Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 04:23 PM EDT

PDB ID	:	1S5X
Title	:	The crystal structure of Trematomus bernacchii hemoglobin oxidized by air
Authors	:	Vitagliano, L.; Bonomi, G.; Riccio, A.; di Prisco, G.; Smulevich, G.; Mazzarella, L.
Deposited on	:	2004-01-22
Resolution	:	2.40 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 (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:

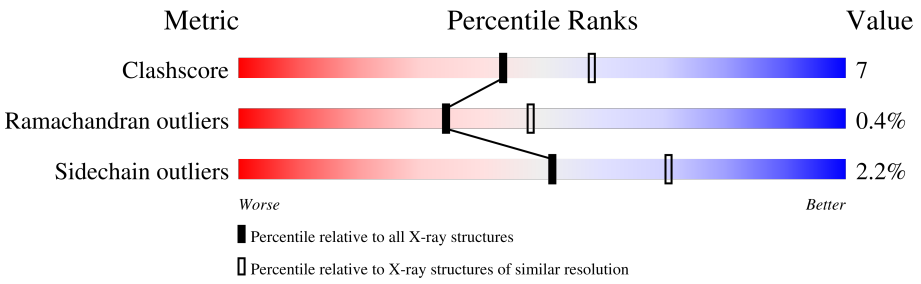
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	143	84% 15% •
2	B	146	77% 14% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2267 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.

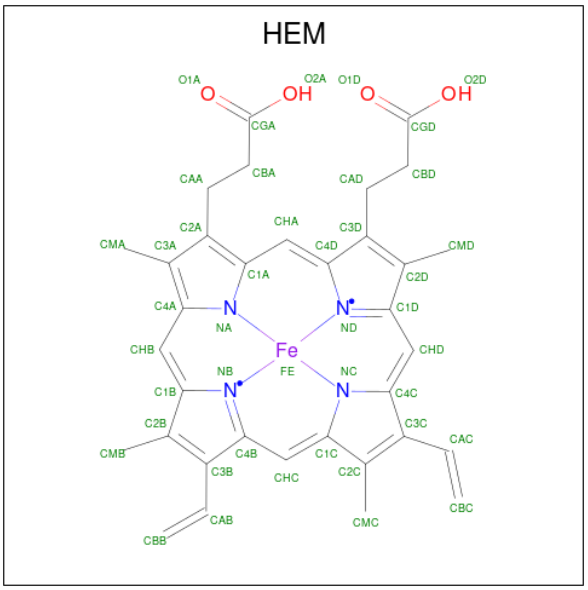
- Molecule 1 is a protein called Hemoglobin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	143	1104	710	190	199	5	0	0	0

- Molecule 2 is a protein called Hemoglobin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	136	1050	669	182	194	5	0	0	0

- 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
			Total	C	Fe	N	O		
3	A	1	43	34	1	4	4	0	0
3	B	1	43	34	1	4	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	15	15	15	0	0
			Total	O		
4	B	12	12	12	0	0

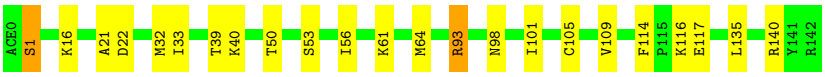
3 Residue-property plots (i)

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.

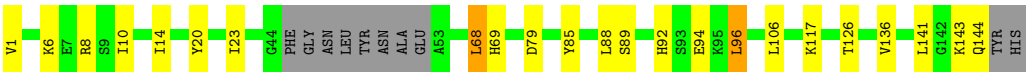
• Molecule 1: Hemoglobin alpha chain

Chain A:



• Molecule 2: Hemoglobin beta chain

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	108.52Å 65.09Å 55.75Å 90.00° 113.48° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2267	wwPDB-VP
Average B, all atoms ($Å^2$)	34.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.46	0/1127	0.68	1/1523 (0.1%)
2	B	0.42	0/1071	0.56	0/1449
All	All	0.44	0/2198	0.63	1/2972 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	SER	O-C-N	-11.73	103.93	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	SER	Mainchain

5.2 Too-close contacts (i)

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	1104	0	1136	15	0
2	B	1050	0	1047	15	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
4	A	15	0	0	1	0
4	B	12	0	0	1	0
All	All	2267	0	2243	30	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 7.

