



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:17 AM UTC

PDB ID : 1MBN / pdb_00001mbn
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

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

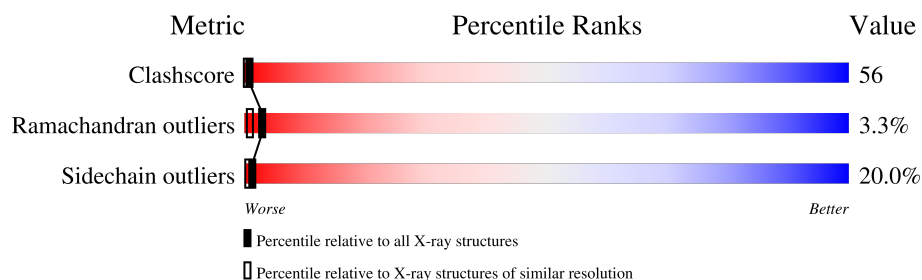
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	153	

2 Entry composition [i](#)

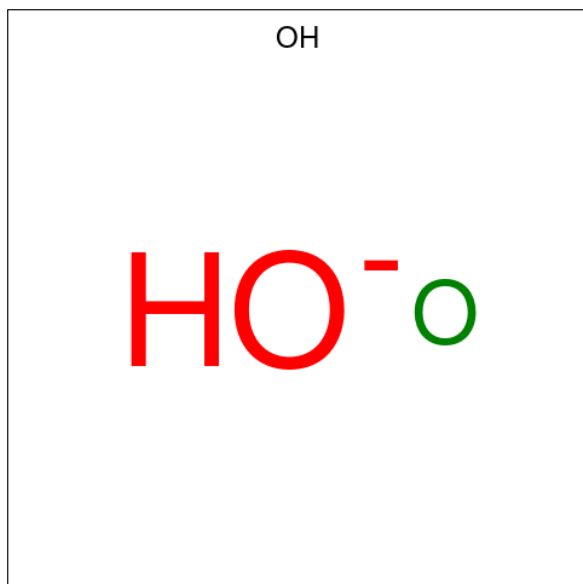
There are 3 unique types of molecules in this entry. The entry contains 1260 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

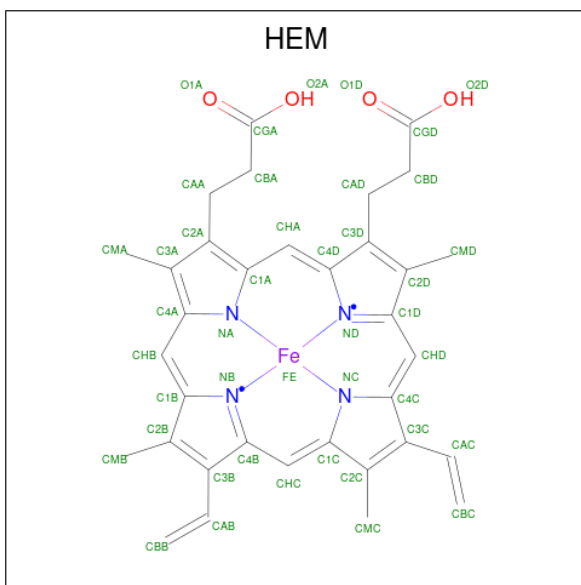
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	0	0	0
			1216	783	216	215	2			

- Molecule 2 is HYDROXIDE ION (CCD ID: 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 (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

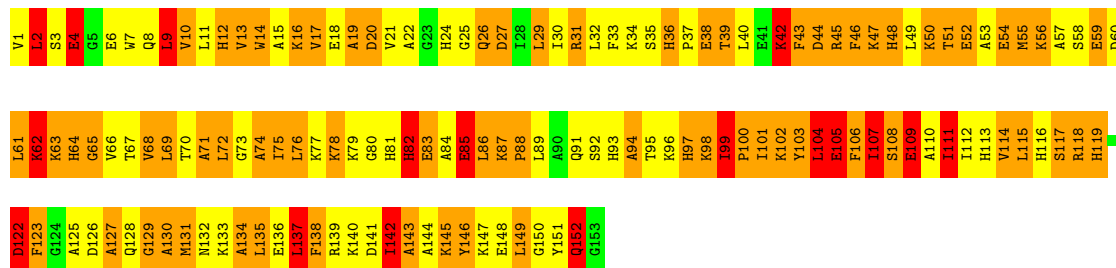
3 Residue-property plots

These plots are drawn for all protein, RNA, 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

