



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:50 PM GMT

PDB ID : 1MBN
Title : The stereochemistry of the protein myoglobin
Authors : Watson, H.C.; Kendrew, J.C.
Deposited on : 1973-04-05
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

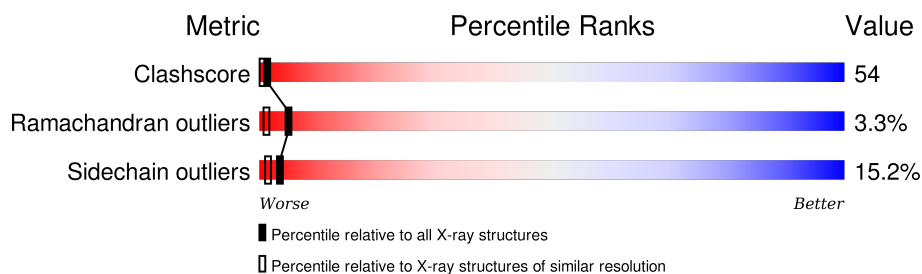
1 Overall quality at a glance

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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	153	

2 Entry composition [i](#)

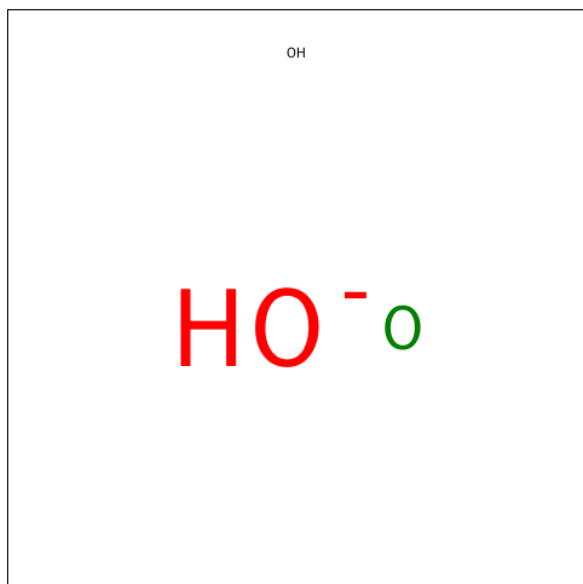
There are 3 unique types of molecules in this entry. The entry contains 1260 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

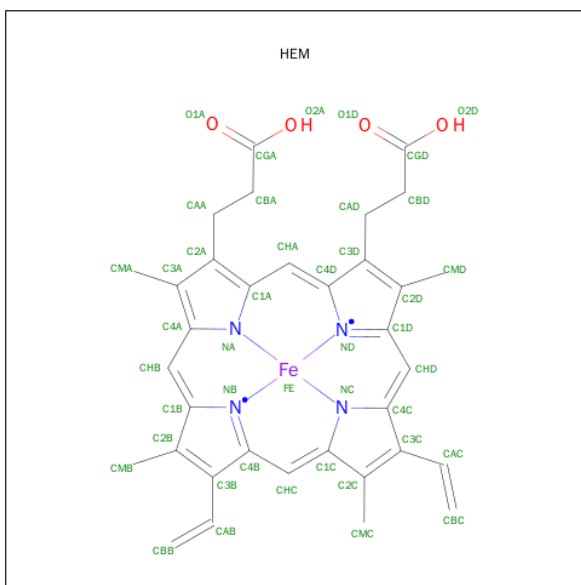
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1216	783	216	215	2			

- Molecule 2 is HYDROXIDE ION (three-letter code: OH) (formula: HO).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



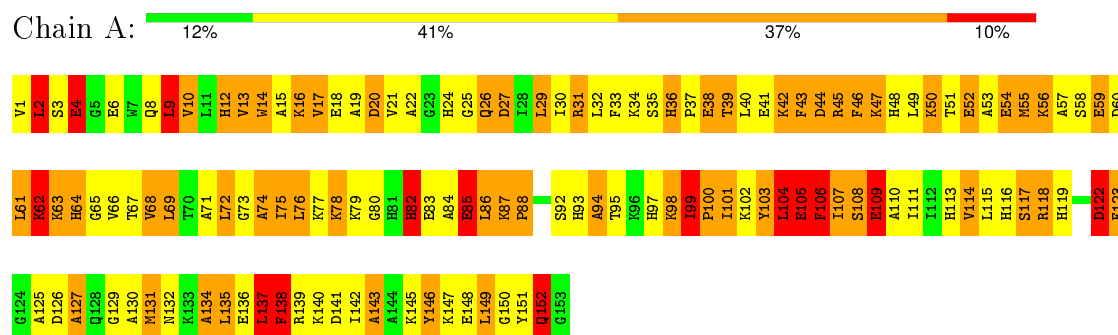
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.50 Å 30.90 Å 34.70 Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1260	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: HEM, OH

