Full wwPDB X-ray Structure Validation Report ⓘ

Feb 3, 2024 – 03:25 PM EST

PDB ID	:	1LHT
Title	:	LOGGERHEAD SEA TURTLE MYOGLOBIN (CYANO-MET)
Authors	:	Nardini, M.; Tarricone, C.; Lania, A.; Desideri, A.; De Sanctis, G.; Coletta, M.; Petruzzelli, R.; Ascenzi, P.; Coda, A.; Bolognesi, M.
Deposited on	:	1995-02-01
Resolution	:	2.00 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:

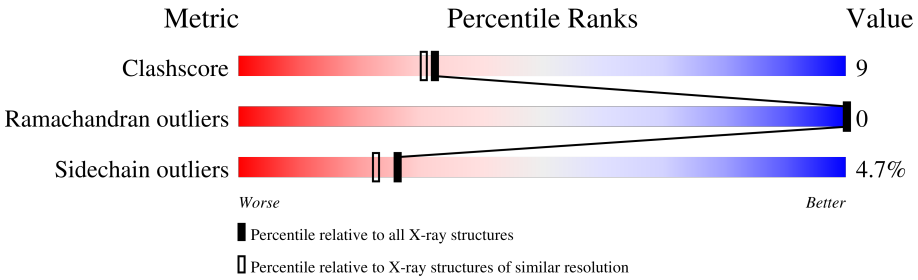
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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	153	61% 33%

2 Entry composition (i)

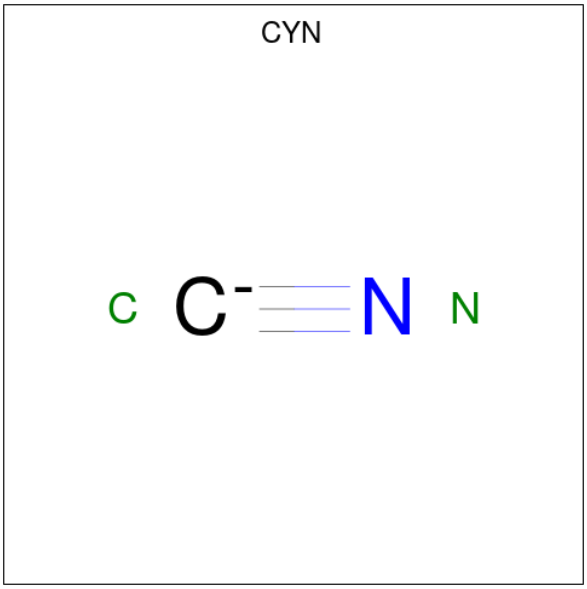
There are 4 unique types of molecules in this entry. The entry contains 1261 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MYOGLOBIN.

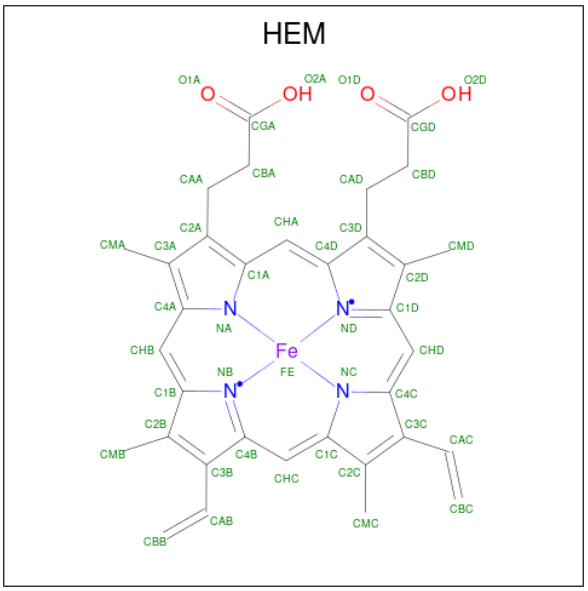
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1148	737	195	213	3	0	0	0

- Molecule 2 is CYANIDE ION (three-letter code: CYN) (formula: CN).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	68	Total	O	0	0
			68	68		

