Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:42 AM EDT

PDB ID	:	6NH7
Title	:	Structure of human endothelial nitric oxide synthase heme domain in complex with 6-(3-(3-(dimethylamino)propyl)-2,5,6-trifluorophenethyl)-4-methylpyridin-2-amine
Authors	:	Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on	:	2018-12-21
Resolution	:	1.90 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 1.90 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

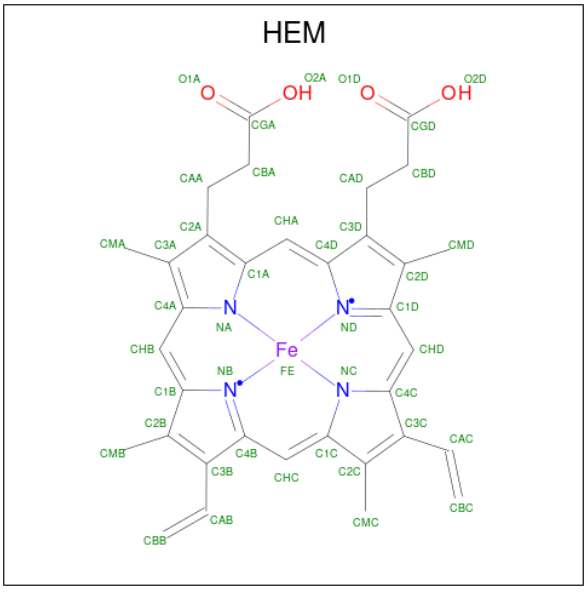
There are 7 unique types of molecules in this entry. The entry contains 7012 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Endothelial nitric oxide synthase splice variant eNOS13A.

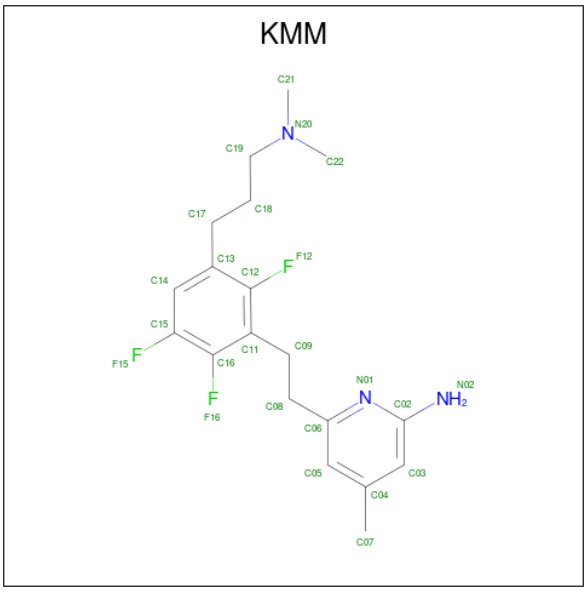
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	401	Total	C	N	O	S	0	4	0
			3220	2051	566	587	16			
1	B	402	Total	C	N	O	S	0	5	0
			3232	2058	569	588	17			

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



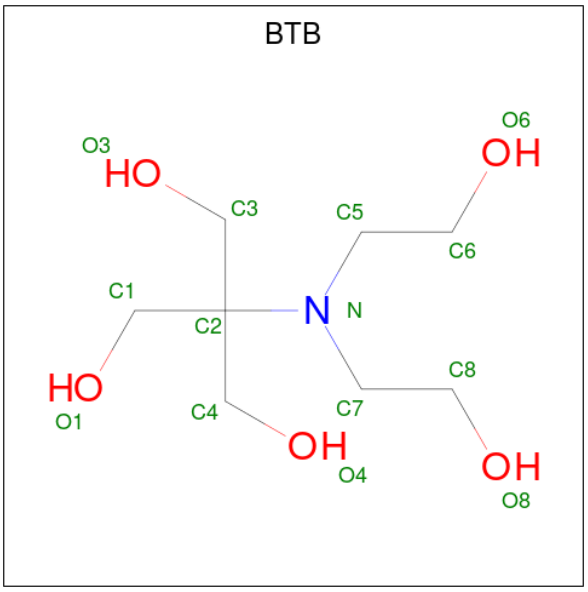
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 6-(2-{3-[3-(dimethylamino)propyl]-2,5,6-trifluorophenyl}ethyl)-4-methylpyridin-2-amine (three-letter code: KMM) (formula: $C_{19}H_{24}F_3N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	N	0	0
			25	19	3	3		
3	A	1	Total	C	F	N	0	0
			25	19	3	3		
3	B	1	Total	C	F	N	0	0
			25	19	3	3		
3	B	1	Total	C	F	N	0	0
			25	19	3	3		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0

