Full wwPDB Geometry-Only Validation Report (i)

Oct 31, 2023 – 10:08 PM EDT

PDB ID	:	3KMF
Title	:	Room Temperature Time-of-Flight Neutron Diffraction Study of Deoxy Human Normal Adult Hemoglobin
Authors	:	Kovalevsky, A.Y.; Morimoto, Y.; Chatake, T.
Deposited on	:	2009-11-10
Resolution	:	2.00 Å(reported)

This is a Full wwPDB Geometry-Only 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 (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 (i)) were used in the production of this report:

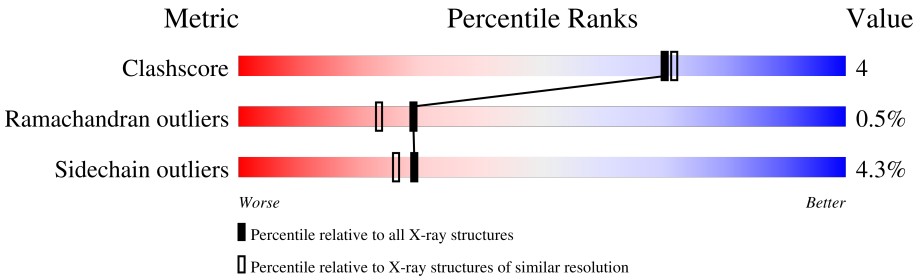
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
NEUTRON DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	141	93% 7%
1	E	141	82% 18%
2	C	146	87% 12%
2	G	146	88% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9975 atoms, of which 3579 are hydrogens and 1531 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.

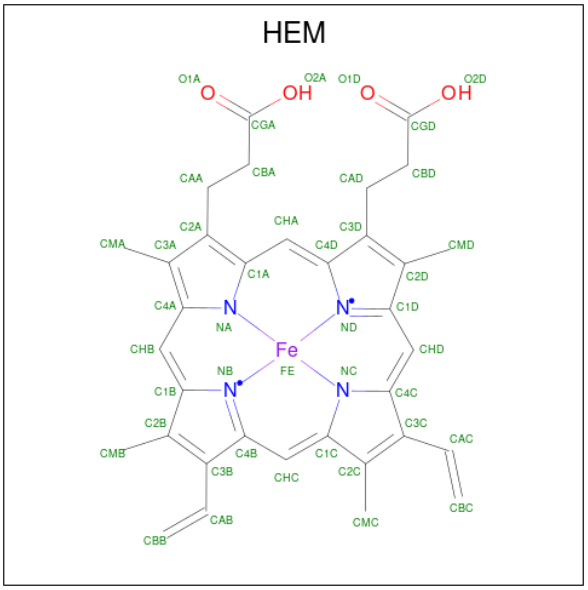
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	141	Total	C	D	H	N	O	S	3	0	0
			2140	685	227	844	187	194	3			
1	E	141	Total	C	D	H	N	O	S	3	0	0
			2146	685	233	844	187	194	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	C	146	Total	C	D	H	N	O	S	1	1	0
			2260	730	239	888	198	202	3			
2	G	146	Total	C	D	H	N	O	S	1	0	0
			2240	724	234	883	195	201	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	E	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
3	G	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	69	Total	D	O		0	0
			207	138	69			
4	C	73	Total	D	O		0	0
			219	146	73			
4	E	86	Total	D	O		0	0
			258	172	86			
4	G	71	Total	D	O		0	0
			213	142	71			

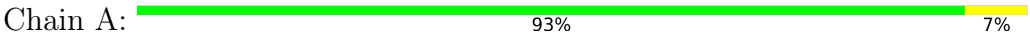
3 Residue-property plots (i)

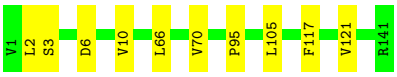
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: Hemoglobin subunit alpha

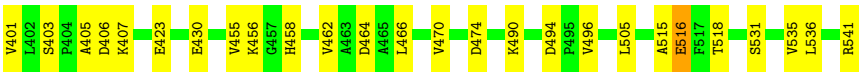
Chain A:





