Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 10:39 AM EST

PDB ID : 2LH3
Title : X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI. STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESOLUTION OF 2.0 ANGSTROMS (RUSSIAN)
Authors : Vainshtein, B.K.; Harutyunyan, E.H.; Kuranova, I.P.; Borisov, V.V.; Sosfenov, N.I.; Pavlovsky, A.G.; Grebenko, A.I.; Konareva, N.V.
Deposited on : 1982-04-23
Resolution : 2.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

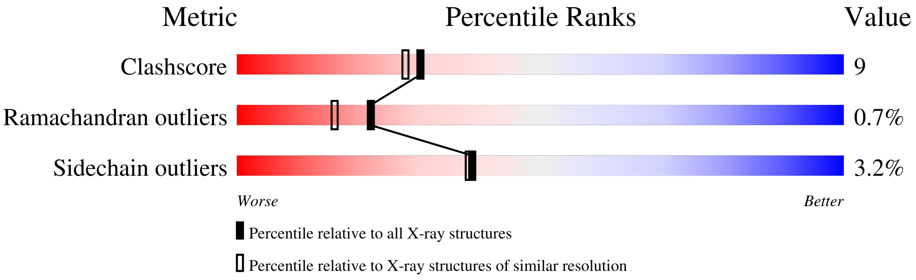
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

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

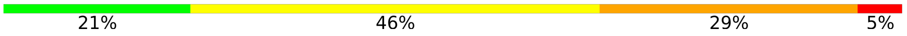
The reported resolution of this entry is 2.00 Å.

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%

Mol	Chain	Length	Quality of chain
1	A	153	

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 1291 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.

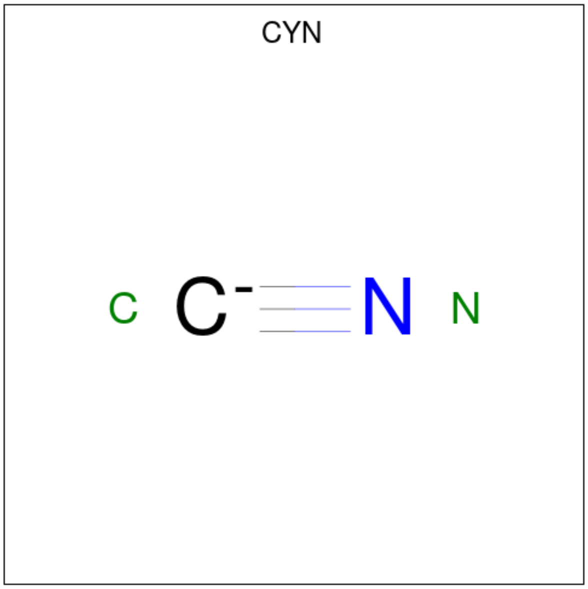
- Molecule 1 is a protein called LEGHEMOGLOBIN (CYANO MET).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1180	761	193	225	1	35	1	0

There are 2 discrepancies between the modelled and reference sequences:

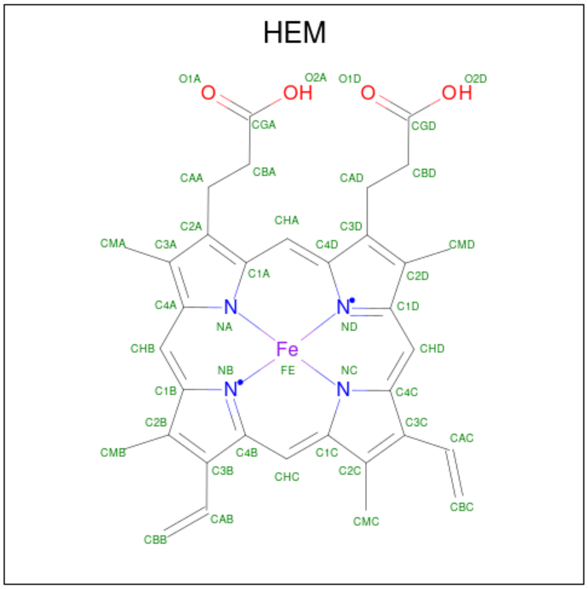
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLU	GLN	conflict	UNP P02240
A	150	ASP	ASN	conflict	UNP P02240