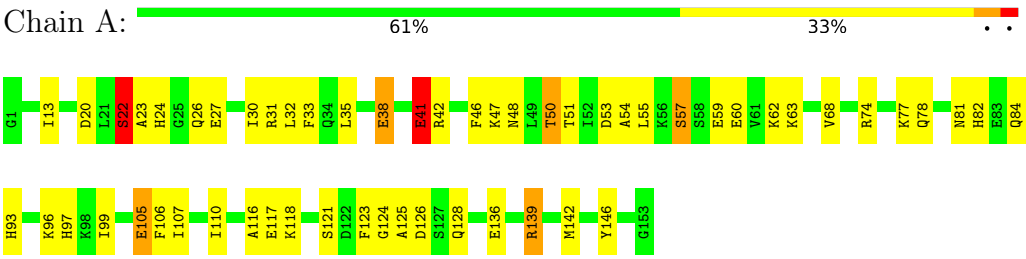
3 Residue-property plots (i)

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: MYOGLOBIN

Chain A:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	37.57Å 61.27Å 75.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, X-PLOR 3.1	Depositor
R, R_{free}	0.178 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1261	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CYN, 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	2.67	52/1174 (4.4%)	1.86	32/1588 (2.0%)

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ARG	NE-CZ	23.86	1.64	1.33
1	A	60	GLU	CD-OE2	21.66	1.49	1.25
1	A	41	GLU	CD-OE1	21.60	1.49	1.25
1	A	57	SER	CA-CB	16.21	1.77	1.52
1	A	38	GLU	CB-CG	-13.86	1.25	1.52
1	A	60	GLU	CD-OE1	13.40	1.40	1.25
1	A	42	ARG	CZ-NH2	11.23	1.47	1.33
1	A	38	GLU	CG-CD	-10.78	1.35	1.51
1	A	139	ARG	NE-CZ	-10.31	1.19	1.33
1	A	139	ARG	CD-NE	9.70	1.62	1.46
1	A	41	GLU	CG-CD	9.53	1.66	1.51
1	A	121	SER	CA-CB	9.38	1.67	1.52
1	A	74	ARG	NE-CZ	8.89	1.44	1.33
1	A	105	GLU	CG-CD	8.68	1.65	1.51
1	A	139	ARG	CZ-NH1	-8.52	1.22	1.33
1	A	20	ASP	CG-OD2	8.29	1.44	1.25
1	A	91	GLU	CD-OE1	8.12	1.34	1.25
1	A	117	GLU	CD-OE2	7.87	1.34	1.25
1	A	53	ASP	CA-CB	7.64	1.70	1.53
1	A	42	ARG	CD-NE	-7.55	1.33	1.46
1	A	117	GLU	CD-OE1	7.53	1.33	1.25
1	A	78	GLN	CG-CD	7.37	1.68	1.51
1	A	27	GLU	CB-CG	7.00	1.65	1.52
1	A	146	TYR	CA-C	6.85	1.70	1.52
1	A	105	GLU	CB-CG	-6.68	1.39	1.52
1	A	26	GLN	CD-NE2	-6.59	1.16	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLU	CB-CG	-6.57	1.39	1.52
1	A	24	HIS	CA-C	6.52	1.70	1.52
1	A	139	ARG	CZ-NH2	-6.42	1.24	1.33
1	A	50	THR	CB-CG2	6.32	1.73	1.52
1	A	85	GLU	CA-CB	6.29	1.67	1.53
1	A	48	ASN	N-CA	-6.26	1.33	1.46
1	A	84	GLN	CA-CB	5.95	1.67	1.53
1	A	125	ALA	CA-CB	5.93	1.65	1.52
1	A	136	GLU	CD-OE1	5.93	1.32	1.25
1	A	74	ARG	CD-NE	5.87	1.56	1.46
1	A	59	GLU	CA-CB	5.78	1.66	1.53
1	A	30	ILE	CA-CB	5.78	1.68	1.54
1	A	55	LEU	N-CA	-5.64	1.35	1.46
1	A	142	MET	CA-C	5.58	1.67	1.52
1	A	22	SER	CA-CB	5.56	1.61	1.52
1	A	54	ALA	C-O	-5.55	1.12	1.23
1	A	118	LYS	CD-CE	5.41	1.64	1.51
1	A	47	LYS	C-O	-5.32	1.13	1.23
1	A	13	ILE	CA-CB	5.16	1.66	1.54
1	A	85	GLU	CD-OE1	5.12	1.31	1.25
1	A	50	THR	C-N	-5.12	1.22	1.34
1	A	126	ASP	CG-OD1	-5.10	1.13	1.25
1	A	105	GLU	CD-OE1	-5.06	1.20	1.25
1	A	121	SER	C-O	5.05	1.32	1.23
1	A	42	ARG	NE-CZ	5.01	1.39	1.33
1	A	93	HIS	CG-CD2	5.00	1.44	1.35

