wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 02:14 PM EDT

PDB ID	:	6NLK
Title	:	1.85 A resolution structure of WT BfrB from Pseudomonas aeruginosa in complex with a protein-protein interaction inhibitor (analog 13)
Authors	:	Lovell, S.; Punchi-Hewage, A.; Battaile, K.P.; Yao, H.; Nammalwar, B.; Gnanasekaran, K.K.; Bunce, R.A.; Reitz, A.B.; Rivera, M.
Deposited on	:	2019-01-08
Resolution	:	1.85 Å(reported)

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

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

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

The following versions of software and data (see references (1)) 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 1.85 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 6 unique types of molecules in this entry. The entry contains 17552 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 Ferroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	2	0
			1278	809	218	244	7			
1	B	156	Total	C	N	O	S	0	2	0
			1275	807	217	244	7			
1	C	156	Total	C	N	O	S	0	2	0
			1267	802	216	242	7			
1	D	156	Total	C	N	O	S	0	2	0
			1277	807	217	246	7			
1	E	156	Total	C	N	O	S	0	3	0
			1280	811	218	244	7			
1	F	156	Total	C	N	O	S	0	2	0
			1267	804	216	240	7			
1	G	156	Total	C	N	O	S	0	2	0
			1272	806	216	243	7			
1	H	156	Total	C	N	O	S	0	3	0
			1274	808	217	242	7			
1	I	156	Total	C	N	O	S	0	2	0
			1270	805	215	243	7			
1	J	156	Total	C	N	O	S	0	2	0
			1274	806	217	244	7			
1	K	156	Total	C	N	O	S	0	2	0
			1277	809	218	243	7			
1	L	156	Total	C	N	O	S	0	3	0
			1280	811	218	244	7			

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		

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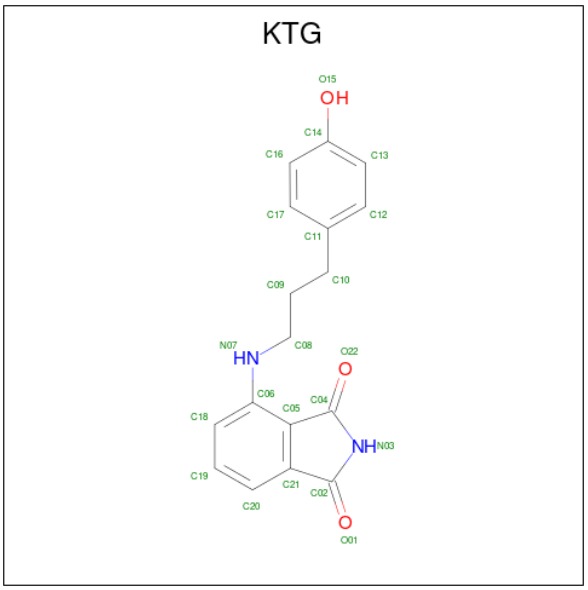
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is 4-{[3-(4-hydroxyphenyl)propyl]amino}-1H-isoindole-1,3(2H)-dione (three-letter code: KTG) (formula: $C_{17}H_{16}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 13 9 2 2	0	0
3	B	1	Total C N O 22 17 2 3	0	0
3	C	1	Total C N O 22 17 2 3	0	0
3	D	1	Total C N O 13 9 2 2	0	0
3	E	1	Total C N O 22 17 2 3	0	0
3	F	1	Total C N O 22 17 2 3	0	0
3	G	1	Total C N O 22 17 2 3	0	0
3	H	1	Total C N O 15 11 2 2	0	0
3	I	1	Total C N O 22 17 2 3	0	0
3	J	1	Total C N O 22 17 2 3	0	0

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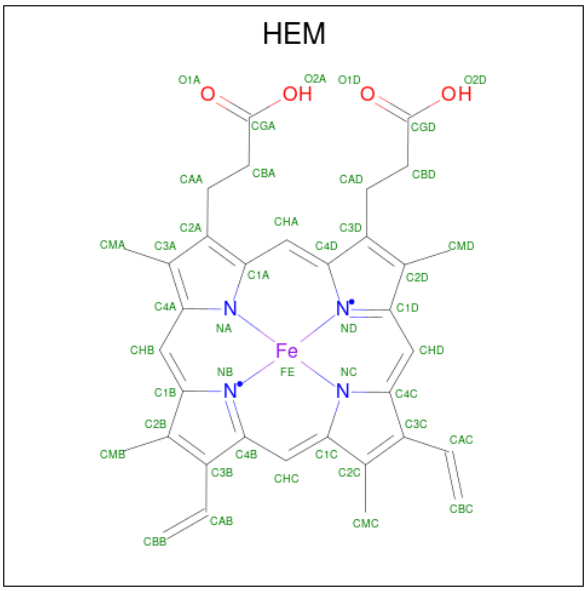
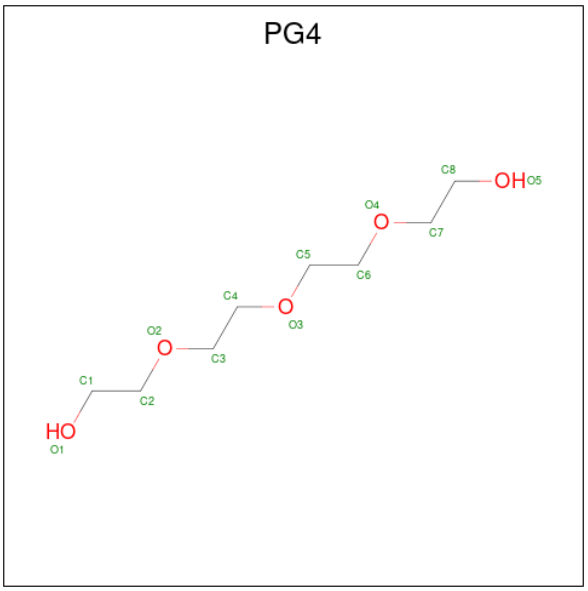
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total C N O 22 17 2 3	0	0
3	L	1	Total C N O 22 17 2 3	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 8 5	0	0
5	A	1	Total C O 13 8 5	0	0
5	C	1	Total C O 11 7 4	0	0
5	C	1	Total C O 10 6 4	0	0
5	D	1	Total C O 13 8 5	0	0
5	D	1	Total C O 10 6 4	0	0
5	E	1	Total C O 13 8 5	0	0
5	E	1	Total C O 8 5 3	0	0
5	G	1	Total C O 13 8 5	0	0
5	H	1	Total C O 13 8 5	0	0
5	H	1	Total C O 8 5 3	0	0
5	I	1	Total C O 13 8 5	0	0
5	I	1	Total C O 8 5 3	0	0
5	J	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total C O 13 8 5	0	0
5	K	1	Total C O 13 8 5	0	0
5	L	1	Total C O 13 8 5	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	124	Total O 124 124	0	0
6	B	135	Total O 135 135	0	0
6	C	144	Total O 144 144	0	0
6	D	109	Total O 109 109	0	0
6	E	156	Total O 156 156	0	0
6	F	133	Total O 133 133	0	0
6	G	115	Total O 115 115	0	0
6	H	122	Total O 122 122	0	0
6	I	104	Total O 104 104	0	0
6	J	127	Total O 127 127	0	0
6	K	133	Total O 133 133	0	0
6	L	118	Total O 118 118	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	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	129.81Å 194.56Å 203.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.31 – 1.85	Depositor
% Data completeness (in resolution range)	99.6 (47.31-1.85)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.86Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.162 , 0.195	Depositor
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.571	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17552	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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 39 ligands modelled in this entry, 3 are monoatomic - leaving 36 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	KTG	K	201	-	24,24,24	1.83	4 (16%)	33,33,33	1.08	2 (6%)
5	PG4	I	202	-	12,12,12	0.36	0	11,11,11	0.81	0
5	PG4	G	202	-	12,12,12	0.50	0	11,11,11	0.57	0
4	HEM	C	202	1	41,50,50	1.44	6 (14%)	45,82,82	1.89	16 (35%)
3	KTG	H	201	-	16,16,24	1.94	5 (31%)	22,22,33	1.66	3 (13%)
3	KTG	B	202	-	24,24,24	1.70	6 (25%)	33,33,33	1.07	2 (6%)
5	PG4	A	205	-	12,12,12	0.48	0	11,11,11	0.39	0
5	PG4	D	204	-	12,12,12	0.52	0	11,11,11	0.35	0
5	PG4	I	203	-	7,7,12	0.56	0	6,6,11	0.21	0
3	KTG	C	201	-	24,24,24	1.71	4 (16%)	33,33,33	1.19	3 (9%)
3	KTG	A	202	-	14,14,24	2.53	5 (35%)	19,20,33	1.35	2 (10%)
4	HEM	D	203	1	41,50,50	1.46	5 (12%)	45,82,82	1.55	9 (20%)
3	KTG	G	201	-	24,24,24	1.73	5 (20%)	33,33,33	1.09	2 (6%)
5	PG4	K	202	-	12,12,12	0.59	0	11,11,11	0.35	0
4	HEM	L	202	1	41,50,50	1.40	3 (7%)	45,82,82	1.58	9 (20%)
3	KTG	J	201	-	24,24,24	1.84	5 (20%)	33,33,33	1.25	3 (9%)
4	HEM	E	202	1	41,50,50	1.44	7 (17%)	45,82,82	1.75	14 (31%)
5	PG4	L	203	-	12,12,12	0.47	0	11,11,11	0.42	0
5	PG4	A	204	-	12,12,12	0.62	0	11,11,11	0.49	0
5	PG4	E	203	-	12,12,12	0.59	0	11,11,11	0.53	0
4	HEM	A	203	1	41,50,50	1.50	4 (9%)	45,82,82	1.72	12 (26%)
5	PG4	J	203	-	12,12,12	0.39	0	11,11,11	0.58	0
5	PG4	J	202	-	12,12,12	0.53	0	11,11,11	0.43	0
3	KTG	I	201	-	24,24,24	1.78	4 (16%)	33,33,33	0.95	1 (3%)
3	KTG	L	201	-	24,24,24	1.84	4 (16%)	33,33,33	1.21	2 (6%)
5	PG4	H	203	-	12,12,12	0.47	0	11,11,11	0.49	0
3	KTG	D	202	-	14,14,24	2.35	5 (35%)	19,20,33	1.26	2 (10%)
5	PG4	E	204	-	7,7,12	0.63	0	6,6,11	0.17	0
3	KTG	F	201	-	24,24,24	1.66	5 (20%)	33,33,33	1.02	3 (9%)
5	PG4	H	204	-	7,7,12	0.58	0	6,6,11	0.31	0
5	PG4	D	205	-	9,9,12	0.63	0	8,8,11	0.29	0
5	PG4	C	203	-	10,10,12	0.53	0	9,9,11	0.46	0
4	HEM	H	202	1	41,50,50	1.51	4 (9%)	45,82,82	1.83	11 (24%)
3	KTG	E	201	-	24,24,24	1.72	4 (16%)	33,33,33	1.12	3 (9%)
4	HEM	F	202	1	41,50,50	1.45	4 (9%)	45,82,82	1.69	10 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	PG4	C	204	-	9,9,12	0.57	0	8,8,11	0.47	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	KTG	K	201	-	-	0/7/19/19	0/3/3/3
5	PG4	I	202	-	-	3/10/10/10	-
5	PG4	G	202	-	-	5/10/10/10	-
4	HEM	C	202	1	-	4/12/54/54	-
3	KTG	H	201	-	-	1/4/16/19	0/2/2/3
3	KTG	B	202	-	-	2/7/19/19	0/3/3/3
5	PG4	A	205	-	-	1/10/10/10	-
5	PG4	D	204	-	-	3/10/10/10	-
5	PG4	I	203	-	-	1/5/5/10	-
3	KTG	C	201	-	-	1/7/19/19	0/3/3/3
3	KTG	A	202	-	-	0/2/14/19	0/2/2/3
4	HEM	D	203	1	-	4/12/54/54	-
3	KTG	G	201	-	-	0/7/19/19	0/3/3/3
5	PG4	K	202	-	-	2/10/10/10	-
4	HEM	L	202	1	-	4/12/54/54	-
3	KTG	J	201	-	-	0/7/19/19	0/3/3/3
4	HEM	E	202	1	-	4/12/54/54	-
5	PG4	L	203	-	-	3/10/10/10	-
5	PG4	A	204	-	-	5/10/10/10	-
5	PG4	E	203	-	-	1/10/10/10	-
4	HEM	A	203	1	-	4/12/54/54	-
5	PG4	J	203	-	-	0/10/10/10	-
5	PG4	J	202	-	-	1/10/10/10	-
3	KTG	I	201	-	-	0/7/19/19	0/3/3/3
3	KTG	L	201	-	-	0/7/19/19	0/3/3/3
5	PG4	H	203	-	-	4/10/10/10	-
3	KTG	D	202	-	-	0/2/14/19	0/2/2/3
5	PG4	E	204	-	-	0/5/5/10	-
3	KTG	F	201	-	-	0/7/19/19	0/3/3/3
5	PG4	H	204	-	-	0/5/5/10	-
5	PG4	D	205	-	-	0/7/7/10	-
5	PG4	C	203	-	-	0/8/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	H	202	1	-	4/12/54/54	-
3	KTG	E	201	-	-	0/7/19/19	0/3/3/3
4	HEM	F	202	1	-	4/12/54/54	-
5	PG4	C	204	-	-	3/7/7/10	-

