Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 10:50 PM EDT

PDB ID	:	6Q2C
Title	:	Domain-swapped dimer of Acanthamoeba castellanii CYP51
Authors	:	Sharma, V.; Podust, L.M.
Deposited on	:	2019-08-07
Resolution	:	1.80 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 1.80 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 7890 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	4	0
			3601	2327	600	656	18			
1	B	449	Total	C	N	O	S	0	3	0
			3583	2317	597	651	18			

There are 32 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
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

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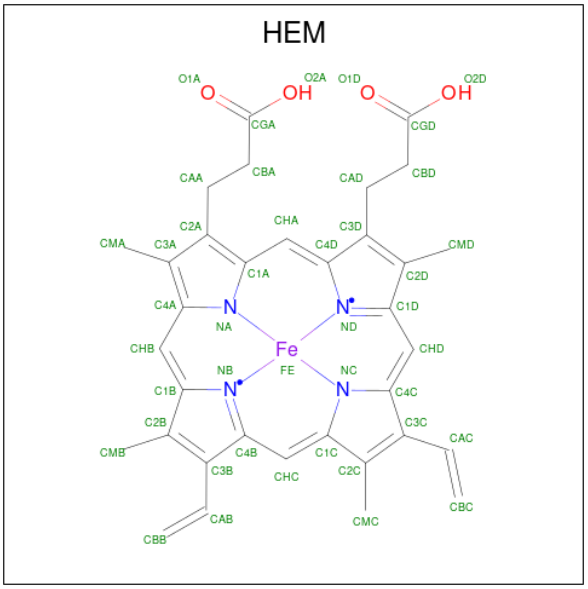
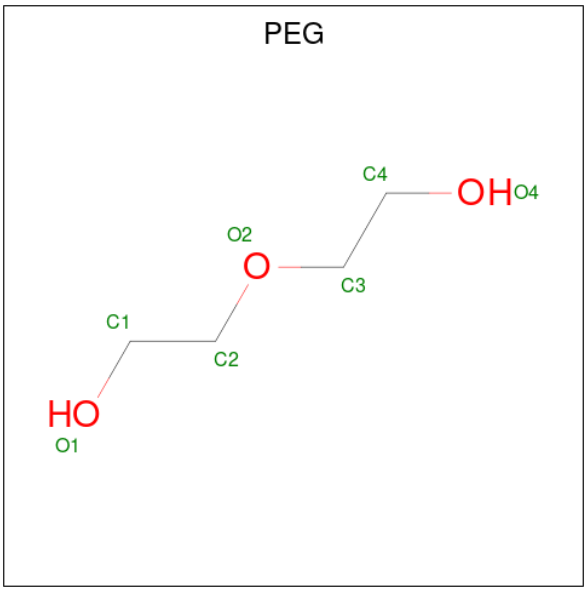
Chain	Residue	Modelled	Actual	Comment	Reference
B	42	LYS	-	expression tag	UNP L8GJB3
B	487	HIS	-	expression tag	UNP L8GJB3
B	488	HIS	-	expression tag	UNP L8GJB3
B	489	HIS	-	expression tag	UNP L8GJB3
B	490	HIS	-	expression tag	UNP L8GJB3
B	491	HIS	-	expression tag	UNP L8GJB3
B	492	HIS	-	expression tag	UNP L8GJB3