- 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	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

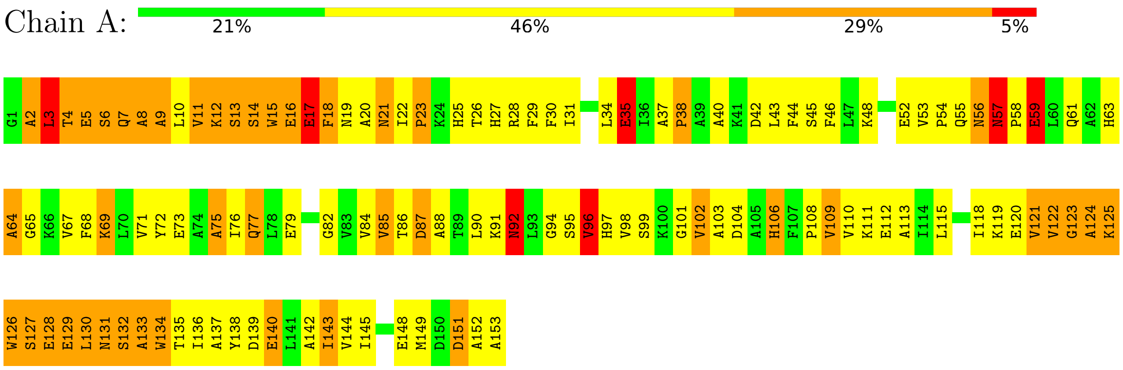
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	66	66	66	0	0

3 Residue-property plots ⓘ

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.

- Molecule 1: LEGHEMOGLOBIN (CYANO MET)



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α, β, γ	93.19Å 38.41Å 52.07Å 90.00° 90.00° 98.90°	Depositor
Resolution (Å)	(Not available) – 2.00 9.94 – 1.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 92.5 (9.94-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.489 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	20.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	1.17 , 256.3	EDS
L-test for twinning[1]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.51	EDS
Total number of atoms	1291	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.59% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] 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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	3.23	135/1214 (11.1%)	2.13	41/1648 (2.5%)