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	2.45	47/1244 (3.8%)	3.08	162/1671 (9.7%)

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	1	0

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GLU	CD-OE2	-13.82	1.10	1.25
1	A	14	TRP	NE1-CE2	-12.20	1.21	1.37
1	A	105	GLU	CD-OE2	-11.77	1.12	1.25
1	A	132	ASN	CG-OD1	10.98	1.48	1.24
1	A	52	GLU	CD-OE2	-10.56	1.14	1.25
1	A	139	ARG	NE-CZ	9.21	1.45	1.33
1	A	103	TYR	CE2-CZ	8.90	1.50	1.38
1	A	6	GLU	CD-OE1	-8.58	1.16	1.25
1	A	18	GLU	CD-OE2	-8.58	1.16	1.25
1	A	136	GLU	CD-OE2	-8.58	1.16	1.25
1	A	37	PRO	N-CD	-8.39	1.36	1.47
1	A	4	GLU	CG-CD	8.34	1.64	1.51
1	A	122	ASP	CG-OD1	7.79	1.43	1.25
1	A	150	GLY	C-O	7.78	1.36	1.23
1	A	105	GLU	C-O	7.67	1.38	1.23
1	A	105	GLU	CG-CD	7.32	1.62	1.51
1	A	103	TYR	CE1-CZ	-7.12	1.29	1.38
1	A	85	GLU	CD-OE2	-7.02	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	ARG	CZ-NH1	-6.85	1.24	1.33
1	A	41	GLU	CG-CD	6.70	1.62	1.51
1	A	106	PHE	CG-CD1	-6.57	1.28	1.38
1	A	35	SER	CB-OG	6.56	1.50	1.42
1	A	46	PHE	C-O	6.32	1.35	1.23
1	A	99	ILE	C-O	6.32	1.35	1.23
1	A	131	MET	C-O	6.32	1.35	1.23
1	A	18	GLU	CG-CD	6.29	1.61	1.51
1	A	31	ARG	NE-CZ	6.24	1.41	1.33
1	A	14	TRP	CD2-CE2	-6.24	1.33	1.41
1	A	14	TRP	CE2-CZ2	6.10	1.50	1.39
1	A	38	GLU	CG-CD	6.08	1.61	1.51
1	A	132	ASN	CG-ND2	-5.97	1.18	1.32
1	A	14	TRP	CD1-NE1	5.97	1.48	1.38
1	A	6	GLU	CD-OE2	-5.87	1.19	1.25
1	A	146	TYR	CG-CD2	-5.81	1.31	1.39
1	A	34	LYS	C-O	5.73	1.34	1.23
1	A	134	ALA	CA-CB	5.72	1.64	1.52
1	A	129	GLY	CA-C	5.57	1.60	1.51
1	A	80	GLY	N-CA	5.57	1.54	1.46
1	A	3	SER	CB-OG	5.54	1.49	1.42
1	A	26	GLN	C-O	5.54	1.33	1.23
1	A	101	ILE	N-CA	5.47	1.57	1.46
1	A	24	HIS	CB-CG	5.43	1.59	1.50
1	A	146	TYR	CE1-CZ	-5.35	1.31	1.38
1	A	27	ASP	CG-OD1	-5.11	1.13	1.25
1	A	43	PHE	CD1-CE1	5.10	1.49	1.39
1	A	88	PRO	N-CD	-5.03	1.40	1.47
1	A	100	PRO	C-N	-5.01	1.22	1.34