- 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	1
			86	68	2	8	8		
2	B	1	Total	C	Fe	N	O	0	1
			86	68	2	8	8		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	279	Total O 279 279	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	231	Total O 231 231	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	100.35Å 101.57Å 123.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.51 – 1.80	Depositor
% Data completeness (in resolution range)	98.1 (78.51-1.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.185 , 0.227	Depositor
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.235	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for k,h,-l	Xtriage
Total number of atoms	7890	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
2	HEM	A	501[A]	1,6	41,50,50	1.42	7 (17%)	45,82,82	1.95	16 (35%)
2	HEM	A	501[B]	1,6	41,50,50	1.36	6 (14%)	45,82,82	2.13	15 (33%)
3	PEG	B	502	-	6,6,6	1.01	0	5,5,5	1.26	0
2	HEM	B	501[B]	1,6	41,50,50	1.23	3 (7%)	45,82,82	1.95	16 (35%)
2	HEM	B	501[A]	1,6	41,50,50	1.28	5 (12%)	45,82,82	1.78	12 (26%)
3	PEG	A	503	-	6,6,6	0.61	0	5,5,5	0.72	0
3	PEG	A	502	-	6,6,6	0.84	0	5,5,5	0.84	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
2	HEM	A	501[A]	1,6	-	0/12/54/54	-
2	HEM	A	501[B]	1,6	-	0/12/54/54	-
3	PEG	B	502	-	-	1/4/4/4	-
2	HEM	B	501[B]	1,6	-	4/12/54/54	-
2	HEM	B	501[A]	1,6	-	0/12/54/54	-
3	PEG	A	503	-	-	2/4/4/4	-
3	PEG	A	502	-	-	2/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	HEM	C1B-NB	-4.74	1.32	1.40
2	B	501[A]	HEM	C1B-NB	-3.98	1.33	1.40
2	B	501[B]	HEM	C1B-NB	-3.95	1.33	1.40
2	A	501[A]	HEM	C1B-NB	-3.86	1.33	1.40
2	A	501[B]	HEM	C4B-NB	-3.16	1.32	1.38
2	A	501[A]	HEM	C4B-NB	-2.87	1.32	1.38
2	A	501[A]	HEM	C4D-ND	-2.80	1.35	1.40
2	B	501[A]	HEM	CHB-C1B	2.54	1.41	1.35
2	A	501[B]	HEM	CHB-C1B	2.53	1.41	1.35
2	A	501[A]	HEM	CHB-C1B	2.53	1.41	1.35
2	A	501[A]	HEM	C4D-C3D	2.50	1.49	1.45
2	B	501[A]	HEM	FE-NB	2.43	2.08	1.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501[B]	HEM	C4B-NB	-2.42	1.33	1.38
2	B	501[A]	HEM	C4B-NB	-2.40	1.33	1.38
2	A	501[A]	HEM	FE-NB	2.32	2.08	1.96
2	A	501[B]	HEM	C1B-C2B	-2.32	1.40	1.44
2	A	501[B]	HEM	C4D-ND	-2.16	1.36	1.40
2	B	501[B]	HEM	CHB-C1B	2.10	1.40	1.35
2	B	501[A]	HEM	C4D-C3D	2.09	1.48	1.45
2	A	501[A]	HEM	CBD-CGD	2.08	1.55	1.50
2	A	501[B]	HEM	C1D-C2D	2.04	1.48	1.44