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.50Å 30.90Å 34.70Å 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: OH, 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	3.14	141/1244 (11.3%)	3.82	233/1671 (13.9%)

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 (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	TRP	NE1-CE2	-14.32	1.21	1.37
1	A	132	ASN	CG-OD1	12.92	1.48	1.23
1	A	105	GLU	C-O	11.92	1.38	1.24
1	A	139	ARG	NE-CZ	10.88	1.45	1.33
1	A	99	ILE	CA-C	-10.65	1.45	1.53
1	A	131	MET	C-O	9.62	1.35	1.24
1	A	20	ASP	CA-C	9.46	1.64	1.53
1	A	122	ASP	CG-OD1	9.44	1.43	1.25
1	A	150	GLY	C-O	9.04	1.36	1.24
1	A	101	ILE	N-CA	8.76	1.57	1.46
1	A	34	LYS	C-O	8.73	1.34	1.24
1	A	46	PHE	C-O	8.65	1.35	1.24
1	A	26	GLN	C-O	8.47	1.33	1.24
1	A	37	PRO	N-CD	-8.32	1.36	1.47
1	A	126	ASP	N-CA	8.31	1.56	1.46
1	A	100	PRO	C-N	-8.18	1.22	1.33
1	A	99	ILE	C-O	8.18	1.35	1.24
1	A	130	ALA	N-CA	8.09	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	PHE	C-N	-8.06	1.24	1.33
1	A	46	PHE	C-N	-8.00	1.23	1.33
1	A	129	GLY	CA-C	7.96	1.60	1.52
1	A	6	GLU	C-N	7.94	1.44	1.33
1	A	4	GLU	CD-OE2	-7.84	1.10	1.25
1	A	38	GLU	CA-C	-7.79	1.43	1.52
1	A	40	LEU	N-CA	7.71	1.56	1.46
1	A	91	GLN	CA-C	7.62	1.62	1.52
1	A	24	HIS	ND1-CE1	-7.60	1.25	1.32
1	A	93	HIS	ND1-CE1	-7.60	1.25	1.32
1	A	89	LEU	C-N	-7.48	1.24	1.33
1	A	81	HIS	CG-ND1	7.41	1.46	1.38
1	A	119	HIS	CG-CD2	-7.38	1.27	1.35
1	A	31	ARG	NE-CZ	7.38	1.41	1.33
1	A	37	PRO	C-N	-7.36	1.24	1.33
1	A	56	LYS	C-N	-7.36	1.24	1.33
1	A	132	ASN	CG-ND2	-7.30	1.18	1.33
1	A	2	LEU	CA-C	7.25	1.62	1.52
1	A	26	GLN	CA-C	-7.24	1.43	1.52
1	A	3	SER	CA-C	7.24	1.61	1.52
1	A	132	ASN	CA-C	7.23	1.62	1.52
1	A	114	VAL	C-O	7.22	1.32	1.24
1	A	116	HIS	ND1-CE1	7.18	1.39	1.32
1	A	38	GLU	C-O	7.18	1.32	1.24
1	A	38	GLU	CA-CB	7.17	1.64	1.53
1	A	93	HIS	CG-ND1	7.09	1.46	1.38
1	A	21	VAL	C-O	-7.05	1.16	1.24
1	A	139	ARG	CA-CB	7.03	1.64	1.53
1	A	111	ILE	N-CA	6.99	1.54	1.46
1	A	24	HIS	CB-CG	6.91	1.59	1.50
1	A	141	ASP	N-CA	6.91	1.54	1.46
1	A	116	HIS	CA-C	6.89	1.62	1.52
1	A	134	ALA	CA-CB	6.88	1.64	1.53
1	A	57	ALA	C-O	6.85	1.31	1.24
1	A	52	GLU	CA-C	-6.84	1.44	1.52
1	A	36	HIS	ND1-CE1	6.82	1.39	1.32
1	A	16	LYS	C-O	6.78	1.31	1.24
1	A	113	HIS	CG-CD2	6.75	1.43	1.35
1	A	143	ALA	N-CA	6.74	1.54	1.46
1	A	93	HIS	C-O	6.72	1.31	1.24
1	A	105	GLU	CD-OE2	-6.66	1.12	1.25
1	A	112	ILE	CA-CB	6.55	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	ALA	C-O	6.54	1.31	1.24
1	A	75	ILE	CA-CB	6.50	1.62	1.54
1	A	74	ALA	CA-C	6.48	1.61	1.52
1	A	105	GLU	CA-CB	6.43	1.63	1.53