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203	HEM	C3C-C2C	-4.96	1.33	1.40
3	I	201	KTG	C21-C02	4.87	1.56	1.48
3	D	202	KTG	C06-N07	4.80	1.46	1.37
3	A	202	KTG	C06-N07	4.76	1.46	1.37
3	C	201	KTG	C21-C02	4.75	1.55	1.48

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	201	KTG	C05-C06-N07	-4.96	115.44	121.32
4	A	203	HEM	CMC-C2C-C3C	4.44	132.98	124.68
4	C	202	HEM	C4D-ND-C1D	4.33	109.54	105.07
4	H	202	HEM	C4B-CHC-C1C	4.23	128.13	122.56
3	L	201	KTG	C04-N03-C02	-4.20	108.94	112.52

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	204	PG4	O2-C3-C4-O3
5	H	203	PG4	O4-C7-C8-O5
3	B	202	KTG	N07-C08-C09-C10
5	C	204	PG4	O3-C5-C6-O4
5	D	204	PG4	O1-C1-C2-O2

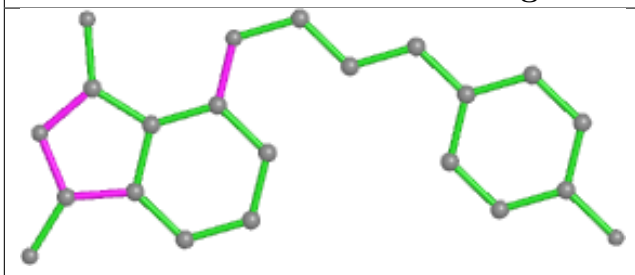
There are no ring outliers.

No monomer is involved in short contacts.

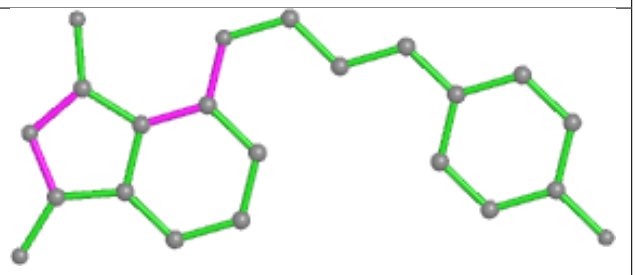
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