All (30) 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)
1:A:93:ARG:HH11	1:A:93:ARG:HB3	1.43	0.82
2:B:23:ILE:HD11	2:B:117:LYS:HD2	1.62	0.80
1:A:140:ARG:HH11	1:A:140:ARG:HB3	1.53	0.72
2:B:89:SER:OG	2:B:144:GLN:HB2	1.91	0.70
2:B:20:TYR:HA	2:B:68:LEU:HD23	1.73	0.70
1:A:140:ARG:HB3	1:A:140:ARG:NH1	2.12	0.65
1:A:116:LYS:HD2	1:A:117:GLU:OE2	1.97	0.65
1:A:22:ASP:OD1	1:A:61:LYS:HE3	2.05	0.56
2:B:1:VAL:HG11	2:B:136:VAL:HG22	1.88	0.56
2:B:8:ARG:HH12	2:B:79:ASP:CG	2.10	0.54
1:A:93:ARG:HB3	1:A:93:ARG:NH1	2.17	0.53
2:B:106:LEU:HD23	3:B:400:HEM:HBB2	1.90	0.52
1:A:105:CYS:O	1:A:109:VAL:HG23	2.12	0.49
2:B:69:HIS:HE1	4:B:516:HOH:O	1.93	0.49
2:B:85:TYR:HD2	2:B:88:LEU:HD12	1.79	0.47
1:A:116:LYS:HB3	4:A:502:HOH:O	2.15	0.47
2:B:141:LEU:CD1	3:B:400:HEM:HAB	2.45	0.46
2:B:89:SER:CB	2:B:144:GLN:HB2	2.46	0.46
1:A:33:ILE:HG23	1:A:40:LYS:HG2	1.97	0.45
2:B:6:LYS:O	2:B:10:ILE:HG13	2.16	0.44
1:A:114:PHE:HB3	1:A:117:GLU:OE1	2.17	0.44
1:A:50:THR:O	1:A:56:ILE:HD12	2.18	0.44
2:B:14:ILE:HD11	2:B:126:THR:HG23	2.00	0.43
2:B:92:HIS:HA	2:B:96:LEU:HB2	2.01	0.43
1:A:98:ASN:HD22	1:A:101:ILE:HD12	1.83	0.43
2:B:143:LYS:HE3	2:B:144:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:O	1:A:64:MET:HG3	2.20	0.41
1:A:32:MET:HE3	1:A:39:THR:HB	2.03	0.41
2:B:94:GLU:HA	2:B:94:GLU:OE2	2.20	0.40
1:A:140:ARG:HH11	1:A:140:ARG:CB	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 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	141/143 (99%)	137 (97%)	3 (2%)	1 (1%)	22 32
2	B	132/146 (90%)	127 (96%)	5 (4%)	0	100 100
All	All	273/289 (94%)	264 (97%)	8 (3%)	1 (0%)	34 48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER

5.3.2 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	119/119 (100%)	116 (98%)	3 (2%)	47 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	112/120 (93%)	110 (98%)	2 (2%)	59 76
All	All	231/239 (97%)	226 (98%)	5 (2%)	52 71

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	93	ARG
1	A	135	LEU
2	B	68	LEU
2	B	96	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	103	ASN
2	B	41	HIS
2	B	69	HIS
2	B	144	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	B	400	2	42,50,50	2.02	13 (30%)	46,82,82	2.16	18 (39%)
3	HEM	A	200	1,4	42,50,50	2.15	14 (33%)	46,82,82	2.30	15 (32%)

