Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 11:44 PM EDT

PDB ID	:	6UW2
Title	:	Clotrimazole bound complex of Acanthamoeba castellanii CYP51
Authors	:	Sharma, V.; Podust, L.M.
Deposited on	:	2019-11-04
Resolution	:	2.92 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 2.92 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.

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
4	GAI	C	503	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 21601 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	449	Total	C	N	O	S	0	0	0
			3543	2291	591	643	18			
1	B	447	Total	C	N	O	S	0	0	0
			3528	2282	580	648	18			
1	C	446	Total	C	N	O	S	0	0	0
			3460	2239	577	627	17			
1	D	447	Total	C	N	O	S	0	0	0
			3531	2287	586	640	18			
1	E	448	Total	C	N	O	S	0	0	0
			3545	2295	591	641	18			
1	F	448	Total	C	N	O	S	0	0	0
			3528	2284	586	640	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

Continued on next page...

Continued from previous page...

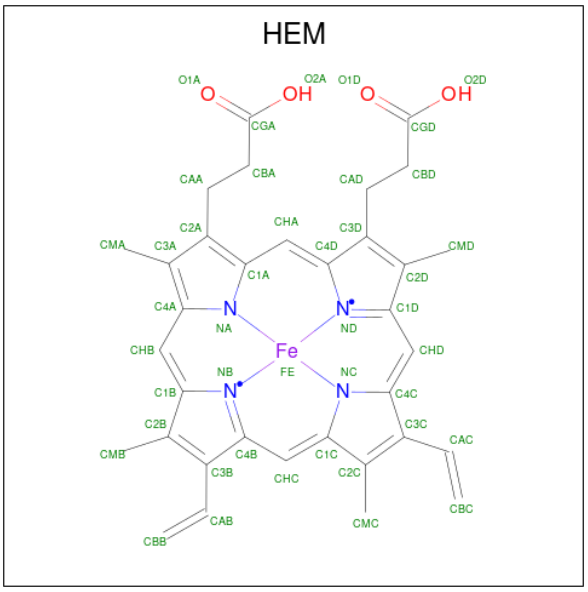
Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ALA	-	expression tag	UNP L8GJB3
B	35	LYS	-	expression tag	UNP L8GJB3
B	36	LYS	-	expression tag	UNP L8GJB3
B	37	THR	-	expression tag	UNP L8GJB3
B	38	SER	-	expression tag	UNP L8GJB3
B	39	SER	-	expression tag	UNP L8GJB3
B	40	LYS	-	expression tag	UNP L8GJB3
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

Continued on next page...

Continued from previous page...

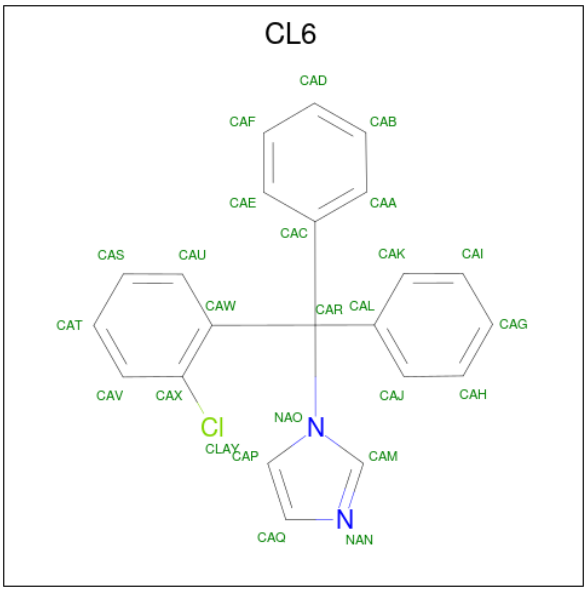
Chain	Residue	Modelled	Actual	Comment	Reference
D	488	HIS	-	expression tag	UNP L8GJB3
D	489	HIS	-	expression tag	UNP L8GJB3
D	490	HIS	-	expression tag	UNP L8GJB3
D	491	HIS	-	expression tag	UNP L8GJB3
D	492	HIS	-	expression tag	UNP L8GJB3
E	33	MET	-	expression tag	UNP L8GJB3
E	34	ALA	-	expression tag	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: $C_{34}H_{32}FeN_4O_4$).



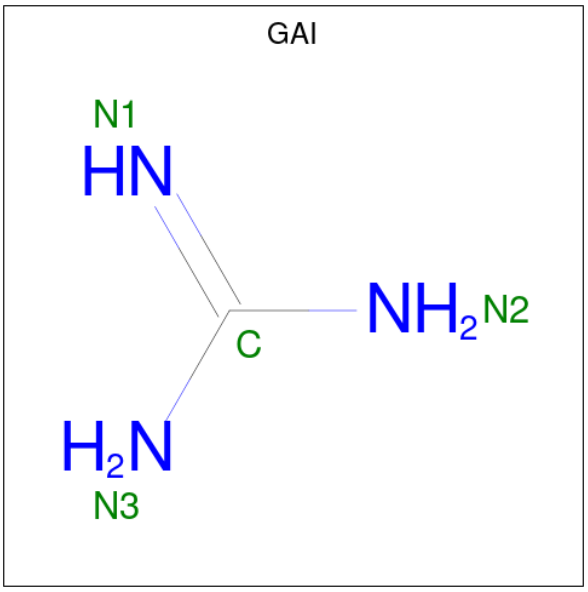
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 1-[(2-CHLOROPHENYL)(DIPHENYL)METHYL]-1H-IMIDAZOLE (three-letter code: CL6) (formula: $C_{22}H_{17}ClN_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	B	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	C	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	D	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	E	1	Total	C	Cl	N	0	0
			25	22	1	2		
3	F	1	Total	C	Cl	N	0	0
			25	22	1	2		

- Molecule 4 is GUANIDINE (three-letter code: GAI) (formula: CH_5N_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N 4 1 3	0	0
4	C	1	Total C N 4 1 3	0	0
4	F	1	Total C N 4 1 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	10	Total O 10 10	0	0
5	C	12	Total O 12 12	0	0
5	D	9	Total O 9 9	0	0
5	E	4	Total O 4 4	0	0
5	F	7	Total O 7 7	0	0

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 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.98Å 177.22Å 181.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.13 – 2.92	Depositor
% Data completeness (in resolution range)	100.0 (127.13-2.92)	Depositor
R_{merge}	0.40	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.44 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.209 , 0.290	Depositor
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.356	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
Total number of atoms	21601	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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

15 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	B	501	3,1	41,50,50	1.45	6 (14%)	45,82,82	1.98	13 (28%)
3	CL6	A	502	2	26,28,28	1.75	4 (15%)	35,39,39	2.10	8 (22%)
2	HEM	E	501	3,1	41,50,50	1.40	5 (12%)	45,82,82	1.88	14 (31%)
2	HEM	C	501	3,1	41,50,50	1.43	4 (9%)	45,82,82	2.19	15 (33%)
4	GAI	B	503	-	3,3,3	3.09	1 (33%)	3,3,3	1.61	1 (33%)
3	CL6	B	502	2	26,28,28	2.17	3 (11%)	35,39,39	2.10	6 (17%)
2	HEM	A	501	3,1	41,50,50	1.40	7 (17%)	45,82,82	1.92	13 (28%)
2	HEM	D	501	3,1	41,50,50	1.43	8 (19%)	45,82,82	2.20	16 (35%)
3	CL6	C	502	2	26,28,28	1.98	4 (15%)	35,39,39	2.32	8 (22%)
2	HEM	F	501	3,1	41,50,50	1.39	6 (14%)	45,82,82	2.03	13 (28%)
3	CL6	D	502	2	26,28,28	1.78	3 (11%)	35,39,39	2.16	6 (17%)
3	CL6	F	502	2	26,28,28	1.88	3 (11%)	35,39,39	2.45	5 (14%)
4	GAI	C	503	-	3,3,3	3.59	3 (100%)	3,3,3	0.91	0
4	GAI	F	503	-	3,3,3	0.68	0	3,3,3	1.33	0
3	CL6	E	502	2	26,28,28	1.93	3 (11%)	35,39,39	2.44	7 (20%)

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	B	501	3,1	-	0/12/54/54	-
3	CL6	A	502	2	-	0/18/24/24	0/4/4/4
2	HEM	E	501	3,1	-	6/12/54/54	-
2	HEM	C	501	3,1	-	6/12/54/54	-
3	CL6	B	502	2	-	0/18/24/24	0/4/4/4
2	HEM	A	501	3,1	-	5/12/54/54	-
2	HEM	D	501	3,1	-	8/12/54/54	-
3	CL6	C	502	2	-	0/18/24/24	0/4/4/4
2	HEM	F	501	3,1	-	4/12/54/54	-
3	CL6	D	502	2	-	0/18/24/24	0/4/4/4
3	CL6	F	502	2	-	0/18/24/24	0/4/4/4
3	CL6	E	502	2	-	0/18/24/24	0/4/4/4