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ALA	N-CA-CB	-17.33	85.84	110.10
1	A	125	ALA	CB-CA-C	14.91	132.47	110.10
1	A	83	GLU	CB-CA-C	14.70	139.81	110.40
1	A	22	ALA	CB-CA-C	14.58	131.97	110.10
1	A	152	GLN	N-CA-CB	14.02	135.84	110.60
1	A	4	GLU	N-CA-CB	13.96	135.72	110.60
1	A	62	LYS	N-CA-CB	13.45	134.81	110.60
1	A	83	GLU	N-CA-CB	-13.21	86.83	110.60
1	A	126	ASP	CB-CA-C	13.14	136.68	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ALA	N-CA-CB	-12.45	92.67	110.10
1	A	8	GLN	N-CA-CB	11.78	131.80	110.60
1	A	126	ASP	CB-CG-OD1	11.68	128.81	118.30
1	A	13	VAL	N-CA-CB	11.62	137.07	111.50
1	A	74	ALA	CB-CA-C	11.35	127.13	110.10
1	A	141	ASP	CB-CG-OD1	11.30	128.47	118.30
1	A	3	SER	CB-CA-C	-11.08	89.04	110.10
1	A	64	HIS	N-CA-CB	10.91	130.24	110.60
1	A	15	ALA	CB-CA-C	-10.36	94.56	110.10
1	A	27	ASP	CB-CA-C	10.21	130.82	110.40
1	A	42	LYS	CB-CA-C	-10.08	90.24	110.40
1	A	3	SER	N-CA-CB	10.07	125.60	110.50
1	A	152	GLN	CB-CA-C	-9.95	90.51	110.40
1	A	103	TYR	CB-CA-C	9.93	130.27	110.40
1	A	17	VAL	CB-CA-C	-9.92	92.55	111.40
1	A	123	PHE	N-CA-CB	-9.88	92.81	110.60
1	A	60	ASP	CB-CG-OD1	9.80	127.12	118.30
1	A	29	LEU	CB-CA-C	9.72	128.67	110.20
1	A	114	VAL	N-CA-CB	9.72	132.88	111.50
1	A	57	ALA	N-CA-CB	9.69	123.66	110.10
1	A	135	LEU	CB-CA-C	9.66	128.56	110.20
1	A	26	GLN	CB-CA-C	9.65	129.71	110.40
1	A	10	VAL	N-CA-CB	9.49	132.38	111.50
1	A	146	TYR	CB-CG-CD1	-9.35	115.39	121.00
1	A	43	PHE	N-CA-CB	-9.34	93.78	110.60
1	A	74	ALA	N-CA-CB	-9.26	97.14	110.10
1	A	45	ARG	N-CA-CB	9.13	127.04	110.60
1	A	130	ALA	CB-CA-C	9.13	123.79	110.10
1	A	98	LYS	N-CA-CB	9.01	126.83	110.60
1	A	122	ASP	CB-CG-OD2	9.01	126.41	118.30
1	A	57	ALA	CB-CA-C	-8.97	96.64	110.10
1	A	105	GLU	OE1-CD-OE2	8.95	134.03	123.30
1	A	139	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	A	108	SER	N-CA-CB	8.69	123.53	110.50
1	A	95	THR	N-CA-C	8.57	134.13	111.00
1	A	47	LYS	N-CA-CB	8.52	125.94	110.60
1	A	135	LEU	N-CA-CB	-8.44	93.53	110.40
1	A	27	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	137	LEU	N-CA-CB	8.42	127.25	110.40
1	A	18	GLU	OE1-CD-OE2	8.39	133.37	123.30
1	A	30	ILE	CB-CA-C	8.32	128.25	111.60
1	A	58	SER	CB-CA-C	-8.26	94.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	HIS	CB-CA-C	-8.21	93.98	110.40
1	A	103	TYR	N-CA-CB	-8.08	96.06	110.60
1	A	9	LEU	CB-CA-C	-8.06	94.89	110.20
1	A	24	HIS	N-CA-CB	-8.00	96.20	110.60
1	A	92	SER	N-CA-CB	7.96	122.44	110.50
1	A	52	GLU	CB-CA-C	-7.89	94.61	110.40
1	A	40	LEU	CB-CA-C	-7.87	95.25	110.20
1	A	14	TRP	CB-CA-C	7.85	126.10	110.40
1	A	151	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	A	146	TYR	CB-CG-CD2	7.79	125.68	121.00
1	A	134	ALA	CB-CA-C	7.74	121.71	110.10
1	A	14	TRP	NE1-CE2-CZ2	-7.69	121.94	130.40
1	A	138	PHE	CB-CA-C	7.62	125.64	110.40
1	A	151	TYR	CB-CA-C	7.46	125.32	110.40
1	A	44	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	105	GLU	CG-CD-OE1	-7.42	103.46	118.30
1	A	86	LEU	CB-CA-C	-7.32	96.30	110.20
1	A	149	LEU	N-CA-CB	-7.22	95.96	110.40
1	A	14	TRP	CD2-CE3-CZ3	-7.21	109.42	118.80
1	A	38	GLU	N-CA-CB	-7.20	97.64	110.60
1	A	3	SER	N-CA-C	7.17	130.35	111.00
1	A	53	ALA	N-CA-CB	7.17	120.13	110.10
1	A	36	HIS	N-CA-CB	-7.16	97.72	110.60
1	A	85	GLU	OE1-CD-OE2	7.05	131.75	123.30
1	A	78	LYS	CB-CA-C	7.04	124.47	110.40
1	A	56	LYS	CB-CA-C	-7.02	96.36	110.40
1	A	41	GLU	OE1-CD-OE2	6.95	131.63	123.30
1	A	117	SER	N-CA-CB	6.92	120.87	110.50
1	A	27	ASP	N-CA-CB	-6.90	98.18	110.60
1	A	125	ALA	N-CA-C	6.88	129.57	111.00