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501[B]	HEM	C1B-NB-C4B	5.64	110.90	105.07
2	A	501[B]	HEM	CHC-C4B-NB	5.35	130.24	124.43
2	B	501[B]	HEM	CAD-C3D-C4D	4.70	132.88	124.66
2	A	501[A]	HEM	C1B-NB-C4B	4.55	109.77	105.07
2	A	501[B]	HEM	O2D-CGD-CBD	4.48	128.42	114.03
2	B	501[B]	HEM	CHC-C4B-NB	4.40	129.21	124.43
2	A	501[A]	HEM	CHC-C4B-NB	4.39	129.20	124.43
2	B	501[A]	HEM	O2A-CGA-O1A	-3.94	113.48	123.30
2	B	501[B]	HEM	C1B-NB-C4B	3.88	109.08	105.07
2	A	501[B]	HEM	O1D-CGD-CBD	-3.62	111.45	123.08
2	A	501[B]	HEM	CHA-C4D-C3D	-3.52	118.72	125.33
2	A	501[B]	HEM	CHA-C4D-ND	3.47	128.67	124.38
2	A	501[A]	HEM	C3D-C4D-ND	3.43	113.98	110.17
2	B	501[A]	HEM	CHC-C4B-NB	3.42	128.15	124.43
2	B	501[A]	HEM	C1B-NB-C4B	3.33	108.52	105.07
2	A	501[A]	HEM	CBA-CAA-C2A	3.28	118.21	112.62
2	B	501[B]	HEM	CAD-C3D-C2D	-3.17	121.97	127.88
2	A	501[A]	HEM	CHA-C4D-C3D	-3.12	119.47	125.33
2	B	501[A]	HEM	C4B-C3B-C2B	-3.04	104.70	107.11
2	A	501[A]	HEM	O2A-CGA-CBA	2.92	123.41	114.03
2	B	501[B]	HEM	CHB-C1B-NB	2.89	127.95	124.38
2	A	501[B]	HEM	C4B-C3B-C2B	-2.87	104.83	107.11
2	A	501[A]	HEM	CAD-C3D-C4D	2.84	129.63	124.66
2	B	501[B]	HEM	CHD-C1D-ND	2.81	127.48	124.43
2	B	501[A]	HEM	O2A-CGA-CBA	2.80	123.01	114.03
2	A	501[B]	HEM	CHB-C1B-NB	2.74	127.76	124.38
2	B	501[A]	HEM	CBA-CAA-C2A	2.69	117.20	112.62
2	A	501[B]	HEM	CMC-C2C-C3C	2.66	129.65	124.68
2	B	501[B]	HEM	CHD-C1D-C2D	-2.65	120.84	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501[A]	HEM	CMC-C2C-C3C	2.62	129.58	124.68
2	B	501[A]	HEM	O2D-CGD-CBD	2.56	122.25	114.03
2	A	501[A]	HEM	CHD-C1D-C2D	-2.52	121.05	124.98
2	A	501[A]	HEM	C4B-CHC-C1C	2.51	125.87	122.56
2	B	501[A]	HEM	CAD-C3D-C4D	2.50	129.02	124.66
2	A	501[A]	HEM	CMC-C2C-C3C	2.49	129.33	124.68
2	B	501[B]	HEM	CAA-CBA-CGA	-2.49	106.79	113.76
2	B	501[A]	HEM	CHA-C4D-C3D	-2.49	120.66	125.33
2	B	501[B]	HEM	CMC-C2C-C3C	2.49	129.33	124.68
2	B	501[B]	HEM	O2A-CGA-CBA	2.46	121.94	114.03
2	A	501[A]	HEM	CAD-CBD-CGD	2.41	118.78	113.60
2	A	501[A]	HEM	O2A-CGA-O1A	-2.31	117.54	123.30
2	A	501[A]	HEM	CHD-C1D-ND	2.26	126.88	124.43
2	A	501[B]	HEM	CHD-C1D-ND	2.24	126.87	124.43
2	B	501[B]	HEM	CBD-CAD-C3D	2.23	118.83	112.63
2	B	501[B]	HEM	O2D-CGD-CBD	2.21	121.13	114.03
2	A	501[B]	HEM	CBD-CAD-C3D	2.21	118.76	112.63
2	A	501[B]	HEM	C3D-C4D-ND	2.16	112.57	110.17
2	A	501[A]	HEM	C4D-ND-C1D	-2.15	102.86	105.07
2	B	501[B]	HEM	CHA-C4D-ND	2.14	127.03	124.38
2	B	501[A]	HEM	C3D-C4D-ND	2.09	112.49	110.17
2	A	501[B]	HEM	C3C-C4C-NC	-2.08	107.02	110.94
2	B	501[A]	HEM	CMD-C2D-C1D	2.08	128.20	125.04
2	B	501[B]	HEM	CHA-C4D-C3D	-2.07	121.44	125.33
2	A	501[B]	HEM	C2C-C3C-C4C	2.07	108.34	106.90
2	A	501[A]	HEM	C4D-C3D-C2D	-2.04	103.92	106.90
2	B	501[B]	HEM	CAD-CBD-CGD	-2.04	109.22	113.60
2	B	501[B]	HEM	O2A-CGA-O1A	-2.03	118.23	123.30
2	A	501[A]	HEM	O2D-CGD-O1D	-2.01	118.29	123.30
2	A	501[B]	HEM	CAB-C3B-C2B	2.01	135.22	128.60

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501[B]	HEM	C2D-C3D-CAD-CBD
2	B	501[B]	HEM	C4D-C3D-CAD-CBD
3	B	502	PEG	C1-C2-O2-C3
3	A	502	PEG	O1-C1-C2-O2
3	A	503	PEG	O1-C1-C2-O2
3	A	503	PEG	C4-C3-O2-C2
2	B	501[B]	HEM	CAD-CBD-CGD-O1D