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	CL6	CAP-NAO	-7.74	1.32	1.38
3	F	502	CL6	CAX-CAW	7.52	1.51	1.39
3	E	502	CL6	CAP-NAO	-6.98	1.33	1.38
3	B	502	CL6	CAX-CAW	6.87	1.50	1.39
3	A	502	CL6	CAX-CAW	6.66	1.50	1.39
3	C	502	CL6	CAX-CAW	6.66	1.50	1.39
3	D	502	CL6	CAX-CAW	6.49	1.50	1.39
3	C	502	CL6	CAP-NAO	-5.80	1.34	1.38
3	E	502	CL6	CAX-CAW	5.54	1.48	1.39
4	B	503	GAI	C-N3	-5.09	1.27	1.36
4	C	503	GAI	C-N3	-4.95	1.27	1.36
2	C	501	HEM	C1B-NB	-4.83	1.32	1.40
2	E	501	HEM	C1B-NB	-4.60	1.32	1.40
3	F	502	CL6	CAP-NAO	-4.46	1.35	1.38
3	D	502	CL6	CAP-NAO	-4.06	1.35	1.38
2	F	501	HEM	C1B-NB	-3.99	1.33	1.40
2	B	501	HEM	C1B-NB	-3.99	1.33	1.40
2	A	501	HEM	C1B-NB	-3.91	1.33	1.40
2	D	501	HEM	C1B-NB	-3.64	1.34	1.40
2	C	501	HEM	C4B-NB	-3.53	1.31	1.38
3	A	502	CL6	CAP-NAO	-3.20	1.36	1.38
2	D	501	HEM	C4B-NB	-3.16	1.32	1.38
2	A	501	HEM	C4B-NB	-3.11	1.32	1.38
2	B	501	HEM	C4D-ND	-3.11	1.34	1.40
2	F	501	HEM	C4B-NB	-3.04	1.32	1.38
2	B	501	HEM	C4B-NB	-2.94	1.32	1.38
2	B	501	HEM	FE-NB	2.89	2.11	1.96
4	C	503	GAI	C-N1	2.80	1.36	1.30
3	C	502	CL6	CAX-CLAY	2.80	1.80	1.73
2	E	501	HEM	C4B-NB	-2.75	1.33	1.38
2	B	501	HEM	CHB-C1B	2.70	1.41	1.35
2	A	501	HEM	FE-NB	2.67	2.10	1.96
2	D	501	HEM	FE-NB	2.65	2.10	1.96
2	A	501	HEM	C4D-ND	-2.62	1.35	1.40
2	D	501	HEM	C1D-ND	-2.52	1.33	1.38
4	C	503	GAI	C-N2	-2.51	1.31	1.36
2	F	501	HEM	FE-NB	2.50	2.09	1.96
3	F	502	CL6	CAX-CLAY	2.47	1.79	1.73
2	D	501	HEM	CHB-C1B	2.44	1.41	1.35
2	E	501	HEM	FE-NB	2.41	2.08	1.96
2	F	501	HEM	CHB-C1B	2.39	1.41	1.35
2	E	501	HEM	C3B-C4B	2.38	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	HEM	C4D-ND	-2.38	1.36	1.40
2	B	501	HEM	C4D-C3D	2.37	1.49	1.45
2	D	501	HEM	C3B-C4B	2.35	1.49	1.44
3	A	502	CL6	CAX-CLAY	2.26	1.79	1.73
2	D	501	HEM	C4D-C3D	2.25	1.48	1.45
3	B	502	CL6	CAX-CLAY	2.24	1.79	1.73
2	A	501	HEM	C3B-C4B	2.20	1.49	1.44
2	F	501	HEM	C1D-ND	-2.18	1.34	1.38
2	C	501	HEM	FE-NB	2.17	2.07	1.96
2	A	501	HEM	CHB-C1B	2.14	1.40	1.35
2	E	501	HEM	C4D-ND	-2.14	1.36	1.40
2	A	501	HEM	C1D-C2D	2.14	1.48	1.44
3	D	502	CL6	CAX-CLAY	2.13	1.78	1.73
3	C	502	CL6	CAA-CAC	2.09	1.42	1.39
3	E	502	CL6	CAX-CLAY	2.07	1.78	1.73
2	C	501	HEM	CHB-C1B	2.05	1.40	1.35
2	F	501	HEM	C4D-ND	-2.04	1.36	1.40
3	A	502	CL6	CAR-NAO	2.00	1.54	1.51

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	CL6	CAM-NAO-CAR	-8.89	119.33	126.71
3	F	502	CL6	CAM-NAO-CAR	-8.87	119.35	126.71
3	D	502	CL6	CAM-NAO-CAR	-8.09	120.00	126.71
3	B	502	CL6	CAM-NAO-CAR	-7.55	120.45	126.71
3	C	502	CL6	CAM-NAO-CAR	-7.47	120.51	126.71
3	A	502	CL6	CAM-NAO-CAR	-7.23	120.71	126.71
3	C	502	CL6	CAL-CAR-CAW	-7.18	102.44	112.00
2	D	501	HEM	CAD-C3D-C4D	6.64	136.27	124.66
3	F	502	CL6	CAL-CAR-CAW	-6.39	103.48	112.00
3	E	502	CL6	CAP-NAO-CAM	6.16	112.16	108.25
3	F	502	CL6	CAP-NAO-CAM	5.97	112.04	108.25
2	C	501	HEM	CAD-C3D-C4D	5.63	134.49	124.66
3	E	502	CL6	CAL-CAR-CAW	-5.60	104.54	112.00
2	F	501	HEM	CAD-C3D-C4D	5.57	134.39	124.66
3	B	502	CL6	CAP-NAO-CAM	5.38	111.67	108.25
3	B	502	CL6	CAL-CAR-CAW	-5.37	104.84	112.00
2	C	501	HEM	C1B-NB-C4B	5.05	110.29	105.07
2	B	501	HEM	CHD-C1D-ND	4.99	129.85	124.43
3	A	502	CL6	CAL-CAR-CAW	-4.98	105.37	112.00
2	C	501	HEM	CHD-C1D-ND	4.76	129.61	124.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	502	CL6	CAW-CAR-NAO	4.76	113.37	106.11
2	A	501	HEM	C1B-NB-C4B	4.73	109.96	105.07
2	E	501	HEM	C1B-NB-C4B	4.72	109.95	105.07
3	C	502	CL6	CAP-NAO-CAM	4.67	111.21	108.25
2	D	501	HEM	C1B-NB-C4B	4.59	109.81	105.07
2	D	501	HEM	CAD-C3D-C2D	-4.57	119.36	127.88
2	F	501	HEM	C1B-NB-C4B	4.38	109.60	105.07
3	D	502	CL6	CAU-CAW-CAR	4.27	124.13	121.05
2	B	501	HEM	C1B-NB-C4B	4.20	109.41	105.07
2	C	501	HEM	C4B-C3B-C2B	-4.10	103.86	107.11
3	D	502	CL6	CAP-NAO-CAM	4.07	110.83	108.25
2	B	501	HEM	CHC-C4B-NB	4.06	128.84	124.43
3	A	502	CL6	CAP-NAO-CAR	3.92	129.58	124.95
2	C	501	HEM	CHC-C4B-NB	3.88	128.65	124.43
2	E	501	HEM	C4B-C3B-C2B	-3.87	104.04	107.11
3	A	502	CL6	CAC-CAR-CAW	3.86	117.14	112.00
3	D	502	CL6	CAL-CAR-CAW	-3.85	106.87	112.00
2	B	501	HEM	CHD-C1D-C2D	-3.84	118.97	124.98
2	F	501	HEM	CHC-C4B-NB	3.79	128.54	124.43
2	E	501	HEM	CAD-C3D-C4D	3.78	131.27	124.66
2	C	501	HEM	CAD-C3D-C2D	-3.77	120.86	127.88
2	A	501	HEM	CAD-CBD-CGD	-3.71	105.63	113.60
2	D	501	HEM	CHD-C1D-ND	3.64	128.39	124.43
2	F	501	HEM	CAD-C3D-C2D	-3.63	121.11	127.88
2	B	501	HEM	C4B-C3B-C2B	-3.57	104.28	107.11
3	D	502	CL6	CAP-NAO-CAR	3.56	129.16	124.95
3	E	502	CL6	CAU-CAW-CAR	3.55	123.61	121.05
3	C	502	CL6	CAW-CAR-NAO	3.55	111.52	106.11
2	A	501	HEM	CHA-C4D-C3D	-3.46	118.83	125.33
2	D	501	HEM	CMA-C3A-C4A	-3.41	123.23	128.46
2	F	501	HEM	CBD-CAD-C3D	3.35	121.94	112.63
2	A	501	HEM	CBD-CAD-C3D	3.27	121.71	112.63
2	A	501	HEM	CHC-C4B-NB	3.23	127.94	124.43
2	D	501	HEM	CHC-C4B-NB	3.23	127.94	124.43
2	E	501	HEM	CHC-C4B-NB	3.22	127.93	124.43
2	A	501	HEM	CHA-C4D-ND	3.22	128.36	124.38
2	A	501	HEM	CAD-C3D-C4D	3.15	130.17	124.66
3	B	502	CL6	CAW-CAR-NAO	3.13	110.88	106.11
2	B	501	HEM	C2C-C3C-C4C	-3.09	104.74	106.90
3	F	502	CL6	CAP-NAO-CAR	3.07	128.58	124.95
2	D	501	HEM	CHD-C1D-C2D	-3.06	120.20	124.98
2	B	501	HEM	C4B-CHC-C1C	3.06	126.59	122.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	502	CL6	CAP-NAO-CAR	3.01	128.51	124.95
2	A	501	HEM	CHD-C1D-ND	2.99	127.68	124.43
2	E	501	HEM	CHD-C1D-ND	2.98	127.66	124.43
2	B	501	HEM	CBD-CAD-C3D	2.93	120.75	112.63
2	A	501	HEM	CMD-C2D-C1D	2.91	129.47	125.04
2	F	501	HEM	C4B-C3B-C2B	-2.89	104.82	107.11
2	F	501	HEM	CHD-C1D-ND	2.89	127.57	124.43
2	D	501	HEM	CBA-CAA-C2A	2.87	117.51	112.62
3	E	502	CL6	CAR-CAW-CAX	-2.86	120.84	122.65
2	F	501	HEM	CHA-C4D-ND	2.82	127.86	124.38
3	C	502	CL6	CAP-NAO-CAR	2.80	128.26	124.95
3	D	502	CL6	CAW-CAR-NAO	2.80	110.38	106.11
2	E	501	HEM	C4B-CHC-C1C	2.74	126.17	122.56
2	F	501	HEM	CMD-C2D-C1D	2.73	129.20	125.04
2	D	501	HEM	CBD-CAD-C3D	2.70	120.13	112.63
2	C	501	HEM	CHD-C1D-C2D	-2.64	120.85	124.98
2	C	501	HEM	CHA-C4D-ND	2.64	127.65	124.38
2	F	501	HEM	CHA-C4D-C3D	-2.64	120.37	125.33
2	B	501	HEM	CAD-C3D-C4D	2.64	129.27	124.66
2	D	501	HEM	CMD-C2D-C1D	2.63	129.05	125.04
3	E	502	CL6	CAC-CAR-CAW	2.58	115.44	112.00
2	A	501	HEM	CHD-C1D-C2D	-2.54	121.01	124.98
2	B	501	HEM	CMA-C3A-C4A	-2.54	124.56	128.46
2	C	501	HEM	O2A-CGA-CBA	2.53	122.16	114.03
2	C	501	HEM	O2A-CGA-O1A	-2.53	117.00	123.30
2	F	501	HEM	CAD-CBD-CGD	-2.52	108.17	113.60
2	C	501	HEM	CBD-CAD-C3D	2.47	119.48	112.63
2	E	501	HEM	CAD-CBD-CGD	-2.45	108.33	113.60
2	A	501	HEM	CHB-C1B-NB	2.45	127.41	124.38
3	B	502	CL6	CAP-NAO-CAR	2.44	127.83	124.95
3	A	502	CL6	CAF-CAE-CAC	2.44	123.32	120.76
2	E	501	HEM	CBD-CAD-C3D	2.43	119.36	112.63
2	D	501	HEM	C4B-CHC-C1C	2.40	125.73	122.56
2	A	501	HEM	C4B-CHC-C1C	2.39	125.71	122.56
2	E	501	HEM	CHD-C1D-C2D	-2.39	121.25	124.98
4	B	503	GAI	N3-C-N2	2.39	121.81	116.13
2	E	501	HEM	O2A-CGA-CBA	2.38	121.69	114.03
2	A	501	HEM	C3D-C4D-ND	2.38	112.82	110.17
2	C	501	HEM	CHB-C1B-NB	2.35	127.28	124.38
3	B	502	CL6	CAU-CAW-CAR	2.34	122.74	121.05
2	D	501	HEM	CHB-C1B-NB	2.32	127.25	124.38
3	A	502	CL6	CAU-CAW-CAX	-2.31	114.03	116.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	HEM	CHB-C1B-NB	2.30	127.22	124.38
3	A	502	CL6	CAP-NAO-CAM	2.29	109.70	108.25
3	C	502	CL6	CAK-CAL-CAR	2.27	125.53	120.94
3	C	502	CL6	CAA-CAC-CAR	2.26	125.52	120.94
2	E	501	HEM	CMD-C2D-C1D	2.20	128.40	125.04
2	D	501	HEM	C2C-C3C-C4C	-2.18	105.38	106.90
2	F	501	HEM	CMA-C3A-C4A	-2.14	125.18	128.46
2	E	501	HEM	CAD-C3D-C2D	-2.14	123.90	127.88
2	C	501	HEM	C3B-C2B-C1B	2.13	108.06	106.49
2	D	501	HEM	C4B-C3B-C2B	-2.12	105.43	107.11
2	E	501	HEM	CAA-CBA-CGA	-2.12	107.83	113.76
2	D	501	HEM	CMA-C3A-C2A	2.12	128.93	124.94
2	B	501	HEM	CAD-CBD-CGD	-2.11	109.06	113.60
2	E	501	HEM	CHA-C4D-C3D	-2.10	121.39	125.33
2	C	501	HEM	CHA-C4D-C3D	-2.09	121.40	125.33
2	B	501	HEM	CMC-C2C-C3C	2.09	128.58	124.68
2	C	501	HEM	C4B-CHC-C1C	2.08	125.30	122.56
3	A	502	CL6	CAA-CAC-CAR	2.07	125.12	120.94
2	D	501	HEM	CAD-CBD-CGD	-2.05	109.19	113.60
2	B	501	HEM	CHC-C4B-C3B	-2.02	121.47	124.57
3	C	502	CL6	CAW-CAX-CLAY	2.00	123.98	121.68