- Molecule 6 is GADOLINIUM ATOM (three-letter code: GD) (formula: Gd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Gd 2 2	0	0
6	B	2	Total Gd 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	111	Total O 111 111	0	0
7	B	160	Total O 160 160	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	55.96Å 109.38Å 153.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.73 – 1.90	Depositor
% Data completeness (in resolution range)	99.8 (76.73-1.90)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.11.1-2575_1496	Depositor
R, R_{free}	0.210 , 0.258	Depositor
Wilson B-factor (Å^2)	29.6	Xtriage
Anisotropy	1.049	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7012	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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 18 ligands modelled in this entry, 5 are monoatomic - leaving 13 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	KMM	A	502	-	26,26,26	0.42	0	36,36,36	2.63	10 (27%)
3	KMM	B	503	-	26,26,26	0.45	0	36,36,36	1.94	6 (16%)
4	BTB	A	505	-	13,13,13	0.46	0	7,16,16	0.56	0
2	HEM	A	501	1	41,50,50	1.57	5 (12%)	45,82,82	1.79	12 (26%)
4	BTB	B	506	-	13,13,13	0.57	0	7,16,16	0.68	0
3	KMM	A	503	-	26,26,26	0.38	0	36,36,36	2.14	9 (25%)
4	BTB	A	504	6	13,13,13	0.43	0	7,16,16	0.68	0
4	BTB	B	504	6	13,13,13	0.51	0	7,16,16	0.51	0
4	BTB	B	505	6	13,13,13	0.53	0	7,16,16	1.06	1 (14%)
4	BTB	A	506	-	13,13,13	0.56	0	7,16,16	0.76	0
3	KMM	B	502	-	26,26,26	0.63	0	36,36,36	2.25	10 (27%)
2	HEM	B	501	1	41,50,50	1.52	7 (17%)	45,82,82	1.61	13 (28%)
4	BTB	A	507	-	13,13,13	0.54	0	7,16,16	0.79	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	KMM	A	502	-	-	3/11/11/11	0/2/2/2
3	KMM	B	503	-	-	4/11/11/11	0/2/2/2
4	BTB	A	505	-	-	8/21/21/21	-
2	HEM	A	501	1	-	1/12/54/54	-
4	BTB	B	506	-	-	2/21/21/21	-
3	KMM	A	503	-	-	6/11/11/11	0/2/2/2
4	BTB	A	504	6	-	5/21/21/21	-
4	BTB	B	504	6	-	0/21/21/21	-
4	BTB	B	505	6	-	16/21/21/21	-
4	BTB	A	506	-	-	11/21/21/21	-
3	KMM	B	502	-	-	6/11/11/11	0/2/2/2
2	HEM	B	501	1	-	1/12/54/54	-
4	BTB	A	507	-	-	4/21/21/21	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	FE-NB	4.29	2.18	1.96
2	B	501	HEM	C3C-C2C	-3.54	1.35	1.40
2	A	501	HEM	C3C-CAC	3.41	1.54	1.47
2	A	501	HEM	C3C-C2C	-3.26	1.35	1.40
2	B	501	HEM	CAB-C3B	3.25	1.56	1.47
2	A	501	HEM	CAB-C3B	2.95	1.55	1.47
2	B	501	HEM	FE-NB	2.74	2.10	1.96
2	B	501	HEM	C3C-CAC	2.71	1.53	1.47
2	B	501	HEM	CMA-C3A	2.38	1.56	1.51
2	B	501	HEM	CMB-C2B	2.21	1.55	1.50
2	A	501	HEM	CMB-C2B	2.17	1.55	1.50
2	B	501	HEM	CMD-C2D	2.17	1.55	1.50