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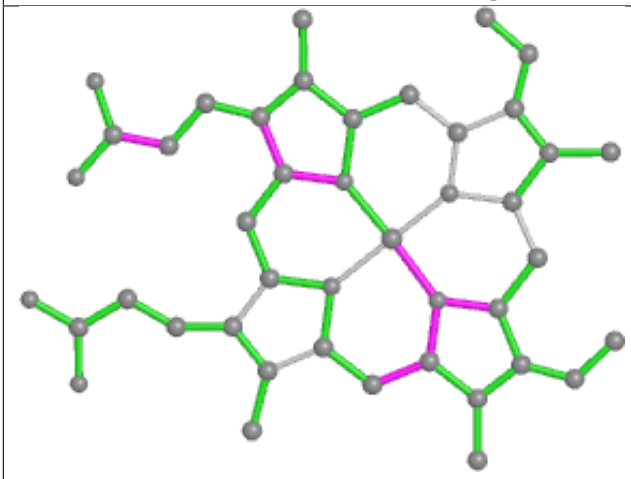
Mol	Chain	Res	Type	Atoms
2	B	501[B]	HEM	CAD-CBD-CGD-O2D
3	A	502	PEG	O2-C3-C4-O4

There are no ring outliers.

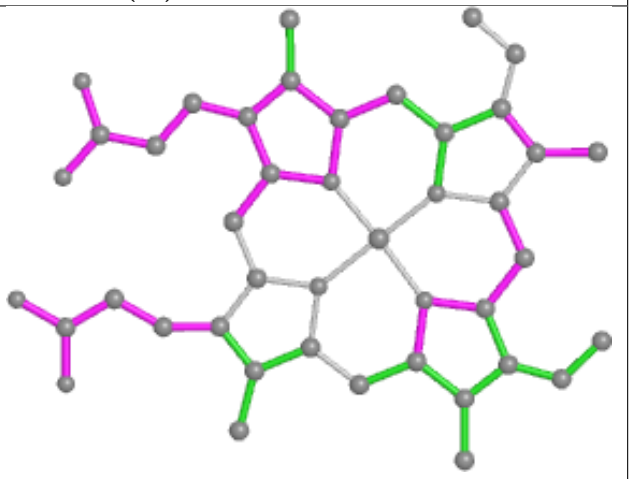
No monomer is involved in short contacts.

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.

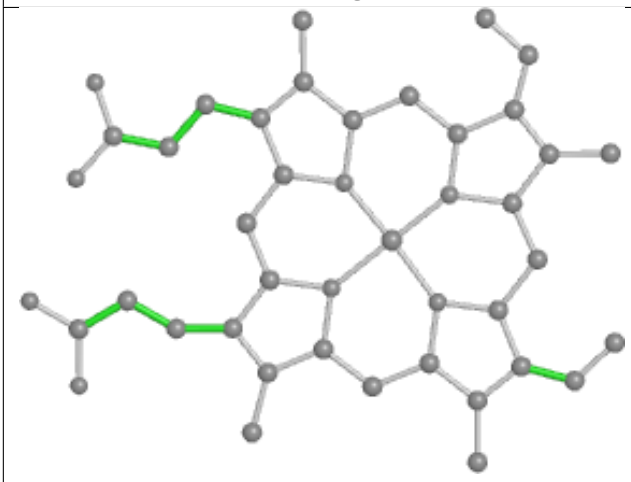
Ligand HEM A 501 (A)