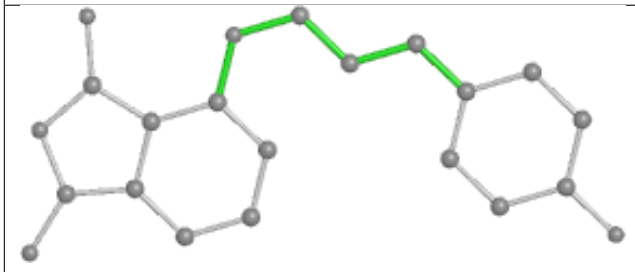
Ligand KTG K 201



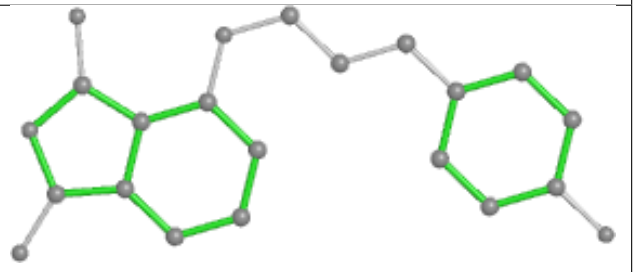
Bond lengths



Bond angles

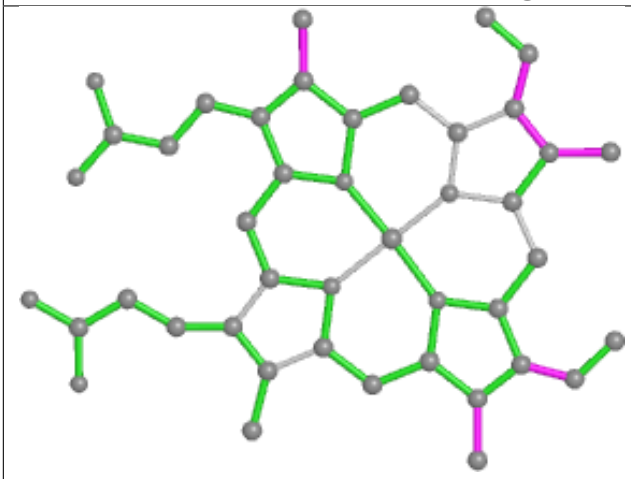


Torsions

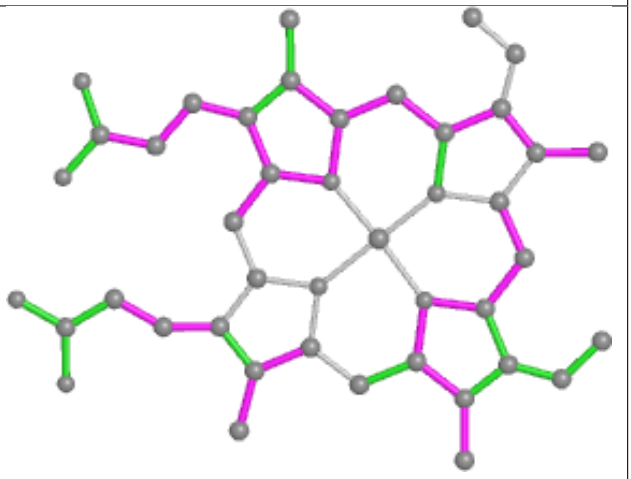


Rings

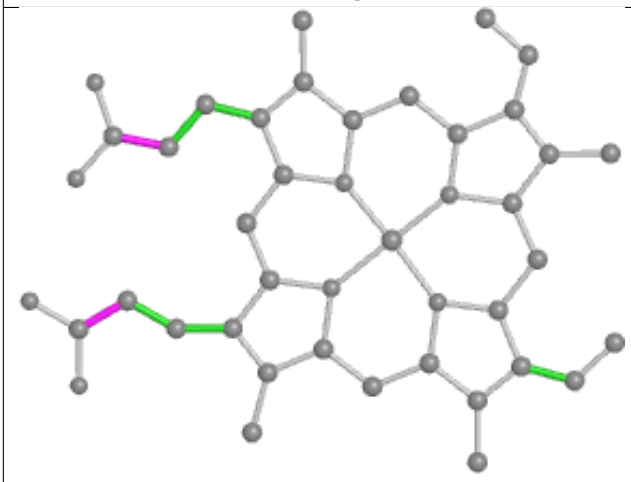
Ligand HEM C 202



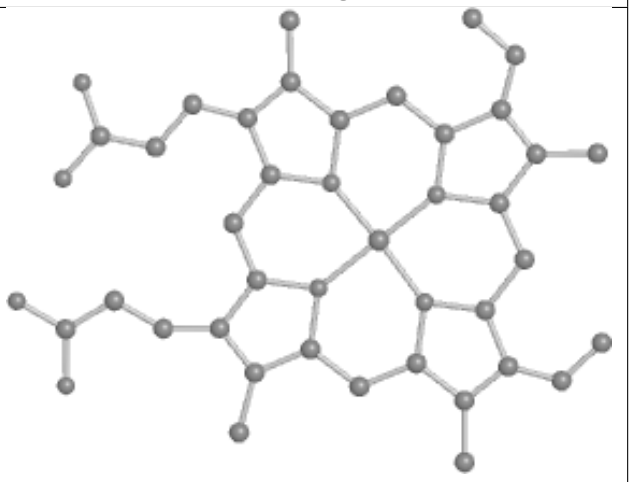
Bond lengths



Bond angles

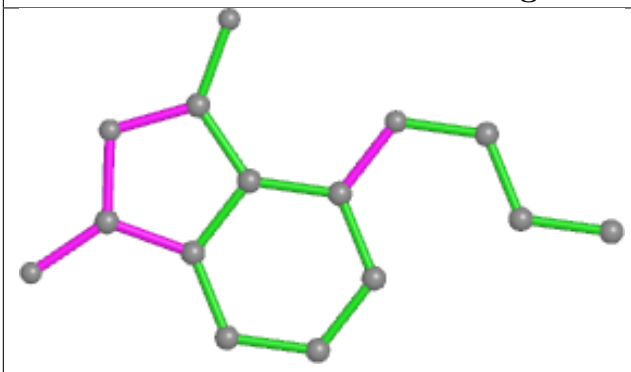


Torsions

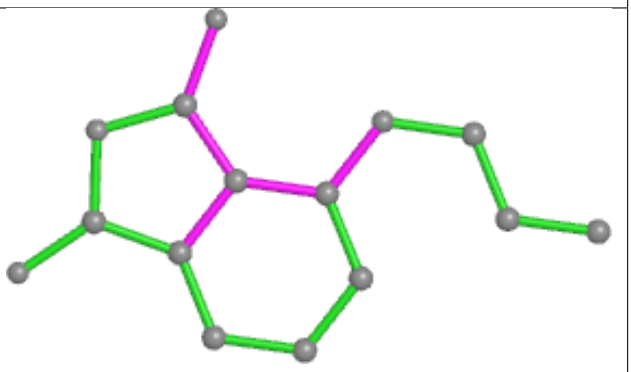


Rings

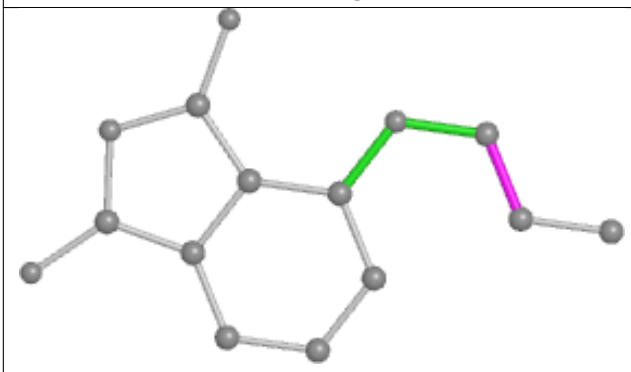
Ligand KTG H 201



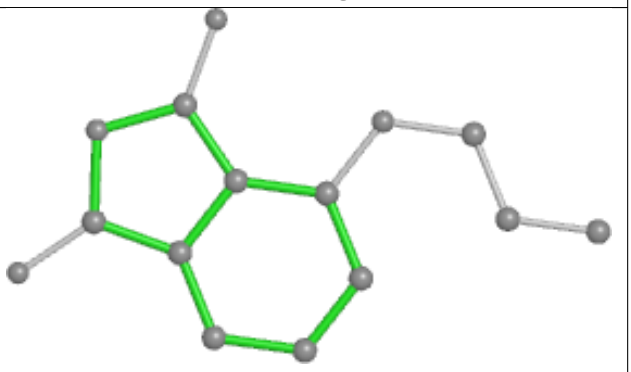
Bond lengths



Bond angles

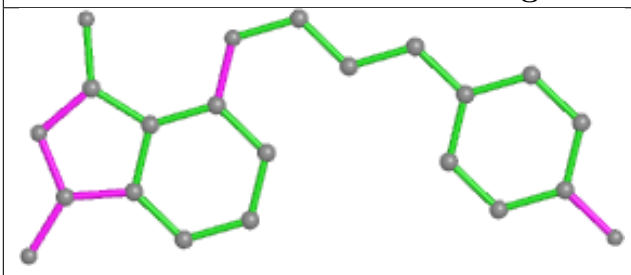


Torsions



Rings

Ligand KTG B 202



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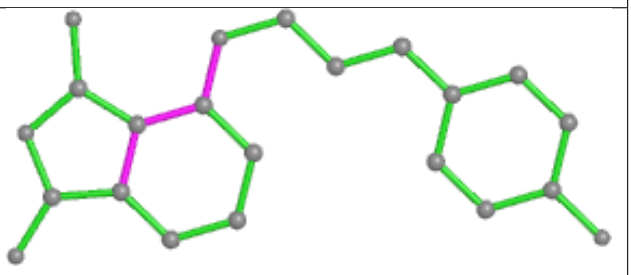
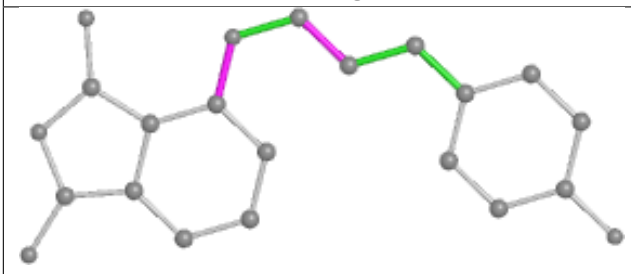


Bond angles



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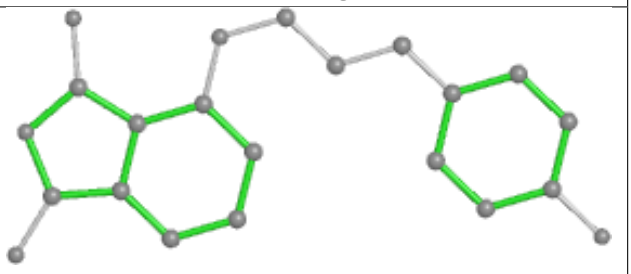
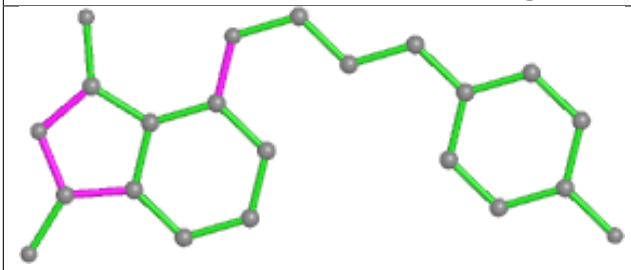


Rings

Ligand KTG C 201



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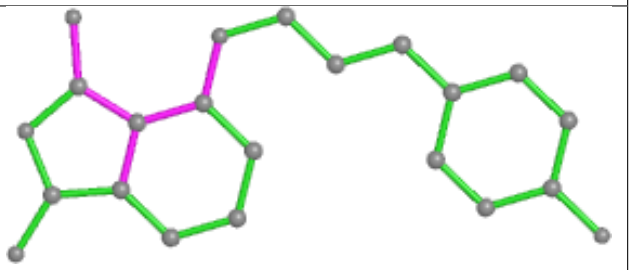
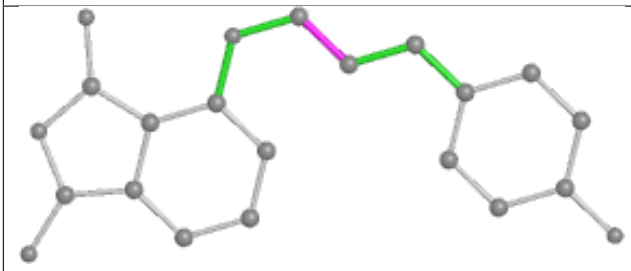