1	A	63	LYS	N-CA-CB	-6.87	98.23	110.60
1	A	60	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	A	4	GLU	OE1-CD-OE2	6.81	131.47	123.30
1	A	15	ALA	N-CA-CB	6.76	119.56	110.10
1	A	118	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	14	TRP	CH2-CZ2-CE2	-6.75	110.66	117.40
1	A	118	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	123	PHE	N-CA-C	6.71	129.11	111.00
1	A	85	GLU	CG-CD-OE1	-6.70	104.90	118.30
1	A	127	ALA	N-CA-CB	-6.69	100.73	110.10
1	A	136	GLU	N-CA-CB	-6.64	98.64	110.60
1	A	14	TRP	CE3-CZ3-CH2	6.62	128.48	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	TYR	CG-CD1-CE1	-6.62	116.00	121.30
1	A	118	ARG	N-CA-CB	-6.62	98.69	110.60
1	A	59	GLU	OE1-CD-OE2	6.59	131.21	123.30
1	A	16	LYS	N-CA-CB	-6.55	98.81	110.60
1	A	38	GLU	OE1-CD-OE2	6.51	131.11	123.30
1	A	50	LYS	N-CA-CB	6.45	122.21	110.60
1	A	93	HIS	CB-CA-C	6.44	123.28	110.40
1	A	14	TRP	CG-CD2-CE3	-6.42	128.12	133.90
1	A	33	PHE	CB-CG-CD1	-6.40	116.32	120.80
1	A	72	LEU	N-CA-CB	6.34	123.08	110.40
1	A	113	HIS	CB-CA-C	-6.29	97.83	110.40
1	A	105	GLU	N-CA-CB	6.28	121.91	110.60
1	A	66	VAL	N-CA-CB	6.25	125.25	111.50
1	A	149	LEU	N-CA-C	6.22	127.78	111.00
1	A	76	LEU	CB-CA-C	6.11	121.81	110.20
1	A	104	LEU	CB-CA-C	6.09	121.77	110.20
1	A	136	GLU	CG-CD-OE1	-6.05	106.19	118.30
1	A	86	LEU	N-CA-C	5.98	127.15	111.00
1	A	122	ASP	N-CA-CB	-5.98	99.84	110.60
1	A	38	GLU	CB-CA-C	5.97	122.34	110.40
1	A	4	GLU	CG-CD-OE1	-5.97	106.36	118.30
1	A	84	ALA	CB-CA-C	5.93	119.00	110.10
1	A	100	PRO	O-C-N	5.92	132.18	122.70
1	A	2	LEU	O-C-N	5.92	132.17	122.70
1	A	116	HIS	N-CA-CB	5.87	121.16	110.60
1	A	83	GLU	CG-CD-OE1	-5.81	106.67	118.30
1	A	69	LEU	CB-CA-C	5.80	121.23	110.20
1	A	34	LYS	N-CA-CB	-5.80	100.16	110.60
1	A	130	ALA	N-CA-C	-5.79	95.37	111.00
1	A	20	ASP	N-CA-CB	5.76	120.97	110.60
1	A	86	LEU	N-CA-CB	5.75	121.90	110.40
1	A	52	GLU	CG-CD-OE1	-5.73	106.83	118.30
1	A	136	GLU	CB-CA-C	-5.71	98.97	110.40
1	A	52	GLU	OE1-CD-OE2	5.58	130.00	123.30
1	A	82	HIS	N-CA-C	5.58	126.06	111.00
1	A	21	VAL	CA-CB-CG1	5.57	119.25	110.90
1	A	37	PRO	CB-CA-C	5.56	125.91	112.00
1	A	134	ALA	N-CA-CB	-5.56	102.31	110.10
1	A	74	ALA	O-C-N	5.55	131.58	122.70
1	A	54	GLU	OE1-CD-OE2	5.53	129.94	123.30
1	A	43	PHE	CB-CG-CD2	5.53	124.67	120.80
1	A	67	THR	CB-CA-C	5.44	126.30	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	LYS	CB-CA-C	5.43	121.27	110.40
1	A	87	LYS	CB-CA-C	5.43	121.26	110.40
1	A	103	TYR	CD1-CE1-CZ	5.43	124.69	119.80
1	A	6	GLU	OE1-CD-OE2	5.42	129.81	123.30
1	A	12	HIS	N-CA-CB	-5.41	100.86	110.60
1	A	68	VAL	N-CA-CB	-5.40	99.62	111.50
1	A	94	ALA	N-CA-CB	5.35	117.59	110.10
1	A	18	GLU	CG-CD-OE1	-5.35	107.60	118.30
1	A	107	ILE	CA-CB-CG2	-5.26	100.37	110.90
1	A	78	LYS	N-CA-CB	-5.25	101.16	110.60
1	A	14	TRP	NE1-CE2-CD2	5.24	112.54	107.30
1	A	39	THR	N-CA-CB	5.23	120.24	110.30
1	A	111	ILE	N-CA-CB	5.23	122.83	110.80
1	A	34	LYS	CB-CA-C	5.21	120.83	110.40
1	A	109	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	A	106	PHE	CZ-CE2-CD2	5.20	126.34	120.10
1	A	101	ILE	O-C-N	5.19	131.01	122.70
1	A	110	ALA	N-CA-CB	-5.18	102.84	110.10
1	A	75	ILE	CA-CB-CG2	-5.17	100.56	110.90
1	A	36	HIS	CB-CA-C	5.13	120.66	110.40
1	A	140	LYS	CB-CA-C	5.12	120.65	110.40
1	A	76	LEU	N-CA-CB	-5.11	100.19	110.40
1	A	55	MET	N-CA-CB	-5.10	101.41	110.60
1	A	143	ALA	CB-CA-C	5.10	117.75	110.10
1	A	54	GLU	O-C-N	5.10	130.85	122.70
1	A	138	PHE	N-CA-CB	-5.05	101.50	110.60
1	A	88	PRO	CB-CA-C	5.01	124.53	112.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	8	GLN	CA