There are no chirality outliers.

All (29) 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	C1A-C2A-CAA-CBA
2	D	501	HEM	C3A-C2A-CAA-CBA
2	D	501	HEM	C2D-C3D-CAD-CBD
2	D	501	HEM	C4D-C3D-CAD-CBD
2	F	501	HEM	C2D-C3D-CAD-CBD
2	F	501	HEM	C4D-C3D-CAD-CBD
2	E	501	HEM	C2D-C3D-CAD-CBD
2	E	501	HEM	C4D-C3D-CAD-CBD
2	A	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O1D
2	F	501	HEM	CAD-CBD-CGD-O2D
2	F	501	HEM	CAD-CBD-CGD-O1D
2	C	501	HEM	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

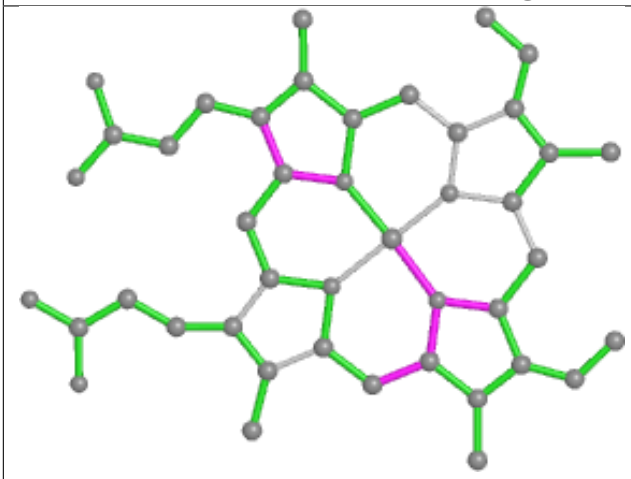
Mol	Chain	Res	Type	Atoms
2	A	501	HEM	C2D-C3D-CAD-CBD
2	D	501	HEM	CAD-CBD-CGD-O2D
2	A	501	HEM	CAA-CBA-CGA-O2A
2	A	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAA-CBA-CGA-O2A
2	E	501	HEM	CAD-CBD-CGD-O2D
2	C	501	HEM	CAA-CBA-CGA-O1A
2	A	501	HEM	CAD-CBD-CGD-O1D
2	E	501	HEM	CAA-CBA-CGA-O1A
2	E	501	HEM	CAD-CBD-CGD-O1D
2	E	501	HEM	CAA-CBA-CGA-O2A
2	D	501	HEM	CAA-CBA-CGA-O1A
2	D	501	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

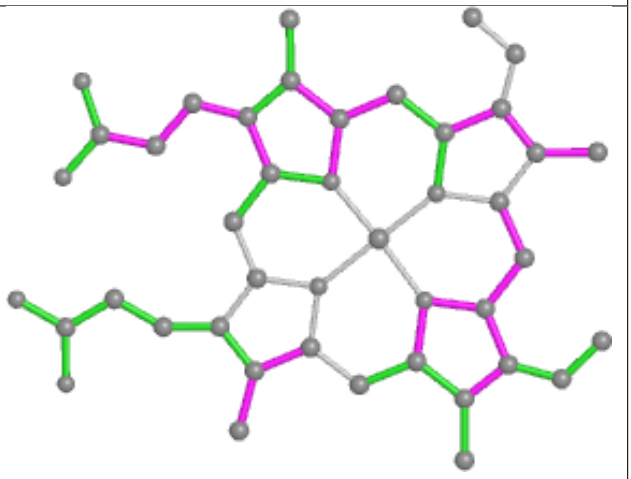
No monomer is involved in short contacts.

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.