• Molecule 1: Hemoglobin subunit alpha

Chain E:

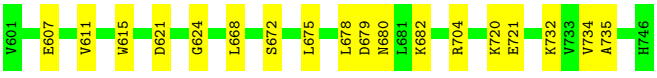


• Molecule 2: Hemoglobin subunit beta

Chain C:

• Molecule 2: Hemoglobin subunit beta

Chain G:



4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOD, HEM

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.33	0/1097	0.53	0/1491
1	E	0.38	0/1097	0.56	0/1491
2	C	0.35	0/1164	0.55	0/1581
2	G	0.34	0/1153	0.53	0/1566
All	All	0.35	0/4511	0.54	0/6129

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	704	ARG	Sidechain

4.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1296	844	1073	3	0
1	E	1302	844	1070	13	0
2	C	1372	888	1121	9	0
2	G	1357	883	1115	8	0
3	A	43	30	30	0	0
3	C	43	30	30	0	0
3	E	43	30	30	0	0
3	G	43	30	30	0	0
4	A	207	0	0	1	0
4	C	219	0	0	3	0
4	E	258	0	0	4	0
4	G	213	0	0	3	0
All	All	6396	3579	4499	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1004:DOD:O	1:E:401:VAL:HG11	1.52	1.02
1:E:494:ASP:OD2	1:E:496:VAL:HG12	1.79	0.77
2:C:207:GLU:O	2:C:211:VAL:HG23	1.95	0.61
1:E:541:ARG:N	4:E:1079:DOD:O	2.33	0.60
1:A:6:ASP:O	1:A:10:VAL:HG23	1.97	0.60
2:G:607:GLU:O	2:G:611:VAL:HG23	1.98	0.59
2:C:201:VAL:HG23	2:C:202:HIS:N	2.14	0.57
2:C:201:VAL:HG22	2:C:203:LEU:CD1	2.33	0.54
2:G:621:ASP:O	4:G:1042:DOD:O	2.22	0.53
1:E:466:LEU:O	1:E:470:VAL:HG23	2.04	0.53
2:C:232:LEU:HD23	2:C:238:THR:OG1	2.02	0.53
2:G:732:LYS:HG2	4:G:1247:DOD:O	2.03	0.53
1:E:518:THR:HG21	4:E:1030:DOD:O	2.05	0.51
2:C:326:VAL:HG21	4:C:1193:DOD:O	2.07	0.50
2:C:333:VAL:O	2:C:337:VAL:HG23	2.07	0.49
1:E:403:SER:O	1:E:406:ASP:HB2	2.08	0.48
1:E:407:LYS:NZ	1:E:474:ASP:OD1	2.47	0.47
1:E:458:HIS:O	1:E:462:VAL:HG23	2.09	0.47
2:G:720:LYS:HG2	2:G:721:GLU:N	2.25	0.45
1:E:405:ALA:HB2	4:E:1151:DOD:O	2.11	0.45
1:E:430:GLU:HG3	4:E:1179:DOD:O	2.12	0.45
2:G:734:VAL:HG23	2:G:735:ALA:N	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:O	1:A:70:VAL:HG23	2.12	0.43
1:E:515:ALA:HB3	1:E:516:GLU:OE1	2.14	0.43
1:E:516:GLU:CD	1:E:516:GLU:N	2.73	0.42
2:G:678:LEU:HB2	4:G:1204:DOD:O	2.15	0.41
1:E:531:SER:O	1:E:535:VAL:HG23	2.15	0.41
2:C:251:PRO:O	2:C:255:MET:HG2	2.15	0.41
2:C:212:THR:HG22	4:C:1290:DOD:O	2.14	0.41
2:G:624:GLY:N	2:G:668:LEU:HD22	2.29	0.41
1:A:3:SER:OG	1:A:6:ASP:OD1	2.36	0.41
2:G:615:TRP:HZ2	2:G:672:SER:HG	1.59	0.41
2:C:277:HIS:CE1	4:C:1066:DOD:O	2.74	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	139/141 (99%)	125 (90%)	12 (9%)	2 (1%)	11 5
1	E	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	22 16
2	C	145/146 (99%)	133 (92%)	12 (8%)	0	100 100
2	G	144/146 (99%)	129 (90%)	15 (10%)	0	100 100
All	All	567/574 (99%)	515 (91%)	49 (9%)	3 (0%)	29 23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	PHE
1	E	536	LEU
1	A	95	PRO

