Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 06:44 AM EDT

PDB ID	:	6UX0
Title	:	Isavuconazole bound complex of Acanthamoeba castellanii CYP51
Authors	:	Sharma, V.; Podust, L.M.
Deposited on	:	2019-11-06
Resolution	:	2.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 ⓘ 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 ⓘ) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
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)	:	2.35.1

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 2.93 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19999 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 Obtusifoliol 14alphademethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3253	2099	540	596	18			
1	B	414	Total	C	N	O	S	0	0	0
			3262	2103	544	597	18			
1	C	414	Total	C	N	O	S	0	0	0
			3256	2103	541	594	18			
1	D	414	Total	C	N	O	S	0	0	0
			3268	2113	544	593	18			
1	E	413	Total	C	N	O	S	0	0	0
			3255	2101	542	594	18			
1	F	413	Total	C	N	O	S	0	0	0
			3258	2101	543	596	18			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	expression tag	UNP L8GJB3
A	34	ALA	-	expression tag	UNP L8GJB3
A	35	LYS	-	expression tag	UNP L8GJB3
A	36	LYS	-	expression tag	UNP L8GJB3
A	37	THR	-	expression tag	UNP L8GJB3
A	38	SER	-	expression tag	UNP L8GJB3
A	39	SER	-	expression tag	UNP L8GJB3
A	40	LYS	-	expression tag	UNP L8GJB3
A	41	GLY	-	expression tag	UNP L8GJB3
A	42	LYS	-	expression tag	UNP L8GJB3
A	487	HIS	-	expression tag	UNP L8GJB3
A	488	HIS	-	expression tag	UNP L8GJB3
A	489	HIS	-	expression tag	UNP L8GJB3
A	490	HIS	-	expression tag	UNP L8GJB3
A	491	HIS	-	expression tag	UNP L8GJB3
A	492	HIS	-	expression tag	UNP L8GJB3
B	33	MET	-	expression tag	UNP L8GJB3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ALA	-	expression tag	UNP L8GJB3
B	35	LYS	-	expression tag	UNP L8GJB3
B	36	LYS	-	expression tag	UNP L8GJB3
B	37	THR	-	expression tag	UNP L8GJB3
B	38	SER	-	expression tag	UNP L8GJB3
B	39	SER	-	expression tag	UNP L8GJB3
B	40	LYS	-	expression tag	UNP L8GJB3
B	41	GLY	-	expression tag	UNP L8GJB3
B	42	LYS	-	expression tag	UNP L8GJB3
B	487	HIS	-	expression tag	UNP L8GJB3
B	488	HIS	-	expression tag	UNP L8GJB3
B	489	HIS	-	expression tag	UNP L8GJB3
B	490	HIS	-	expression tag	UNP L8GJB3
B	491	HIS	-	expression tag	UNP L8GJB3
B	492	HIS	-	expression tag	UNP L8GJB3
C	33	MET	-	expression tag	UNP L8GJB3
C	34	ALA	-	expression tag	UNP L8GJB3
C	35	LYS	-	expression tag	UNP L8GJB3
C	36	LYS	-	expression tag	UNP L8GJB3
C	37	THR	-	expression tag	UNP L8GJB3
C	38	SER	-	expression tag	UNP L8GJB3
C	39	SER	-	expression tag	UNP L8GJB3
C	40	LYS	-	expression tag	UNP L8GJB3
C	41	GLY	-	expression tag	UNP L8GJB3
C	42	LYS	-	expression tag	UNP L8GJB3
C	487	HIS	-	expression tag	UNP L8GJB3
C	488	HIS	-	expression tag	UNP L8GJB3
C	489	HIS	-	expression tag	UNP L8GJB3
C	490	HIS	-	expression tag	UNP L8GJB3
C	491	HIS	-	expression tag	UNP L8GJB3
C	492	HIS	-	expression tag	UNP L8GJB3
D	33	MET	-	expression tag	UNP L8GJB3
D	34	ALA	-	expression tag	UNP L8GJB3
D	35	LYS	-	expression tag	UNP L8GJB3
D	36	LYS	-	expression tag	UNP L8GJB3
D	37	THR	-	expression tag	UNP L8GJB3
D	38	SER	-	expression tag	UNP L8GJB3
D	39	SER	-	expression tag	UNP L8GJB3
D	40	LYS	-	expression tag	UNP L8GJB3
D	41	GLY	-	expression tag	UNP L8GJB3
D	42	LYS	-	expression tag	UNP L8GJB3
D	487	HIS	-	expression tag	UNP L8GJB3

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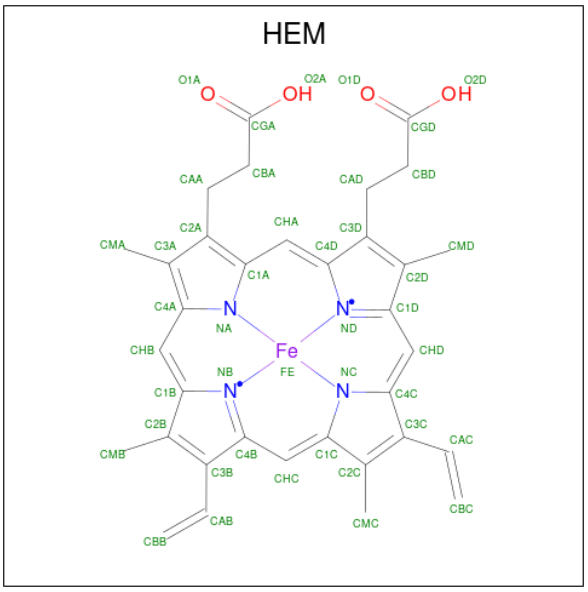
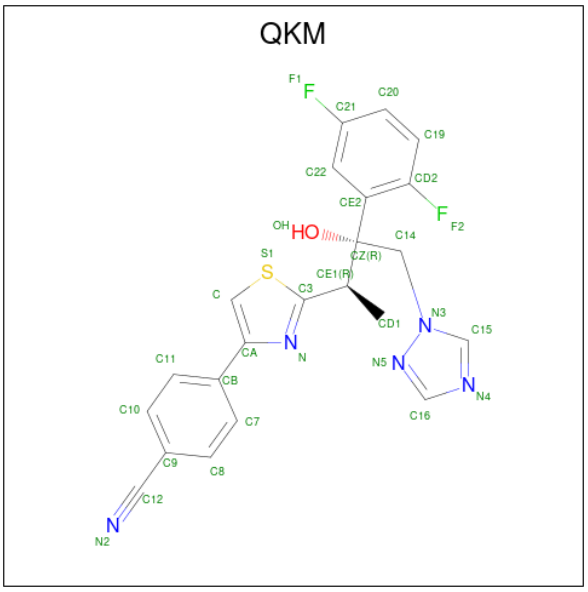
Chain	Residue	Modelled	Actual	Comment	Reference
D	488	HIS	-	expression tag	UNP L8GJB3
D	489	HIS	-	expression tag	UNP L8GJB3
D	490	HIS	-	expression tag	UNP L8GJB3
D	491	HIS	-	expression tag	UNP L8GJB3
D	492	HIS	-	expression tag	UNP L8GJB3
E	33	MET	-	expression tag	UNP L8GJB3
E	34	ALA	-	expression tag	UNP L8GJB3
E	35	LYS	-	expression tag	UNP L8GJB3
E	36	LYS	-	expression tag	UNP L8GJB3
E	37	THR	-	expression tag	UNP L8GJB3
E	38	SER	-	expression tag	UNP L8GJB3
E	39	SER	-	expression tag	UNP L8GJB3
E	40	LYS	-	expression tag	UNP L8GJB3
E	41	GLY	-	expression tag	UNP L8GJB3
E	42	LYS	-	expression tag	UNP L8GJB3
E	487	HIS	-	expression tag	UNP L8GJB3
E	488	HIS	-	expression tag	UNP L8GJB3
E	489	HIS	-	expression tag	UNP L8GJB3
E	490	HIS	-	expression tag	UNP L8GJB3
E	491	HIS	-	expression tag	UNP L8GJB3
E	492	HIS	-	expression tag	UNP L8GJB3
F	33	MET	-	expression tag	UNP L8GJB3
F	34	ALA	-	expression tag	UNP L8GJB3
F	35	LYS	-	expression tag	UNP L8GJB3
F	36	LYS	-	expression tag	UNP L8GJB3
F	37	THR	-	expression tag	UNP L8GJB3
F	38	SER	-	expression tag	UNP L8GJB3
F	39	SER	-	expression tag	UNP L8GJB3
F	40	LYS	-	expression tag	UNP L8GJB3
F	41	GLY	-	expression tag	UNP L8GJB3
F	42	LYS	-	expression tag	UNP L8GJB3
F	487	HIS	-	expression tag	UNP L8GJB3
F	488	HIS	-	expression tag	UNP L8GJB3
F	489	HIS	-	expression tag	UNP L8GJB3
F	490	HIS	-	expression tag	UNP L8GJB3
F	491	HIS	-	expression tag	UNP L8GJB3
F	492	HIS	-	expression tag	UNP L8GJB3

- 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	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 4-{2-[(2R,3R)-3-(2,5-difluorophenyl)-3-hydroxy-4-(1H-1,2,4-triazol-1-yl)butan-2-yl]-1,3-thiazol-4-yl}benzonitrile (three-letter code: QKM) (formula: $C_{22}H_{17}F_2N_5OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			31	22	2	5	1	1		
3	B	1	Total	C	F	N	O	S	0	0
			31	22	2	5	1	1		
3	C	1	Total	C	F	N	O	S	0	0
			31	22	2	5	1	1		
3	D	1	Total	C	F	N	O	S	0	0
			31	22	2	5	1	1		
3	E	1	Total	C	F	N	O	S	0	0
			31	22	2	5	1	1		
3	F	1	Total	C	F	N	O	S	0	0
			31	22	2	5	1	1		