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	B	400	2	-	3/12/54/54	-
3	HEM	A	200	1,4	-	7/12/54/54	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	200	HEM	CBD-CGD	-5.57	1.37	1.50
3	A	200	HEM	CBB-CAB	5.43	1.56	1.30
3	B	400	HEM	CBC-CAC	4.41	1.56	1.29
3	B	400	HEM	CBB-CAB	4.41	1.51	1.30
3	B	400	HEM	CMB-C2B	4.00	1.59	1.50
3	B	400	HEM	O1A-CGA	3.70	1.34	1.22
3	A	200	HEM	CBA-CGA	-3.61	1.42	1.50
3	A	200	HEM	CBC-CAC	3.59	1.51	1.29
3	A	200	HEM	C3C-CAC	3.52	1.55	1.47
3	A	200	HEM	O1A-CGA	3.41	1.33	1.22
3	B	400	HEM	CBA-CGA	-3.35	1.42	1.50
3	B	400	HEM	CHA-C4D	3.26	1.42	1.34
3	A	200	HEM	CBD-CAD	3.26	1.63	1.51
3	B	400	HEM	C3C-CAC	3.14	1.54	1.47
3	A	200	HEM	CHA-C4D	3.01	1.42	1.34
3	B	400	HEM	CBD-CGD	-2.98	1.43	1.50
3	A	200	HEM	C3C-C4C	2.95	1.45	1.41
3	B	400	HEM	CBD-CAD	2.82	1.61	1.51
3	A	200	HEM	C2C-C1C	2.65	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400	HEM	C2C-C1C	2.64	1.48	1.42
3	A	200	HEM	C4D-C3D	2.43	1.49	1.45
3	A	200	HEM	C1A-NA	2.35	1.41	1.36
3	B	400	HEM	O1D-CGD	2.33	1.29	1.22
3	B	400	HEM	C3B-C4B	2.29	1.49	1.44
3	A	200	HEM	CAB-C3B	2.14	1.53	1.47
3	B	400	HEM	CAB-C3B	2.13	1.53	1.47
3	A	200	HEM	CHB-C1B	2.11	1.39	1.34

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	HEM	C4B-CHC-C1C	6.57	131.23	122.56
3	A	200	HEM	C4C-CHD-C1D	6.21	130.75	122.56
3	A	200	HEM	C3B-C4B-NB	5.97	113.76	109.47
3	A	200	HEM	C4B-CHC-C1C	5.34	129.61	122.56
3	B	400	HEM	C2B-C1B-NB	4.55	115.08	109.84
3	B	400	HEM	C4C-CHD-C1D	4.26	128.18	122.56
3	A	200	HEM	C2D-C1D-ND	4.00	114.52	109.90
3	A	200	HEM	CHC-C4B-NB	-3.92	120.22	124.44
3	B	400	HEM	C3B-C2B-C1B	-3.47	103.81	106.41
3	A	200	HEM	CHD-C1D-ND	-3.42	120.75	124.44
3	A	200	HEM	C1D-C2D-C3D	-3.41	103.39	106.98
3	A	200	HEM	C1B-NB-C4B	-3.02	101.62	105.21
3	B	400	HEM	CHC-C4B-NB	-3.00	121.21	124.44
3	A	200	HEM	O1A-CGA-CBA	-2.99	113.60	123.09
3	A	200	HEM	O2A-CGA-CBA	2.80	122.84	114.00
3	B	400	HEM	CAD-CBD-CGD	2.76	120.97	113.67
3	B	400	HEM	O2D-CGD-CBD	2.68	122.47	114.00
3	B	400	HEM	O2D-CGD-O1D	-2.67	116.47	123.33
3	B	400	HEM	C3B-C4B-NB	2.56	111.31	109.47
3	B	400	HEM	O2A-CGA-CBA	2.51	121.94	114.00
3	A	200	HEM	CBD-CAD-C3D	-2.51	105.59	112.53
3	A	200	HEM	CMC-C2C-C3C	2.46	129.59	124.68
3	A	200	HEM	CMA-C3A-C4A	-2.32	125.06	128.46
3	B	400	HEM	C1B-NB-C4B	-2.27	102.52	105.21
3	A	200	HEM	C4B-C3B-C2B	-2.22	105.24	107.28
3	A	200	HEM	C2B-C1B-NB	2.22	112.39	109.84
3	B	400	HEM	CMA-C3A-C2A	2.21	129.11	124.94
3	B	400	HEM	C4A-C3A-C2A	-2.19	105.47	107.00
3	B	400	HEM	CMB-C2B-C1B	2.14	128.38	125.03
3	B	400	HEM	CAD-C3D-C2D	2.14	131.87	127.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400	HEM	CAD-C3D-C4D	-2.13	120.99	124.70
3	B	400	HEM	CBA-CAA-C2A	-2.10	109.00	112.54
3	B	400	HEM	CMA-C3A-C4A	-2.09	125.40	128.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	200	HEM	C2B-C3B-CAB-CBB
3	A	200	HEM	C4B-C3B-CAB-CBB
3	B	400	HEM	C2B-C3B-CAB-CBB
3	B	400	HEM	C4B-C3B-CAB-CBB
3	A	200	HEM	C2A-CAA-CBA-CGA
3	A	200	HEM	CAA-CBA-CGA-O2A
3	A	200	HEM	CAA-CBA-CGA-O1A
3	A	200	HEM	CAD-CBD-CGD-O1D
3	A	200	HEM	CAD-CBD-CGD-O2D
3	B	400	HEM	CAD-CBD-CGD-O1D