4.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	113/113 (100%)	110 (97%)	3 (3%)	44	46
1	E	113/113 (100%)	106 (94%)	7 (6%)	18	13
2	C	119/118 (101%)	113 (95%)	6 (5%)	24	20
2	G	118/118 (100%)	114 (97%)	4 (3%)	37	36
All	All	463/462 (100%)	443 (96%)	20 (4%)	29	26

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	105	LEU
1	A	121	VAL
2	C	212	THR
2	C	226	GLU
2	C	291	LEU
2	C	320	LYS
2	C	331	GLN
2	C	339	ASN
1	E	423	GLU
1	E	455	VAL
1	E	456	LYS
1	E	464	ASP
1	E	490	LYS
1	E	505	LEU
1	E	516	GLU
2	G	675	LEU
2	G	679	ASP
2	G	680	ASN
2	G	682	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS
2	C	263	HIS
2	G	680	ASN

4.3.3 RNA

There are no RNA molecules in this entry.

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

4 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	$\#\|Z\| > 2$
3	HEM	C	347	2	41,50,50	1.44	6 (14%)	45,82,82	1.47	9 (20%)
3	HEM	E	542	1	41,50,50	1.57	6 (14%)	45,82,82	1.07	3 (6%)
3	HEM	G	747	2	41,50,50	1.50	7 (17%)	45,82,82	1.58	8 (17%)
3	HEM	A	142	1	41,50,50	1.47	5 (12%)	45,82,82	1.43	7 (15%)

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	HEM	C	347	2	-	6/12/54/54	-
3	HEM	E	542	1	-	4/12/54/54	-
3	HEM	G	747	2	-	5/12/54/54	-
3	HEM	A	142	1	-	5/12/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	542	HEM	C3C-CAC	-4.54	1.38	1.47
3	A	142	HEM	C3C-CAC	-3.94	1.39	1.47
3	G	747	HEM	C3C-C2C	-3.80	1.35	1.40
3	C	347	HEM	C3C-C2C	-3.57	1.35	1.40
3	E	542	HEM	C3C-C2C	-3.32	1.35	1.40
3	C	347	HEM	CBB-CAB	3.29	1.46	1.30
3	C	347	HEM	C3C-CAC	-3.27	1.41	1.47
3	G	747	HEM	C3C-CAC	-3.24	1.41	1.47
3	E	542	HEM	CBB-CAB	3.06	1.45	1.30
3	G	747	HEM	CBB-CAB	3.01	1.45	1.30
3	A	142	HEM	CBB-CAB	2.97	1.45	1.30
3	E	542	HEM	CAB-C3B	-2.93	1.39	1.47
3	A	142	HEM	C1B-NB	-2.88	1.35	1.40
3	G	747	HEM	CAB-C3B	-2.86	1.39	1.47
3	A	142	HEM	CAB-C3B	-2.83	1.39	1.47
3	E	542	HEM	CAA-C2A	2.80	1.56	1.52
3	E	542	HEM	CBC-CAC	2.54	1.46	1.29
3	G	747	HEM	CBC-CAC	2.53	1.46	1.29
3	G	747	HEM	CAA-C2A	2.52	1.55	1.52
3	C	347	HEM	CBC-CAC	2.50	1.45	1.29
3	C	347	HEM	C4D-ND	-2.32	1.36	1.40
3	A	142	HEM	CBC-CAC	2.29	1.44	1.29
3	C	347	HEM	CAB-C3B	-2.14	1.41	1.47
3	G	747	HEM	C1B-C2B	2.06	1.48	1.44