Bond angles



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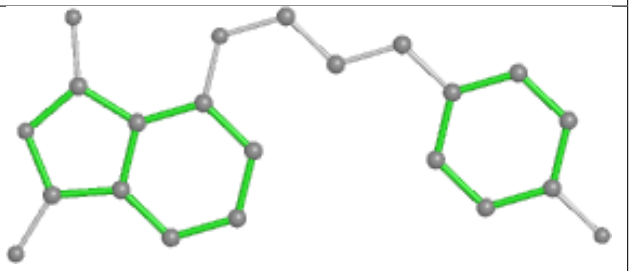

Rings

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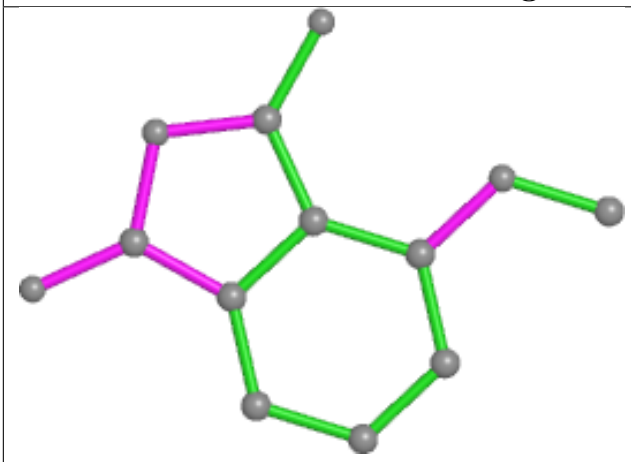

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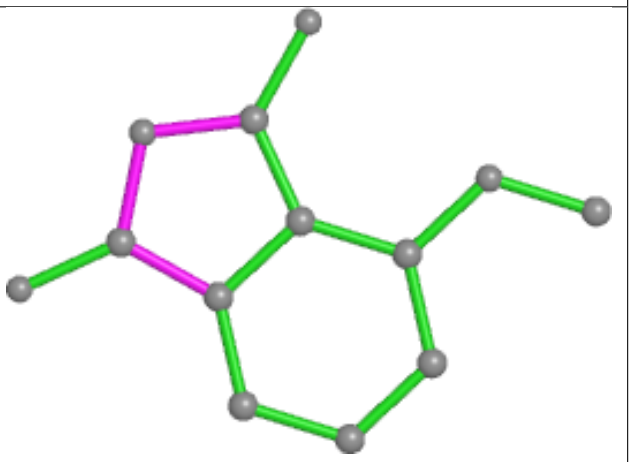

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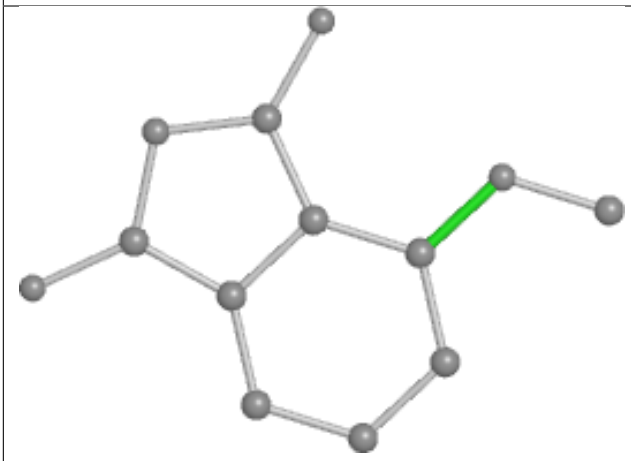

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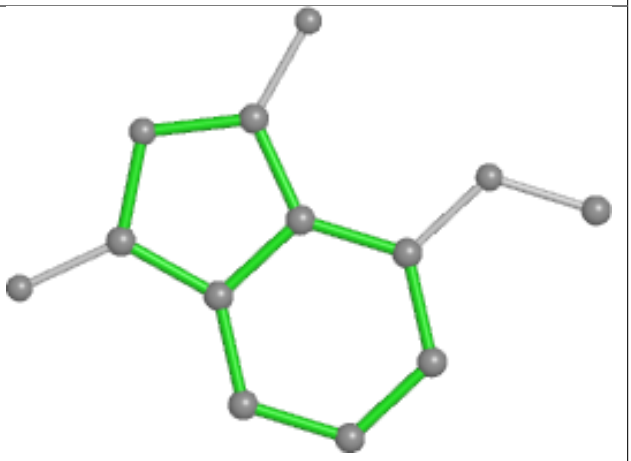
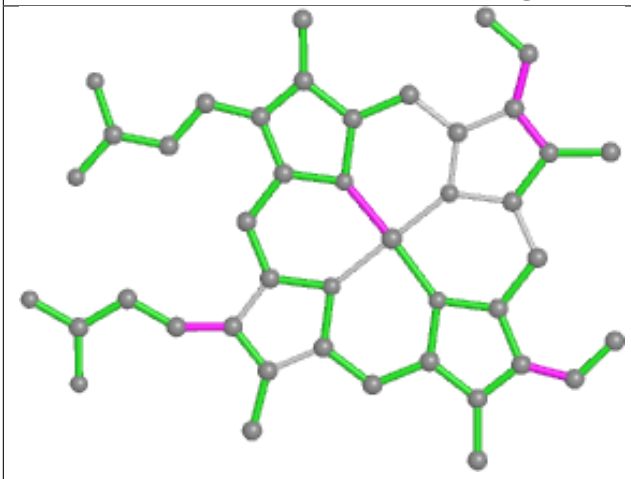


Rings

Ligand HEM D 203



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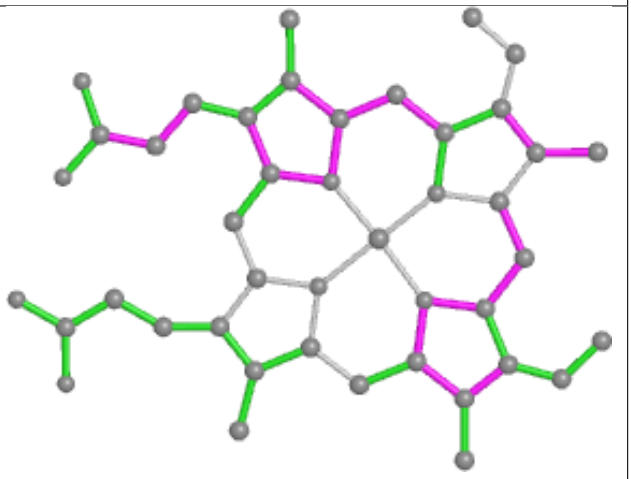

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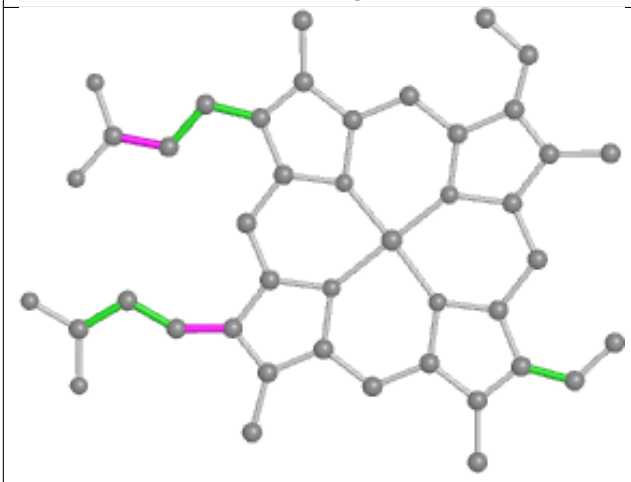

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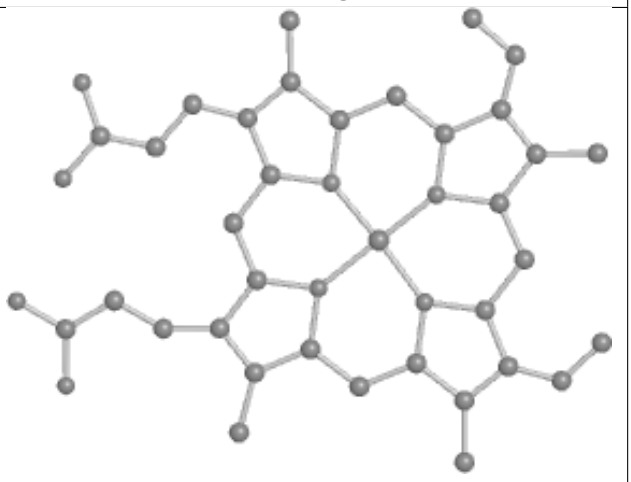
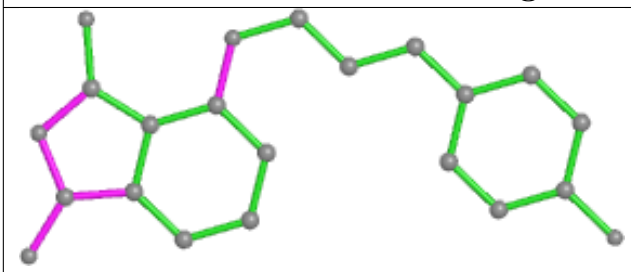