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		
4	F	1	Total	Fe	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	1	Total	O	0	0
			1	1		

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	99.45Å 99.06Å 108.71Å 92.61° 96.20° 120.09°	Depositor
Resolution (Å)	107.35 – 2.93	Depositor
% Data completeness (in resolution range)	94.0 (107.35-2.93)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.213 , 0.308	Depositor
Wilson B-factor (Å^2)	90.4	Xtriage
Anisotropy	0.262	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -k,-h,-l	Xtriage
Total number of atoms	19999	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

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

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	QKM	F	502	2	29,34,34	1.43	4 (13%)	39,49,49	1.47	5 (12%)
2	HEM	A	501	1,3	41,50,50	1.58	5 (12%)	45,82,82	2.09	16 (35%)
3	QKM	C	502	2	29,34,34	1.50	4 (13%)	39,49,49	1.79	10 (25%)
3	QKM	D	502	2	29,34,34	1.31	4 (13%)	39,49,49	1.69	8 (20%)
3	QKM	B	502	2	29,34,34	1.43	5 (17%)	39,49,49	2.36	17 (43%)
3	QKM	A	502	2	29,34,34	1.47	3 (10%)	39,49,49	2.02	13 (33%)
2	HEM	E	501	1,3	41,50,50	1.53	6 (14%)	45,82,82	2.13	18 (40%)
2	HEM	C	501	1,3	41,50,50	1.42	5 (12%)	45,82,82	2.58	15 (33%)
3	QKM	E	502	2	29,34,34	1.40	3 (10%)	39,49,49	1.60	9 (23%)
2	HEM	B	501	1,3	41,50,50	1.57	8 (19%)	45,82,82	1.87	13 (28%)
2	HEM	D	501	1,3	41,50,50	1.47	6 (14%)	45,82,82	2.19	12 (26%)
2	HEM	F	501	1,3	41,50,50	1.53	8 (19%)	45,82,82	1.79	13 (28%)

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	QKM	F	502	2	-	2/24/27/27	0/4/4/4
2	HEM	A	501	1,3	-	2/12/54/54	-
3	QKM	C	502	2	-	7/24/27/27	0/4/4/4
3	QKM	D	502	2	-	2/24/27/27	0/4/4/4
3	QKM	B	502	2	-	6/24/27/27	0/4/4/4
3	QKM	A	502	2	-	8/24/27/27	0/4/4/4
2	HEM	E	501	1,3	-	2/12/54/54	-
2	HEM	C	501	1,3	-	6/12/54/54	-
3	QKM	E	502	2	-	7/24/27/27	0/4/4/4
2	HEM	B	501	1,3	-	0/12/54/54	-
2	HEM	D	501	1,3	-	4/12/54/54	-
2	HEM	F	501	1,3	-	2/12/54/54	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	HEM	C1B-NB	-5.49	1.30	1.40
2	D	501	HEM	C1B-NB	-4.77	1.32	1.40
2	A	501	HEM	C1B-NB	-4.57	1.32	1.40
3	E	502	QKM	CA-N	4.40	1.51	1.37
2	B	501	HEM	C1B-NB	-4.40	1.32	1.40
3	F	502	QKM	CA-N	4.37	1.51	1.37
2	F	501	HEM	C1B-NB	-4.06	1.33	1.40
3	C	502	QKM	C15-N3	4.04	1.37	1.33
2	A	501	HEM	C4B-NB	-3.99	1.30	1.38
2	C	501	HEM	C1B-NB	-3.93	1.33	1.40
3	A	502	QKM	C15-N3	3.90	1.37	1.33
3	B	502	QKM	CB-CA	-3.89	1.42	1.48
3	C	502	QKM	CA-N	3.88	1.49	1.37
3	A	502	QKM	CA-N	3.88	1.49	1.37
3	D	502	QKM	CA-N	3.87	1.49	1.37
3	A	502	QKM	CB-CA	-3.71	1.43	1.48
3	B	502	QKM	CA-N	3.61	1.48	1.37
2	F	501	HEM	C4D-ND	-3.58	1.34	1.40
2	C	501	HEM	C4B-NB	-3.56	1.31	1.38
2	B	501	HEM	C4B-NB	-3.42	1.31	1.38
3	F	502	QKM	C15-N3	3.36	1.37	1.33
3	C	502	QKM	CB-CA	-3.33	1.43	1.48
2	A	501	HEM	C4D-ND	-3.25	1.34	1.40
3	C	502	QKM	CZ-CE1	-3.24	1.50	1.56
2	E	501	HEM	C4B-NB	-3.24	1.32	1.38
3	F	502	QKM	CZ-CE1	-3.19	1.51	1.56
2	F	501	HEM	C4B-NB	-3.00	1.32	1.38
2	D	501	HEM	C4B-NB	-2.90	1.32	1.38
3	D	502	QKM	CB-CA	-2.85	1.44	1.48
3	D	502	QKM	C15-N3	2.81	1.36	1.33
2	D	501	HEM	C4D-ND	-2.80	1.35	1.40
2	C	501	HEM	CHB-C1B	2.73	1.42	1.35
2	B	501	HEM	C4D-ND	-2.71	1.35	1.40
2	D	501	HEM	FE-NB	2.68	2.10	1.96
3	E	502	QKM	CB-CA	-2.67	1.44	1.48
3	B	502	QKM	C15-N3	2.67	1.36	1.33
3	B	502	QKM	CZ-CE1	-2.62	1.52	1.56
2	F	501	HEM	FE-NB	2.60	2.09	1.96
2	E	501	HEM	CHB-C1B	2.60	1.41	1.35
2	C	501	HEM	C4D-ND	-2.58	1.35	1.40
2	A	501	HEM	C4D-C3D	2.56	1.49	1.45
3	E	502	QKM	CZ-CE2	-2.51	1.49	1.53
2	D	501	HEM	C4D-C3D	2.50	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	HEM	FE-NB	2.49	2.09	1.96
2	C	501	HEM	FE-NB	2.47	2.09	1.96
2	A	501	HEM	FE-NB	2.43	2.08	1.96
3	B	502	QKM	CZ-CE2	-2.42	1.49	1.53
2	B	501	HEM	C4D-C3D	2.38	1.49	1.45
2	E	501	HEM	C4D-ND	-2.35	1.36	1.40
2	F	501	HEM	CHB-C1B	2.35	1.41	1.35
2	F	501	HEM	C3D-C2D	-2.35	1.31	1.36
2	B	501	HEM	FE-NB	2.33	2.08	1.96
2	F	501	HEM	C3B-C4B	2.28	1.49	1.44
2	B	501	HEM	C3B-C4B	2.27	1.49	1.44
2	B	501	HEM	O1D-CGD	2.11	1.29	1.22
2	D	501	HEM	CHB-C1B	2.09	1.40	1.35
2	F	501	HEM	C1D-ND	-2.08	1.34	1.38
2	B	501	HEM	CHB-C1B	2.07	1.40	1.35
3	D	502	QKM	CZ-CE1	-2.06	1.52	1.56
2	E	501	HEM	C1D-ND	-2.03	1.34	1.38
3	F	502	QKM	CB-CA	-2.02	1.45	1.48