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	747	HEM	C2C-C3C-C4C	-5.08	103.35	106.90
3	A	142	HEM	C4C-CHD-C1D	4.52	128.52	122.56
3	G	747	HEM	CMD-C2D-C1D	4.04	131.19	125.04
3	C	347	HEM	C2C-C3C-C4C	-3.90	104.17	106.90
3	C	347	HEM	C4B-CHC-C1C	3.41	127.05	122.56
3	E	542	HEM	C4B-CHC-C1C	3.40	127.04	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	747	HEM	C4B-CHC-C1C	3.25	126.85	122.56
3	E	542	HEM	C4C-CHD-C1D	3.17	126.75	122.56
3	C	347	HEM	C3D-C4D-ND	2.72	113.19	110.17
3	G	747	HEM	C4C-CHD-C1D	2.68	126.09	122.56
3	G	747	HEM	CBA-CAA-C2A	2.57	117.00	112.62
3	C	347	HEM	CMB-C2B-C1B	2.48	128.81	125.04
3	A	142	HEM	C4B-C3B-C2B	-2.46	105.16	107.11
3	C	347	HEM	C4C-CHD-C1D	2.45	125.78	122.56
3	A	142	HEM	CBB-CAB-C3B	2.44	139.75	127.62
3	A	142	HEM	C2D-C1D-ND	2.43	112.80	109.88
3	C	347	HEM	CBB-CAB-C3B	2.42	139.66	127.62
3	G	747	HEM	C2D-C1D-ND	2.39	112.74	109.88
3	A	142	HEM	CMC-C2C-C3C	2.32	129.02	124.68
3	G	747	HEM	CBB-CAB-C3B	2.31	139.09	127.62
3	A	142	HEM	CMD-C2D-C1D	2.25	128.47	125.04
3	E	542	HEM	CMD-C2D-C1D	2.21	128.41	125.04
3	A	142	HEM	C4B-CHC-C1C	2.20	125.46	122.56
3	C	347	HEM	CMD-C2D-C1D	2.15	128.31	125.04
3	C	347	HEM	C2B-C1B-NB	2.08	112.31	109.84
3	G	747	HEM	CAD-C3D-C2D	-2.07	124.02	127.88
3	C	347	HEM	CBA-CAA-C2A	-2.05	109.11	112.62

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	747	HEM	C3A-C2A-CAA-CBA
3	A	142	HEM	C3A-C2A-CAA-CBA
3	C	347	HEM	C3D-CAD-CBD-CGD
3	G	747	HEM	CAA-CBA-CGA-O2A
3	G	747	HEM	CAA-CBA-CGA-O1A
3	E	542	HEM	CAD-CBD-CGD-O1D
3	E	542	HEM	CAD-CBD-CGD-O2D
3	A	142	HEM	CAA-CBA-CGA-O2A
3	G	747	HEM	CAD-CBD-CGD-O2D
3	E	542	HEM	CAA-CBA-CGA-O2A
3	A	142	HEM	CAD-CBD-CGD-O1D
3	E	542	HEM	CAA-CBA-CGA-O1A
3	C	347	HEM	CAA-CBA-CGA-O2A
3	G	747	HEM	CAD-CBD-CGD-O1D
3	A	142	HEM	CAA-CBA-CGA-O1A
3	A	142	HEM	CAD-CBD-CGD-O2D

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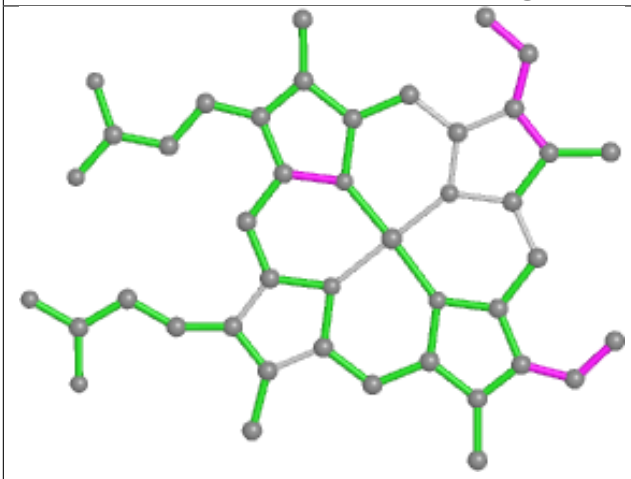
Mol	Chain	Res	Type	Atoms
3	C	347	HEM	CAD-CBD-CGD-O2D
3	C	347	HEM	CAA-CBA-CGA-O1A
3	C	347	HEM	CAD-CBD-CGD-O1D
3	C	347	HEM	C2D-C3D-CAD-CBD

There are no ring outliers.