Rings

Ligand KTG G 201



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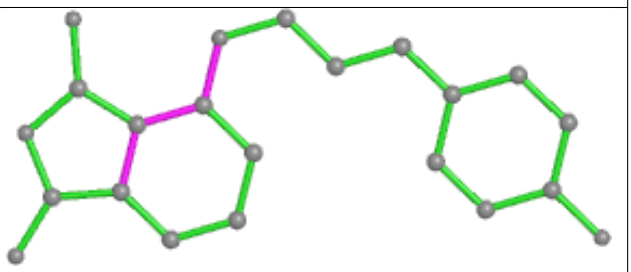

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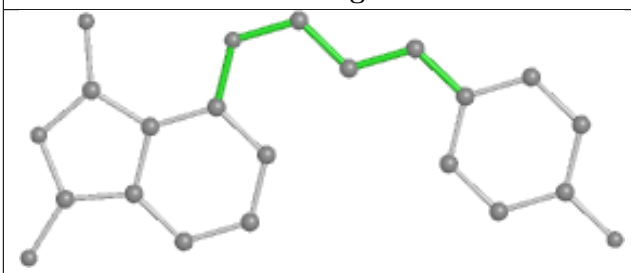

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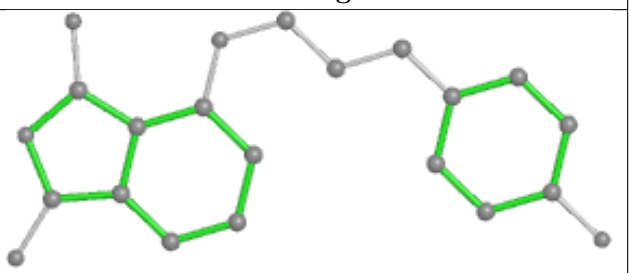
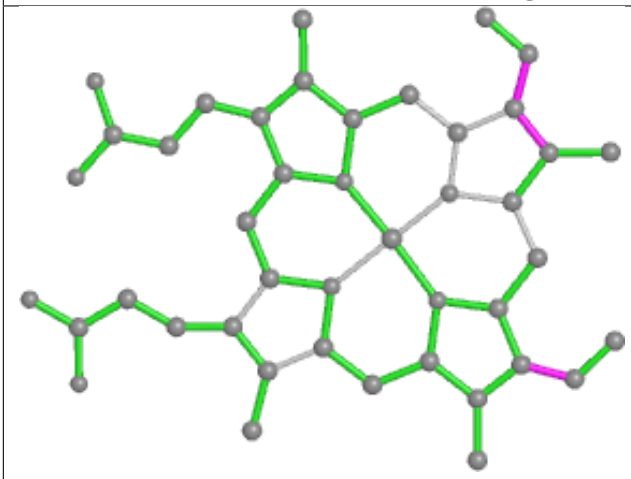


Rings

Ligand HEM L 202



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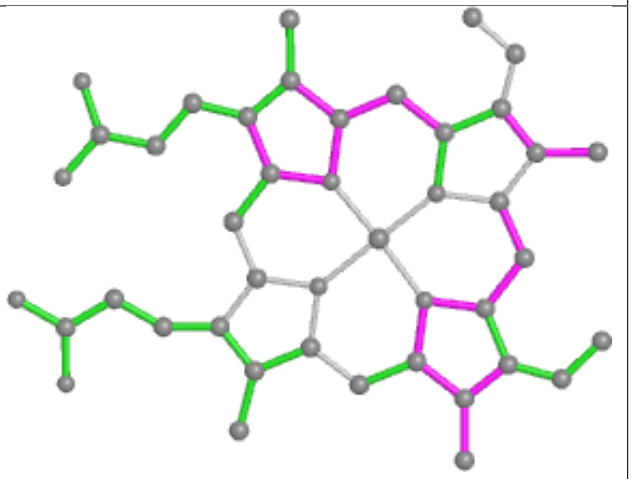
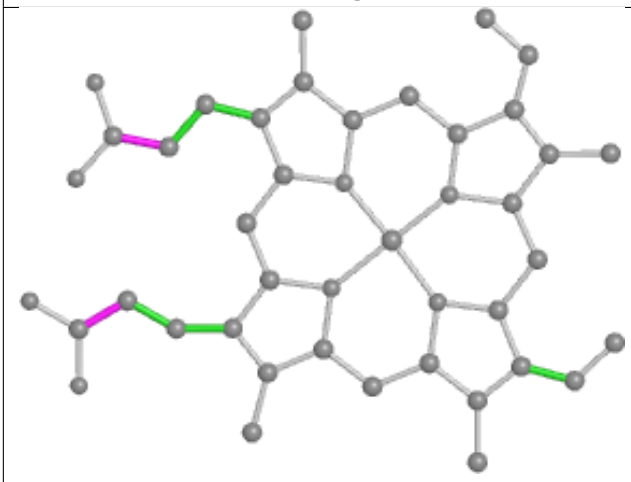


Bond angles



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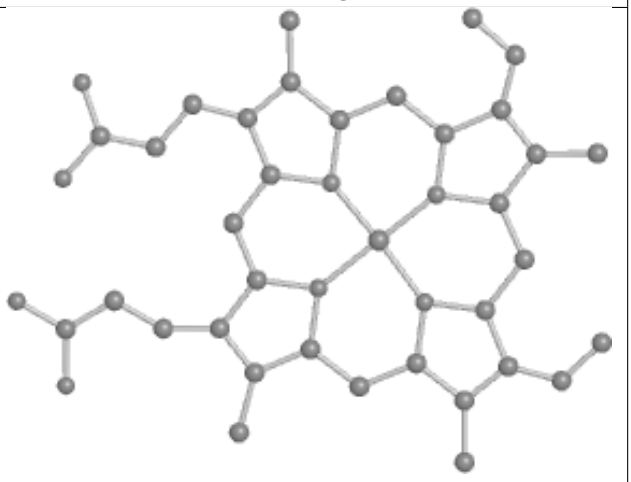
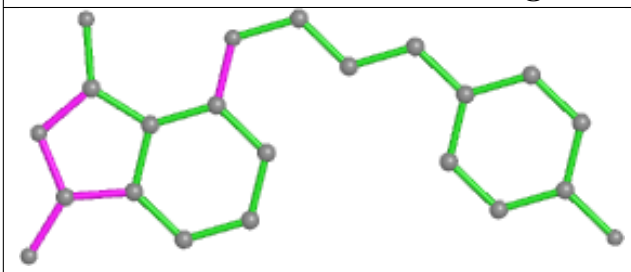


Rings

Ligand KTG J 201



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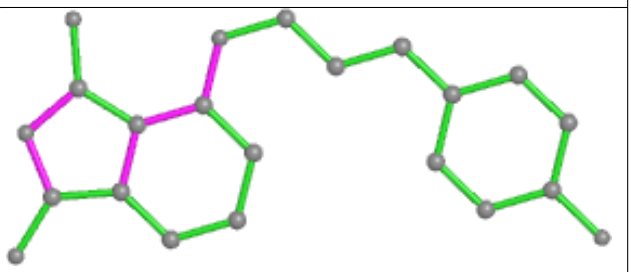

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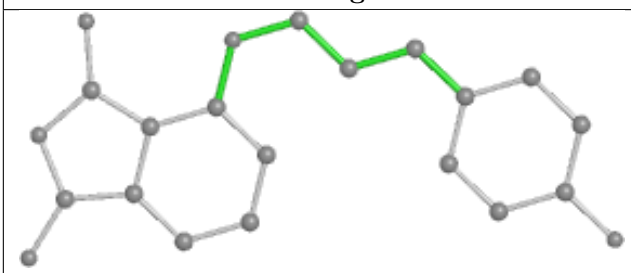

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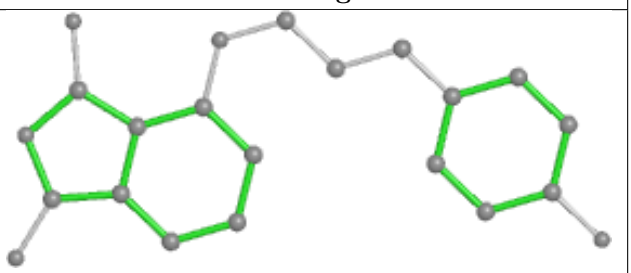
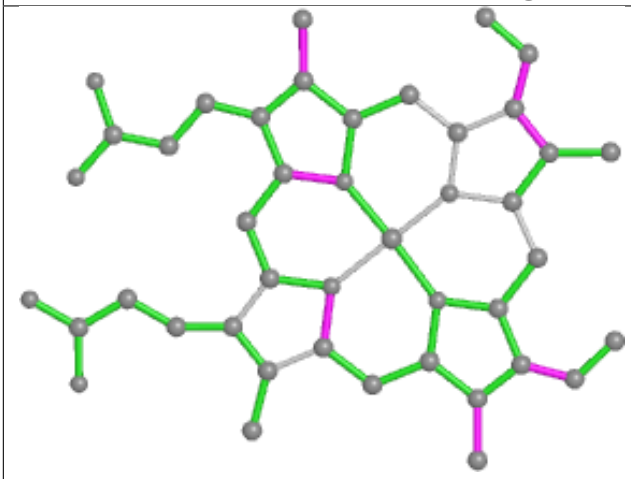


