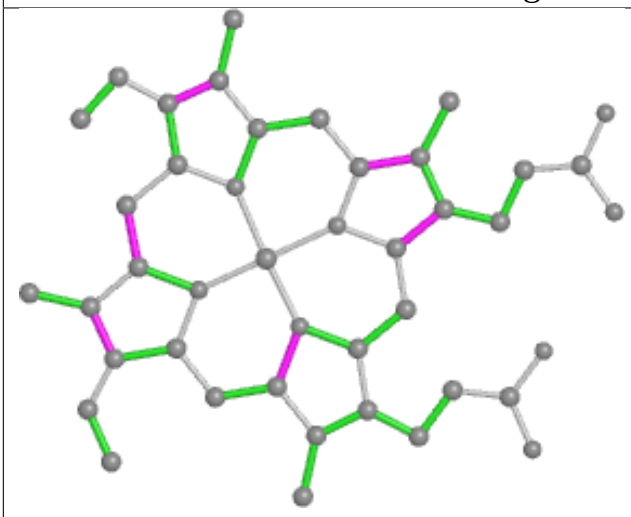


Torsions

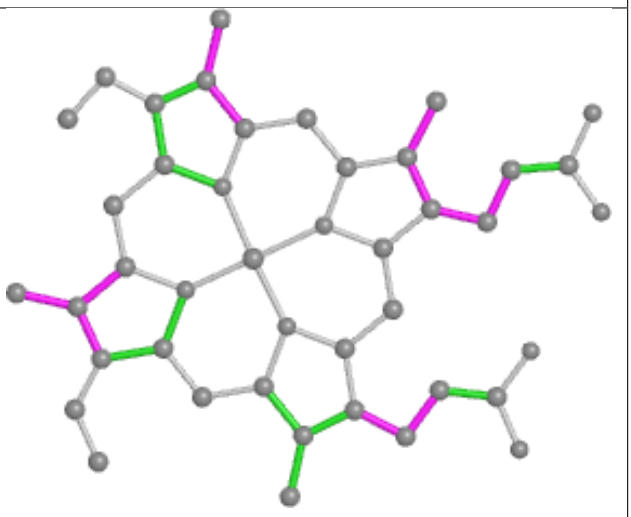


Rings

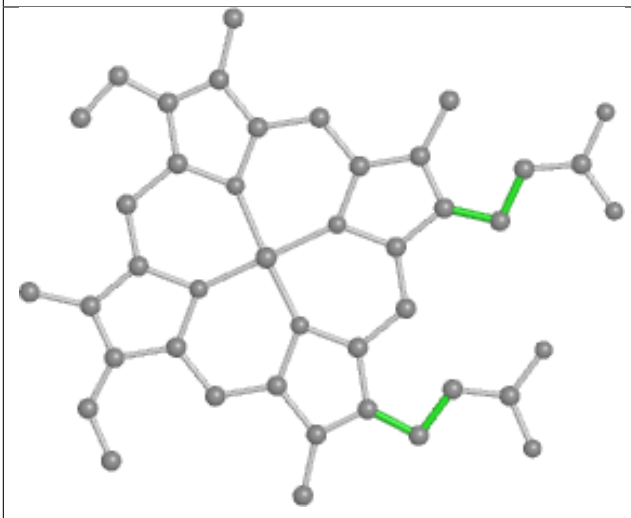
Ligand HEC B 550



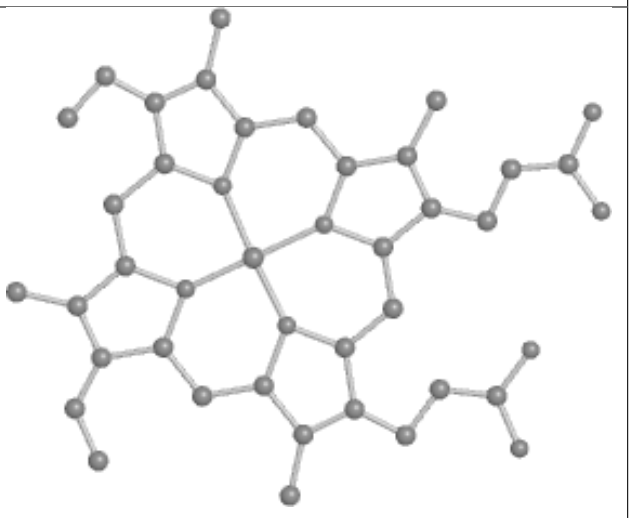
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.