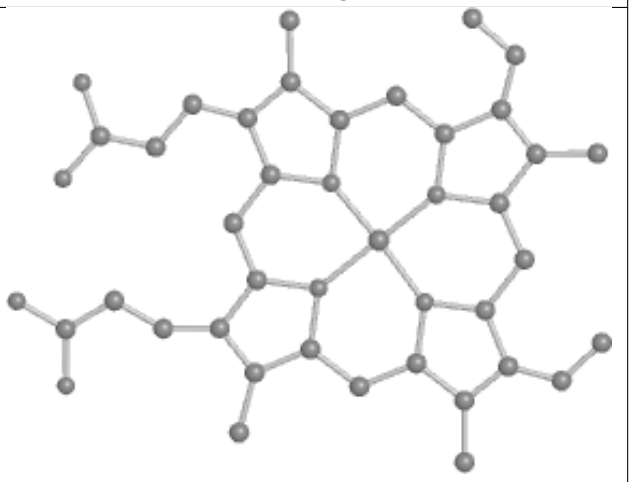
Bond lengths



Bond angles

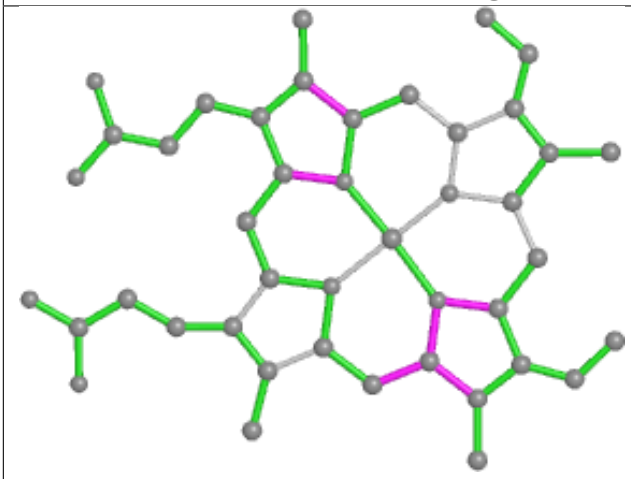


Torsions

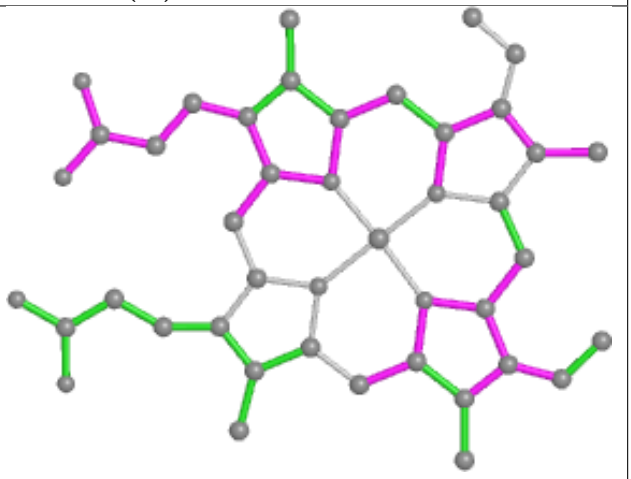


Rings

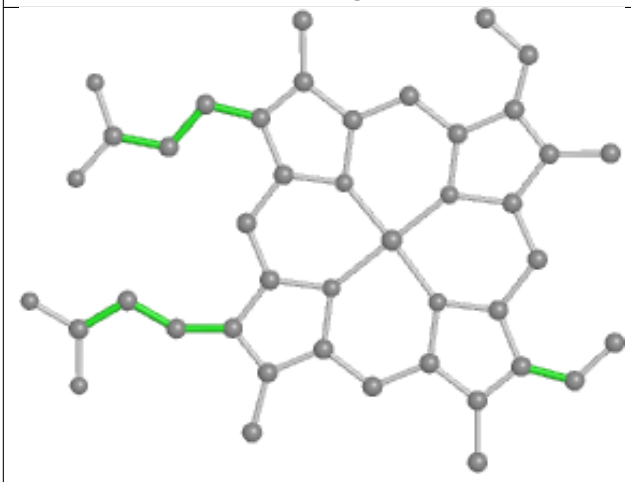
Ligand HEM A 501 (B)