1	A	15	ALA	C-O	6.35	1.31	1.24
1	A	24	HIS	C-N	6.33	1.41	1.33
1	A	102	LYS	C-O	6.31	1.31	1.24
1	A	92	SER	C-N	-6.25	1.25	1.33
1	A	78	LYS	CA-C	-6.19	1.44	1.52
1	A	27	ASP	CG-OD1	-6.19	1.13	1.25
1	A	9	LEU	C-O	6.19	1.31	1.24
1	A	54	GLU	N-CA	6.19	1.53	1.46
1	A	92	SER	C-O	6.19	1.31	1.24
1	A	42	LYS	C-O	6.18	1.31	1.24
1	A	133	LYS	CA-C	-6.16	1.45	1.52
1	A	144	ALA	CA-C	-6.16	1.45	1.52
1	A	82	HIS	CG-ND1	6.15	1.45	1.38
1	A	139	ARG	CZ-NH1	-6.15	1.24	1.32
1	A	101	ILE	C-N	-6.13	1.25	1.34
1	A	115	LEU	C-N	6.10	1.42	1.33
1	A	144	ALA	C-N	6.09	1.41	1.33
1	A	43	PHE	CA-CB	6.07	1.61	1.53
1	A	48	HIS	C-O	6.05	1.31	1.24
1	A	82	HIS	C-O	6.01	1.31	1.24
1	A	19	ALA	C-O	5.97	1.31	1.24
1	A	110	ALA	CA-C	5.96	1.60	1.52
1	A	52	GLU	CD-OE2	-5.96	1.14	1.25
1	A	85	GLU	CA-CB	5.92	1.62	1.53
1	A	135	LEU	N-CA	5.92	1.53	1.46
1	A	81	HIS	CB-CG	-5.91	1.41	1.50
1	A	24	HIS	N-CA	5.88	1.53	1.46
1	A	133	LYS	C-O	5.86	1.30	1.24
1	A	87	LYS	N-CA	-5.83	1.38	1.46
1	A	45	ARG	CD-NE	5.82	1.54	1.46
1	A	55	MET	C-O	5.74	1.31	1.24
1	A	108	SER	C-O	5.74	1.31	1.24
1	A	22	ALA	C-O	5.74	1.30	1.24
1	A	72	LEU	N-CA	-5.67	1.39	1.46
1	A	91	GLN	N-CA	-5.66	1.39	1.46
1	A	125	ALA	CA-CB	5.66	1.62	1.53
1	A	71	ALA	N-CA	-5.58	1.39	1.46
1	A	12	HIS	CD2-NE2	5.57	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	HIS	CA-CB	5.57	1.63	1.53
1	A	20	ASP	C-N	-5.56	1.27	1.33
1	A	89	LEU	CA-C	5.55	1.59	1.52
1	A	48	HIS	CA-C	-5.53	1.45	1.52
1	A	127	ALA	C-N	5.53	1.40	1.33
1	A	51	THR	N-CA	5.51	1.53	1.45
1	A	111	ILE	C-N	-5.50	1.27	1.33
1	A	20	ASP	CG-OD2	-5.50	1.15	1.25
1	A	122	ASP	CG-OD2	-5.50	1.15	1.25
1	A	39	THR	CB-OG1	-5.48	1.34	1.43
1	A	48	HIS	CG-CD2	5.47	1.41	1.35
1	A	78	LYS	CA-CB	5.47	1.62	1.53
1	A	44	ASP	C-N	5.46	1.41	1.33
1	A	47	LYS	C-O	5.46	1.30	1.24
1	A	152	GLN	C-O	5.44	1.30	1.24
1	A	132	ASN	C-N	-5.44	1.27	1.33
1	A	36	HIS	CB-CG	-5.41	1.42	1.50
1	A	53	ALA	N-CA	-5.36	1.40	1.46
1	A	113	HIS	C-O	-5.35	1.18	1.24
1	A	48	HIS	N-CA	5.35	1.53	1.46
1	A	83	GLU	N-CA	-5.34	1.39	1.46
1	A	131	MET	N-CA	-5.34	1.39	1.46
1	A	80	GLY	N-CA	5.32	1.54	1.44
1	A	78	LYS	N-CA	5.28	1.53	1.46
1	A	14	TRP	CA-C	-5.27	1.45	1.52
1	A	60	ASP	CG-OD1	-5.27	1.15	1.25
1	A	17	VAL	N-CA	5.26	1.53	1.46
1	A	40	LEU	C-O	5.24	1.30	1.24
1	A	64	HIS	ND1-CE1	-5.21	1.27	1.32
1	A	12	HIS	CG-ND1	5.21	1.44	1.38
1	A	139	ARG	C-O	5.20	1.30	1.24
1	A	70	THR	C-O	5.19	1.30	1.24
1	A	92	SER	CA-C	5.16	1.59	1.52
1	A	135	LEU	C-N	5.10	1.40	1.34
1	A	9	LEU	CA-C	-5.06	1.46	1.52
1	A	59	GLU	C-N	5.06	1.40	1.33
1	A	22	ALA	C-N	-5.04	1.26	1.33
1	A	27	ASP	C-N	5.01	1.40	1.33
1	A	81	HIS	CA-C	-5.00	1.47	1.53