There are no planarity outliers.

5.2 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	1216	0	1242	135	5
2	A	1	0	0	0	0
3	A	43	0	30	6	0
All	All	1260	0	1272	137	5

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 54.

All (137) 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:78:LYS:NZ	1:A:85:GLU:OE1	1.81	1.13
1:A:143:ALA:HB1	1:A:152:GLN:OE1	1.52	1.09
1:A:87:LYS:HE3	1:A:145:LYS:HE2	1.30	1.07
1:A:1:VAL:HG13	1:A:2:LEU:HD12	1.37	1.03
1:A:1:VAL:CG1	1:A:2:LEU:HD12	1.92	0.98
1:A:2:LEU:H	1:A:2:LEU:HD12	1.26	0.98
1:A:104:LEU:CD1	1:A:142:ILE:HD12	1.94	0.97
1:A:42:LYS:HZ3	1:A:98:LYS:HB2	1.29	0.96
1:A:145:LYS:HZ2	1:A:148:GLU:CD	1.73	0.90
1:A:145:LYS:NZ	1:A:148:GLU:CD	2.24	0.90
1:A:145:LYS:NZ	1:A:148:GLU:OE1	2.08	0.87
1:A:87:LYS:HE3	1:A:145:LYS:CE	2.05	0.85
1:A:49:LEU:HD21	1:A:61:LEU:CD1	2.06	0.85
1:A:49:LEU:HD23	1:A:55:MET:HG2	1.57	0.84
1:A:48:HIS:O	1:A:50:LYS:HE3	1.79	0.82
1:A:94:ALA:HB2	1:A:146:TYR:CE2	2.14	0.82
1:A:38:GLU:HG3	1:A:103:TYR:OH	1.80	0.82
1:A:49:LEU:C	1:A:50:LYS:HE2	2.00	0.81
1:A:51:THR:OG1	1:A:54:GLU:HG3	1.80	0.81
1:A:2:LEU:H	1:A:2:LEU:CD1	1.94	0.80
1:A:100:PRO:O	1:A:103:TYR:HB2	1.82	0.79
1:A:13:VAL:HG21	1:A:123:PHE:CE2	2.17	0.79
1:A:2:LEU:HD12	1:A:2:LEU:N	1.98	0.79
1:A:104:LEU:HD11	1:A:142:ILE:HD12	1.67	0.76
1:A:42:LYS:NZ	1:A:98:LYS:HB2	2.01	0.75
1:A:12:HIS:NE2	1:A:16:LYS:NZ	2.32	0.75
1:A:82:HIS:CE1	1:A:137:LEU:HD21	2.22	0.74
1:A:145:LYS:NZ	1:A:148:GLU:OE2	2.20	0.73
1:A:42:LYS:NZ	1:A:98:LYS:O	2.22	0.72
1:A:49:LEU:CD2	1:A:61:LEU:CD1	2.66	0.72
1:A:4:GLU:OE1	1:A:4:GLU:HA	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:O	1:A:55:MET:HG3	1.90	0.71
1:A:82:HIS:HE1	1:A:137:LEU:HD21	1.55	0.71
1:A:82:HIS:HE1	1:A:137:LEU:CD2	2.03	0.71
1:A:145:LYS:O	1:A:149:LEU:HG	1.92	0.69
1:A:13:VAL:HG21	1:A:123:PHE:HE2	1.59	0.68
3:A:155:HEM:CMD	3:A:155:HEM:HBD1	2.24	0.68
1:A:143:ALA:CB	1:A:152:GLN:OE1	2.36	0.68
1:A:49:LEU:O	1:A:50:LYS:HE2	1.94	0.67
1:A:145:LYS:O	1:A:149:LEU:CG	2.44	0.66
1:A:29:LEU:HD11	1:A:65:GLY:HA2	1.76	0.65
1:A:1:VAL:CG1	1:A:2:LEU:CD1	2.74	0.65
1:A:43:PHE:CE2	3:A:155:HEM:CHD	2.80	0.64