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	9

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	SER	CB-OG	10.49	1.55	1.42
1	A	138	TYR	CZ-OH	10.07	1.54	1.37
1	A	138	TYR	CB-CG	9.92	1.66	1.51
1	A	112	GLU	CG-CD	9.46	1.66	1.51
1	A	15	TRP	CD2-CE2	9.18	1.52	1.41
1	A	132[A]	SER	CA-CB	9.11	1.66	1.52
1	A	132[B]	SER	CA-CB	9.11	1.66	1.52
1	A	132[C]	SER	CA-CB	9.11	1.66	1.52
1	A	120	GLU	CG-CD	9.00	1.65	1.51
1	A	106	HIS	CB-CG	8.46	1.65	1.50
1	A	72	TYR	CE1-CZ	8.31	1.49	1.38
1	A	123	GLY	CA-C	8.23	1.65	1.51
1	A	65	GLY	C-O	8.21	1.36	1.23
1	A	18	PHE	CB-CG	8.16	1.65	1.51
1	A	94	GLY	CA-C	8.12	1.64	1.51
1	A	15	TRP	CB-CG	8.05	1.64	1.50
1	A	72	TYR	CG-CD2	7.78	1.49	1.39
1	A	44	PHE	CB-CG	7.46	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	PHE	CB-CG	7.36	1.63	1.51
1	A	140	GLU	CB-CG	7.29	1.66	1.52
1	A	35	GLU	CD-OE2	7.28	1.33	1.25
1	A	110	VAL	CB-CG2	7.20	1.68	1.52
1	A	13	SER	CA-CB	7.20	1.63	1.52
1	A	128	GLU	CD-OE2	-7.18	1.17	1.25
1	A	101	GLY	CA-C	7.18	1.63	1.51
1	A	144	VAL	CB-CG2	7.07	1.67	1.52
1	A	11	VAL	CB-CG1	6.97	1.67	1.52
1	A	113	ALA	CA-CB	6.97	1.67	1.52
1	A	61	GLN	C-O	6.95	1.36	1.23
1	A	15	TRP	CZ3-CH2	6.93	1.51	1.40
1	A	121	VAL	CB-CG2	6.92	1.67	1.52
1	A	85	VAL	CB-CG2	6.90	1.67	1.52
1	A	72	TYR	C-O	6.88	1.36	1.23
1	A	5	GLU	CD-OE2	6.85	1.33	1.25
1	A	138	TYR	CD2-CE2	6.84	1.49	1.39
1	A	79	GLU	CB-CG	6.84	1.65	1.52
1	A	88	ALA	N-CA	6.83	1.60	1.46
1	A	102	VAL	CB-CG1	6.72	1.67	1.52
1	A	134	TRP	N-CA	6.71	1.59	1.46
1	A	152	ALA	C-O	6.70	1.36	1.23
1	A	27	HIS	CE1-NE2	6.69	1.48	1.32
1	A	35	GLU	CD-OE1	-6.69	1.18	1.25
1	A	104	ASP	N-CA	6.63	1.59	1.46
1	A	40	ALA	CA-CB	6.62	1.66	1.52
1	A	111	LYS	N-CA	6.62	1.59	1.46
1	A	129	GLU	CD-OE1	6.59	1.32	1.25
1	A	124	ALA	N-CA	6.57	1.59	1.46
1	A	14	SER	CB-OG	-6.53	1.33	1.42
1	A	13	SER	CB-OG	-6.52	1.33	1.42
1	A	145	ILE	N-CA	6.48	1.59	1.46
1	A	15	TRP	C-O	6.48	1.35	1.23
1	A	15	TRP	NE1-CE2	-6.48	1.29	1.37
1	A	138	TYR	CD1-CE1	6.44	1.49	1.39
1	A	11	VAL	N-CA	6.43	1.59	1.46
1	A	68	PHE	C-O	6.40	1.35	1.23
1	A	124	ALA	C-O	6.40	1.35	1.23
1	A	149	MET	C-O	6.36	1.35	1.23
1	A	59	GLU	CD-OE2	6.34	1.32	1.25
1	A	28	ARG	CZ-NH1	6.32	1.41	1.33
1	A	86	THR	N-CA	6.31	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	SER	C-O	6.24	1.35	1.23
1	A	148	GLU	CB-CG	6.23	1.64	1.52
1	A	111	LYS	CD-CE	6.20	1.66	1.51
1	A	6	SER	CA-CB	6.19	1.62	1.52
1	A	67	VAL	CB-CG2	6.19	1.65	1.52