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	VAL	N-CA-CB	22.67	137.07	110.55
1	A	114	VAL	N-CA-CB	20.15	132.88	110.51
1	A	10	VAL	N-CA-CB	17.52	132.38	110.47
1	A	83	GLU	CB-CA-C	17.51	139.81	110.74
1	A	95	THR	N-CA-C	17.31	134.13	113.18
1	A	4	GLU	N-CA-CB	17.04	135.72	109.82
1	A	126	ASP	CB-CA-C	16.17	136.68	110.81
1	A	125	ALA	N-CA-CB	-16.14	85.84	110.06
1	A	3	SER	N-CA-C	15.47	130.35	110.24
1	A	125	ALA	N-CA-C	15.08	129.57	111.33
1	A	152	GLN	N-CA-CB	15.00	135.84	110.49
1	A	123	PHE	N-CA-C	14.59	129.11	108.54
1	A	86	LEU	N-CA-C	14.56	127.15	111.28
1	A	62	LYS	N-CA-CB	14.39	134.81	110.49
1	A	83	GLU	N-CA-CB	-14.08	86.83	109.78
1	A	64	HIS	N-CA-CB	13.95	130.24	110.01
1	A	66	VAL	N-CA-CB	13.94	125.25	110.62
1	A	8	GLN	N-CA-CB	12.99	131.80	109.72
1	A	130	ALA	N-CA-C	-12.83	95.37	111.02
1	A	125	ALA	CB-CA-C	12.82	132.47	110.68
1	A	30	ILE	CB-CA-C	12.79	128.25	111.88
1	A	22	ALA	CB-CA-C	12.76	131.97	110.79
1	A	17	VAL	CB-CA-C	-12.65	92.55	112.16
1	A	149	LEU	N-CA-C	12.63	127.78	112.38
1	A	113	HIS	N-CA-C	-12.28	97.58	110.97
1	A	103	TYR	CB-CA-C	12.26	130.27	110.90
1	A	75	ILE	N-CA-C	11.91	121.86	110.42
1	A	137	LEU	N-CA-CB	11.89	127.25	110.01
1	A	22	ALA	N-CA-CB	-11.87	92.67	110.12
1	A	26	GLN	CB-CA-C	11.81	129.71	110.92
1	A	3	SER	CB-CA-C	-11.64	89.04	109.64
1	A	111	ILE	N-CA-CB	11.62	122.83	110.62
1	A	135	LEU	N-CA-CB	-11.37	93.53	110.01
1	A	135	LEU	CB-CA-C	11.26	128.56	110.88
1	A	29	LEU	CB-CA-C	11.16	128.67	110.92
1	A	11	LEU	N-CA-C	10.96	123.31	111.36
1	A	21	VAL	N-CA-C	10.55	121.21	110.23
1	A	99	ILE	N-CA-C	10.45	117.06	107.56
1	A	82	HIS	N-CA-C	10.40	126.06	113.16
1	A	27	ASP	CB-CA-C	10.25	130.82	110.42
1	A	74	ALA	CB-CA-C	10.20	127.13	110.81
1	A	9	LEU	CB-CA-C	-10.18	94.89	110.88
1	A	43	PHE	N-CA-CB	-10.05	93.78	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	GLN	CB-CA-C	-10.01	90.51	110.42
1	A	58	SER	CB-CA-C	-9.93	94.41	109.90
1	A	47	LYS	N-CA-CB	9.91	125.94	109.78
1	A	135	LEU	N-CA-C	9.90	121.66	111.07
1	A	123	PHE	N-CA-CB	-9.88	92.81	110.60
1	A	68	VAL	N-CA-CB	-9.81	99.62	110.51
1	A	3	SER	N-CA-CB	9.80	125.60	109.92