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	KMM	C11-C12-C13	-8.67	119.71	124.98
3	A	503	KMM	C11-C12-C13	-7.85	120.21	124.98
3	B	502	KMM	C11-C12-C13	-7.63	120.34	124.98
3	A	502	KMM	C02-N01-C06	7.61	123.87	118.10
3	B	503	KMM	C11-C12-C13	-7.11	120.66	124.98
3	B	502	KMM	C02-N01-C06	5.76	122.47	118.10
3	A	502	KMM	C08-C09-C11	-4.79	103.66	112.49
3	A	503	KMM	C02-N01-C06	4.37	121.41	118.10
3	B	503	KMM	C02-N01-C06	4.24	121.31	118.10
2	B	501	HEM	C1B-NB-C4B	3.99	109.19	105.07
3	B	502	KMM	C08-C09-C11	-3.97	105.17	112.49
3	A	503	KMM	C09-C11-C12	-3.83	118.29	122.06
3	A	502	KMM	C09-C11-C16	-3.80	118.33	122.06
3	B	502	KMM	C05-C06-N01	-3.75	118.92	122.90
2	A	501	HEM	C4D-ND-C1D	3.75	108.95	105.07
2	A	501	HEM	C4B-CHC-C1C	3.74	127.50	122.56
3	A	502	KMM	C05-C06-N01	-3.71	118.96	122.90
3	B	503	KMM	C14-C13-C12	3.68	120.13	116.76
2	A	501	HEM	CBA-CAA-C2A	-3.66	106.37	112.62
3	A	502	KMM	C14-C13-C12	3.65	120.11	116.76
3	A	503	KMM	C14-C13-C12	3.63	120.08	116.76
3	B	503	KMM	C05-C06-N01	-3.55	119.14	122.90
2	A	501	HEM	C1B-NB-C4B	3.37	108.56	105.07
3	A	502	KMM	C16-C11-C12	3.36	119.88	115.90
3	B	502	KMM	C14-C13-C12	3.26	119.74	116.76
2	B	501	HEM	C4D-ND-C1D	3.13	108.31	105.07
3	B	502	KMM	C16-C11-C12	3.09	119.56	115.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	KMM	C16-C11-C12	3.01	119.46	115.90
3	B	502	KMM	C08-C06-C05	2.93	125.10	121.22
3	B	503	KMM	C08-C06-N01	2.90	120.26	115.95
2	A	501	HEM	CHC-C4B-C3B	2.87	128.96	124.57
2	A	501	HEM	C4C-CHD-C1D	2.77	126.21	122.56
2	B	501	HEM	C4C-CHD-C1D	2.75	126.19	122.56
2	B	501	HEM	CBA-CAA-C2A	-2.75	107.93	112.62
2	B	501	HEM	C4B-CHC-C1C	2.71	126.13	122.56
3	A	503	KMM	C05-C06-N01	-2.67	120.07	122.90
3	A	502	KMM	C08-C06-C05	2.60	124.66	121.22
2	B	501	HEM	CBD-CAD-C3D	-2.60	105.40	112.63
2	B	501	HEM	C3B-C2B-C1B	2.55	108.38	106.49
3	B	503	KMM	C16-C11-C12	2.54	118.91	115.90
2	A	501	HEM	CMC-C2C-C3C	2.53	129.41	124.68
2	A	501	HEM	CMA-C3A-C4A	-2.52	124.59	128.46
2	A	501	HEM	C3D-C4D-ND	-2.50	107.38	110.17
3	B	502	KMM	C11-C16-C15	-2.37	120.23	121.92
3	B	502	KMM	C09-C11-C16	-2.37	119.73	122.06
2	B	501	HEM	C2B-C1B-NB	-2.36	107.04	109.84
3	A	502	KMM	C04-C05-C06	-2.34	118.79	120.32
3	A	503	KMM	C11-C16-C15	-2.32	120.27	121.92
4	B	505	BTB	O4-C4-C2	-2.31	105.12	111.44
3	A	503	KMM	C08-C06-N01	2.29	119.36	115.95
2	A	501	HEM	CHD-C1D-C2D	2.27	128.53	124.98
3	A	503	KMM	F12-C12-C13	2.22	120.20	117.85
3	A	502	KMM	C11-C16-C15	-2.10	120.42	121.92
3	B	502	KMM	F12-C12-C13	2.08	120.05	117.85
2	B	501	HEM	CHC-C4B-C3B	2.08	127.75	124.57
2	A	501	HEM	C3B-C2B-C1B	2.08	108.03	106.49
2	B	501	HEM	CMA-C3A-C4A	-2.07	125.28	128.46
2	B	501	HEM	C3D-C4D-ND	-2.05	107.88	110.17
2	A	501	HEM	C2D-C1D-ND	-2.04	107.44	109.88
2	B	501	HEM	C2C-C3C-C4C	2.03	108.32	106.90
2	B	501	HEM	CHB-C1B-NB	2.02	126.88	124.38