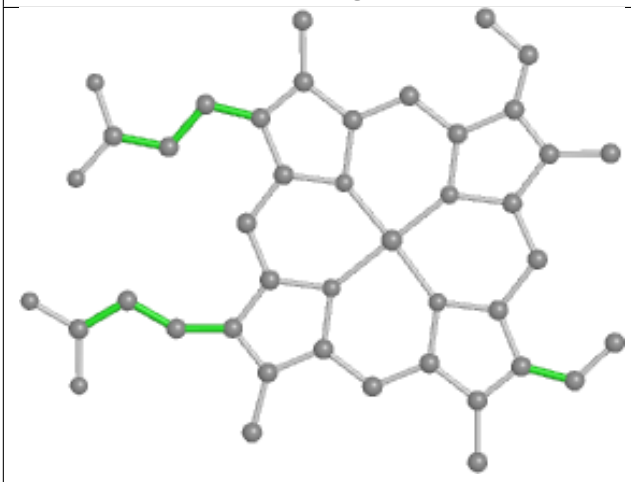
Ligand HEM B 501



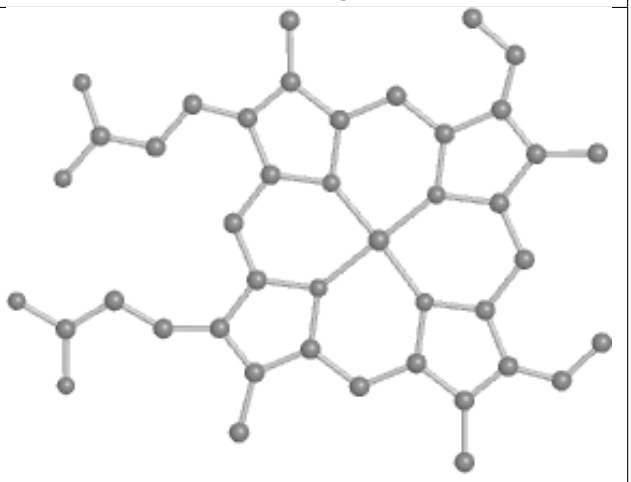
Bond lengths



Bond angles

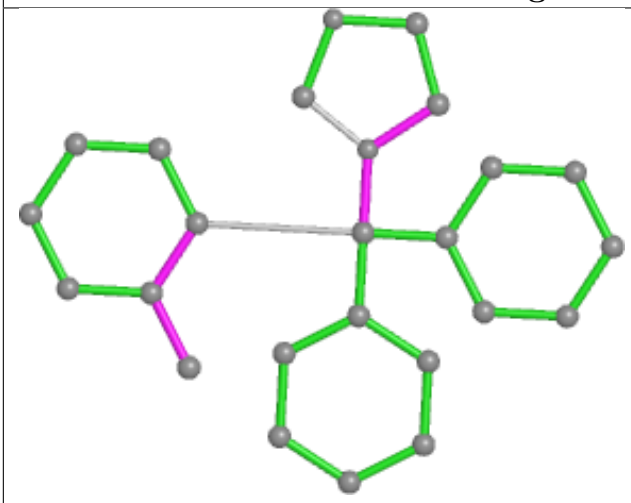


Torsions

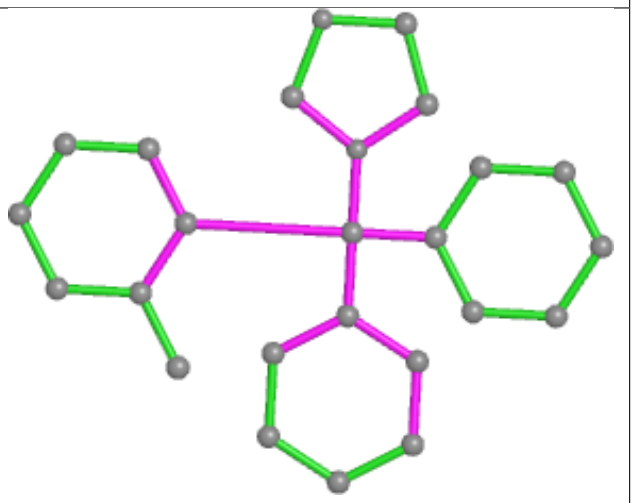


Rings

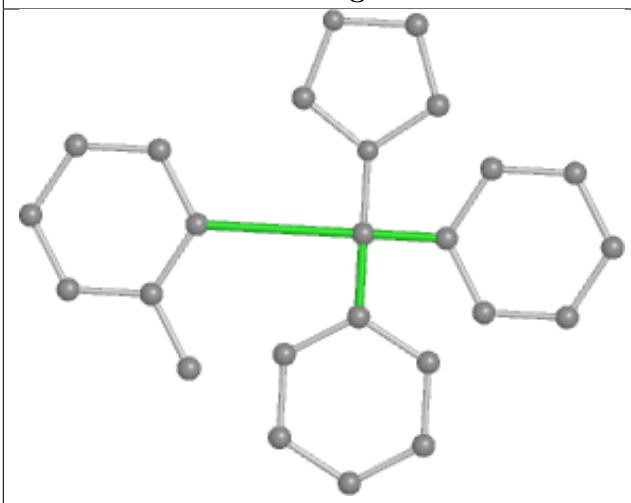
Ligand CL6 A 502



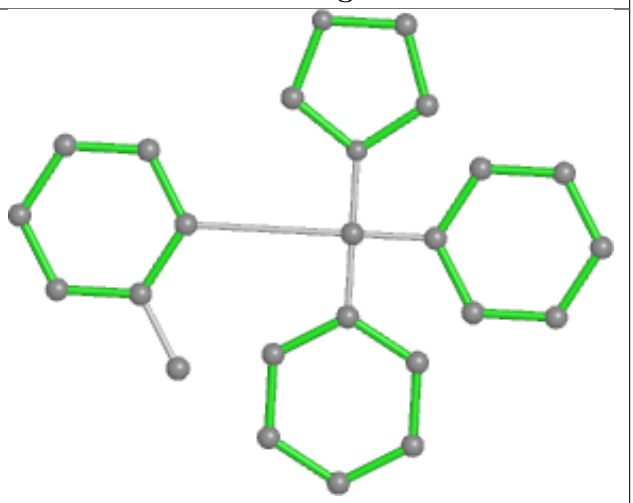
Bond lengths



Bond angles

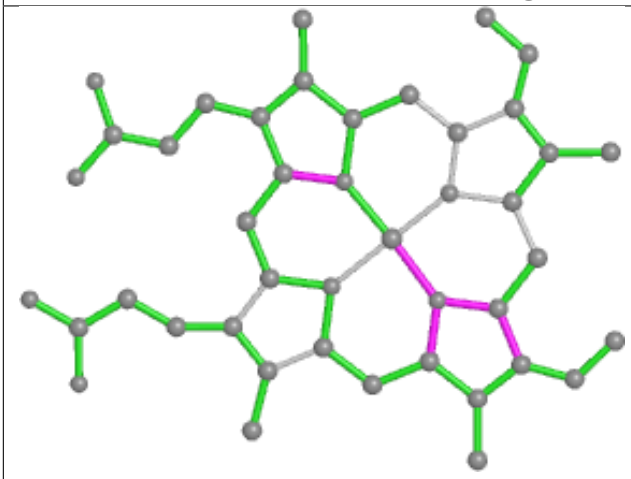


Torsions

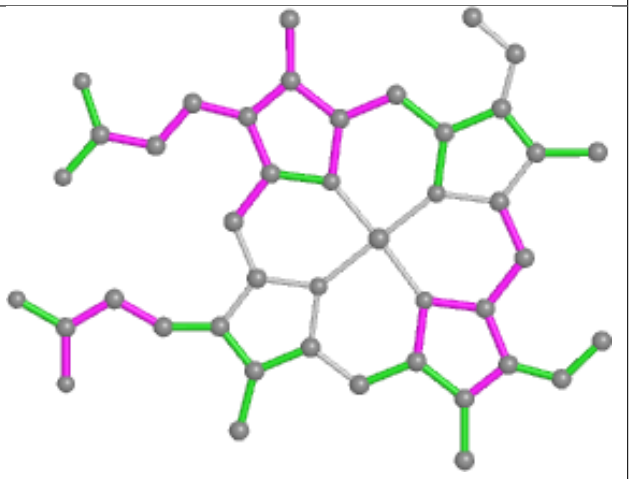


Rings

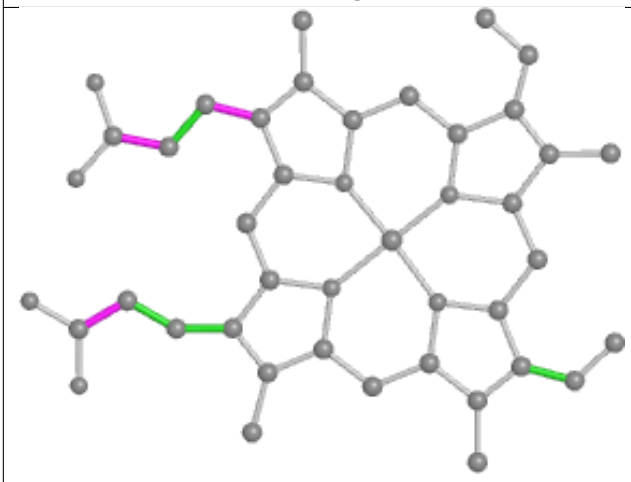
Ligand HEM E 501



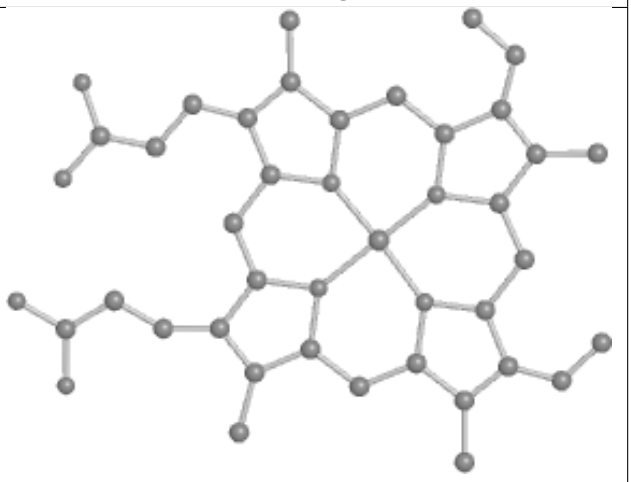