1:A:47:LYS:O	1:A:50:LYS:NZ	2.25	0.64
1:A:100:PRO:O	1:A:103:TYR:N	2.24	0.64
1:A:1:VAL:HG12	1:A:2:LEU:HD12	1.79	0.63
1:A:32:LEU:HD22	1:A:107:ILE:HG13	1.80	0.62
1:A:44:ASP:OD1	1:A:47:LYS:CE	2.47	0.62
1:A:49:LEU:HD21	1:A:61:LEU:HD13	1.80	0.62
1:A:103:TYR:HD1	3:A:155:HEM:HBC1	1.65	0.61
1:A:99:ILE:HD13	1:A:99:ILE:N	2.14	0.61
1:A:29:LEU:HD11	1:A:65:GLY:CA	2.31	0.61
1:A:49:LEU:CD2	1:A:61:LEU:HD11	2.29	0.61
1:A:146:TYR:O	1:A:149:LEU:HB2	2.02	0.60
1:A:42:LYS:HZ3	1:A:98:LYS:CB	2.11	0.60
1:A:44:ASP:OD1	1:A:47:LYS:HE2	2.02	0.60
1:A:13:VAL:HG21	1:A:123:PHE:CD2	2.36	0.60
1:A:147:LYS:O	1:A:148:GLU:C	2.42	0.58
3:A:155:HEM:HBC2	3:A:155:HEM:CMC	2.33	0.58
1:A:48:HIS:C	1:A:50:LYS:HE3	2.26	0.56
1:A:145:LYS:O	1:A:149:LEU:HD12	2.06	0.56
1:A:131:MET:O	1:A:135:LEU:HG	2.05	0.56
1:A:87:LYS:HB3	1:A:88:PRO:HD3	1.88	0.56
1:A:1:VAL:HG13	1:A:2:LEU:N	2.20	0.56
1:A:87:LYS:CE	1:A:145:LYS:HE2	2.21	0.56
1:A:104:LEU:HD11	1:A:142:ILE:CD1	2.34	0.56
1:A:26:GLN:OE1	1:A:56:LYS:HA	2.07	0.55
1:A:42:LYS:HD2	1:A:99:ILE:CD1	2.37	0.55
1:A:39:THR:HG22	1:A:103:TYR:CD1	2.42	0.54
1:A:42:LYS:NZ	1:A:98:LYS:CB	2.69	0.54
1:A:46:PHE:O	1:A:49:LEU:HB2	2.08	0.54
1:A:101:ILE:HD11	1:A:146:TYR:CD1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LYS:O	1:A:149:LEU:CD1	2.57	0.53
1:A:44:ASP:HA	1:A:47:LYS:HE2	1.90	0.53
1:A:31:ARG:HD2	1:A:31:ARG:O	2.08	0.53
1:A:14:TRP:CZ2	1:A:73:GLY:CA	2.92	0.52
1:A:105:GLU:O	1:A:108:SER:HB2	2.11	0.51
1:A:1:VAL:HG12	1:A:2:LEU:CD1	2.39	0.50
1:A:138:PHE:O	1:A:142:ILE:HG13	2.11	0.50
1:A:98:LYS:C	1:A:99:ILE:HD13	2.32	0.50
1:A:52:GLU:O	1:A:56:LYS:HG3	2.11	0.50
1:A:87:LYS:HE3	1:A:145:LYS:NZ	2.27	0.49
1:A:119:HIS:HB3	1:A:122:ASP:HB2	1.93	0.49
1:A:2:LEU:HD21	1:A:134:ALA:N	2.28	0.49
1:A:109:GLU:OE2	1:A:109:GLU:HA	2.13	0.49
1:A:103:TYR:N	1:A:103:TYR:CD2	2.81	0.49
1:A:9:LEU:HG	1:A:127:ALA:HA	1.94	0.48
1:A:32:LEU:HD22	1:A:107:ILE:HB	1.95	0.48
1:A:64:HIS:O	1:A:68:VAL:HG23	2.14	0.48
1:A:17:VAL:O	1:A:17:VAL:HG12	2.13	0.47
1:A:97:HIS:O	1:A:99:ILE:HD13	2.15	0.47
1:A:43:PHE:CE2	3:A:155:HEM:HHD	2.49	0.47
1:A:71:ALA:O	1:A:74:ALA:HB3	2.14	0.47