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CBA-CAA-C2A	-6.85	100.93	112.62
2	C	501	HEM	CAD-C3D-C4D	6.37	135.80	124.66
2	D	501	HEM	CAD-C3D-C4D	6.36	135.77	124.66
3	B	502	QKM	C-CA-CB	-6.26	120.73	129.44
2	D	501	HEM	C1B-NB-C4B	5.63	110.89	105.07
2	C	501	HEM	C4B-C3B-C2B	-5.26	102.94	107.11
2	E	501	HEM	C1B-NB-C4B	5.05	110.29	105.07
2	C	501	HEM	CHD-C1D-ND	4.83	129.68	124.43
3	A	502	QKM	OH-CZ-CE1	-4.82	100.64	110.59
2	B	501	HEM	C1B-NB-C4B	4.75	109.98	105.07
2	A	501	HEM	C1B-NB-C4B	4.64	109.87	105.07
2	C	501	HEM	C1B-NB-C4B	4.56	109.78	105.07
2	D	501	HEM	CAD-C3D-C2D	-4.55	119.40	127.88
2	F	501	HEM	CHD-C1D-ND	4.54	129.37	124.43
2	C	501	HEM	CAD-C3D-C2D	-4.35	119.78	127.88
3	D	502	QKM	C7-CB-CA	-4.30	114.50	121.28
3	D	502	QKM	C8-C9-C12	-4.29	112.84	119.99
2	F	501	HEM	C1B-NB-C4B	4.27	109.48	105.07
3	A	502	QKM	C7-CB-CA	-4.08	114.84	121.28
2	E	501	HEM	C4B-C3B-C2B	-4.08	103.88	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	QKM	C20-C21-C22	-4.06	118.01	123.29
2	D	501	HEM	CHD-C1D-ND	4.06	128.84	124.43
2	A	501	HEM	CBD-CAD-C3D	4.05	123.89	112.63
2	F	501	HEM	C4B-C3B-C2B	-3.84	104.06	107.11
3	B	502	QKM	F1-C21-C22	3.78	123.65	118.25
2	D	501	HEM	CHC-C4B-NB	3.78	128.53	124.43
2	E	501	HEM	CHD-C1D-ND	3.77	128.52	124.43
2	C	501	HEM	CBD-CAD-C3D	3.76	123.08	112.63
3	F	502	QKM	C-CA-CB	-3.72	124.27	129.44
3	A	502	QKM	CE2-C22-C21	3.70	122.66	117.56
2	C	501	HEM	C4B-CHC-C1C	3.69	127.42	122.56
2	E	501	HEM	CHA-C4D-ND	3.56	128.78	124.38
2	E	501	HEM	C4A-C3A-C2A	3.55	109.47	107.00
2	E	501	HEM	CHC-C4B-NB	3.53	128.27	124.43
2	A	501	HEM	CHD-C1D-C2D	-3.53	119.47	124.98
3	A	502	QKM	CE2-CZ-CE1	3.52	115.90	110.74
2	D	501	HEM	CHD-C1D-C2D	-3.52	119.49	124.98
2	D	501	HEM	C4B-C3B-C2B	-3.50	104.34	107.11
2	B	501	HEM	CHC-C4B-NB	3.48	128.22	124.43
3	C	502	QKM	CE2-C22-C21	3.47	122.33	117.56
3	E	502	QKM	CB-CA-N	-3.46	114.97	120.78
2	A	501	HEM	C4B-C3B-C2B	-3.44	104.39	107.11
3	F	502	QKM	CE2-C22-C21	3.41	122.25	117.56
3	C	502	QKM	C7-CB-CA	-3.40	115.91	121.28
3	C	502	QKM	C7-C8-C9	-3.40	115.96	120.35
2	F	501	HEM	CHC-C4B-NB	3.40	128.12	124.43
2	B	501	HEM	C4B-C3B-C2B	-3.39	104.42	107.11
2	B	501	HEM	CHD-C1D-ND	3.38	128.10	124.43
3	B	502	QKM	CE2-C22-C21	3.37	122.20	117.56
2	A	501	HEM	C4B-CHC-C1C	3.36	126.99	122.56
3	D	502	QKM	C10-C9-C12	3.35	125.58	119.99
3	B	502	QKM	CE2-CZ-CE1	3.31	115.58	110.74
3	A	502	QKM	C10-C9-C8	3.30	124.92	118.96
3	A	502	QKM	CB-CA-N	-3.30	115.24	120.78
2	E	501	HEM	CHA-C4D-C3D	-3.29	119.15	125.33
2	C	501	HEM	CHC-C4B-NB	3.28	128.00	124.43
2	A	501	HEM	O2D-CGD-O1D	-3.28	115.13	123.30
2	B	501	HEM	C4B-CHC-C1C	3.28	126.88	122.56
2	E	501	HEM	O2A-CGA-CBA	3.23	124.41	114.03
3	C	502	QKM	OH-CZ-CE1	-3.21	103.97	110.59
3	C	502	QKM	CD1-CE1-C3	-3.19	104.24	108.59
3	D	502	QKM	OH-CZ-CE1	-3.10	104.20	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	502	QKM	C10-C11-CB	-3.10	116.67	121.13
2	A	501	HEM	CHC-C4B-NB	3.09	127.79	124.43
2	F	501	HEM	CHD-C1D-C2D	-3.08	120.16	124.98
3	B	502	QKM	C8-C9-C12	-3.08	114.86	119.99
2	B	501	HEM	CBD-CAD-C3D	3.04	121.09	112.63
2	A	501	HEM	CHD-C1D-ND	3.03	127.72	124.43
2	A	501	HEM	CAD-C3D-C4D	2.99	129.88	124.66
3	F	502	QKM	CD1-CE1-CZ	-2.98	106.01	111.57
2	F	501	HEM	CAD-CBD-CGD	-2.97	107.21	113.60
2	D	501	HEM	CBD-CAD-C3D	2.97	120.88	112.63
3	B	502	QKM	CD1-CE1-CZ	-2.97	106.03	111.57
2	C	501	HEM	C3B-C2B-C1B	2.97	108.69	106.49
3	B	502	QKM	CZ-CE2-CD2	-2.95	119.06	123.07
2	D	501	HEM	C4B-CHC-C1C	2.94	126.44	122.56
3	A	502	QKM	C8-C9-C12	-2.91	115.13	119.99
3	F	502	QKM	CZ-CE1-C3	2.91	117.88	112.77
2	B	501	HEM	CAD-C3D-C4D	2.90	129.73	124.66
2	A	501	HEM	CHB-C1B-NB	2.89	127.96	124.38
3	B	502	QKM	F2-CD2-CE2	2.88	122.45	118.98
3	E	502	QKM	C14-CZ-CE1	-2.87	104.36	110.08
3	B	502	QKM	CZ-CE1-C3	2.86	117.80	112.77
3	E	502	QKM	OH-CZ-CE2	-2.85	103.08	107.11
3	B	502	QKM	OH-CZ-CE1	-2.84	104.74	110.59
2	A	501	HEM	CBA-CAA-C2A	-2.83	107.78	112.62
2	E	501	HEM	C4B-CHC-C1C	2.83	126.29	122.56
3	B	502	QKM	C19-CD2-CE2	-2.83	119.49	123.44
2	C	501	HEM	CAD-CBD-CGD	-2.82	107.52	113.60
2	B	501	HEM	CMD-C2D-C1D	2.81	129.32	125.04
2	C	501	HEM	CMA-C3A-C4A	-2.80	124.16	128.46
2	C	501	HEM	CHD-C1D-C2D	-2.78	120.63	124.98
2	A	501	HEM	CMA-C3A-C4A	-2.76	124.22	128.46
3	A	502	QKM	C7-C8-C9	-2.76	116.79	120.35
2	B	501	HEM	CHD-C1D-C2D	-2.71	120.74	124.98
2	F	501	HEM	CHA-C4D-ND	2.71	127.73	124.38
3	E	502	QKM	F2-CD2-C19	-2.70	112.58	118.59
3	A	502	QKM	C11-CB-C7	2.70	122.96	117.59
2	D	501	HEM	CAD-CBD-CGD	-2.61	107.98	113.60
2	E	501	HEM	CAD-CBD-CGD	-2.61	107.98	113.60
2	B	501	HEM	CHA-C4D-C3D	-2.59	120.47	125.33
2	A	501	HEM	CAD-CBD-CGD	-2.57	108.07	113.60
3	C	502	QKM	C10-C9-C8	2.56	123.59	118.96
3	B	502	QKM	C22-CE2-CZ	2.56	122.54	118.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	QKM	F2-CD2-CE2	2.55	122.05	118.98
2	E	501	HEM	CHD-C1D-C2D	-2.55	121.00	124.98
2	F	501	HEM	C4B-CHC-C1C	2.54	125.91	122.56
2	A	501	HEM	C2D-C1D-ND	2.44	112.81	109.88
2	B	501	HEM	CHA-C4D-ND	2.41	127.36	124.38
2	A	501	HEM	CMD-C2D-C1D	2.41	128.72	125.04
2	E	501	HEM	CMD-C2D-C1D	2.40	128.70	125.04
3	E	502	QKM	CZ-CE2-CD2	2.39	126.32	123.07
2	E	501	HEM	CAD-C3D-C4D	2.39	128.84	124.66
3	B	502	QKM	C11-CB-C7	2.38	122.34	117.59
3	F	502	QKM	OH-CZ-C14	2.38	111.88	108.24
2	E	501	HEM	O2A-CGA-O1A	-2.38	117.38	123.30
2	B	501	HEM	O2A-CGA-O1A	-2.37	117.38	123.30
2	E	501	HEM	CMA-C3A-C4A	-2.35	124.84	128.46
3	D	502	QKM	C11-CB-CA	2.30	124.92	121.28
3	E	502	QKM	N4-C15-N3	-2.30	109.46	112.24
2	E	501	HEM	CBA-CAA-C2A	-2.29	108.72	112.62
3	E	502	QKM	CE2-CZ-CE1	2.26	114.06	110.74
3	C	502	QKM	C11-CB-C7	2.26	122.10	117.59
3	D	502	QKM	CD1-CE1-C3	-2.26	105.51	108.59
3	A	502	QKM	F1-C21-C20	2.26	122.38	118.54
3	D	502	QKM	OH-CZ-C14	2.23	111.66	108.24
2	F	501	HEM	O2A-CGA-CBA	2.23	121.19	114.03
3	C	502	QKM	C22-CE2-CZ	2.22	122.01	118.61
3	B	502	QKM	N4-C15-N3	-2.21	109.57	112.24
2	B	501	HEM	O2A-CGA-CBA	2.20	121.11	114.03
3	E	502	QKM	C10-C9-C8	2.20	122.94	118.96
3	A	502	QKM	OH-CZ-CE2	2.18	110.20	107.11
2	C	501	HEM	CMC-C2C-C3C	2.17	128.75	124.68
3	C	502	QKM	OH-CZ-CE2	2.15	110.16	107.11
2	D	501	HEM	CAA-CBA-CGA	-2.13	107.78	113.76
2	F	501	HEM	CHA-C4D-C3D	-2.13	121.33	125.33
3	A	502	QKM	C11-C10-C9	-2.12	117.61	120.35
2	F	501	HEM	CAD-C3D-C4D	2.11	128.35	124.66
2	E	501	HEM	O2D-CGD-CBD	2.10	120.77	114.03
2	C	501	HEM	CHC-C4B-C3B	-2.09	121.38	124.57
2	A	501	HEM	CHA-C4D-C3D	-2.08	121.42	125.33
2	F	501	HEM	CAA-CBA-CGA	-2.08	107.93	113.76
2	E	501	HEM	CAA-CBA-CGA	2.07	119.57	113.76
3	B	502	QKM	C20-C19-CD2	2.06	121.53	119.05
3	B	502	QKM	C10-C9-C8	2.05	122.67	118.96
2	D	501	HEM	CHB-C1B-NB	2.05	126.91	124.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	HEM	CMC-C2C-C3C	2.04	128.50	124.68
3	A	502	QKM	C10-C11-CB	-2.04	118.20	121.13
3	D	502	QKM	CE2-C22-C21	2.03	120.36	117.56