Bond lengths



Bond angles

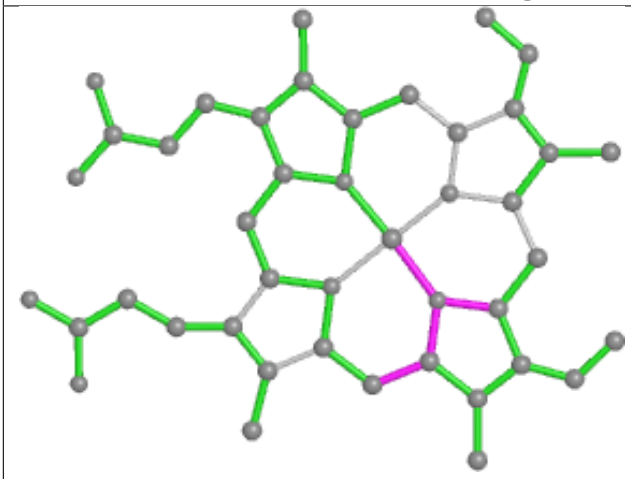


Torsions

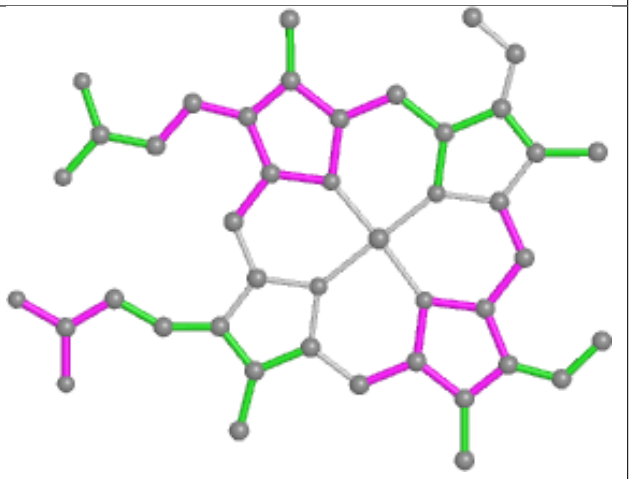


Rings

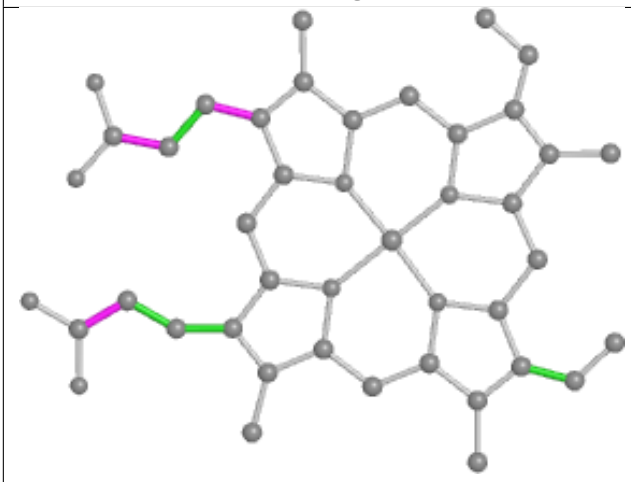
Ligand HEM C 501



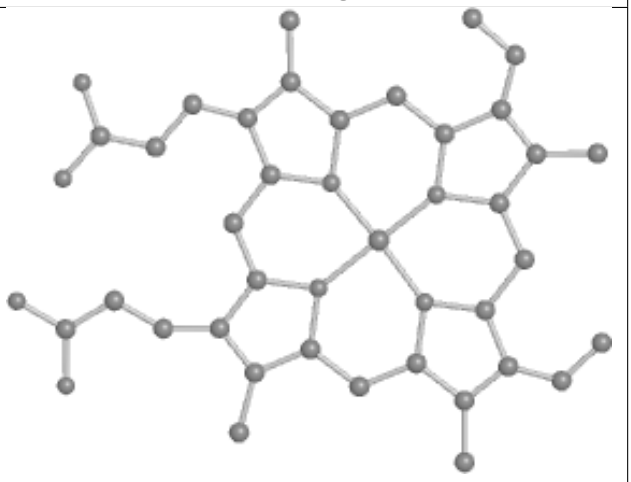
Bond lengths



Bond angles

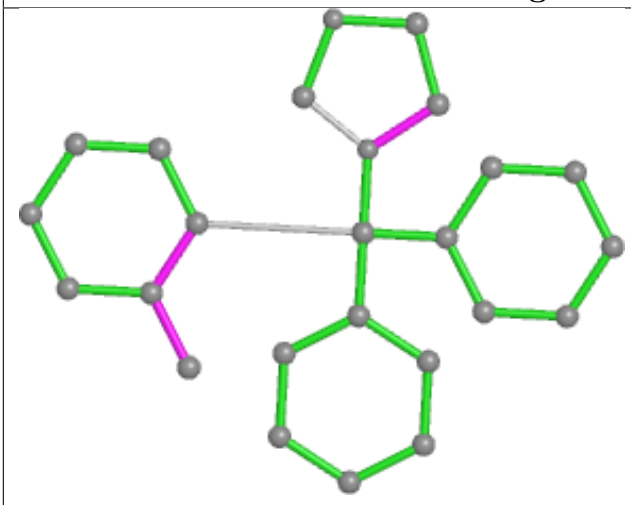


Torsions

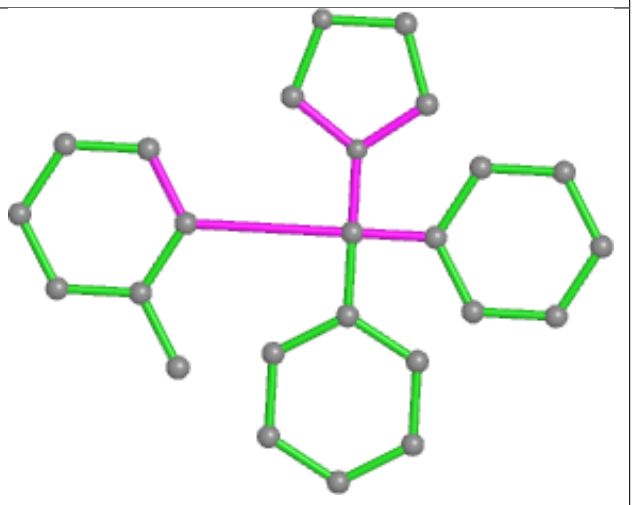


Rings

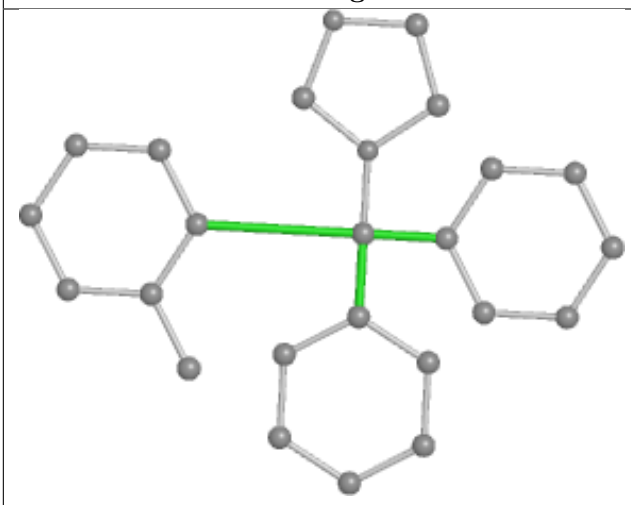
Ligand CL6 B 502



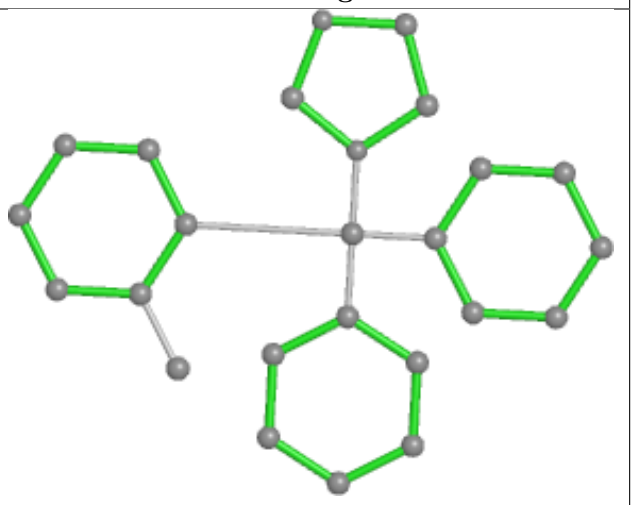
Bond lengths



Bond angles

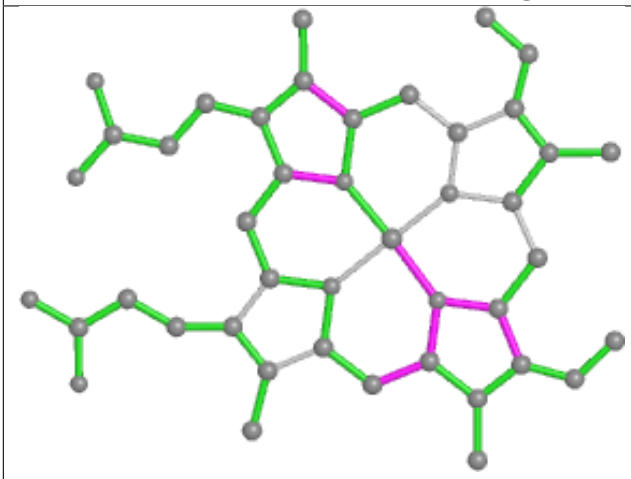