1	A	102	VAL	N-CA	6.19	1.58	1.46
1	A	95	SER	N-CA	6.17	1.58	1.46
1	A	98	VAL	CB-CG2	6.16	1.65	1.52
1	A	68	PHE	CG-CD2	6.15	1.48	1.38
1	A	68	PHE	CE1-CZ	6.09	1.49	1.37
1	A	84	VAL	CB-CG1	6.00	1.65	1.52
1	A	15	TRP	CD1-NE1	5.99	1.48	1.38
1	A	73	GLU	CG-CD	5.98	1.60	1.51
1	A	55	GLN	C-O	5.97	1.34	1.23
1	A	109	VAL	CA-CB	5.96	1.67	1.54
1	A	27	HIS	CG-ND1	5.95	1.51	1.38
1	A	16	GLU	CG-CD	5.94	1.60	1.51
1	A	122	VAL	N-CA	5.94	1.58	1.46
1	A	9	ALA	CA-CB	5.92	1.64	1.52
1	A	75	ALA	C-O	5.91	1.34	1.23
1	A	97	HIS	CG-CD2	-5.90	1.25	1.35
1	A	75	ALA	N-CA	5.90	1.58	1.46
1	A	2	ALA	CA-CB	5.89	1.64	1.52
1	A	106	HIS	ND1-CE1	5.84	1.49	1.34
1	A	8	ALA	C-O	5.82	1.34	1.23
1	A	97	HIS	CA-CB	5.82	1.66	1.53
1	A	120	GLU	CA-CB	5.81	1.66	1.53
1	A	99	SER	N-CA	5.80	1.57	1.46
1	A	52	GLU	CG-CD	-5.78	1.43	1.51
1	A	76	ILE	C-O	5.78	1.34	1.23
1	A	79	GLU	CD-OE2	5.75	1.31	1.25
1	A	58	PRO	N-CD	5.68	1.55	1.47
1	A	18	PHE	N-CA	5.68	1.57	1.46
1	A	152	ALA	N-CA	5.67	1.57	1.46
1	A	79	GLU	C-O	5.66	1.34	1.23
1	A	148	GLU	CD-OE2	5.66	1.31	1.25
1	A	69	LYS	C-O	5.62	1.34	1.23
1	A	77	GLN	CG-CD	5.62	1.64	1.51
1	A	96	VAL	CB-CG1	5.56	1.64	1.52
1	A	125	LYS	CD-CE	5.54	1.65	1.51
1	A	90	LEU	CA-CB	5.53	1.66	1.53
1	A	111	LYS	CB-CG	5.53	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	PHE	N-CA	5.51	1.57	1.46
1	A	45	SER	N-CA	5.50	1.57	1.46
1	A	82	GLY	CA-C	5.45	1.60	1.51
1	A	153	ALA	C-OXT	5.43	1.33	1.23
1	A	5	GLU	CD-OE1	-5.42	1.19	1.25
1	A	130	LEU	N-CA	5.41	1.57	1.46
1	A	115	LEU	N-CA	5.41	1.57	1.46
1	A	52	GLU	N-CA	5.39	1.57	1.46
1	A	30	PHE	CG-CD2	-5.38	1.30	1.38
1	A	4	THR	C-O	5.37	1.33	1.23
1	A	43	LEU	CA-CB	5.33	1.66	1.53
1	A	71	VAL	CB-CG1	5.33	1.64	1.52
1	A	127	SER	CA-CB	5.31	1.60	1.52
1	A	127	SER	C-O	5.30	1.33	1.23
1	A	53	VAL	CA-CB	5.28	1.65	1.54
1	A	133	ALA	CA-C	5.28	1.66	1.52
1	A	140	GLU	CD-OE2	5.26	1.31	1.25
1	A	148	GLU	C-O	5.24	1.33	1.23
1	A	143	ILE	CA-CB	5.22	1.66	1.54
1	A	134	TRP	CD2-CE2	-5.18	1.35	1.41
1	A	3	LEU	CA-CB	5.16	1.65	1.53
1	A	128	GLU	CG-CD	5.16	1.59	1.51
1	A	92	ASN	C-O	5.13	1.33	1.23
1	A	45	SER	CB-OG	5.12	1.49	1.42
1	A	12	LYS	C-O	5.11	1.33	1.23
1	A	38	PRO	N-CA	5.11	1.55	1.47
1	A	64	ALA	N-CA	5.10	1.56	1.46
1	A	20	ALA	CA-CB	5.08	1.63	1.52
1	A	92	ASN	CB-CG	5.08	1.62	1.51
1	A	57	ASN	C-O	5.03	1.32	1.23
1	A	64	ALA	C-O	5.02	1.32	1.23
1	A	87	ASP	CA-C	5.01	1.66	1.52
1	A	148	GLU	CD-OE1	5.01	1.31	1.25