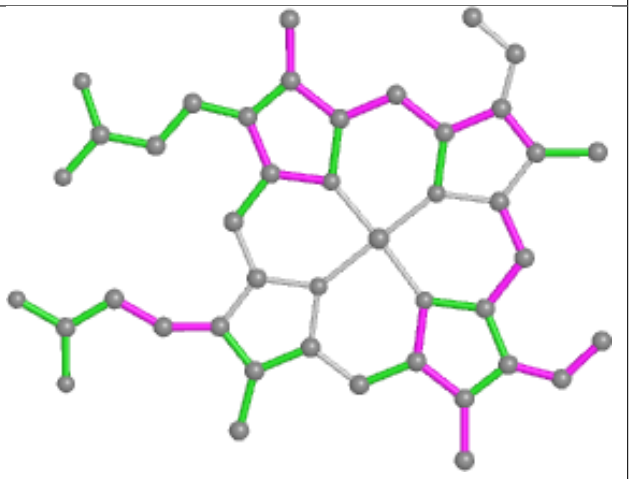
No monomer is involved in short contacts.

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.

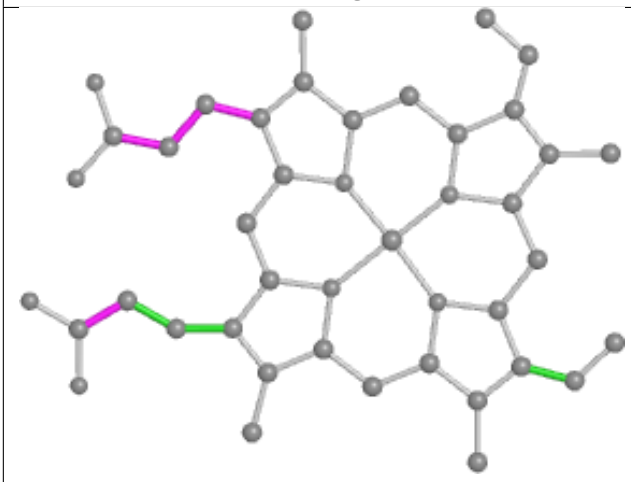
Ligand HEM C 347