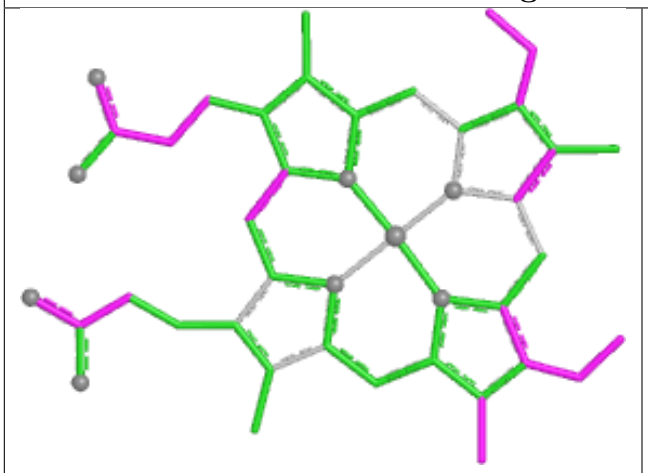
There are no ring outliers.

1 monomer is involved in 2 short contacts:

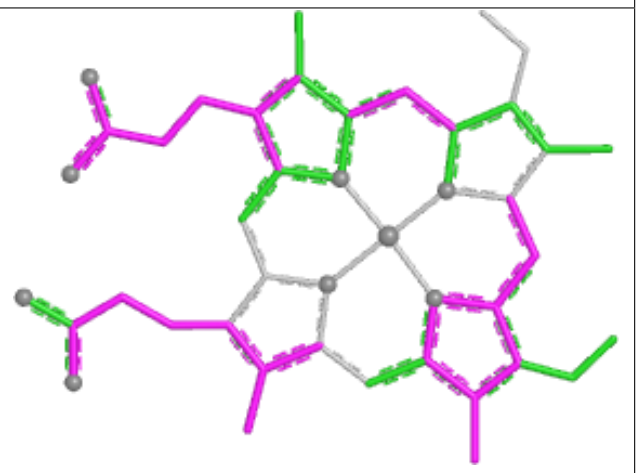
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