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	TYR	CB-CG-CD1	-9.85	115.09	121.00
1	A	112	GLU	OE1-CD-OE2	-9.48	111.92	123.30
1	A	28	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	73	GLU	OE1-CD-OE2	-8.09	113.59	123.30
1	A	16	GLU	OE1-CD-OE2	-7.72	114.03	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	TRP	CG-CD2-CE3	-7.60	127.06	133.90
1	A	128	GLU	OE1-CD-OE2	-7.08	114.80	123.30
1	A	108	PRO	N-CA-CB	6.98	111.67	103.30
1	A	54	PRO	N-CA-CB	6.93	111.61	103.30
1	A	138	TYR	CB-CG-CD2	6.83	125.10	121.00
1	A	29	PHE	CB-CG-CD1	-6.81	116.03	120.80
1	A	46	PHE	CB-CG-CD2	6.78	125.55	120.80
1	A	126	TRP	CE2-CD2-CG	-6.64	101.99	107.30
1	A	17	GLU	OE1-CD-OE2	-6.52	115.47	123.30
1	A	120	GLU	OE1-CD-OE2	-6.47	115.53	123.30
1	A	30	PHE	CB-CG-CD2	-6.39	116.32	120.80
1	A	29	PHE	CD1-CG-CD2	6.20	126.36	118.30
1	A	134	TRP	CG-CD1-NE1	-6.15	103.95	110.10
1	A	72	TYR	CG-CD1-CE1	-6.04	116.47	121.30
1	A	87	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	A	15	TRP	CH2-CZ2-CE2	-5.98	111.42	117.40
1	A	48	LYS	CB-CA-C	-5.97	98.46	110.40
1	A	131	ASN	O-C-N	5.87	132.10	122.70
1	A	126	TRP	NE1-CE2-CD2	5.80	113.10	107.30
1	A	142	ALA	O-C-N	5.74	131.89	122.70
1	A	8	ALA	O-C-N	5.71	131.83	122.70
1	A	124	ALA	CB-CA-C	-5.69	101.57	110.10
1	A	5	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	23	PRO	N-CA-CB	5.65	110.08	103.30
1	A	138	TYR	CD1-CE1-CZ	5.63	124.87	119.80
1	A	15	TRP	CD2-CE3-CZ3	-5.61	111.50	118.80
1	A	76	ILE	O-C-N	5.61	131.67	122.70
1	A	12	LYS	O-C-N	5.40	131.34	122.70
1	A	68	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	A	65	GLY	O-C-N	5.18	130.99	122.70
1	A	15	TRP	CD1-NE1-CE2	-5.17	104.34	109.00
1	A	45	SER	O-C-N	5.15	130.94	122.70
1	A	15	TRP	NE1-CE2-CZ2	-5.14	124.75	130.40
1	A	149	MET	O-C-N	5.13	130.91	122.70
1	A	29	PHE	CG-CD1-CE1	-5.06	115.24	120.80
1	A	104	ASP	CB-CG-OD2	5.05	122.85	118.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	A	17	GLU	Sidechain
1	A	35	GLU	Sidechain
1	A	42	ASP	Sidechain
1	A	56	ASN	Sidechain
1	A	57	ASN	Sidechain
1	A	59	GLU	Sidechain
1	A	7	GLN	Sidechain
1	A	92	ASN	Sidechain