1	A	98	LYS	N-CA-CB	9.73	126.83	112.13
1	A	67	THR	CB-CA-C	9.67	126.30	110.92
1	A	103	TYR	N-CA-CB	-9.66	96.06	110.07
1	A	42	LYS	CB-CA-C	-9.60	90.24	110.31
1	A	36	HIS	N-CA-CB	-9.56	97.72	111.20
1	A	52	GLU	CB-CA-C	-9.55	94.61	110.85
1	A	7	TRP	N-CA-C	-9.50	100.91	111.07
1	A	57	ALA	N-CA-CB	9.42	123.66	110.01
1	A	24	HIS	N-CA-CB	-9.22	96.20	109.94
1	A	45	ARG	N-CA-CB	9.19	127.04	110.32
1	A	42	LYS	N-CA-C	9.18	123.75	112.54
1	A	118	ARG	N-CA-C	9.18	124.48	113.28
1	A	74	ALA	O-C-N	9.13	131.58	122.09
1	A	57	ALA	CB-CA-C	-9.07	96.64	110.88
1	A	138	PHE	CB-CA-C	8.94	125.64	110.79
1	A	82	HIS	CB-CA-C	-8.91	93.98	110.01
1	A	60	ASP	N-CA-C	-8.87	101.69	111.36
1	A	68	VAL	N-CA-C	8.77	119.57	110.36
1	A	86	LEU	CB-CA-C	-8.73	96.30	110.79
1	A	72	LEU	N-CA-CB	8.72	123.08	109.82
1	A	74	ALA	N-CA-CB	-8.59	97.14	109.94
1	A	75	ILE	N-CA-CB	-8.54	100.56	110.55
1	A	38	GLU	N-CA-CB	-8.53	97.64	110.01
1	A	113	HIS	CB-CA-C	-8.53	97.83	110.96
1	A	149	LEU	N-CA-CB	-8.45	95.96	110.32
1	A	40	LEU	CB-CA-C	-8.44	95.25	110.70
1	A	99	ILE	CA-C-N	8.40	128.42	119.76
1	A	99	ILE	C-N-CA	8.40	128.42	119.76
1	A	75	ILE	O-C-N	8.33	130.07	121.91
1	A	92	SER	N-CA-CB	8.30	122.44	109.82
1	A	105	GLU	N-CA-CB	8.23	121.91	109.98
1	A	37	PRO	CB-CA-C	8.17	125.91	112.26
1	A	68	VAL	O-C-N	8.12	130.06	121.94
1	A	130	ALA	CB-CA-C	8.10	123.79	110.92
1	A	91	GLN	O-C-N	8.05	130.40	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	LYS	N-CA-CB	8.02	122.21	110.26
1	A	86	LEU	N-CA-CB	8.01	121.90	110.12
1	A	115	LEU	CA-C-O	7.99	129.20	120.82
1	A	98	LYS	CB-CA-C	-7.97	100.41	111.73
1	A	15	ALA	CB-CA-C	-7.97	94.56	110.42
1	A	14	TRP	CB-CA-C	7.88	126.10	110.42
1	A	88	PRO	CB-CA-C	7.86	124.53	111.56
1	A	46	PHE	N-CA-C	7.86	124.44	114.31
1	A	2	LEU	N-CA-C	7.82	121.73	110.24
1	A	16	LYS	N-CA-CB	-7.77	98.81	110.07
1	A	128	GLN	O-C-N	7.77	130.17	122.09
1	A	56	LYS	CB-CA-C	-7.72	96.36	110.63
1	A	108	SER	N-CA-CB	7.72	123.53	110.49
1	A	13	VAL	CB-CA-C	-7.71	102.11	111.97
1	A	136	GLU	N-CA-C	-7.61	102.96	111.71
1	A	2	LEU	O-C-N	7.59	132.17	123.06
1	A	100	PRO	O-C-N	7.56	132.18	123.03
1	A	78	LYS	CB-CA-C	7.56	124.47	110.11