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	KMM	C08-C09-C11-C12
3	A	503	KMM	C12-C13-C17-C18
3	B	503	KMM	C12-C13-C17-C18

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Mol	Chain	Res	Type	Atoms
4	A	504	BTB	O1-C1-C2-C3
4	A	504	BTB	O1-C1-C2-C4
4	A	505	BTB	O1-C1-C2-C3
4	A	505	BTB	O1-C1-C2-C4
4	A	505	BTB	O1-C1-C2-N
4	A	505	BTB	C6-C5-N-C7
4	A	506	BTB	O1-C1-C2-C3
4	A	506	BTB	O1-C1-C2-C4
4	A	506	BTB	O1-C1-C2-N
4	A	506	BTB	C1-C2-C3-O3
4	A	506	BTB	C4-C2-C3-O3
4	A	506	BTB	C6-C5-N-C7
4	A	507	BTB	C4-C2-C3-O3
4	A	507	BTB	N-C2-C3-O3
4	A	507	BTB	C6-C5-N-C7
4	B	505	BTB	O1-C1-C2-C4
4	B	505	BTB	N-C2-C3-O3
4	B	505	BTB	C1-C2-C4-O4
4	B	505	BTB	C1-C2-N-C5
4	B	505	BTB	C1-C2-N-C7
4	B	505	BTB	C3-C2-N-C5
4	B	505	BTB	C3-C2-N-C7
4	B	505	BTB	C4-C2-N-C5
4	B	505	BTB	C4-C2-N-C7
4	B	505	BTB	C8-C7-N-C5
4	B	506	BTB	C8-C7-N-C5
4	B	506	BTB	N-C7-C8-O8
3	B	502	KMM	C18-C19-N20-C22
4	A	506	BTB	N-C7-C8-O8
3	B	503	KMM	C18-C19-N20-C22
3	B	502	KMM	C17-C18-C19-N20
4	B	505	BTB	N-C7-C8-O8
3	B	502	KMM	C18-C19-N20-C21
3	B	503	KMM	C18-C19-N20-C21
4	B	505	BTB	N-C5-C6-O6
3	A	503	KMM	C17-C18-C19-N20
3	A	502	KMM	C17-C18-C19-N20
4	A	506	BTB	N-C5-C6-O6
3	A	503	KMM	C18-C19-N20-C22
3	B	503	KMM	C17-C18-C19-N20
2	A	501	HEM	C4B-C3B-CAB-CBB
2	B	501	HEM	C4B-C3B-CAB-CBB

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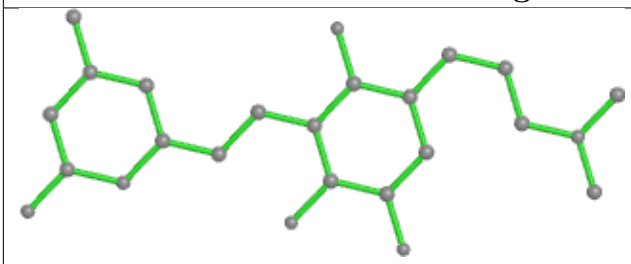
Mol	Chain	Res	Type	Atoms
4	A	504	BTB	C1-C2-C3-O3
4	A	504	BTB	C4-C2-C3-O3
4	A	507	BTB	C1-C2-C3-O3
4	B	505	BTB	O1-C1-C2-C3
4	B	505	BTB	C1-C2-C3-O3
4	B	505	BTB	C4-C2-C3-O3
4	A	504	BTB	O1-C1-C2-N
4	A	505	BTB	N-C2-C3-O3
4	A	505	BTB	C3-C2-N-C5
4	A	506	BTB	N-C2-C3-O3
4	A	506	BTB	C1-C2-N-C5
4	A	506	BTB	C3-C2-N-C5
4	B	505	BTB	O1-C1-C2-N
3	B	502	KMM	N01-C06-C08-C09
3	A	502	KMM	C05-C06-C08-C09
3	A	503	KMM	C05-C06-C08-C09
3	B	502	KMM	C05-C06-C08-C09
3	A	502	KMM	N01-C06-C08-C09
3	A	503	KMM	N01-C06-C08-C09
3	B	502	KMM	C12-C13-C17-C18
4	A	505	BTB	C1-C2-C3-O3
4	A	505	BTB	C4-C2-C3-O3

There are no ring outliers.