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	HEM	C2D-C3D-CAD-CBD
2	C	501	HEM	C4D-C3D-CAD-CBD
2	D	501	HEM	C2D-C3D-CAD-CBD
2	D	501	HEM	C4D-C3D-CAD-CBD
3	A	502	QKM	N-CA-CB-C7
3	A	502	QKM	N-CA-CB-C11
3	A	502	QKM	C-CA-CB-C7
3	A	502	QKM	CD2-CE2-CZ-CE1
3	A	502	QKM	CZ-C14-N3-C15
3	B	502	QKM	N-CA-CB-C7
3	B	502	QKM	N-CA-CB-C11
3	B	502	QKM	C-CA-CB-C7
3	B	502	QKM	C-CA-CB-C11
3	B	502	QKM	CZ-C14-N3-C15
3	C	502	QKM	CD2-CE2-CZ-CE1
3	C	502	QKM	CZ-C14-N3-C15
3	D	502	QKM	CZ-C14-N3-C15
3	E	502	QKM	N-CA-CB-C7
3	E	502	QKM	N-CA-CB-C11
3	E	502	QKM	C-CA-CB-C7
3	E	502	QKM	C-CA-CB-C11
3	E	502	QKM	CZ-C14-N3-C15
3	F	502	QKM	CZ-C14-N3-C15
3	A	502	QKM	C-CA-CB-C11
3	C	502	QKM	N-CA-CB-C7
3	A	502	QKM	CZ-C14-N3-N5
3	F	502	QKM	CZ-C14-N3-N5
2	C	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAD-CBD-CGD-O1D
2	F	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAD-CBD-CGD-O1D
2	D	501	HEM	CAD-CBD-CGD-O2D
3	C	502	QKM	N-CA-CB-C11

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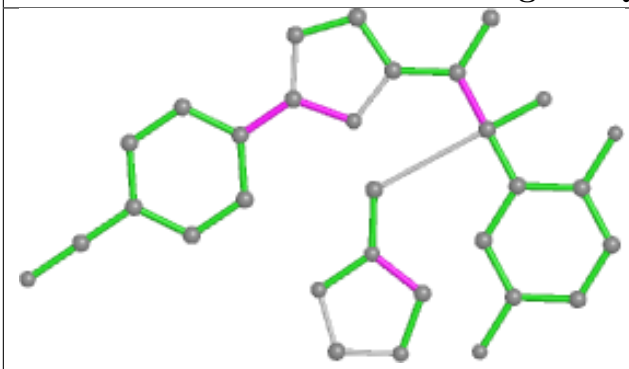
Mol	Chain	Res	Type	Atoms
3	D	502	QKM	N-CA-CB-C7
2	C	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAA-CBA-CGA-O1A
2	C	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAA-CBA-CGA-O2A
2	E	501	HEM	CAA-CBA-CGA-O1A
3	B	502	QKM	CZ-C14-N3-N5
3	C	502	QKM	CZ-C14-N3-N5
3	E	502	QKM	CZ-C14-N3-N5
2	E	501	HEM	CAA-CBA-CGA-O2A
3	E	502	QKM	N3-C14-CZ-CE2
3	C	502	QKM	N-C3-CE1-CD1
3	C	502	QKM	C-CA-CB-C7
3	A	502	QKM	C22-CE2-CZ-CE1

There are no ring outliers.

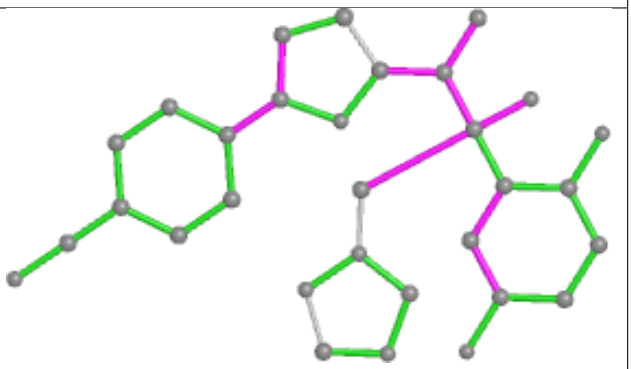
No monomer is involved in short contacts.

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.