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	ARG	NE-CZ-NH1	15.45	128.03	120.30
1	A	42	ARG	NE-CZ-NH1	15.15	127.87	120.30
1	A	74	ARG	NE-CZ-NH2	-12.99	113.81	120.30
1	A	146	TYR	CB-CG-CD2	-8.76	115.75	121.00
1	A	139	ARG	NH1-CZ-NH2	-7.28	111.39	119.40
1	A	35	LEU	CB-CG-CD2	-7.17	98.81	111.00
1	A	53	ASP	CB-CA-C	7.13	124.65	110.40
1	A	38	GLU	CB-CG-CD	6.86	132.72	114.20
1	A	81	ASN	N-CA-CB	-6.77	98.42	110.60
1	A	55	LEU	CB-CG-CD1	-6.67	99.67	111.00
1	A	38	GLU	CB-CA-C	-6.62	97.16	110.40
1	A	105	GLU	CG-CD-OE1	6.49	131.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	22	SER	CA-CB-OG	-6.23	94.37	111.20
1	A	54	ALA	CB-CA-C	-6.20	100.80	110.10
1	A	50	THR	CA-CB-CG2	-6.13	103.82	112.40
1	A	42	ARG	NH1-CZ-NH2	-6.11	112.68	119.40
1	A	46	PHE	CD1-CE1-CZ	-6.08	112.81	120.10
1	A	33	PHE	CB-CG-CD2	-6.01	116.59	120.80
1	A	31	ARG	CB-CG-CD	6.01	127.22	111.60
1	A	51	THR	N-CA-CB	-5.86	99.17	110.30
1	A	68	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	A	86	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	105	GLU	CG-CD-OE2	-5.45	107.41	118.30
1	A	33	PHE	CG-CD2-CE2	-5.35	114.91	120.80
1	A	77	LYS	CA-CB-CG	-5.30	101.74	113.40
1	A	63	LYS	CA-CB-CG	5.28	125.01	113.40
1	A	20	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	46	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	A	126	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	13	ILE	CA-CB-CG2	-5.04	100.82	110.90
1	A	23	ALA	CB-CA-C	-5.04	102.55	110.10
1	A	146	TYR	CB-CG-CD1	5.03	124.02	121.00

There are no chirality outliers.

There are no planarity outliers.

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	1148	0	1064	18	0
2	A	2	0	0	0	0
3	A	43	0	30	2	0
4	A	68	0	0	3	0
All	All	1261	0	1094	20	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 9.