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles ⓘ

5.2.1 Protein backbone ⓘ

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	153/153 (100%)	147 (96%)	5 (3%)	1 (1%)	22 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU

5.2.2 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	127/125 (102%)	123 (97%)	4 (3%)	40 40

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	34	LEU
1	A	96	VAL
1	A	151	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	25	HIS
1	A	61	GLN
1	A	77	GLN

5.2.3 RNA ⓘ

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.4 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.5 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	$\#\|Z\|>2$
3	HEM	A	155	1,2	41,50,50	3.99	27 (65%)	45,82,82	2.25	19 (42%)
2	CYN	A	154	3	0,1,1	-	-	-		

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

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C1D-C2D	7.38	1.58	1.44
3	A	155	HEM	C1B-C2B	7.03	1.58	1.44
3	A	155	HEM	C4D-C3D	6.79	1.56	1.45
3	A	155	HEM	FE-NB	6.78	2.30	1.96
3	A	155	HEM	C3B-C4B	6.47	1.57	1.44
3	A	155	HEM	CBD-CGD	6.25	1.65	1.50
3	A	155	HEM	CAB-C3B	6.22	1.64	1.47
3	A	155	HEM	CAA-C2A	5.94	1.60	1.52
3	A	155	HEM	C1A-NA	5.81	1.48	1.36
3	A	155	HEM	CAD-C3D	4.99	1.64	1.51
3	A	155	HEM	FE-ND	4.92	2.21	1.96
3	A	155	HEM	CMD-C2D	4.62	1.60	1.50
3	A	155	HEM	C3C-CAC	4.61	1.57	1.47
3	A	155	HEM	CMB-C2B	4.48	1.60	1.50
3	A	155	HEM	C3C-C2C	4.26	1.46	1.40
3	A	155	HEM	C4A-NA	3.94	1.44	1.36
3	A	155	HEM	CMC-C2C	3.63	1.60	1.51
3	A	155	HEM	C4A-CHB	3.63	1.51	1.41
3	A	155	HEM	O1A-CGA	3.49	1.33	1.22
3	A	155	HEM	C2A-C3A	3.35	1.47	1.37
3	A	155	HEM	CBA-CGA	3.26	1.58	1.50
3	A	155	HEM	C1A-CHA	3.08	1.49	1.41
3	A	155	HEM	CMA-C3A	2.73	1.57	1.51
3	A	155	HEM	O1D-CGD	2.58	1.30	1.22
3	A	155	HEM	CBD-CAD	-2.50	1.44	1.52
3	A	155	HEM	CHB-C1B	2.29	1.40	1.35
3	A	155	HEM	C4B-NB	2.01	1.42	1.38

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	155	HEM	CMA-C3A-C4A	-5.07	120.67	128.46
3	A	155	HEM	C4C-CHD-C1D	4.78	128.86	122.56
3	A	155	HEM	C4A-C3A-C2A	4.30	109.99	107.00
3	A	155	HEM	C2C-C3C-C4C	3.97	109.67	106.90
3	A	155	HEM	C3C-C4C-NC	-3.43	104.47	110.94
3	A	155	HEM	C4B-C3B-C2B	-3.39	104.42	107.11
3	A	155	HEM	O2D-CGD-O1D	-3.06	115.68	123.30
3	A	155	HEM	CMC-C2C-C3C	3.01	130.30	124.68
3	A	155	HEM	CHD-C1D-ND	-2.95	121.22	124.43
3	A	155	HEM	CAD-C3D-C4D	2.91	129.75	124.66
3	A	155	HEM	CHC-C4B-NB	-2.89	121.29	124.43
3	A	155	HEM	CAD-CBD-CGD	-2.87	107.42	113.60
3	A	155	HEM	C4B-CHC-C1C	2.81	126.27	122.56
3	A	155	HEM	CHB-C1B-NB	-2.73	121.01	124.38
3	A	155	HEM	CHA-C4D-ND	-2.45	121.36	124.38
3	A	155	HEM	C3D-C4D-ND	2.37	112.80	110.17
3	A	155	HEM	CMA-C3A-C2A	2.33	129.34	124.94
3	A	155	HEM	CMD-C2D-C1D	2.15	128.32	125.04
3	A	155	HEM	C2B-C1B-NB	2.09	112.31	109.84