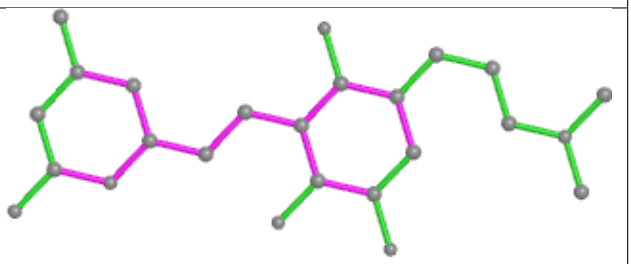
No monomer is involved in short contacts.

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.

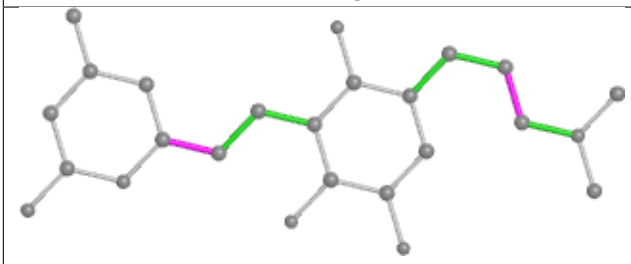
Ligand KMM A 502



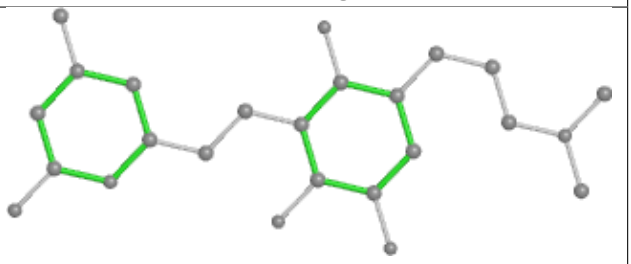
Bond lengths



Bond angles

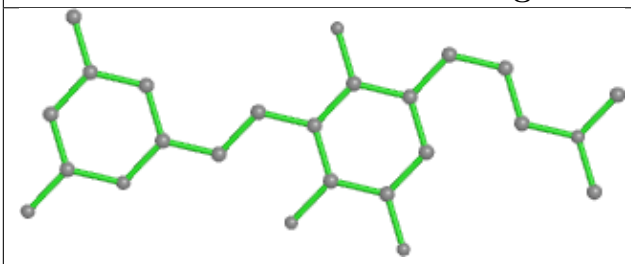


Torsions

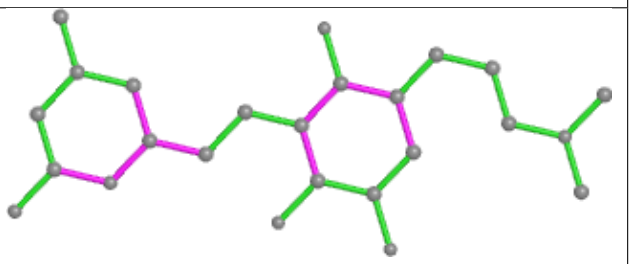