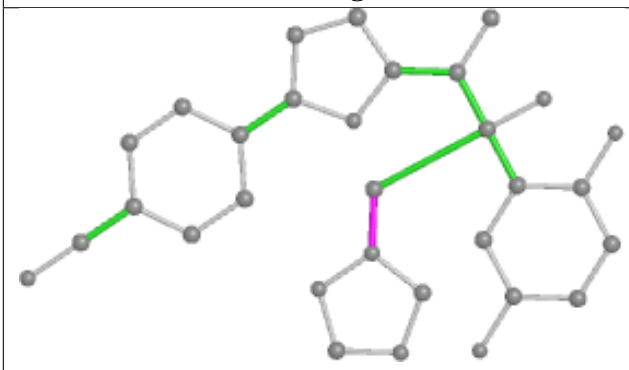
Ligand QKM F 502



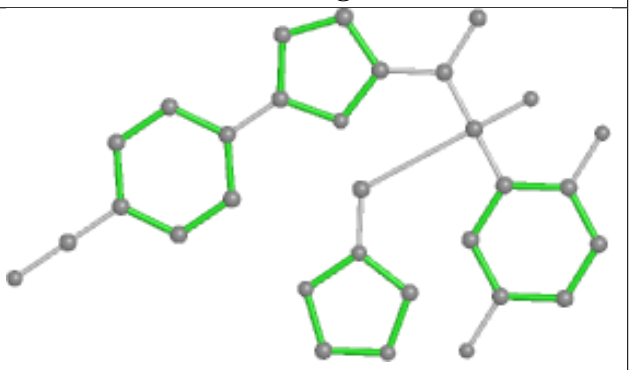
Bond lengths



Bond angles

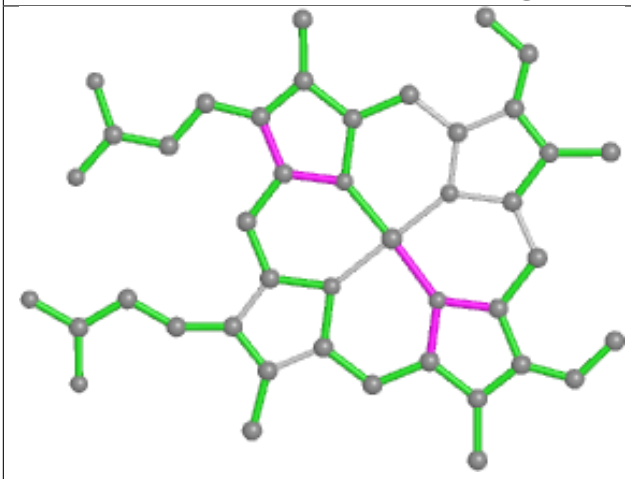


Torsions

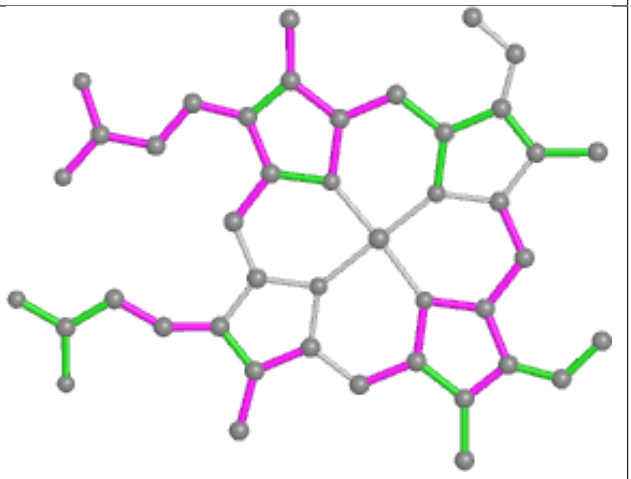


Rings

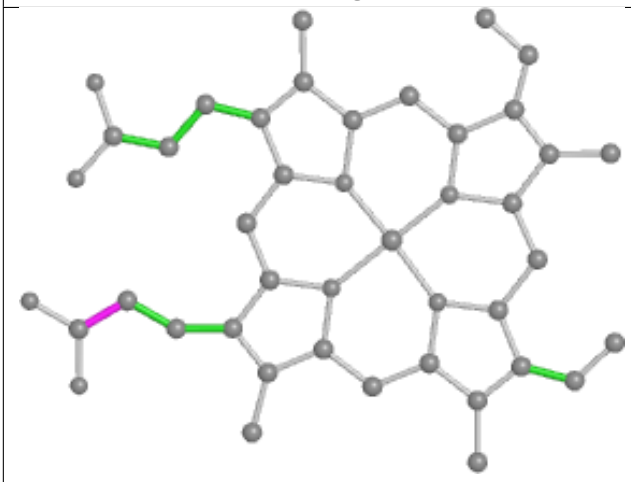
Ligand HEM A 501



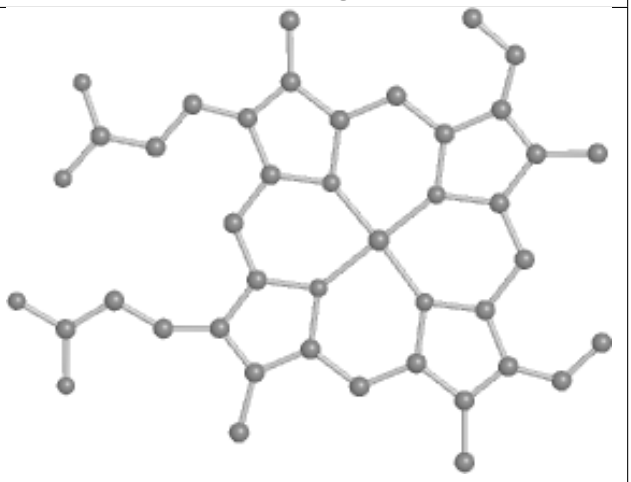
Bond lengths



Bond angles

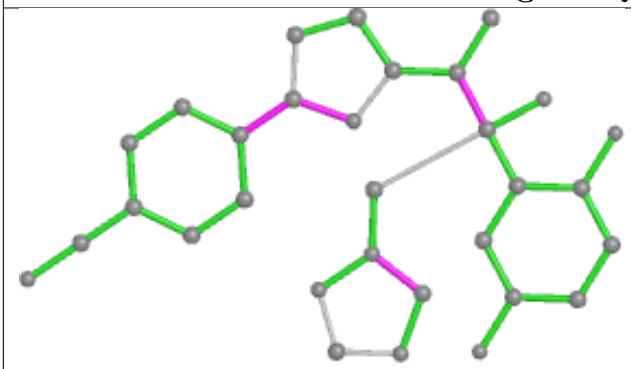


Torsions

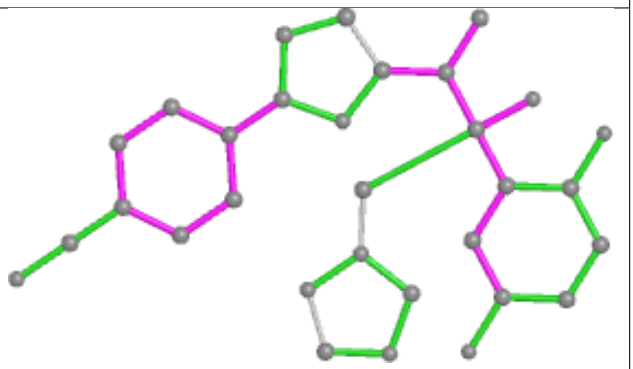


Rings

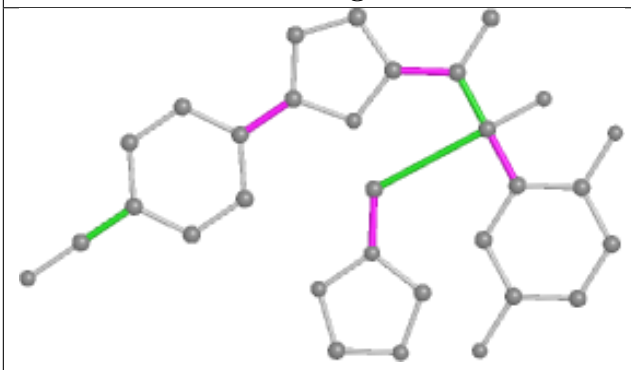
Ligand QKM C 502



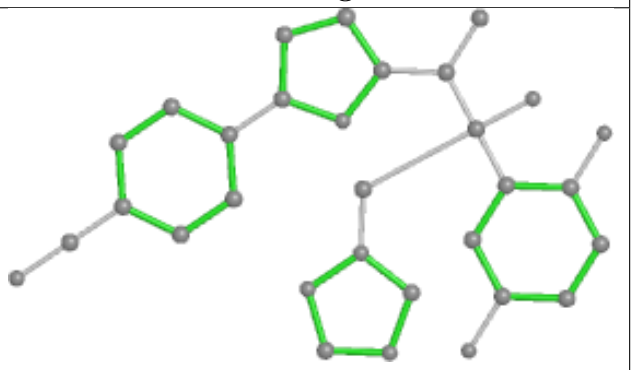
Bond lengths



Bond angles

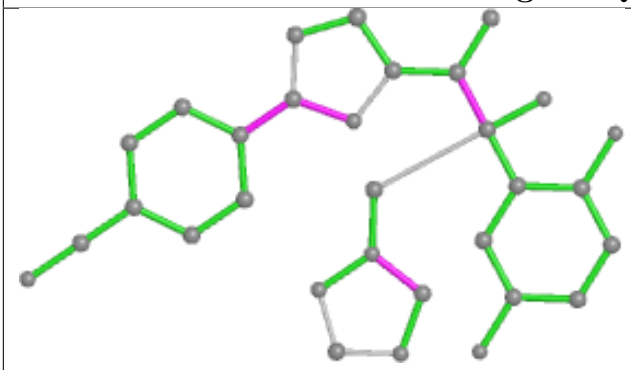


Torsions

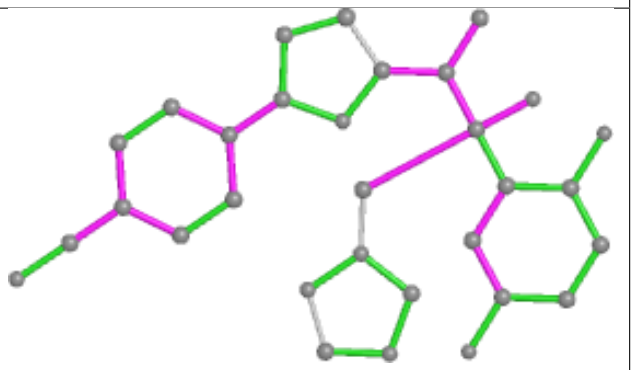


Rings

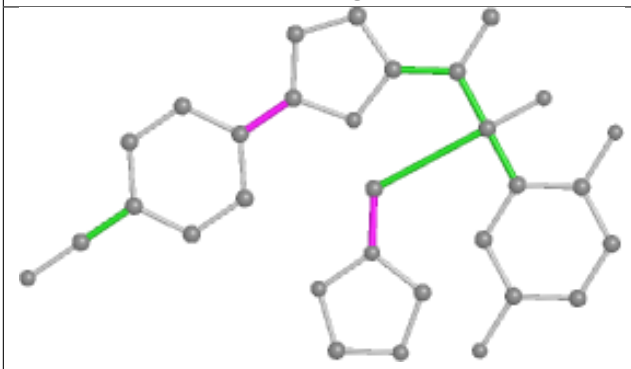
Ligand QKM D 502