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

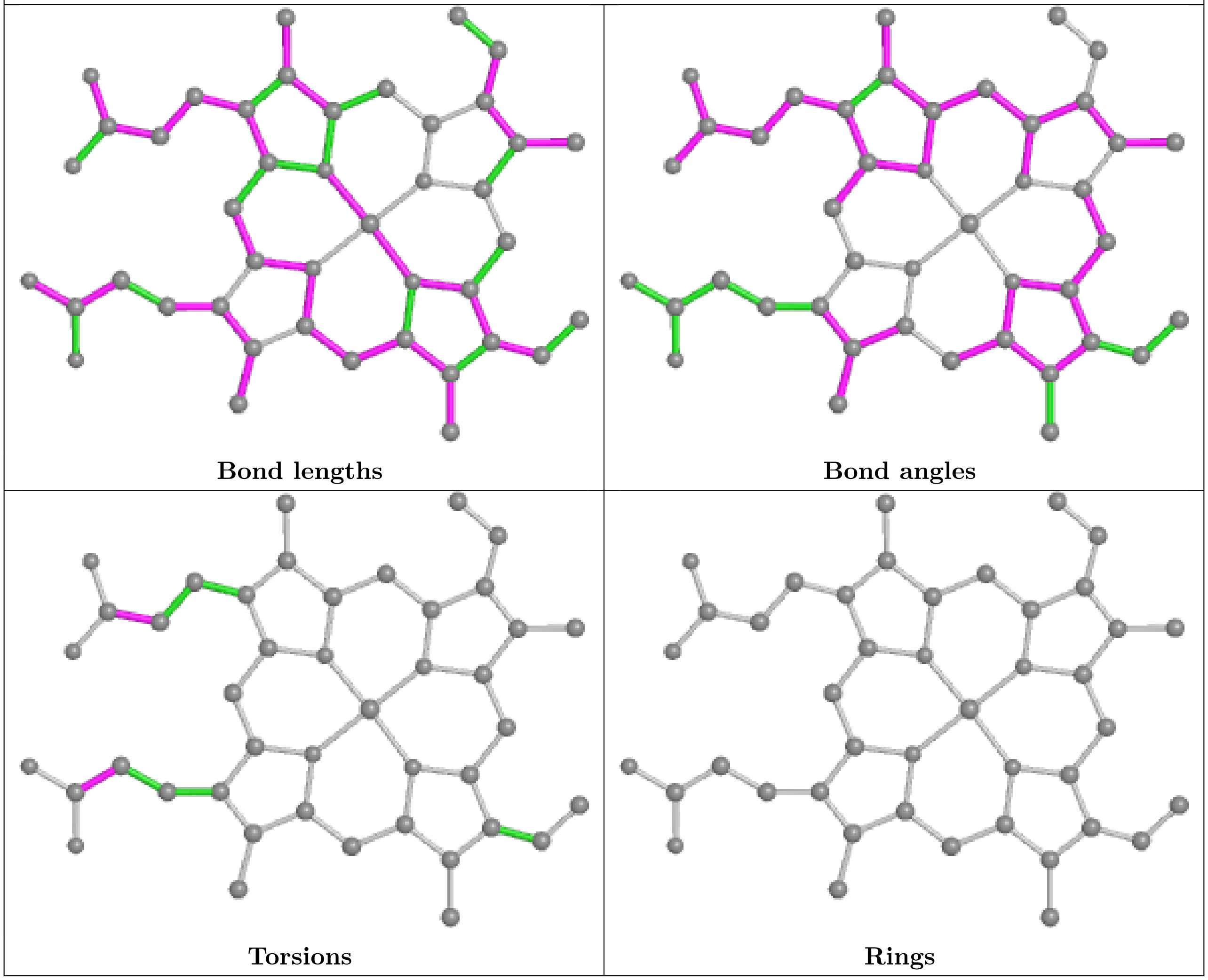
There are no ring outliers.