Rings

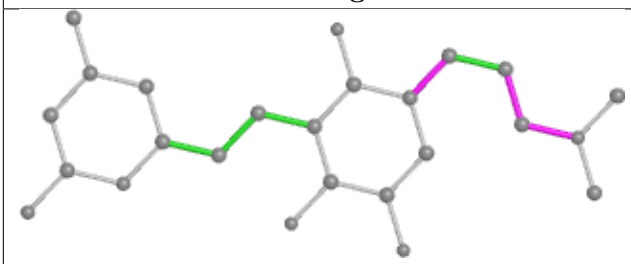
Ligand KMM B 503



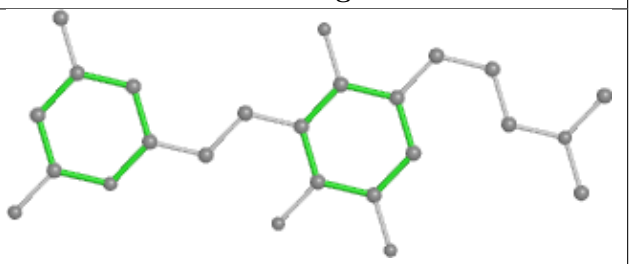
Bond lengths



Bond angles

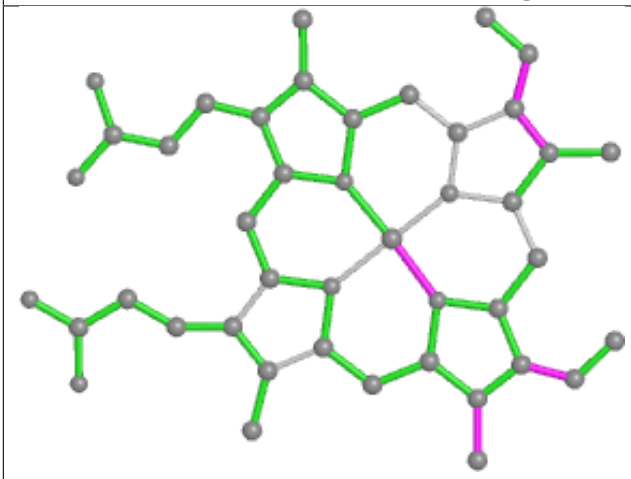


Torsions

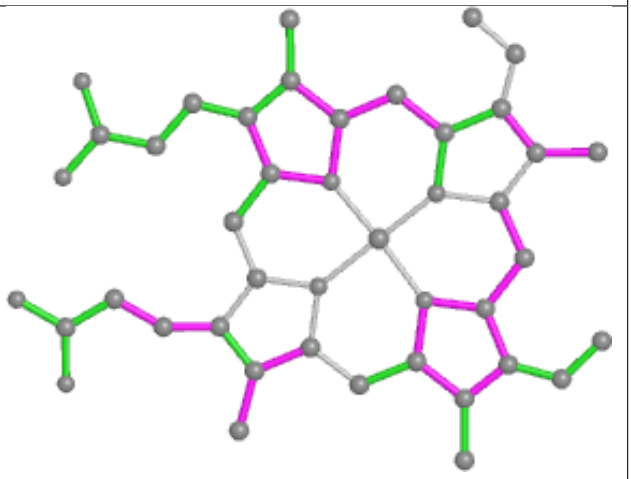


Rings

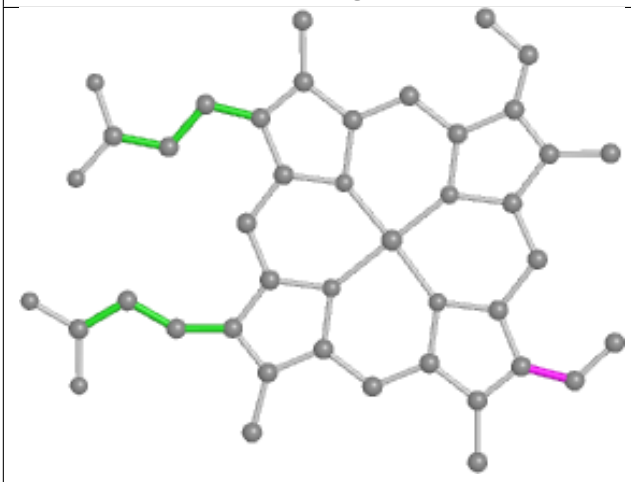
Ligand HEM A 501



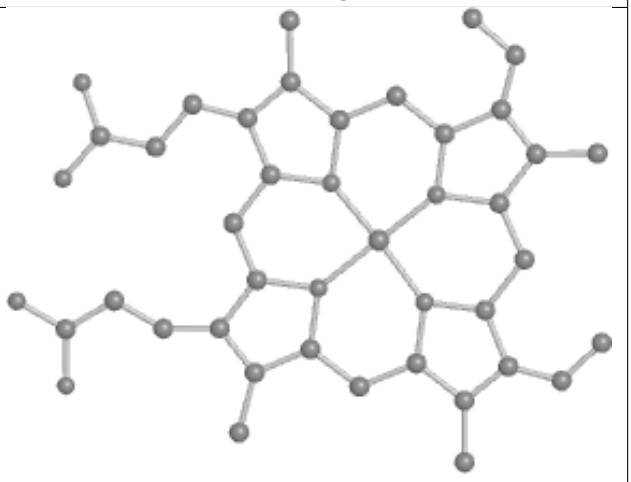
Bond lengths



Bond angles