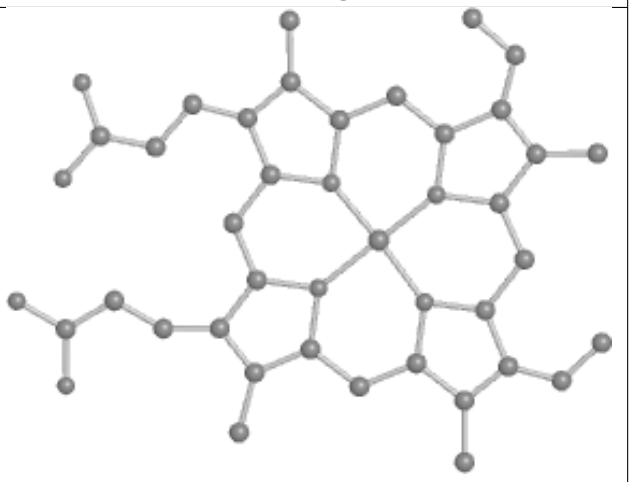
Bond lengths



Bond angles

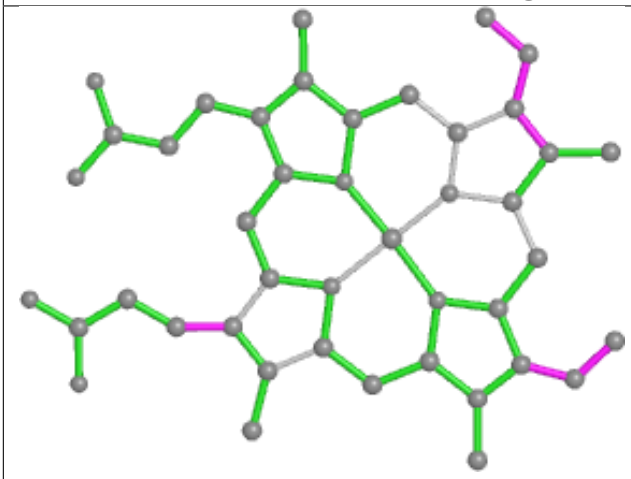


Torsions

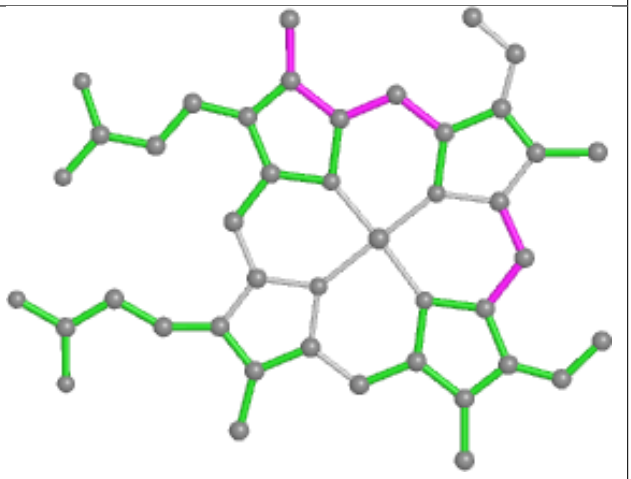


Rings

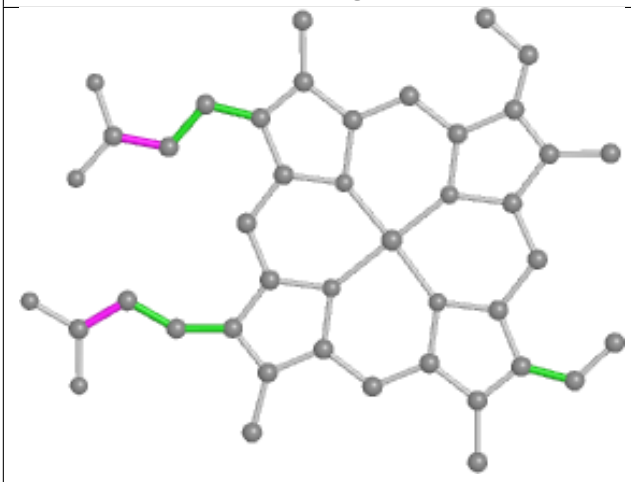
Ligand HEM E 542