Rings

Ligand HEM E 202



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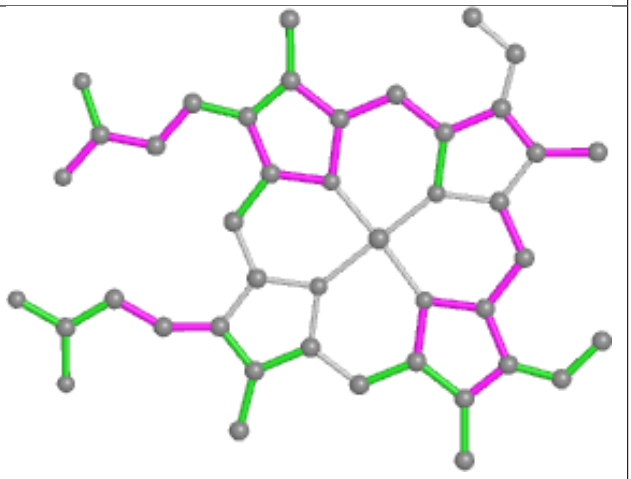
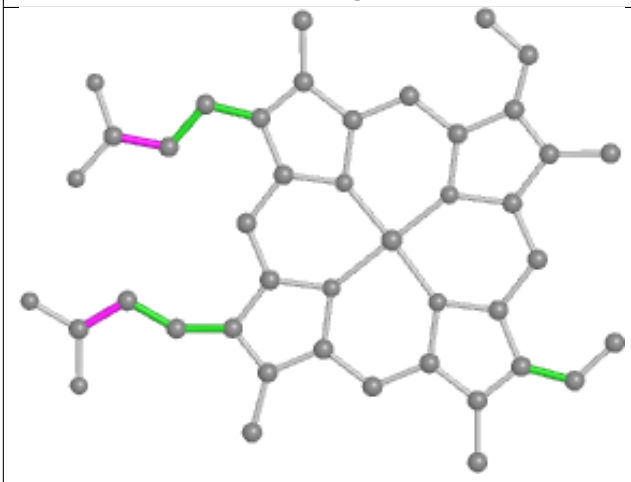
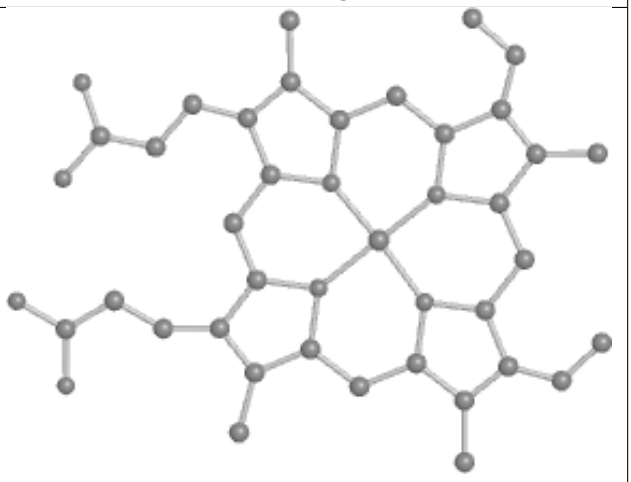


Bond angles

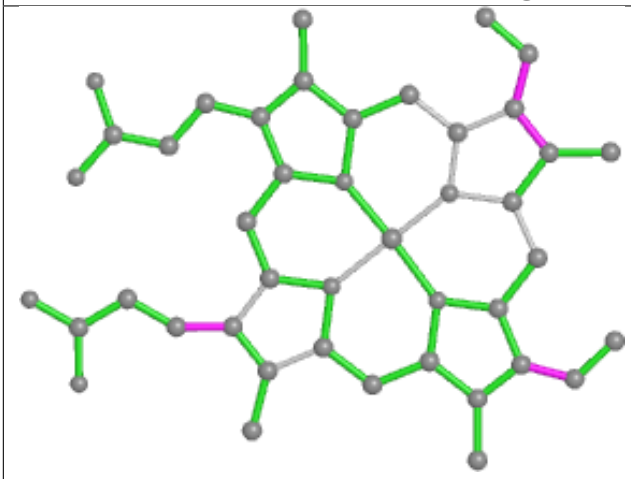


Torsions



Rings

Ligand HEM A 203



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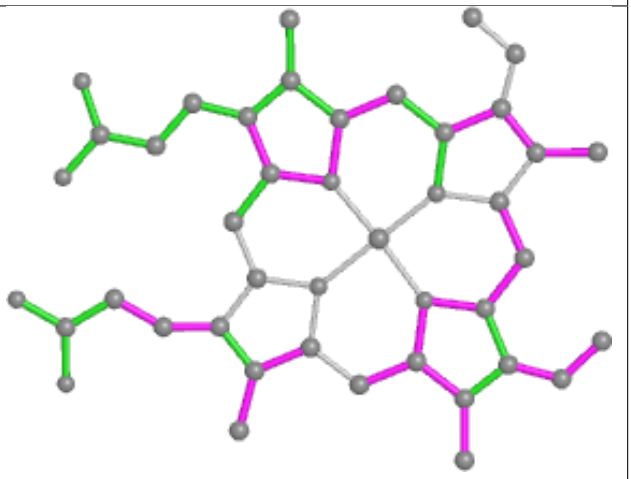
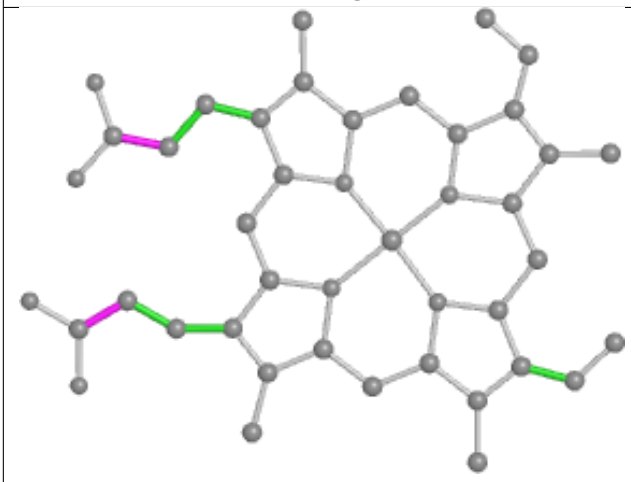
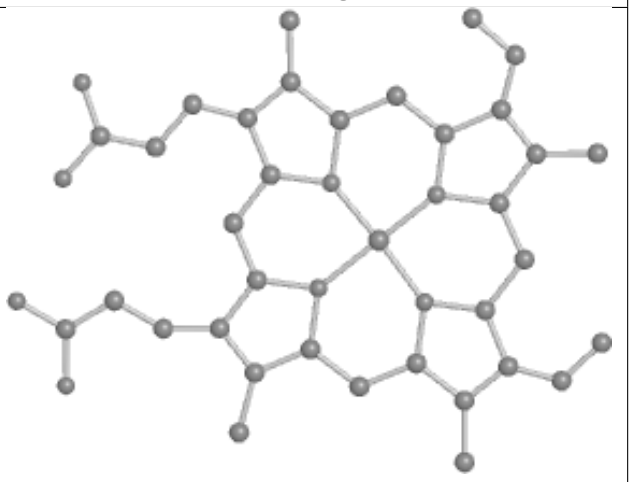


Bond angles

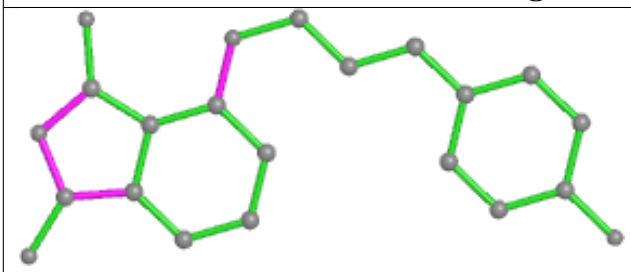


Torsions



Rings

Ligand KTG I 201



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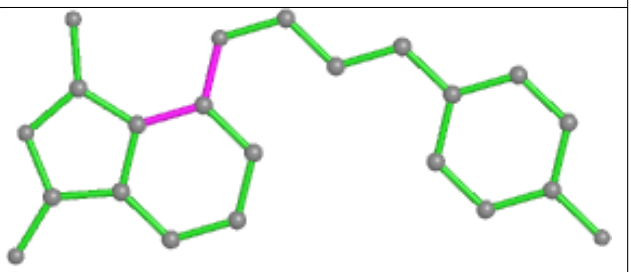

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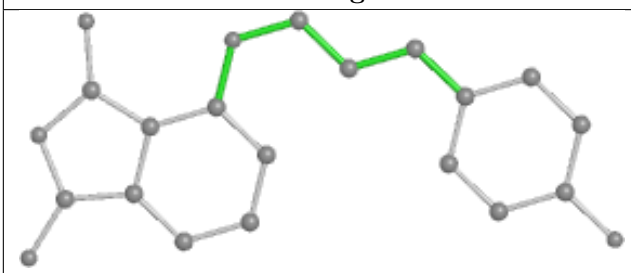

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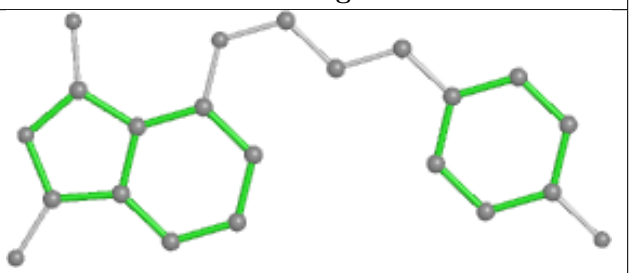
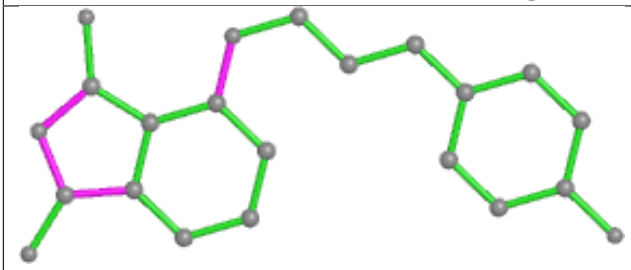