All (20) 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:57:SER:CA	1:A:57:SER:CB	1.77	1.61
1:A:97:HIS:HB2	1:A:99:ILE:HD11	1.49	0.94
1:A:97:HIS:HB2	1:A:99:ILE:CD1	2.04	0.85
1:A:97:HIS:CB	1:A:99:ILE:HD11	2.08	0.84
1:A:128:GLN:OE1	4:A:254:HOH:O	2.08	0.71
1:A:41:GLU:HB3	4:A:243:HOH:O	1.93	0.68
1:A:57:SER:CB	1:A:57:SER:N	2.55	0.67
3:A:155:HEM:HBC2	3:A:155:HEM:HMC1	1.80	0.62
1:A:124:GLY:O	1:A:128:GLN:HG3	2.06	0.56
1:A:105:GLU:HA	1:A:139:ARG:HD3	1.89	0.55
1:A:106:PHE:O	1:A:110:ILE:HD12	2.08	0.54
1:A:22:SER:HB3	1:A:62:LYS:HE3	1.90	0.54
1:A:22:SER:HB3	1:A:62:LYS:CE	2.39	0.53
1:A:123:PHE:CE2	1:A:128:GLN:HG2	2.44	0.52
3:A:155:HEM:HBC2	3:A:155:HEM:CMC	2.40	0.51
1:A:82:HIS:CD2	1:A:86:LEU:HD12	2.45	0.51
1:A:97:HIS:HB3	1:A:99:ILE:HD11	1.91	0.50
1:A:96:LYS:CG	4:A:253:HOH:O	2.62	0.48
1:A:32:LEU:HD22	1:A:107:ILE:HD12	2.01	0.41
1:A:116:ALA:HA	1:A:123:PHE:HD2	1.87	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	151/153 (99%)	148 (98%)	3 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	107/132 (81%)	102 (95%)	5 (5%)	26 22

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

Mol	Chain	Res	Type
1	A	22	SER
1	A	38	GLU
1	A	41	GLU
1	A	50	THR
1	A	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
2	CYN	A	158	3	0,1,1	-	-	-		
3	HEM	A	155	2,1	41,50,50	2.76	14 (34%)	45,82,82	2.45	18 (40%)

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	A	155	2,1	-	4/12/54/54	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	CMB-C2B	7.07	1.65	1.50
3	A	155	HEM	O2D-CGD	-5.61	1.11	1.30
3	A	155	HEM	CBD-CGD	5.59	1.63	1.50
3	A	155	HEM	C3D-C2D	-5.12	1.25	1.36
3	A	155	HEM	C3C-C2C	-4.54	1.34	1.40
3	A	155	HEM	C4D-C3D	4.19	1.52	1.45
3	A	155	HEM	CAB-C3B	4.14	1.58	1.47
3	A	155	HEM	C1B-NB	-4.05	1.33	1.40
3	A	155	HEM	CAA-C2A	3.98	1.57	1.52
3	A	155	HEM	CMD-C2D	3.90	1.59	1.50
3	A	155	HEM	C4D-ND	-3.38	1.34	1.40
3	A	155	HEM	C3C-CAC	2.82	1.53	1.47
3	A	155	HEM	O2A-CGA	-2.23	1.23	1.30
3	A	155	HEM	FE-ND	-2.13	1.86	1.96

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	155	HEM	C4A-C3A-C2A	-6.93	102.18	107.00
3	A	155	HEM	C4D-ND-C1D	-6.76	98.09	105.07
3	A	155	HEM	CMA-C3A-C2A	4.54	133.51	124.94
3	A	155	HEM	CHD-C1D-C2D	-3.99	118.75	124.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	155	HEM	CMA-C3A-C4A	-3.42	123.20	128.46
3	A	155	HEM	C4B-C3B-C2B	-3.33	104.47	107.11
3	A	155	HEM	C2D-C1D-ND	3.30	113.84	109.88
3	A	155	HEM	C1D-C2D-C3D	-2.95	103.86	106.96
3	A	155	HEM	C1B-NB-C4B	-2.82	102.16	105.07
3	A	155	HEM	CAA-CBA-CGA	-2.76	106.01	113.76
3	A	155	HEM	CHC-C4B-C3B	-2.63	120.55	124.57
3	A	155	HEM	CMC-C2C-C3C	2.58	129.51	124.68
3	A	155	HEM	C2B-C1B-NB	2.45	112.74	109.84
3	A	155	HEM	C3D-C4D-ND	2.44	112.88	110.17
3	A	155	HEM	CBA-CAA-C2A	2.34	116.61	112.62
3	A	155	HEM	CAA-C2A-C3A	2.28	133.81	127.25
3	A	155	HEM	O2D-CGD-CBD	2.24	121.24	114.03
3	A	155	HEM	O1A-CGA-CBA	-2.15	116.18	123.08