1:A:16:LYS:HZ2	1:A:122:ASP:HB3	1.80	0.47
1:A:99:ILE:O	1:A:99:ILE:HG22	2.13	0.47
1:A:78:LYS:HZ1	1:A:85:GLU:CD	2.00	0.46
1:A:10:VAL:HG22	1:A:131:MET:HA	1.97	0.46
1:A:1:VAL:HG13	1:A:2:LEU:H	1.80	0.46
1:A:14:TRP:NE1	1:A:73:GLY:HA3	2.31	0.46
1:A:14:TRP:CE2	1:A:73:GLY:CA	2.99	0.46
1:A:51:THR:HG1	1:A:54:GLU:HG3	1.78	0.46
1:A:26:GLN:OE1	1:A:56:LYS:O	2.34	0.45
1:A:98:LYS:O	1:A:100:PRO:HD3	2.15	0.45
1:A:99:ILE:N	1:A:99:ILE:CD1	2.79	0.45
1:A:14:TRP:CE2	1:A:73:GLY:HA2	2.51	0.45
1:A:61:LEU:O	1:A:62:LYS:C	2.54	0.45
1:A:1:VAL:CG1	1:A:2:LEU:N	2.79	0.45
1:A:32:LEU:HD22	1:A:107:ILE:CG1	2.46	0.45
1:A:32:LEU:HD13	1:A:107:ILE:HA	1.97	0.45
1:A:36:HIS:HA	1:A:38:GLU:OE2	2.17	0.45
1:A:14:TRP:O	1:A:17:VAL:HB	2.17	0.45
1:A:72:LEU:O	1:A:76:LEU:HG	2.17	0.44
1:A:145:LYS:HZ3	1:A:148:GLU:CD	2.02	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:HA	1:A:106:PHE:HB2	1.99	0.44
1:A:1:VAL:CG1	1:A:2:LEU:H	2.30	0.44
1:A:104:LEU:HD13	1:A:142:ILE:HD12	1.95	0.43
1:A:94:ALA:HB2	1:A:146:TYR:CD2	2.54	0.43
1:A:100:PRO:C	1:A:102:LYS:N	2.67	0.43
1:A:103:TYR:N	1:A:103:TYR:HD2	2.17	0.43
1:A:14:TRP:CZ2	1:A:73:GLY:N	2.86	0.43
1:A:50:LYS:HE2	1:A:50:LYS:HA	2.00	0.43
1:A:12:HIS:NE2	1:A:16:LYS:CE	2.81	0.43
1:A:1:VAL:HG13	1:A:2:LEU:CD1	2.27	0.42
1:A:76:LEU:O	1:A:79:LYS:N	2.44	0.42
1:A:12:HIS:CE1	1:A:16:LYS:HE3	2.55	0.42
1:A:114:VAL:O	1:A:118:ARG:HB2	2.20	0.42
1:A:103:TYR:O	1:A:107:ILE:N	2.44	0.41
1:A:71:ALA:O	1:A:75:ILE:HG13	2.21	0.41
1:A:59:GLU:OE2	1:A:62:LYS:HE3	2.21	0.41
1:A:25:GLY:O	1:A:29:LEU:HG	2.21	0.41
1:A:43:PHE:CZ	3:A:155:HEM:CHD	3.04	0.41
1:A:102:LYS:HD2	1:A:102:LYS:HA	1.76	0.40
1:A:50:LYS:N	1:A:50:LYS:HE2	2.36	0.40
1:A:85:GLU:HG2	1:A:85:GLU:H	1.71	0.40
1:A:48:HIS:O	1:A:50:LYS:CE	2.60	0.40
1:A:75:ILE:HG23	1:A:82:HIS:HB3	2.04	0.40
1:A:14:TRP:HE1	1:A:73:GLY:HA3	1.87	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:O	1:A:63:LYS:NZ[2_646]	1.01	1.19
1:A:48:HIS:CB	1:A:56:LYS:NZ[2_655]	1.64	0.56
1:A:19:ALA:C	1:A:63:LYS:NZ[2_646]	2.03	0.17
1:A:48:HIS:CG	1:A:56:LYS:NZ[2_655]	2.14	0.06
1:A:19:ALA:O	1:A:63:LYS:CE[2_646]	2.15	0.05