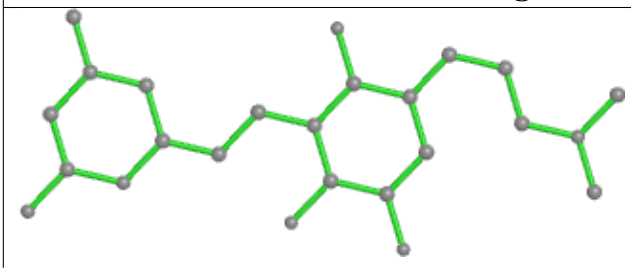


Torsions

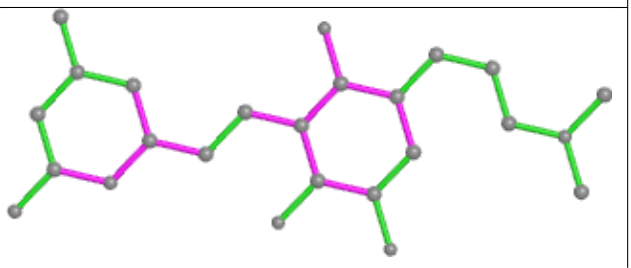


Rings

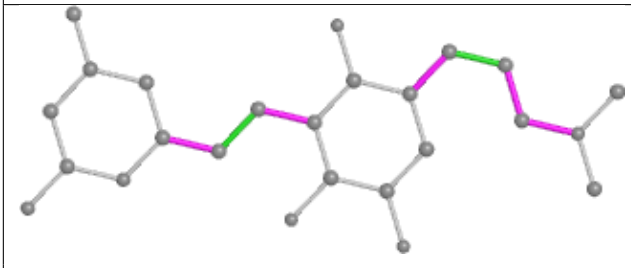
Ligand KMM A 503



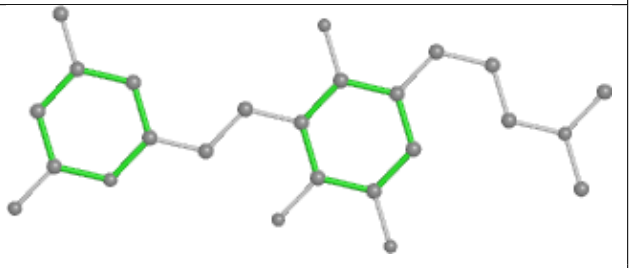
Bond lengths



Bond angles

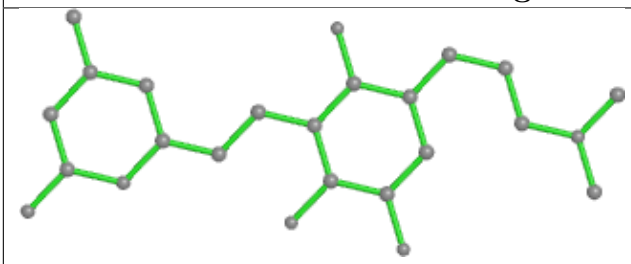


Torsions

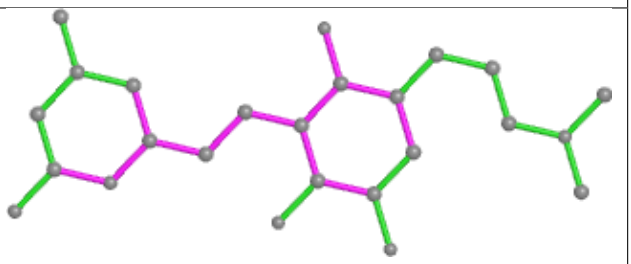


Rings

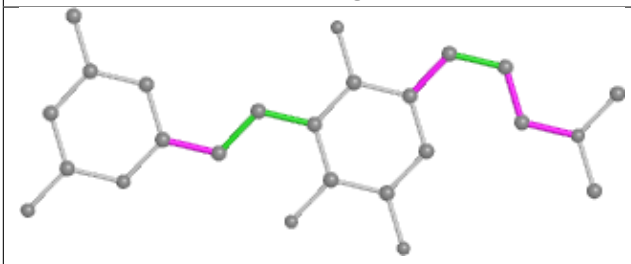