1	A	93	HIS	CB-CA-C	7.52	123.28	110.79
1	A	136	GLU	N-CA-CB	-7.52	98.64	110.22
1	A	118	ARG	N-CA-CB	-7.50	98.69	110.46
1	A	35	SER	N-CA-C	7.37	119.39	111.36
1	A	85	GLU	N-CA-C	7.34	120.71	111.69
1	A	38	GLU	CB-CA-C	7.30	122.34	110.88
1	A	27	ASP	N-CA-CB	-7.29	98.18	110.49
1	A	30	ILE	N-CA-CB	-7.26	102.45	110.51
1	A	63	LYS	N-CA-CB	-7.25	98.23	110.49
1	A	151	TYR	CB-CA-C	7.25	125.32	111.48
1	A	54	GLU	O-C-N	7.15	130.85	122.20
1	A	14	TRP	CD2-CE3-CZ3	-7.06	109.42	118.60
1	A	146	TYR	N-CA-C	-7.02	102.46	111.02
1	A	89	LEU	O-C-N	7.01	129.66	122.09
1	A	151	TYR	N-CA-C	-6.97	99.91	109.95
1	A	71	ALA	CA-C-N	6.90	130.38	120.79
1	A	71	ALA	C-N-CA	6.90	130.38	120.79
1	A	30	ILE	O-C-N	6.88	128.82	121.94
1	A	34	LYS	N-CA-CB	-6.84	100.16	110.07
1	A	50	LYS	N-CA-C	6.82	121.92	112.45
1	A	39	THR	N-CA-CB	6.79	120.24	110.06
1	A	53	ALA	N-CA-CB	6.78	120.13	109.82
1	A	58	SER	N-CA-C	6.75	120.16	110.10
1	A	59	GLU	N-CA-C	6.75	120.74	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ILE	O-C-N	6.75	131.01	122.57
1	A	122	ASP	N-CA-CB	-6.74	99.84	110.22
1	A	98	LYS	CA-C-N	6.73	127.18	122.60
1	A	98	LYS	C-N-CA	6.73	127.18	122.60
1	A	26	GLN	N-CA-C	-6.71	102.84	111.02
1	A	142	ILE	CB-CA-C	-6.70	102.97	112.22
1	A	81	HIS	N-CA-CB	6.67	118.86	110.45
1	A	134	ALA	CB-CA-C	6.61	121.71	110.74
1	A	129	GLY	O-C-N	6.60	128.53	122.19
1	A	12	HIS	CA-C-N	6.57	128.84	120.56
1	A	12	HIS	C-N-CA	6.57	128.84	120.56
1	A	16	LYS	CB-CA-C	6.56	121.27	110.90
1	A	39	THR	CB-CA-C	-6.56	99.53	110.68
1	A	104	LEU	CB-CA-C	6.52	121.77	110.68
1	A	127	ALA	CA-C-O	6.50	127.39	120.70
1	A	105	GLU	CG-CD-OE1	-6.49	103.46	118.40
1	A	39	THR	N-CA-C	6.47	119.16	111.33
1	A	31	ARG	O-C-N	6.45	128.98	122.08
1	A	127	ALA	N-CA-CB	-6.44	100.73	110.07
1	A	38	GLU	CA-C-N	6.43	129.19	120.38
1	A	38	GLU	C-N-CA	6.43	129.19	120.38
1	A	70	THR	CA-C-N	6.40	128.76	120.44
1	A	70	THR	C-N-CA	6.40	128.76	120.44
1	A	127	ALA	N-CA-C	6.40	118.05	111.14
1	A	81	HIS	CA-CB-CG	6.39	120.19	113.80
1	A	142	ILE	N-CA-C	-6.33	104.33	110.72
1	A	116	HIS	N-CA-CB	6.31	121.16	110.49
1	A	136	GLU	CB-CA-C	-6.30	98.97	110.63