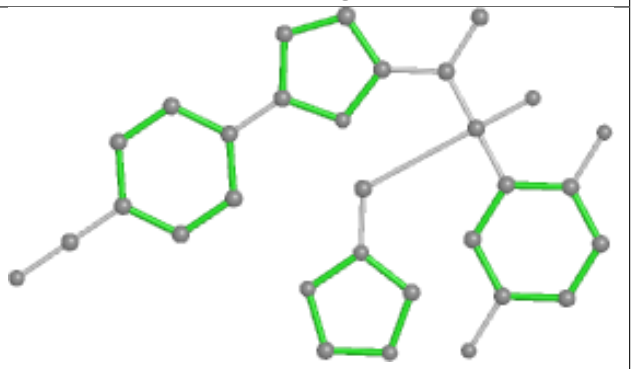
Bond lengths



Bond angles

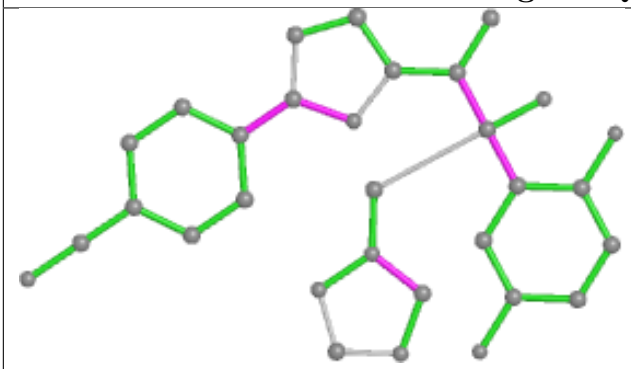


Torsions

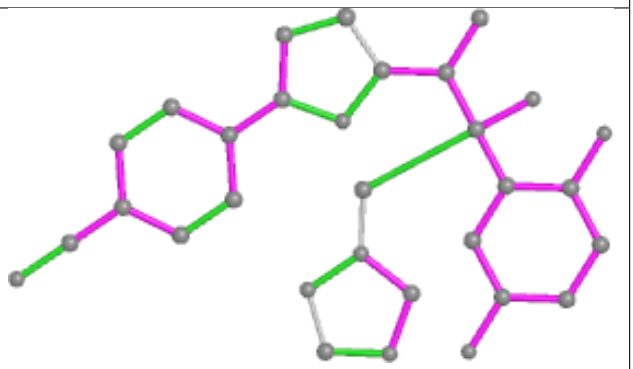


Rings

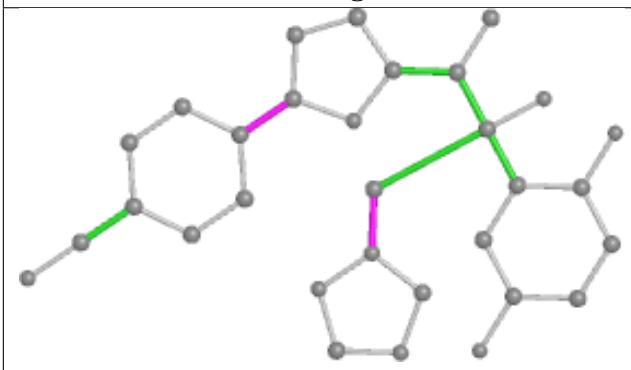
Ligand QKM B 502



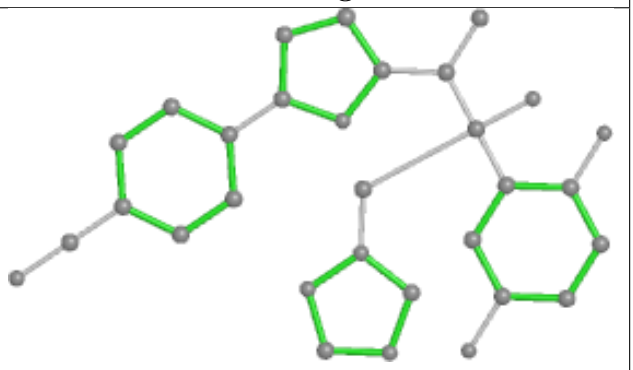
Bond lengths



Bond angles

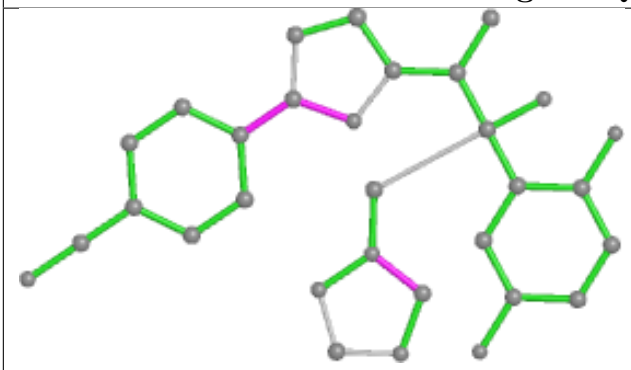


Torsions

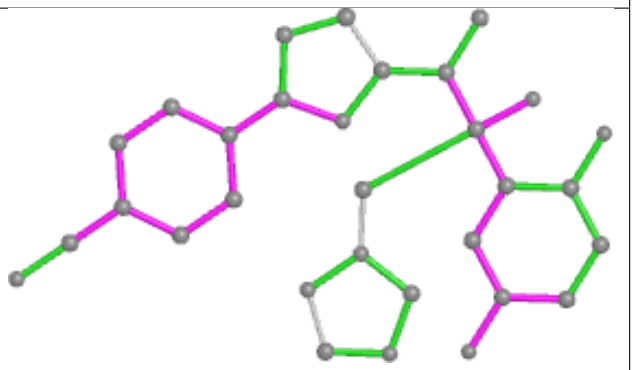


Rings

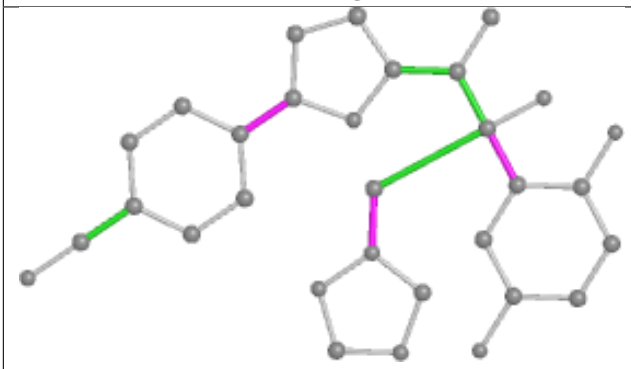
Ligand QKM A 502



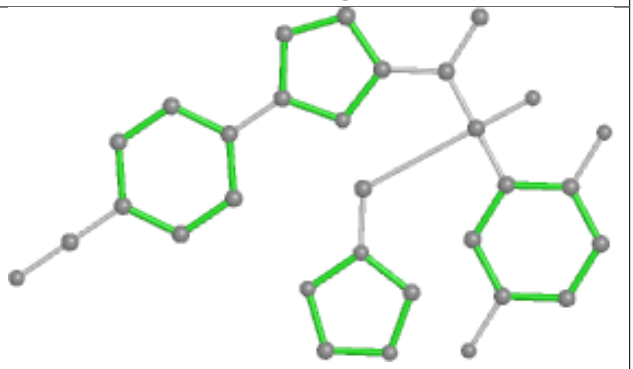
Bond lengths



Bond angles

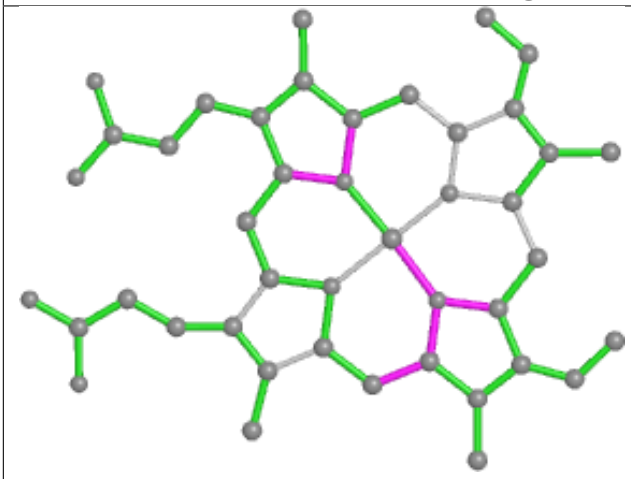


Torsions

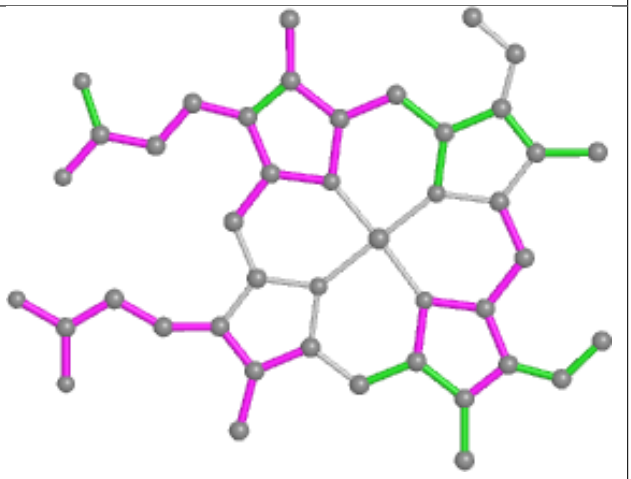


Rings

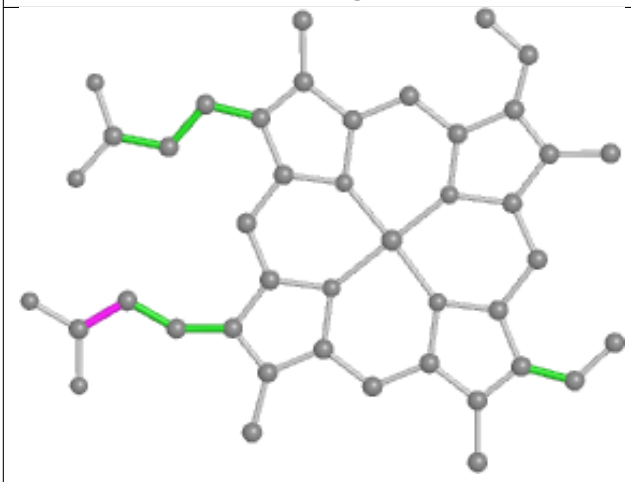
Ligand HEM E 501



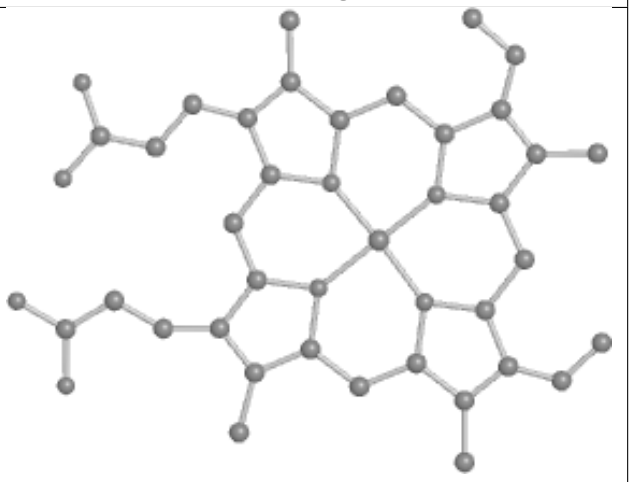
Bond lengths



Bond angles