Ligand KMM B 502



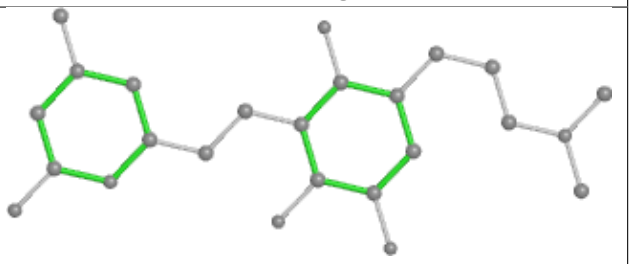
Bond lengths



Bond angles

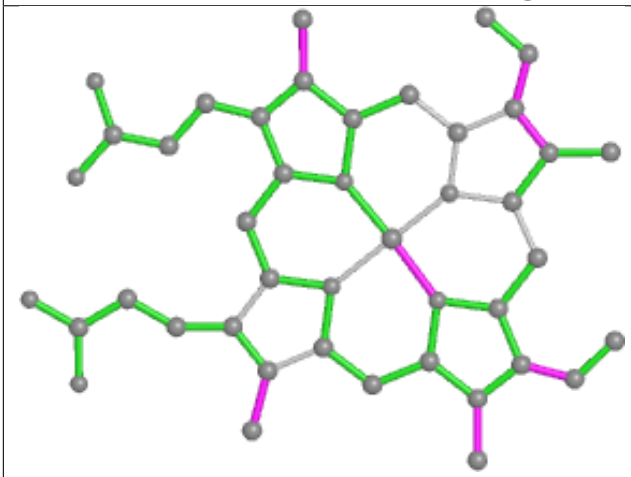


Torsions

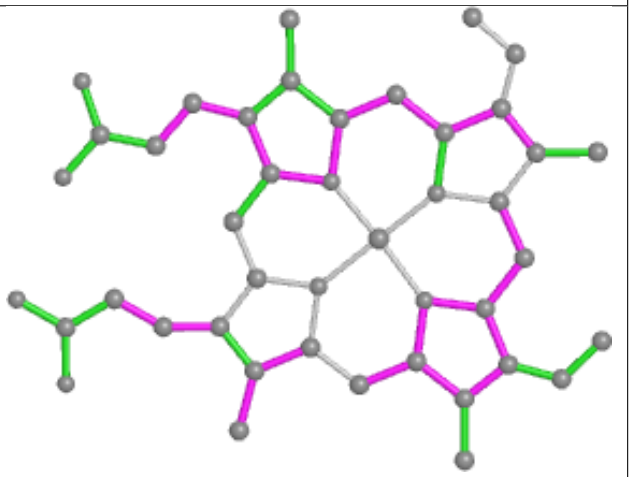


Rings

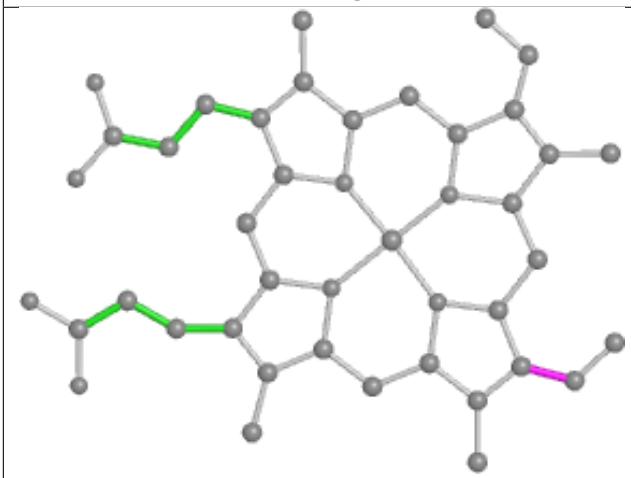
Ligand HEM B 501



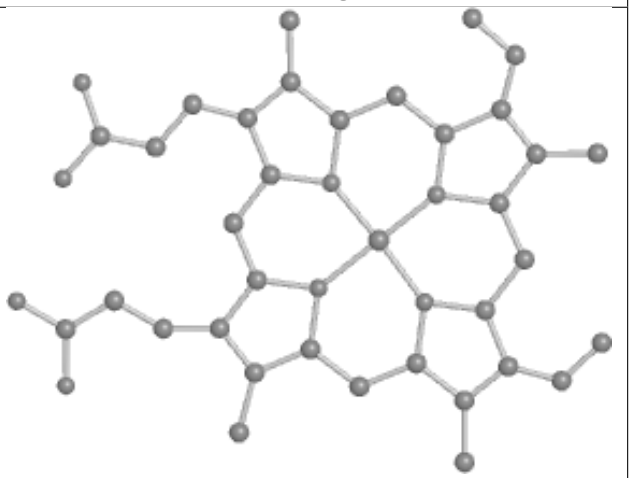
Bond lengths



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.