Torsions

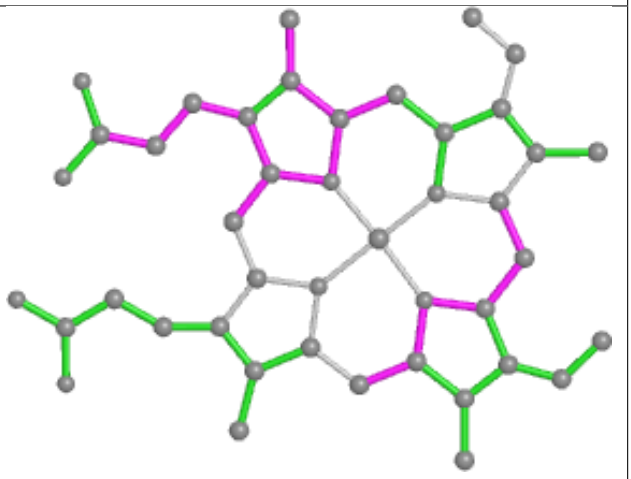


Rings

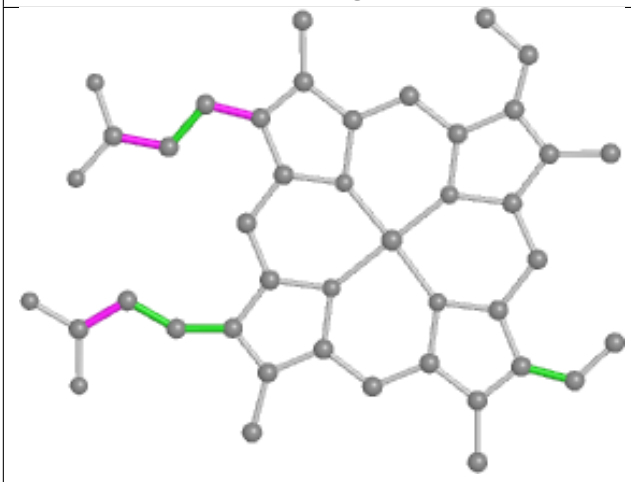
Ligand HEM A 501



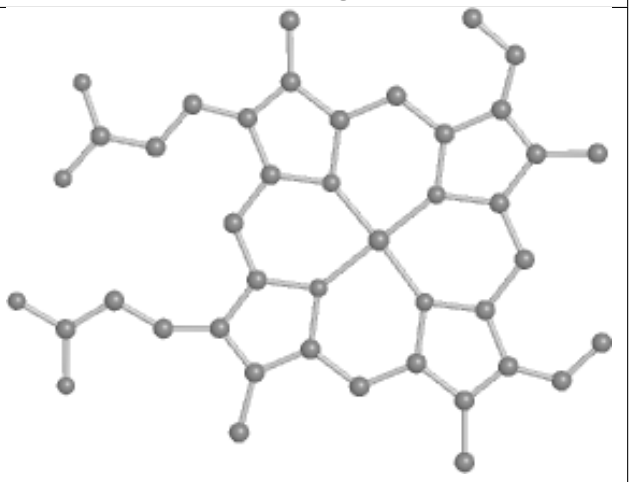
Bond lengths



Bond angles

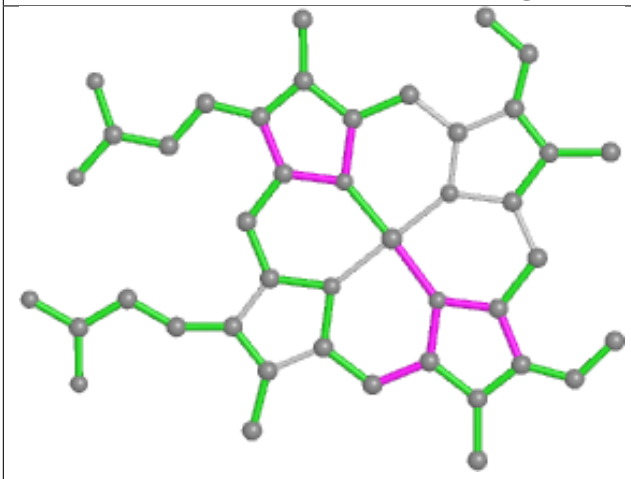


Torsions

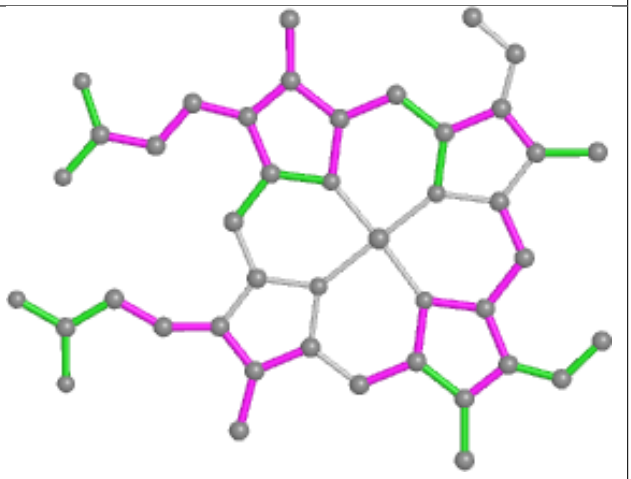


Rings

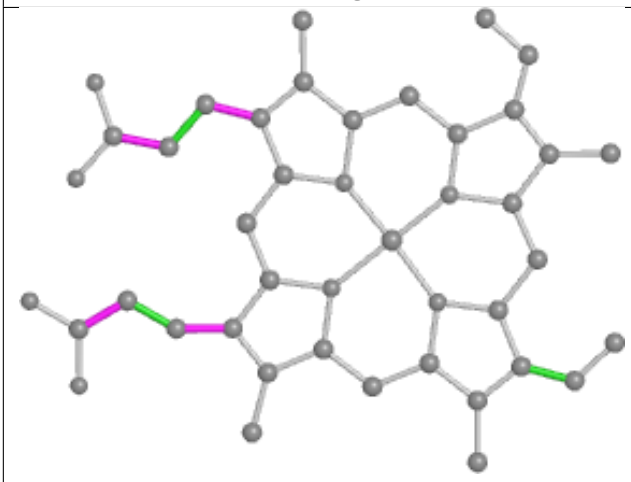
Ligand HEM D 501



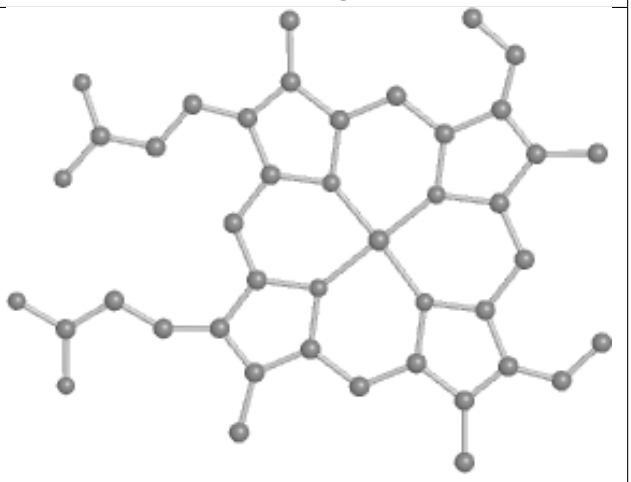
Bond lengths



Bond angles

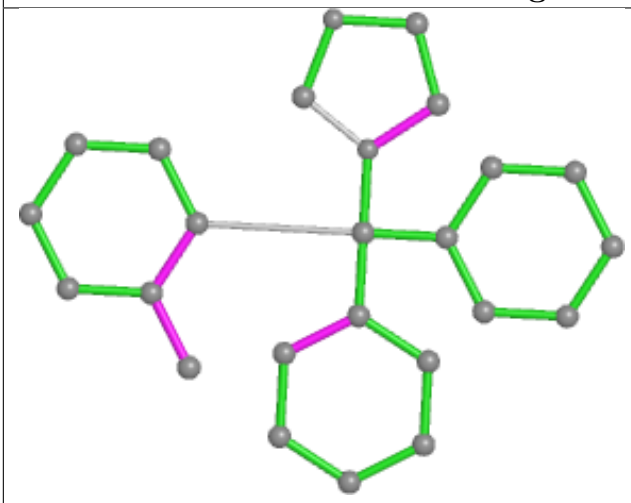


Torsions

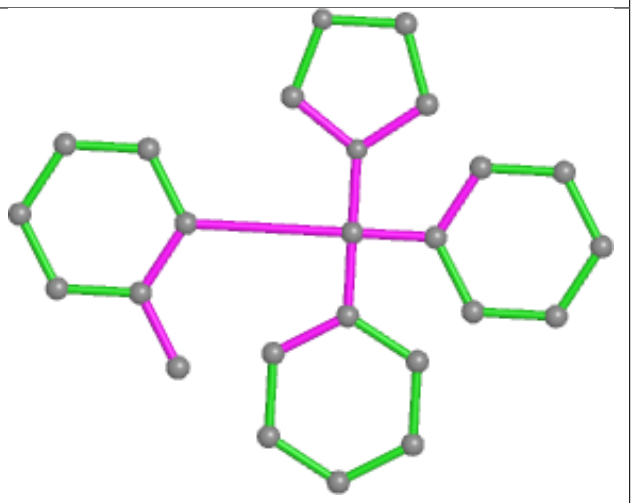


Rings

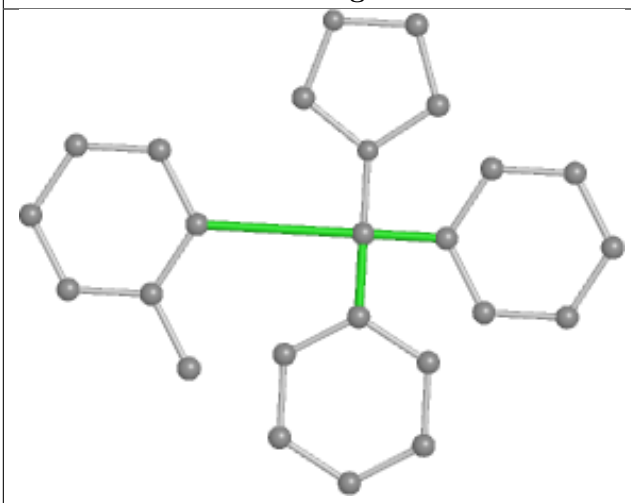