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	155	HEM	CAD-CBD-CGD-O2D
3	A	155	HEM	CAD-CBD-CGD-O1D
3	A	155	HEM	CAA-CBA-CGA-O2A
3	A	155	HEM	CAA-CBA-CGA-O1A

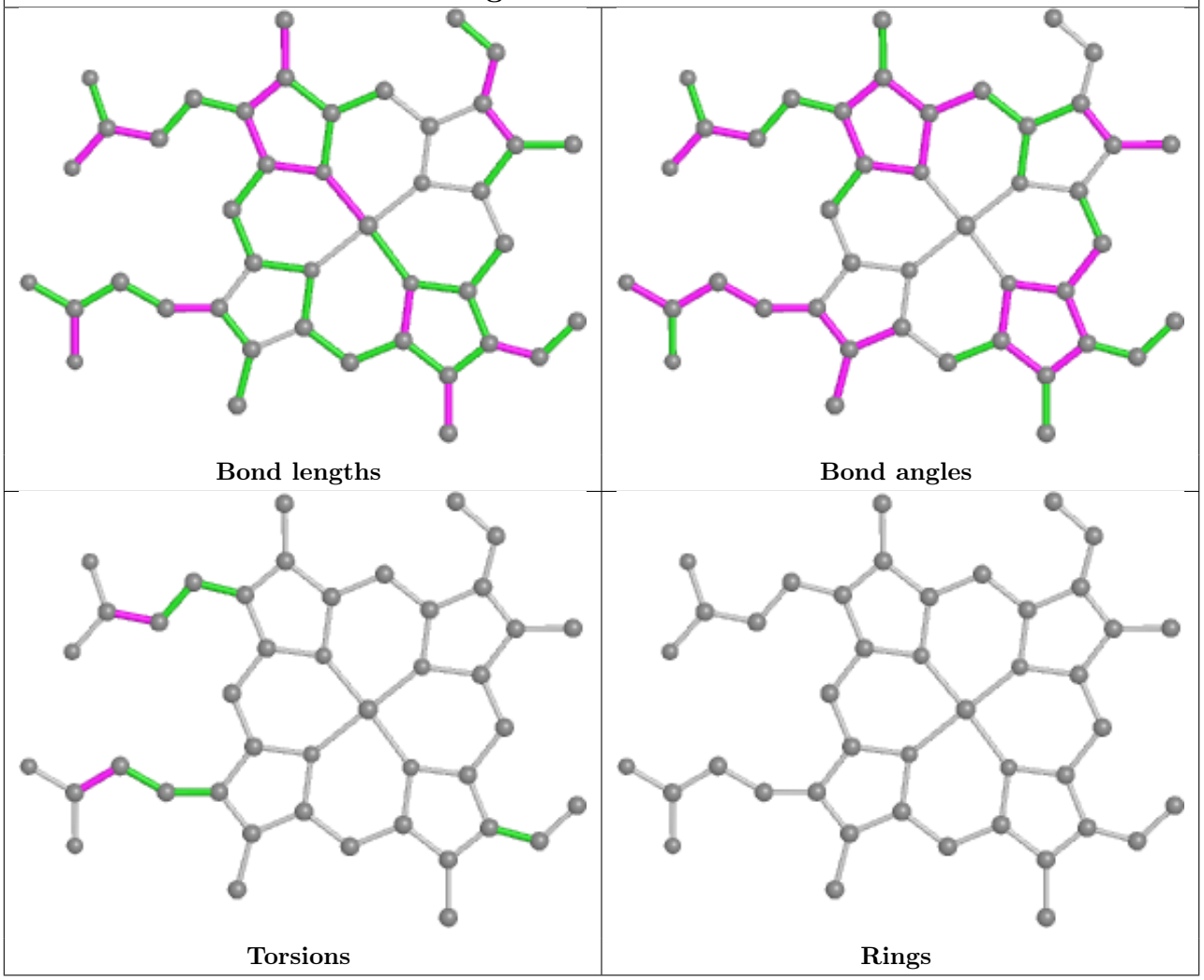
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	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 A 155



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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.