Rings

Ligand KTG L 201



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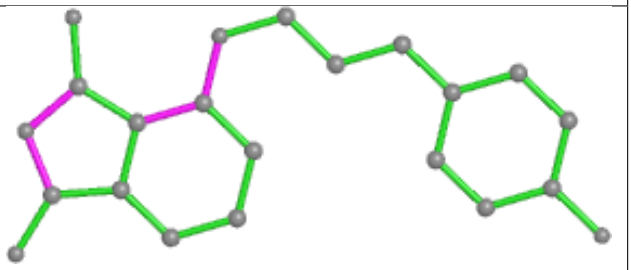
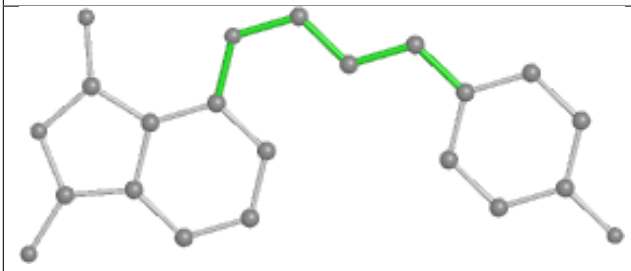


Bond angles



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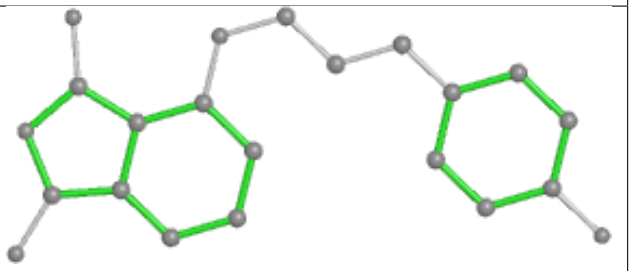
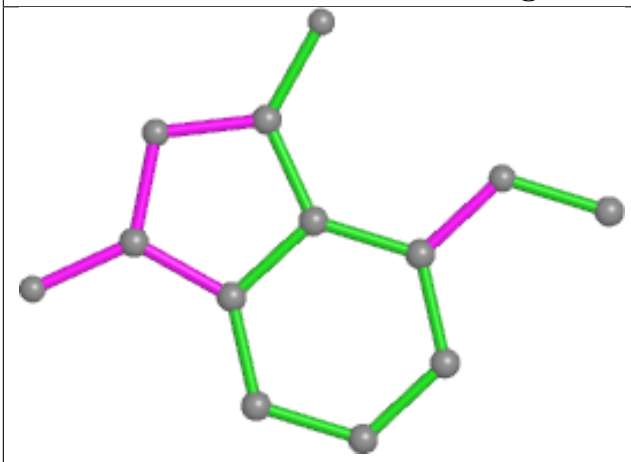


Rings

Ligand KTG D 202



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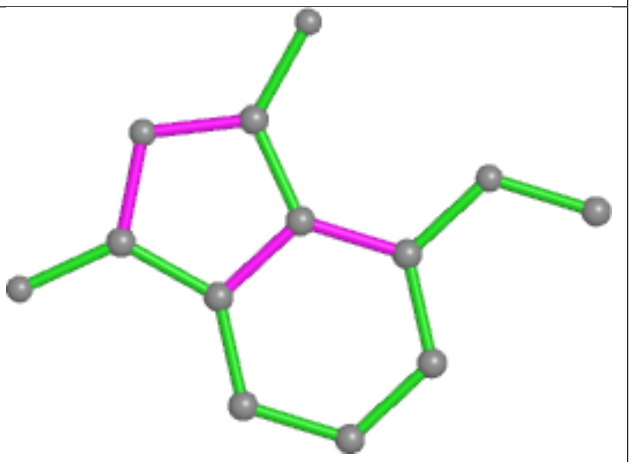
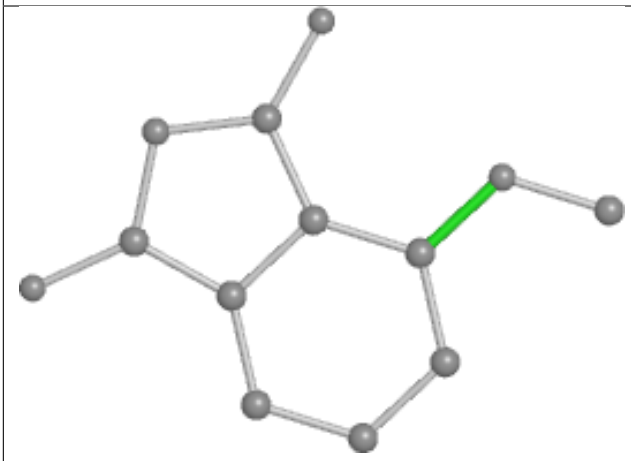


Bond angles



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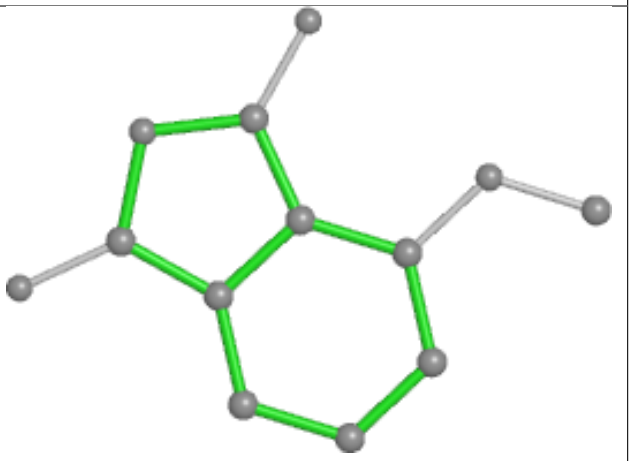
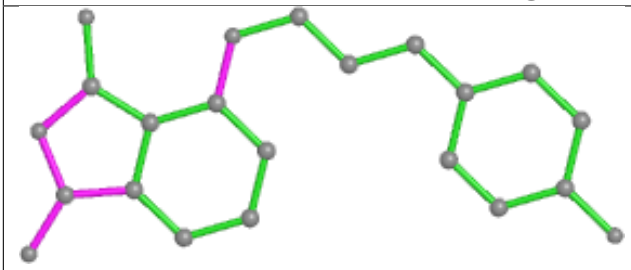


Rings

Ligand KTG F 201



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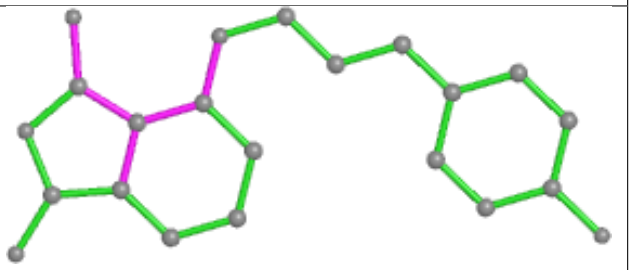
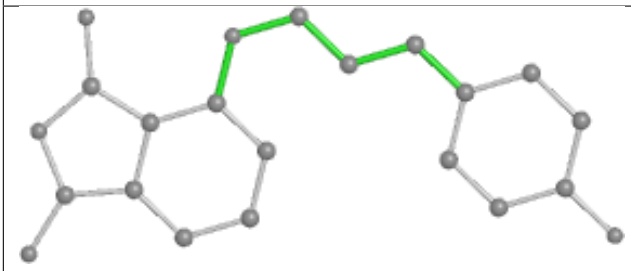
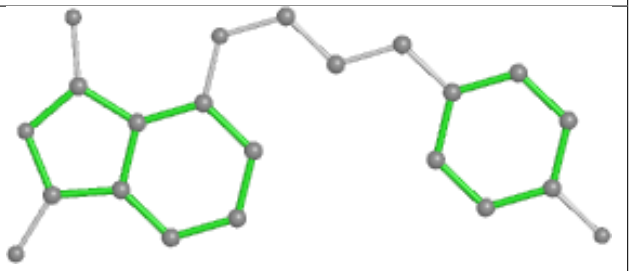