Ligand CL6 C 502



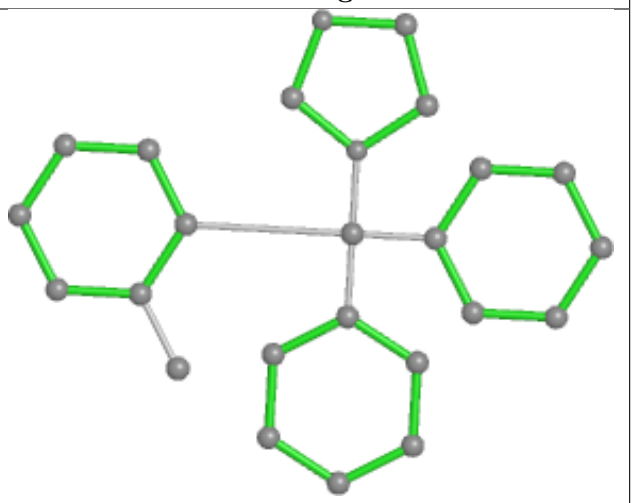
Bond lengths



Bond angles

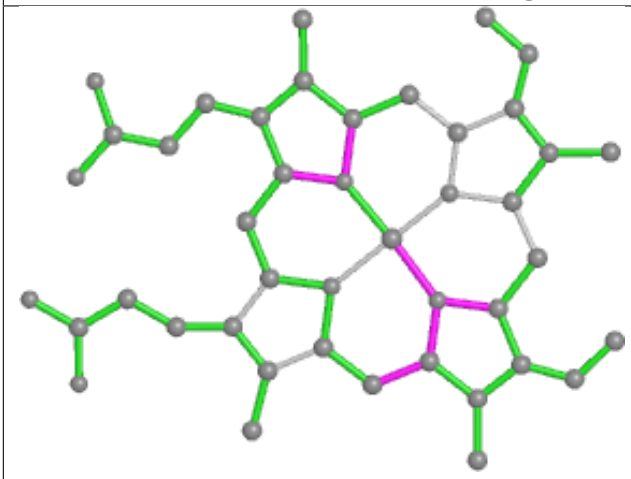


Torsions

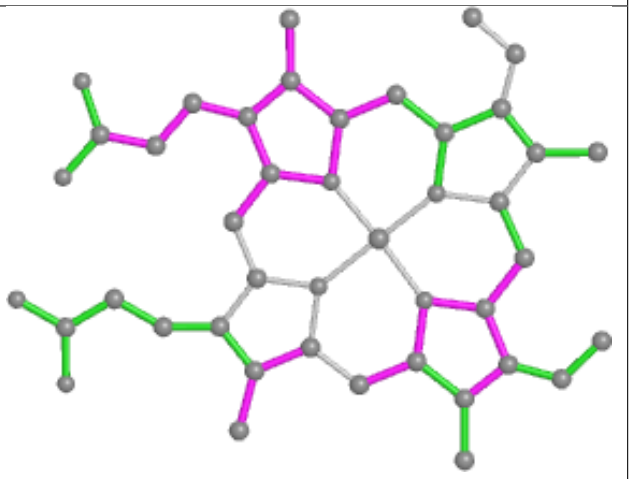


Rings

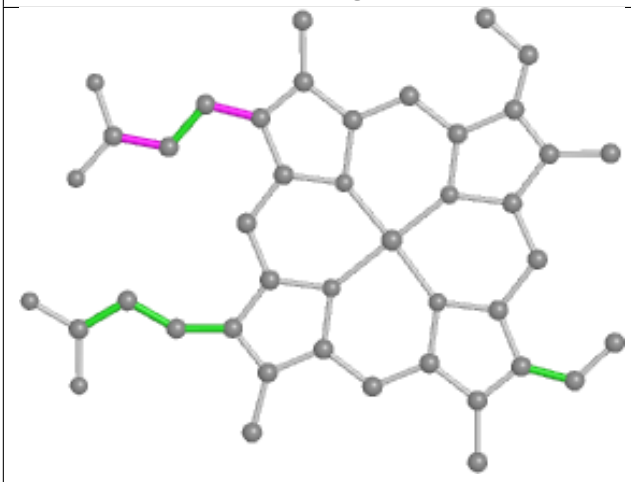
Ligand HEM F 501



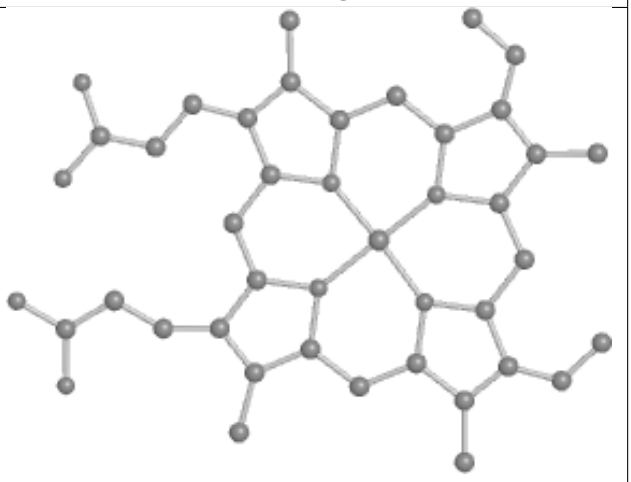
Bond lengths



Bond angles

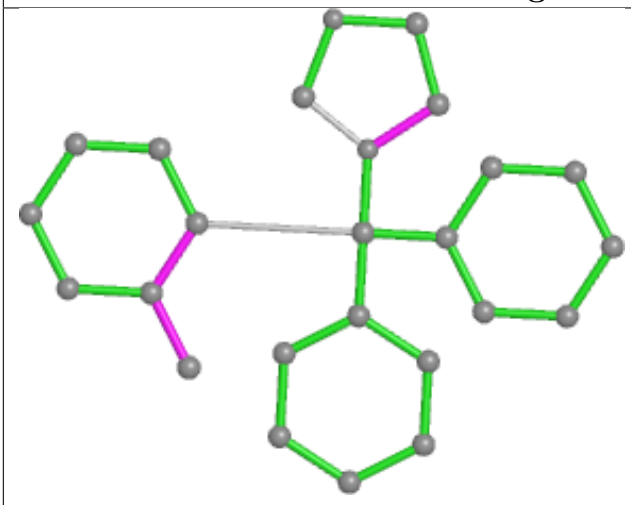


Torsions

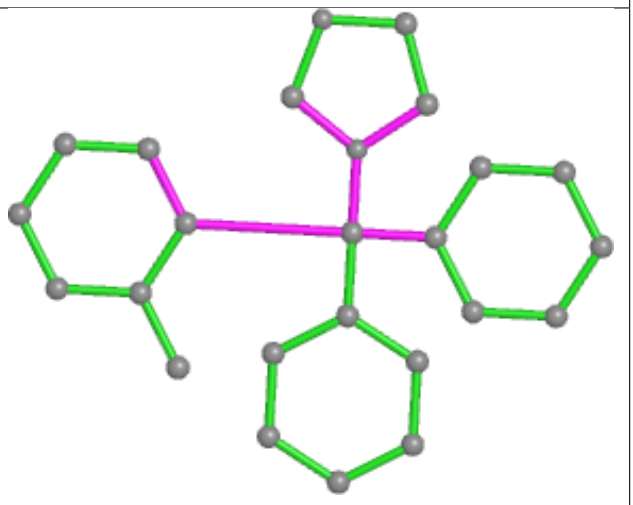


Rings

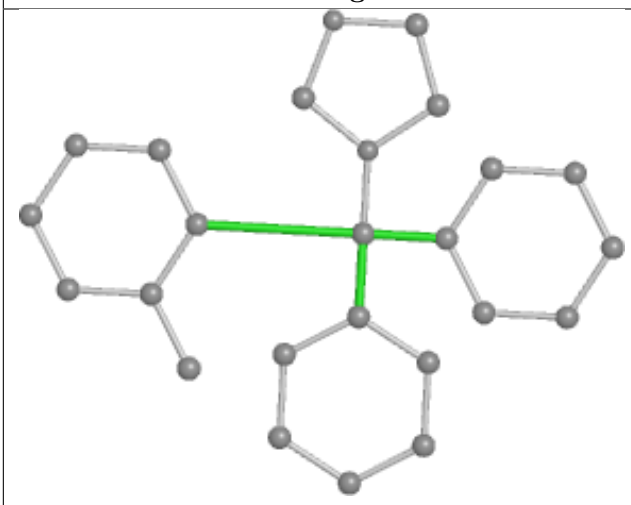
Ligand CL6 D 502



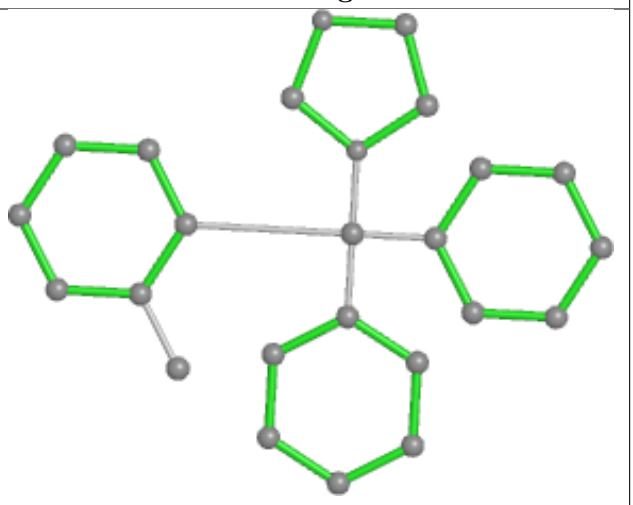
Bond lengths