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%)	115 (76%)	31 (20%)	5 (3%)	5 1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	LYS
1	A	152	GLN
1	A	27	ASP
1	A	62	LYS
1	A	106	PHE

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	125/125 (100%)	106 (85%)	19 (15%)	3 1

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	4	GLU
1	A	9	LEU
1	A	20	ASP
1	A	45	ARG
1	A	61	LEU

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Mol	Chain	Res	Type
1	A	69	LEU
1	A	82	HIS
1	A	85	GLU
1	A	86	LEU
1	A	99	ILE
1	A	104	LEU
1	A	105	GLU
1	A	109	GLU
1	A	115	LEU
1	A	117	SER
1	A	122	ASP
1	A	137	LEU
1	A	138	PHE

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

Mol	Chain	Res	Type
1	A	8	GLN
1	A	82	HIS
1	A	91	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is modelled with single atom - leaving 1 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	$\# Z > 2$
3	HEM	A	155	1,2	30,50,50	3.58	19 (63%)	24,82,82	5.43	15 (62%)

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	-	0/10/54/54	0/0/8/8

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C3C-CAC	-7.73	1.36	1.51
3	A	155	HEM	C2C-C1C	-6.76	1.39	1.52
3	A	155	HEM	CAA-C2A	-6.34	1.41	1.52
3	A	155	HEM	C3D-C4D	-5.92	1.44	1.51
3	A	155	HEM	C3B-C4B	-4.98	1.47	1.51
3	A	155	HEM	C2D-C3D	-4.11	1.42	1.54
3	A	155	HEM	C3B-CAB	-4.10	1.43	1.51
3	A	155	HEM	CAD-C3D	-2.49	1.49	1.54
3	A	155	HEM	C2D-C1D	-2.41	1.44	1.51
3	A	155	HEM	CMA-C3A	-2.09	1.47	1.51
3	A	155	HEM	FE-ND	2.04	2.08	1.97
3	A	155	HEM	FE-NC	2.55	2.05	1.95
3	A	155	HEM	C1A-CHA	2.75	1.47	1.39
3	A	155	HEM	CHC-C1C	3.08	1.43	1.36
3	A	155	HEM	C1C-NC	3.31	1.40	1.36
3	A	155	HEM	C4C-NC	3.31	1.40	1.36
3	A	155	HEM	C2A-C3A	3.40	1.47	1.37
3	A	155	HEM	CHD-C4C	5.01	1.48	1.36
3	A	155	HEM	CBC-CAC	5.02	1.58	1.29

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	155	HEM	CBD-CAD-C3D	-15.00	69.89	113.55
3	A	155	HEM	C3C-CAC-CBC	-11.73	106.47	124.46
3	A	155	HEM	CAA-CBA-CGA	-11.08	92.45	112.75
3	A	155	HEM	CAD-CBD-CGD	-6.57	86.22	113.02
3	A	155	HEM	CMA-C3A-C4A	-3.98	121.78	128.36
3	A	155	HEM	CHC-C4B-NB	-2.38	118.79	124.52
3	A	155	HEM	C3B-CAB-CBB	2.68	128.57	124.46
3	A	155	HEM	CMD-C2D-C3D	2.70	126.28	114.35
3	A	155	HEM	C3B-C4B-CHC	2.73	127.01	123.16
3	A	155	HEM	C4B-CHC-C1C	2.77	130.45	125.82
3	A	155	HEM	CAD-C3D-C4D	3.24	123.90	112.47
3	A	155	HEM	CMC-C2C-C3C	3.28	124.72	116.53
3	A	155	HEM	CBA-CAA-C2A	4.26	120.16	112.53
3	A	155	HEM	CMB-C2B-C3B	5.33	129.83	116.53
3	A	155	HEM	CAD-C3D-C2D	7.04	133.47	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	HEM	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.