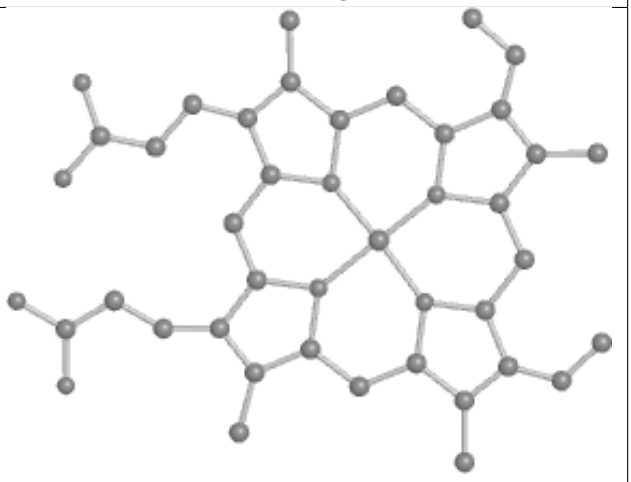
Bond lengths



Bond angles

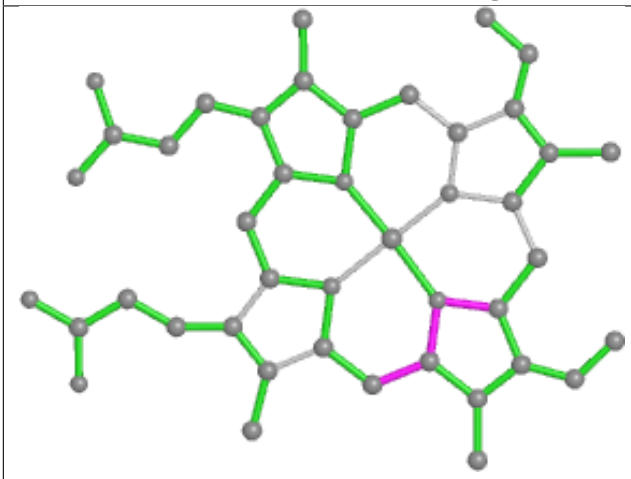


Torsions

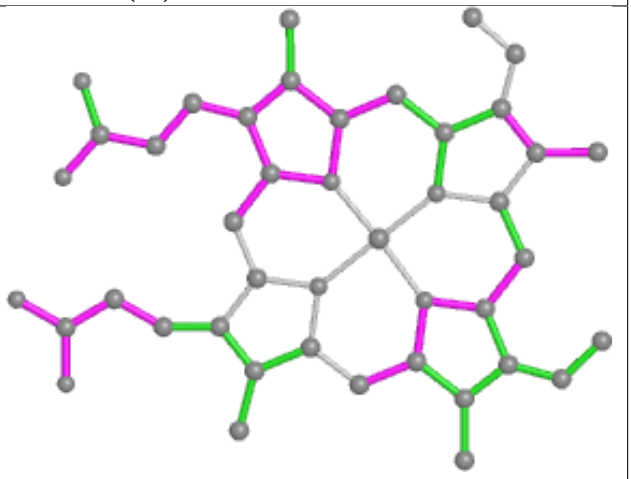


Rings

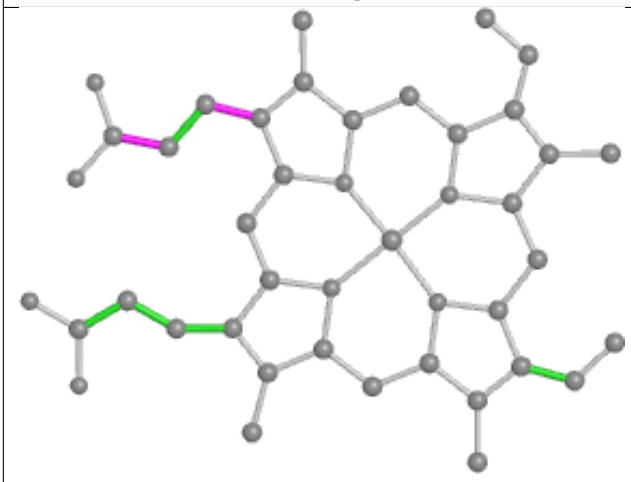
Ligand HEM B 501 (B)