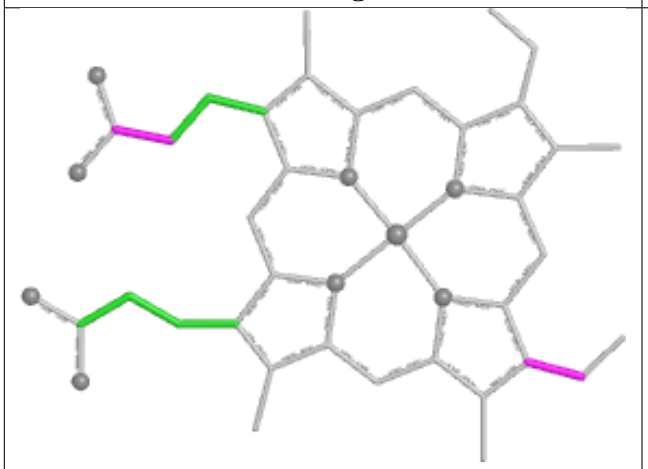
Ligand HEM B 400



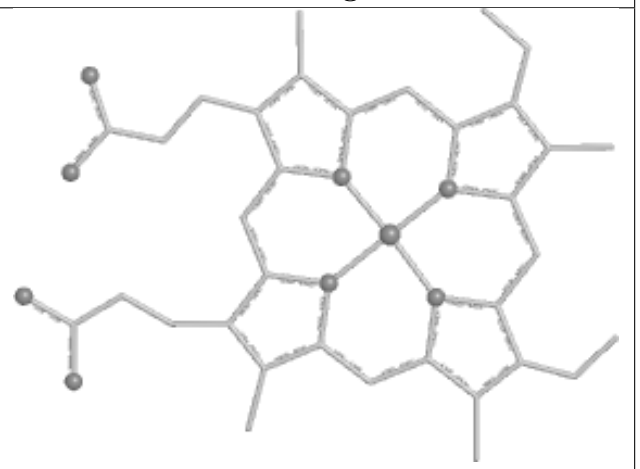
Bond lengths



Bond angles

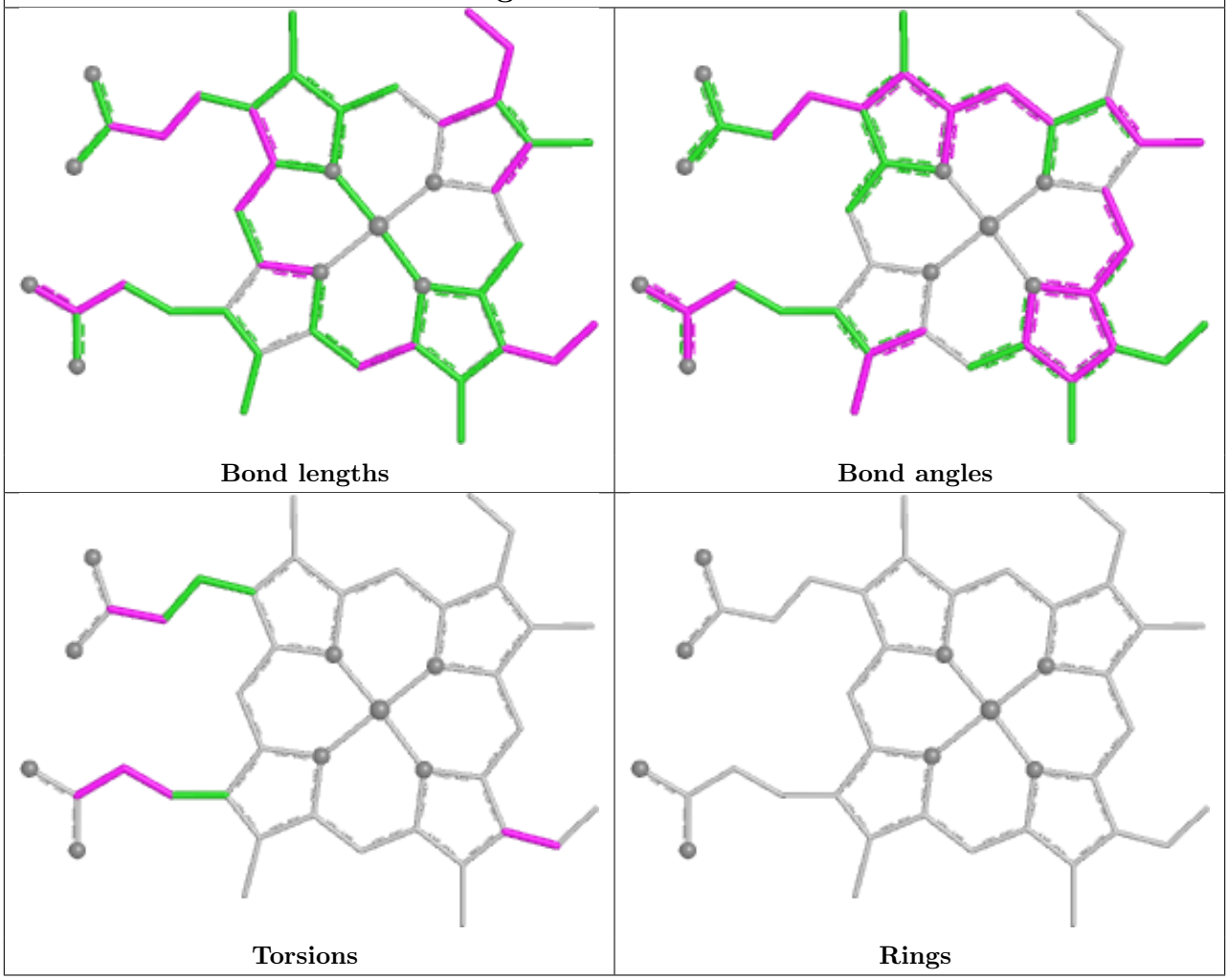


Torsions



Rings

Ligand HEM A 200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.