Bond angles

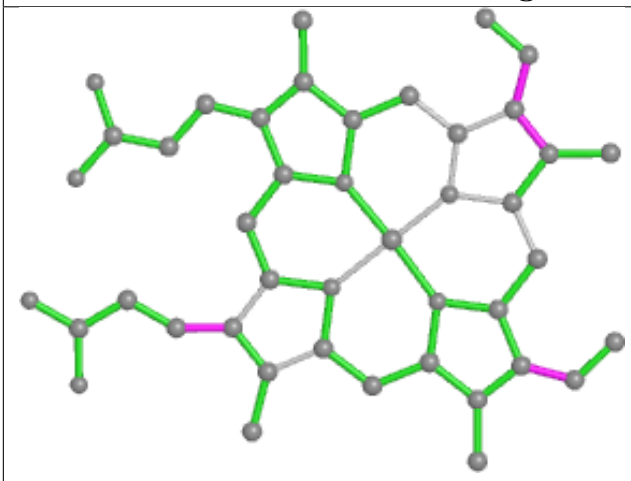


Torsions

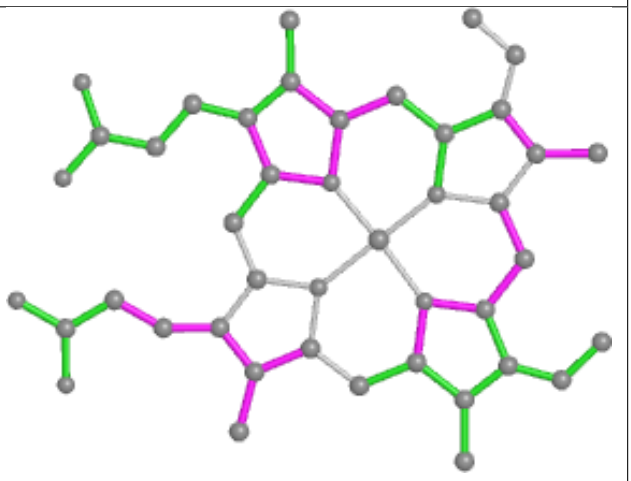


Rings

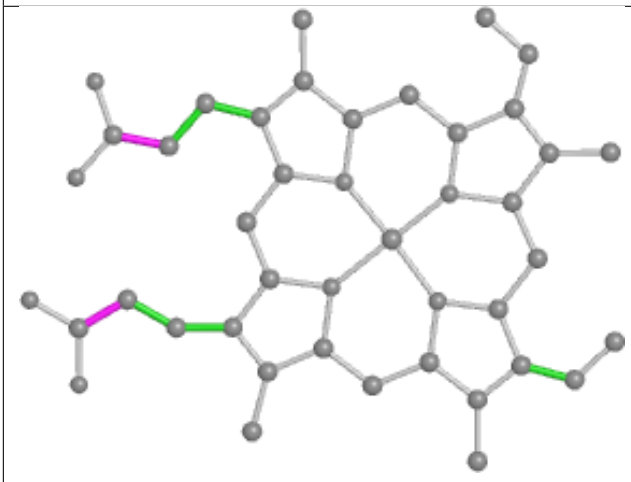
Ligand HEM H 202



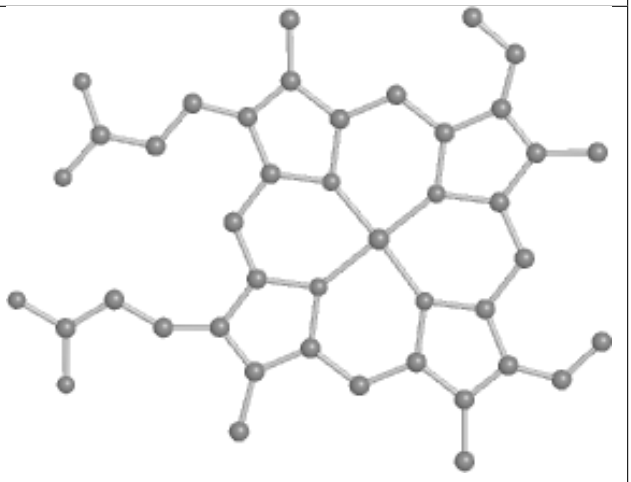
Bond lengths



Bond angles

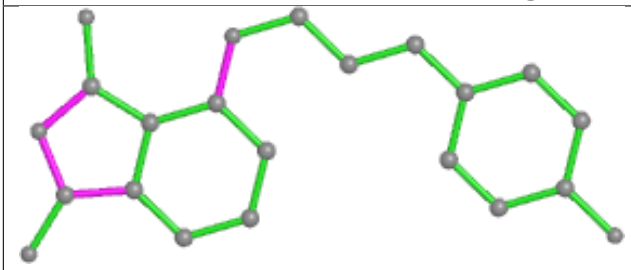


Torsions

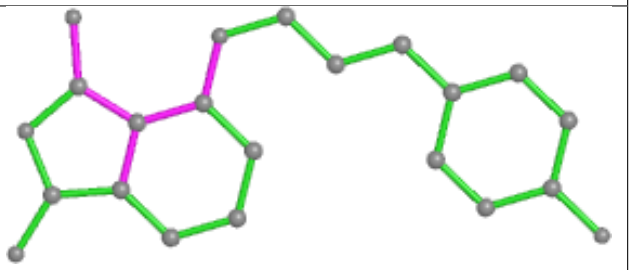


Rings

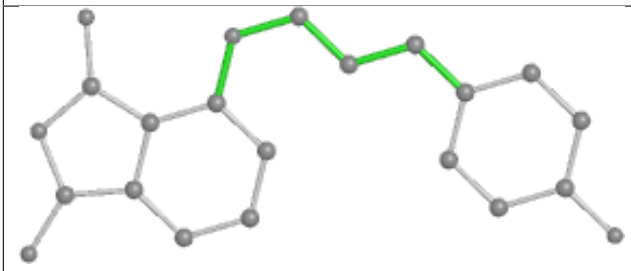
Ligand KTG E 201



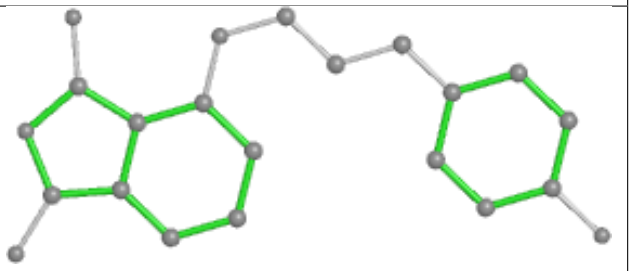
Bond lengths



Bond angles

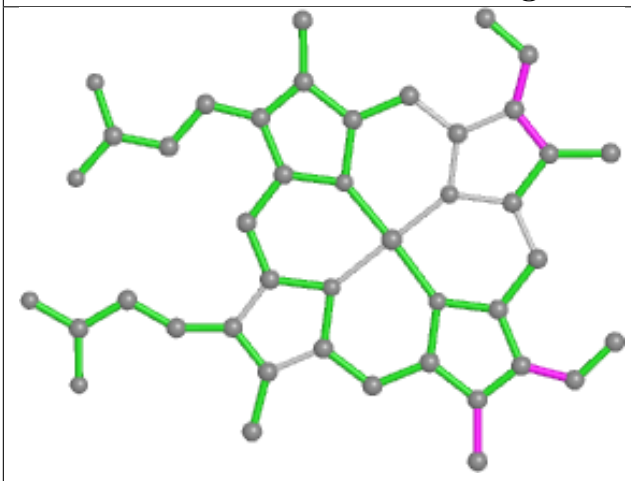


Torsions

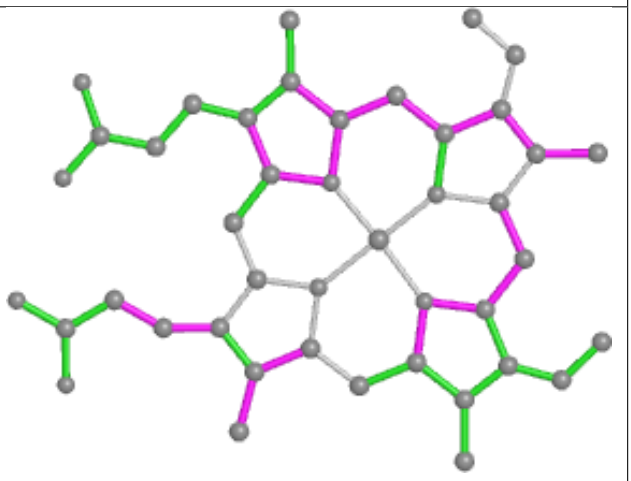


Rings

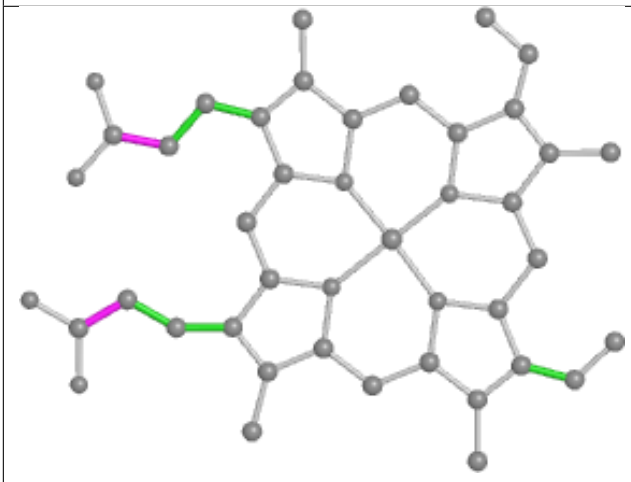
Ligand HEM F 202



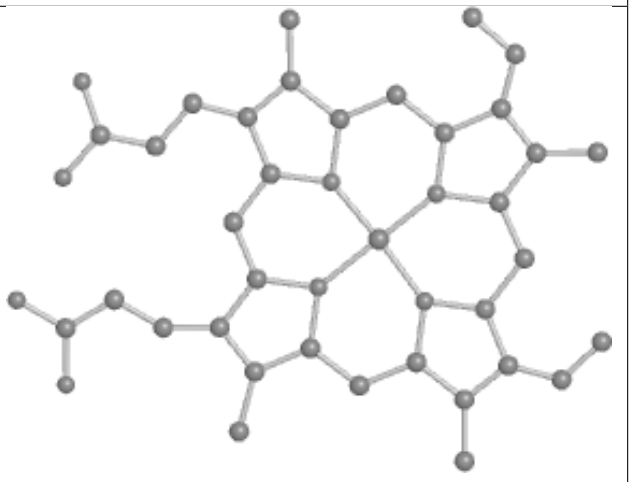
Bond lengths



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.