Bond angles

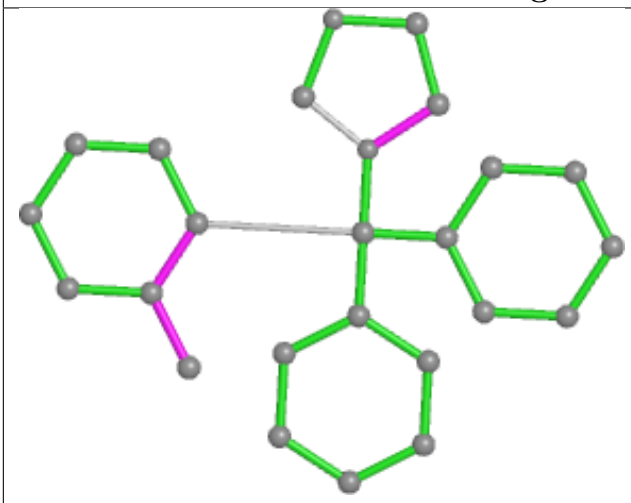


Torsions

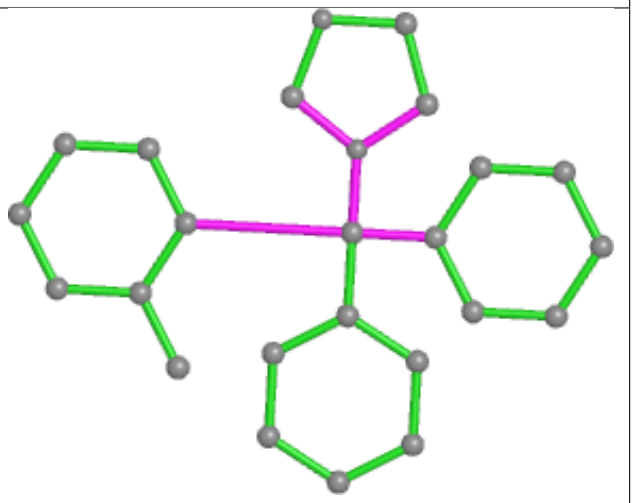


Rings

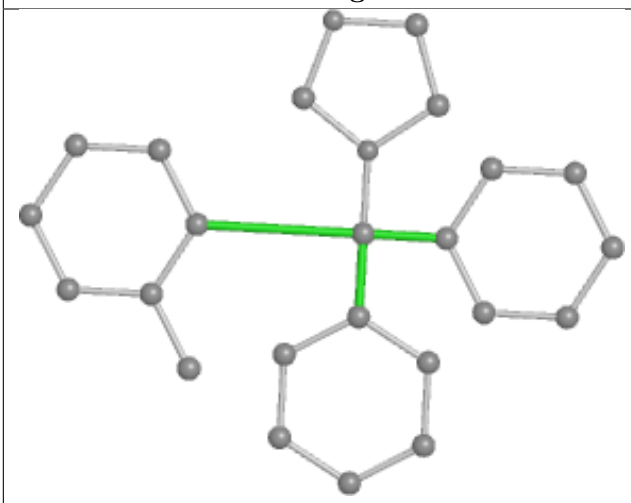
Ligand CL6 F 502



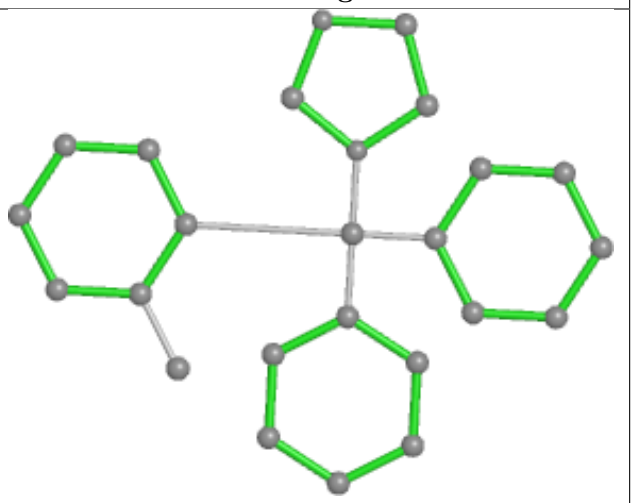
Bond lengths



Bond angles

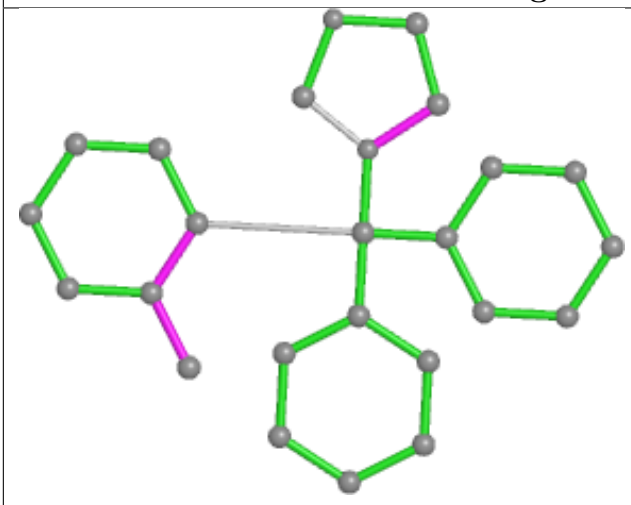


Torsions

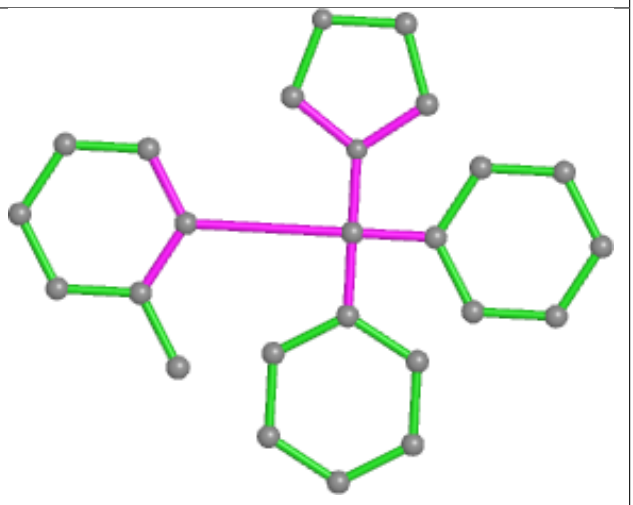


Rings

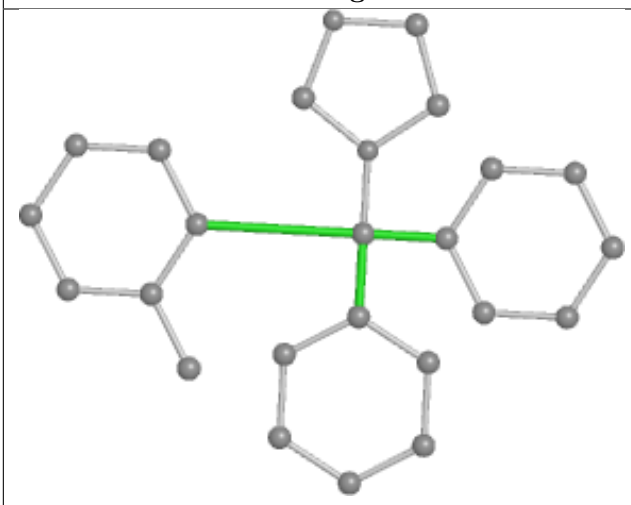
Ligand CL6 E 502



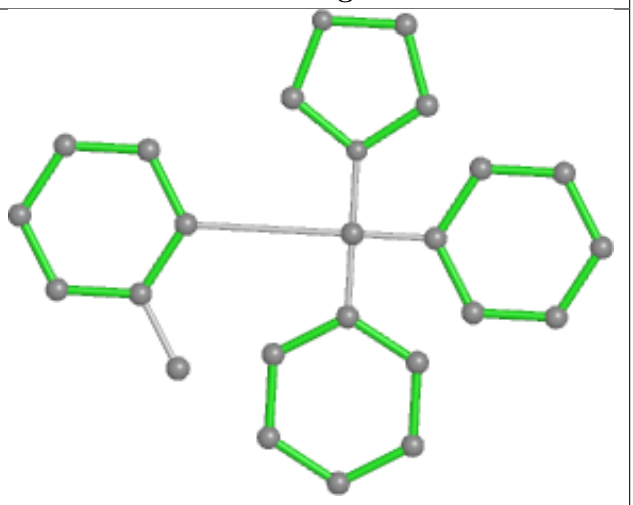
Bond lengths



Bond angles



Torsions



Rings

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.