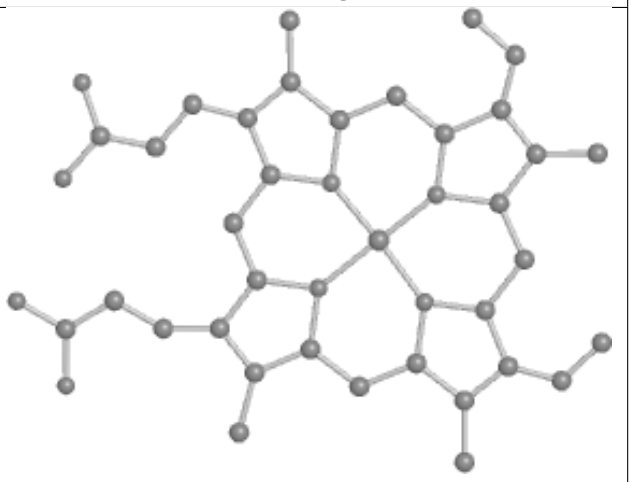
Bond lengths



Bond angles

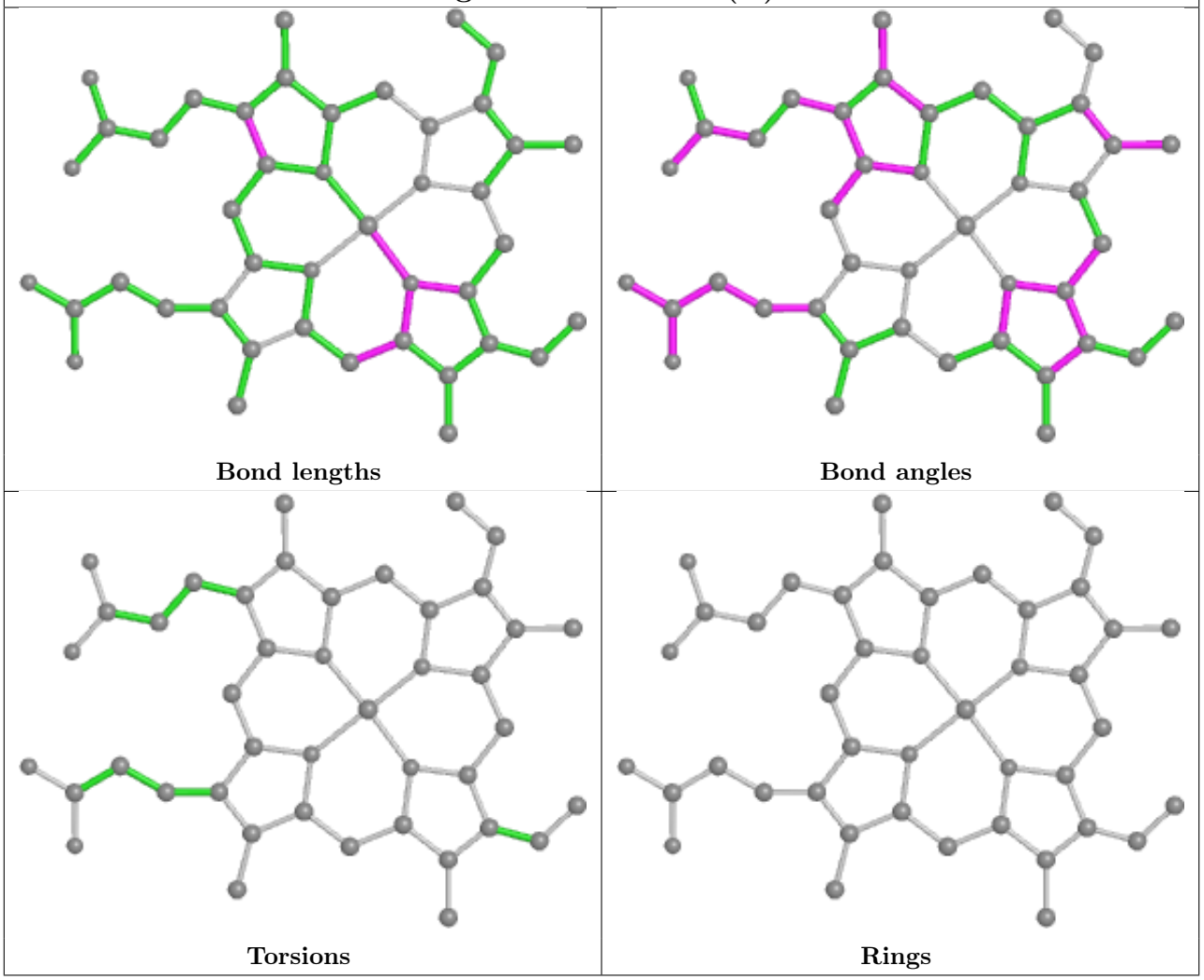


Torsions



Rings

Ligand HEM B 501 (A)



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.