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



Bond lengths

Bond angles

Torsions

Rings

5.6 Other polymers

There are no such residues in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

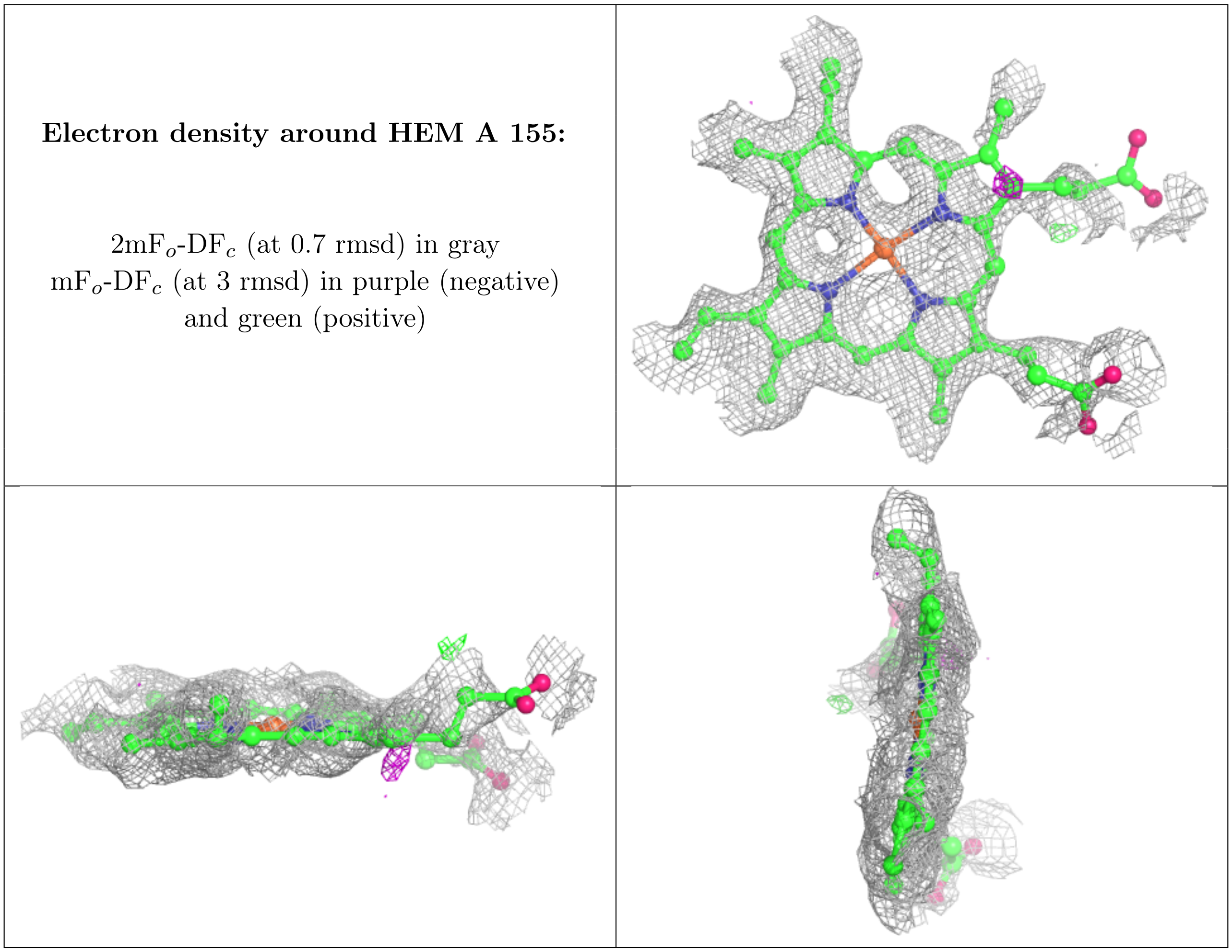
6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 155:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.