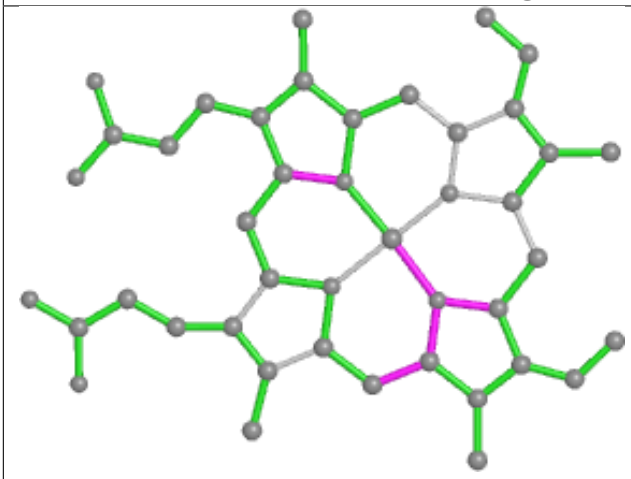


Torsions

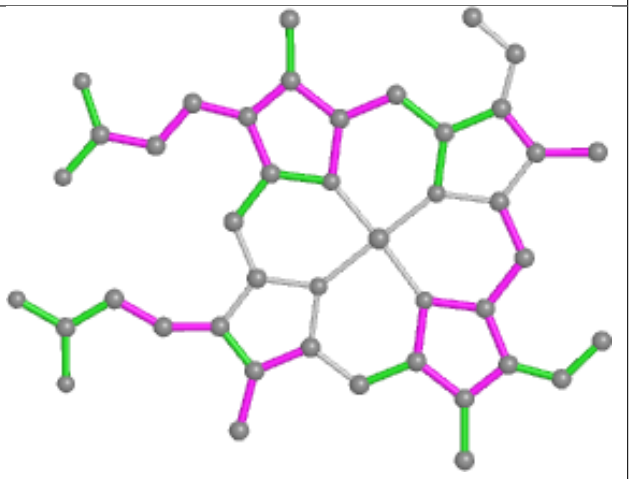


Rings

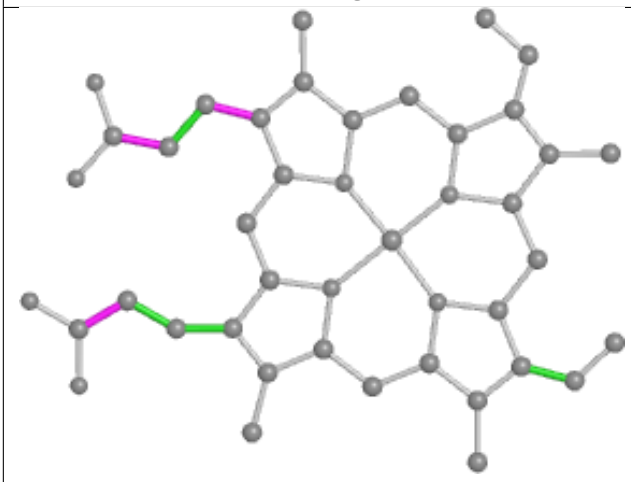
Ligand HEM C 501



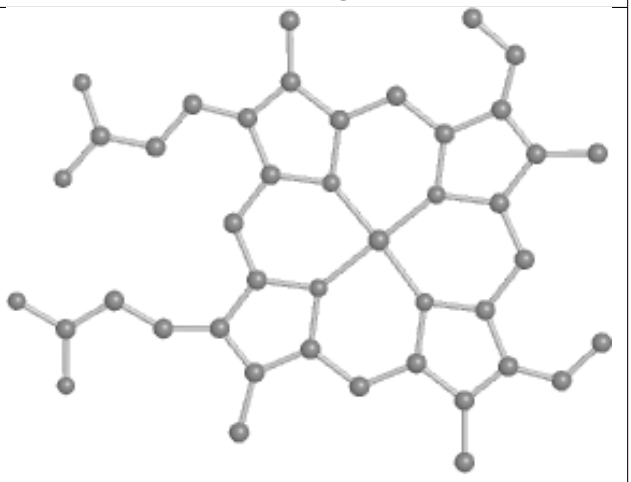
Bond lengths



Bond angles

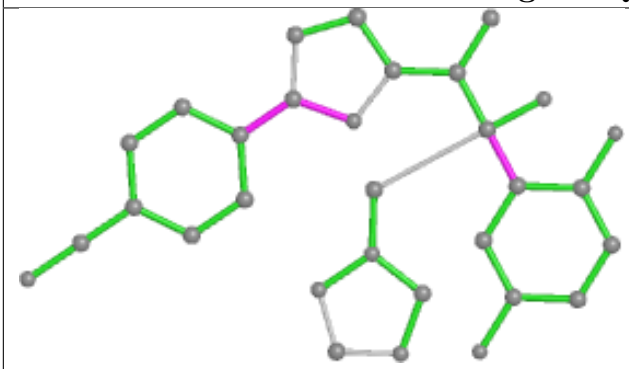


Torsions



Rings

Ligand QKM E 502



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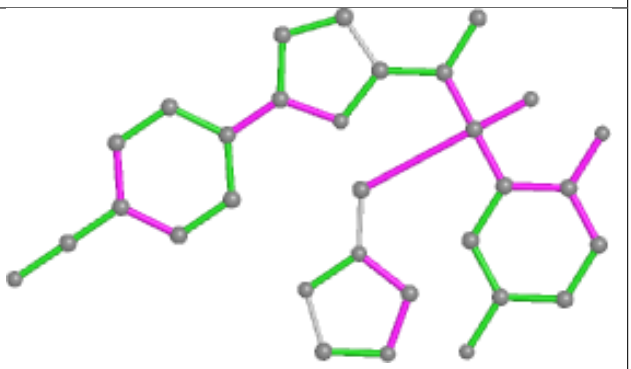
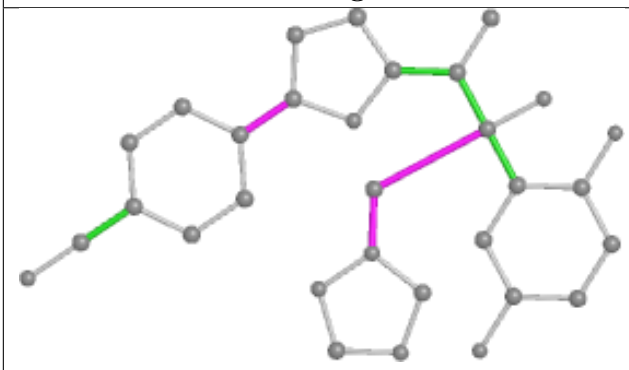


Bond angles



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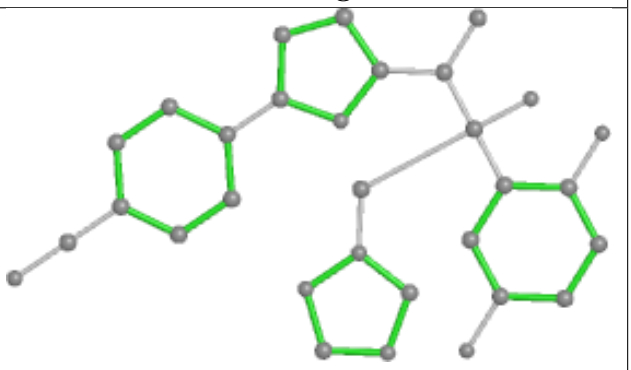
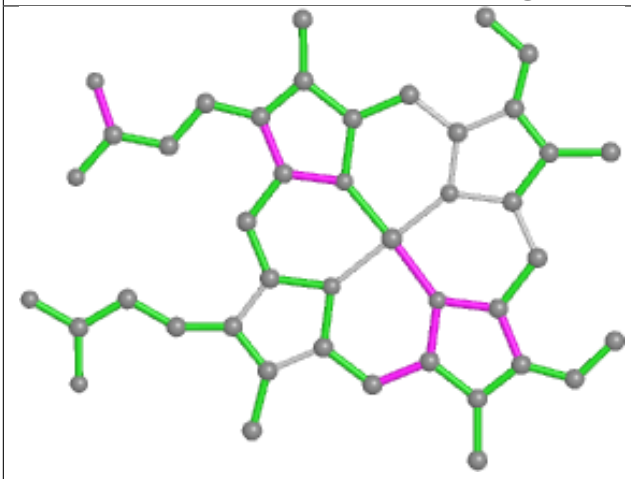


Rings

Ligand HEM B 501



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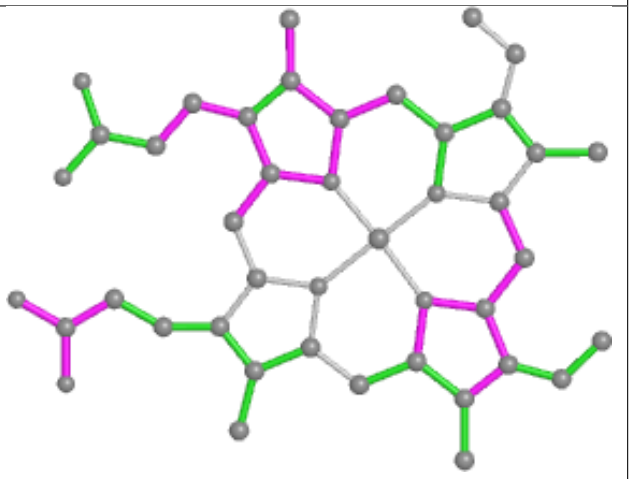
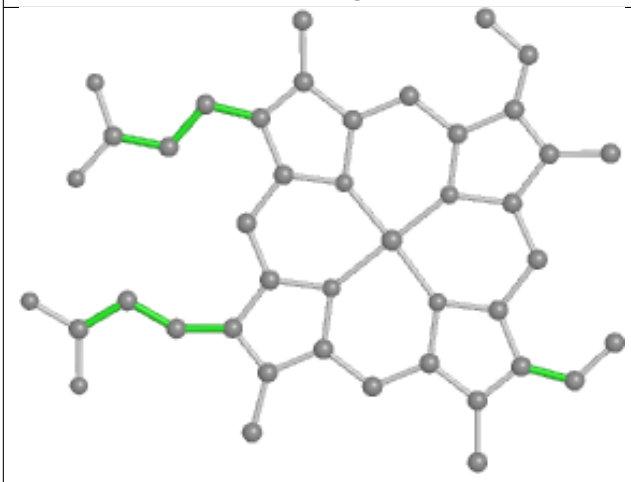