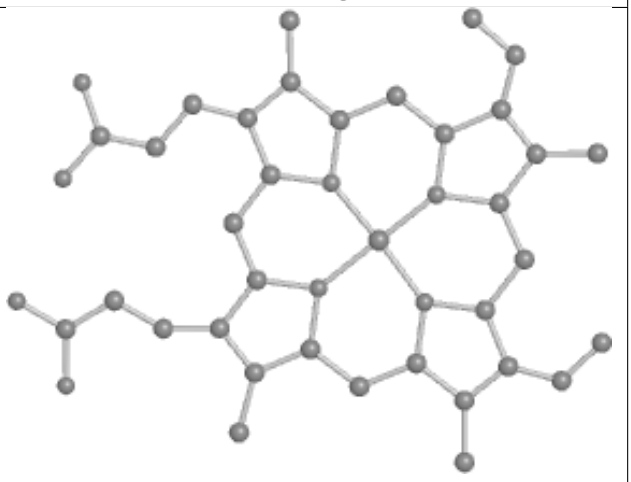
Bond lengths



Bond angles

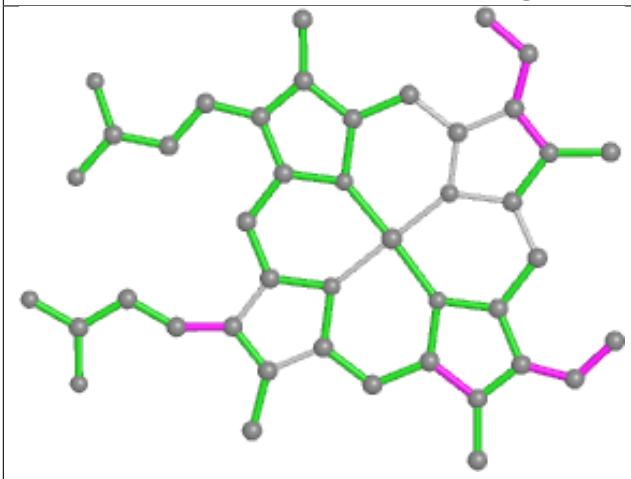


Torsions

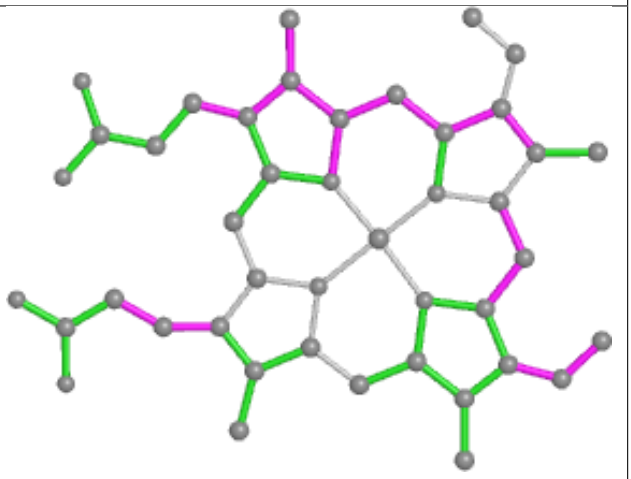


Rings

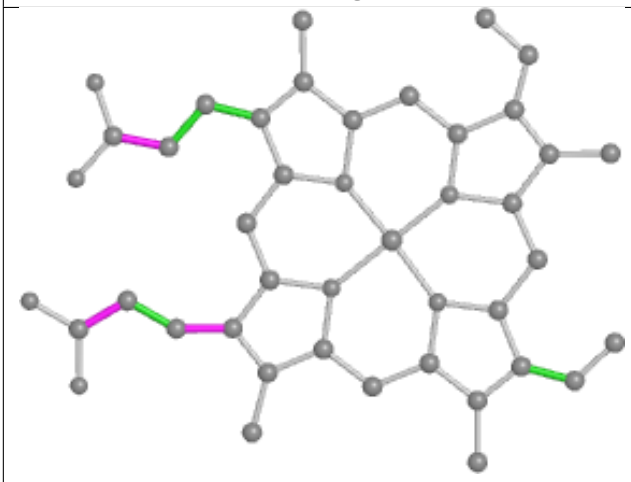
Ligand HEM G 747



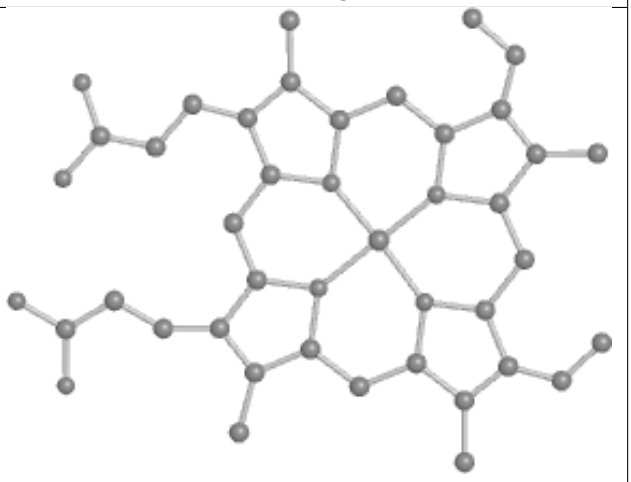
Bond lengths



Bond angles

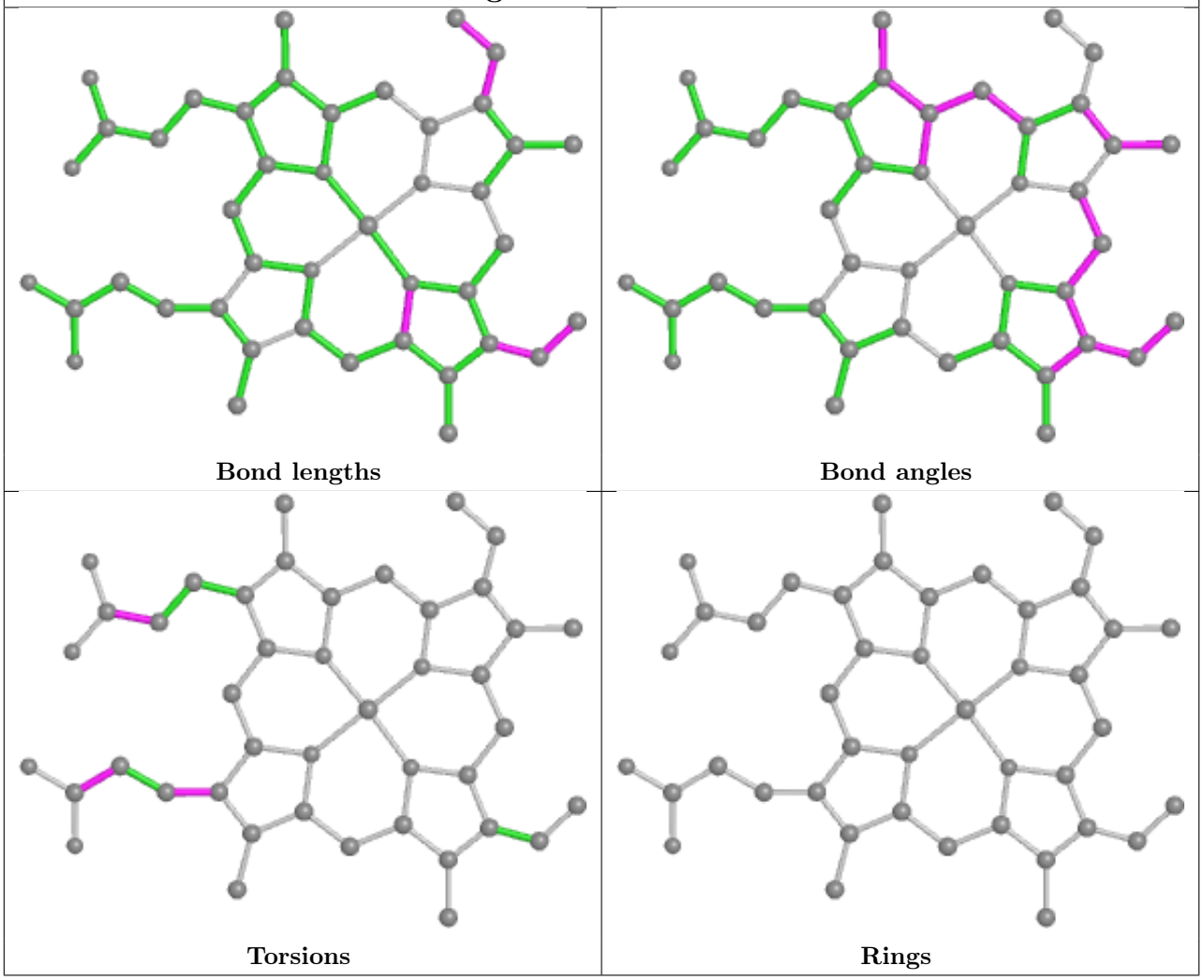


Torsions



Rings

Ligand HEM A 142



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.