Bond angles



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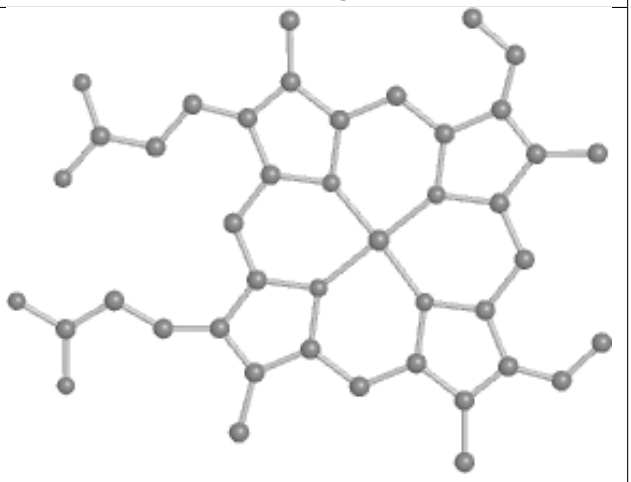
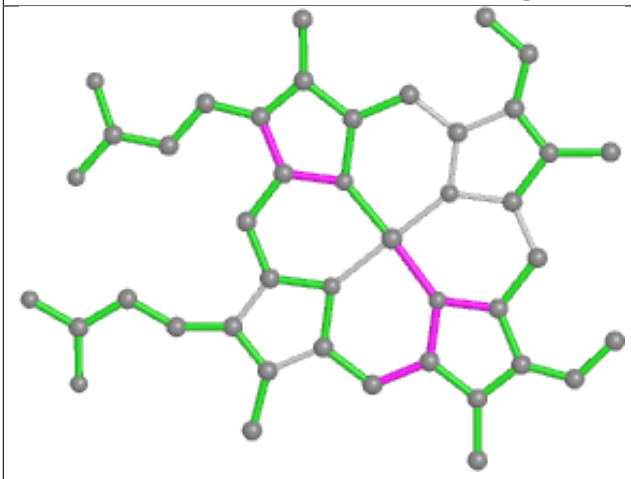


Rings

Ligand HEM D 501



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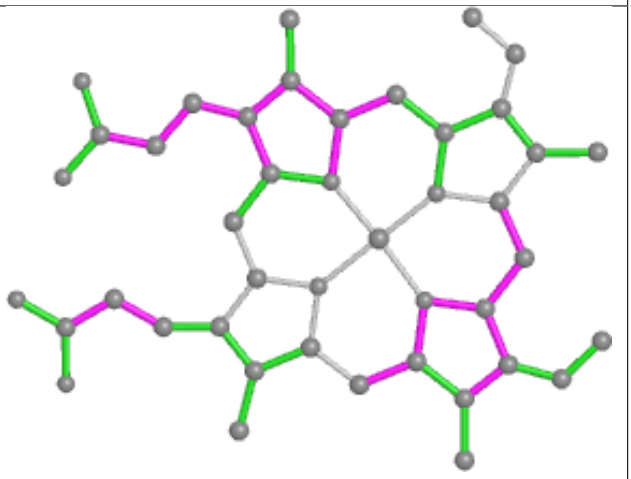
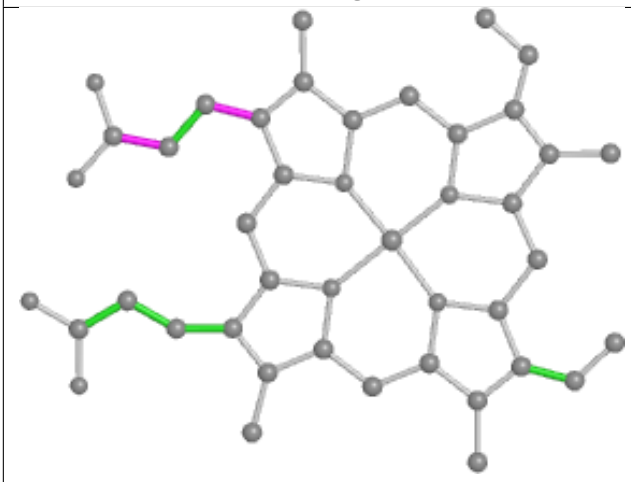
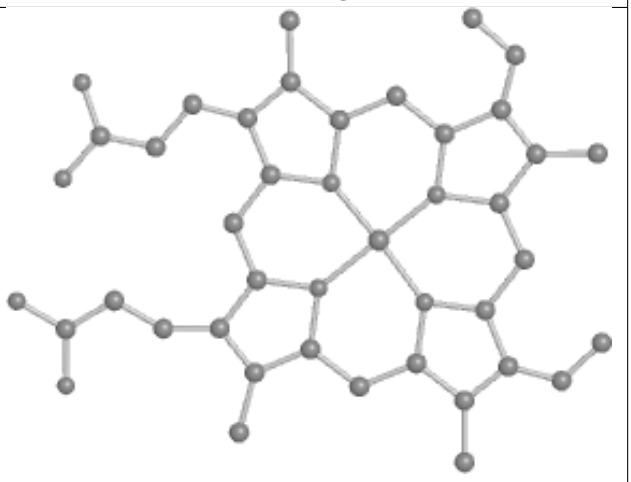


Bond angles

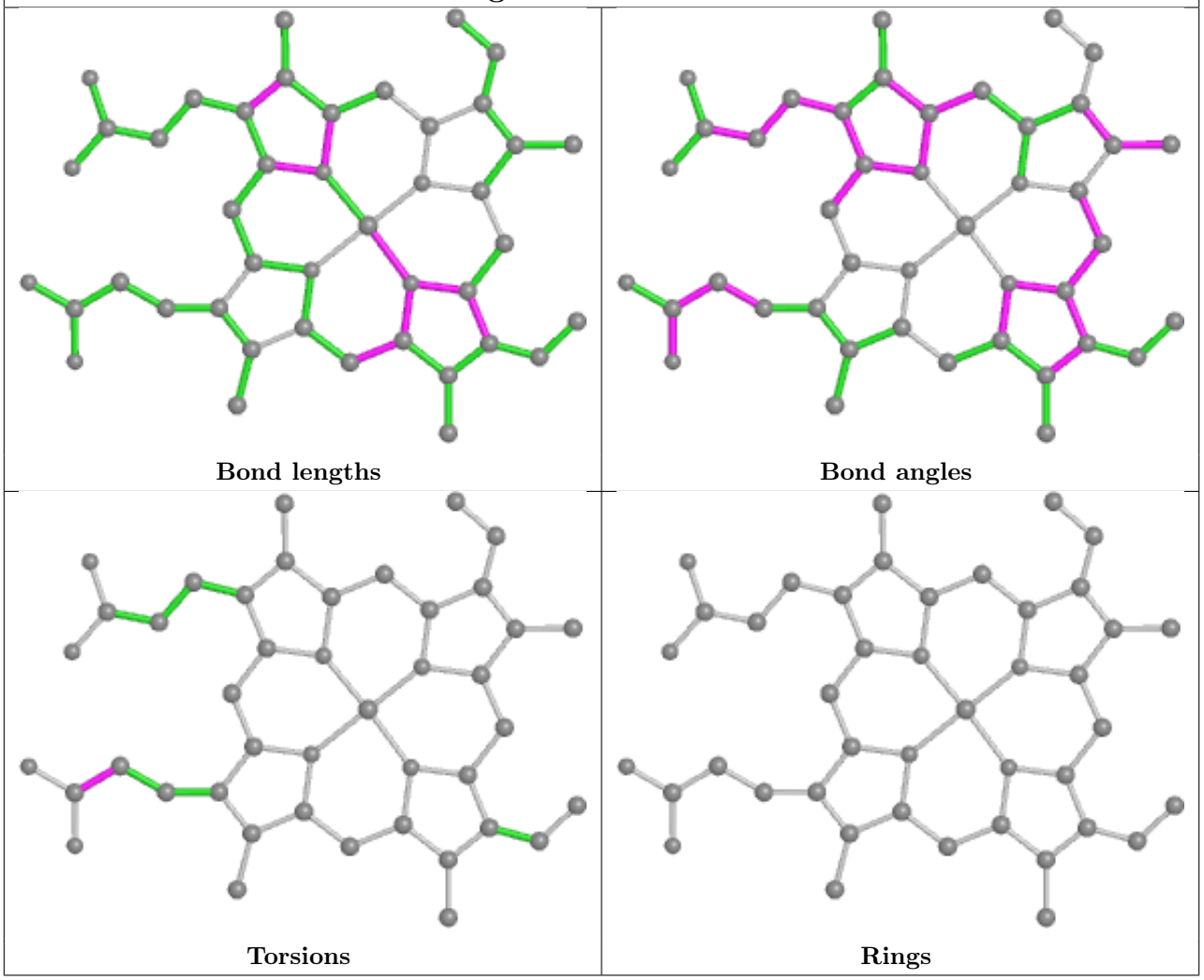


Torsions



Rings

Ligand HEM F 501



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.