1	A	65	GLY	N-CA-C	-6.29	105.16	112.83
1	A	12	HIS	N-CA-CB	-6.28	100.86	110.16
1	A	34	LYS	CB-CA-C	6.28	120.83	110.90
1	A	81	HIS	N-CA-C	-6.23	102.02	110.68
1	A	69	LEU	CB-CA-C	6.20	121.23	110.68
1	A	47	LYS	CB-CA-C	-6.14	100.54	110.74
1	A	117	SER	N-CA-CB	6.14	120.87	110.49
1	A	47	LYS	O-C-N	6.14	129.17	122.11
1	A	76	LEU	N-CA-CB	-6.10	100.19	110.49
1	A	4	GLU	CB-CA-C	-6.04	101.31	110.92
1	A	67	THR	O-C-N	6.04	128.54	122.08
1	A	11	LEU	N-CA-CB	6.00	119.04	110.16
1	A	31	ARG	N-CA-CB	5.99	118.92	109.82
1	A	44	ASP	N-CA-CB	5.98	118.91	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ILE	CA-CB-CG2	-5.96	100.37	110.50
1	A	141	ASP	N-CA-C	5.95	117.77	111.28
1	A	140	LYS	CB-CA-C	5.91	120.65	110.84
1	A	53	ALA	O-C-N	5.88	128.37	122.08
1	A	35	SER	O-C-N	5.87	128.85	122.15
1	A	85	GLU	CG-CD-OE1	-5.87	104.90	118.40
1	A	138	PHE	N-CA-CB	-5.86	101.50	110.12
1	A	75	ILE	CA-CB-CG2	-5.85	100.56	110.50
1	A	82	HIS	ND1-CG-CD2	-5.80	100.30	106.10
1	A	43	PHE	CA-C-O	5.80	126.57	120.54
1	A	133	LYS	N-CA-C	-5.79	103.95	111.02
1	A	14	TRP	CG-CD2-CE3	-5.78	128.12	133.90
1	A	109	GLU	O-C-N	5.78	130.28	122.59
1	A	100	PRO	CB-CA-C	5.78	118.92	111.46
1	A	67	THR	CA-C-O	-5.77	114.72	121.07
1	A	76	LEU	CB-CA-C	5.72	121.81	110.42
1	A	78	LYS	N-CA-CB	-5.72	101.16	110.42
1	A	43	PHE	CA-C-N	5.71	127.93	120.28
1	A	43	PHE	C-N-CA	5.71	127.93	120.28
1	A	14	TRP	CE3-CZ3-CH2	5.68	128.48	121.10
1	A	59	GLU	CA-C-O	5.65	126.46	119.79
1	A	139	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	87	LYS	CB-CA-C	5.63	121.26	110.17
1	A	107	ILE	N-CA-CB	5.61	120.48	111.23
1	A	3	SER	O-C-N	5.59	129.97	122.82
1	A	67	THR	N-CA-C	-5.57	104.22	111.02
1	A	2	LEU	CB-CA-C	-5.54	101.54	109.84
1	A	33	PHE	CA-C-N	5.48	127.89	120.44
1	A	33	PHE	C-N-CA	5.48	127.89	120.44
1	A	80	GLY	N-CA-C	5.46	121.35	114.25
1	A	99	ILE	O-C-N	-5.46	117.68	121.55
1	A	14	TRP	NE1-CE2-CZ2	-5.44	121.94	130.10
1	A	99	ILE	CA-CB-CG2	-5.39	101.34	110.50
1	A	55	MET	N-CA-CB	-5.37	101.41	110.49
1	A	29	LEU	O-C-N	5.37	127.82	122.08
1	A	15	ALA	N-CA-CB	5.37	119.56	110.49
1	A	48	HIS	ND1-CE1-NE2	5.33	113.72	108.40
1	A	136	GLU	CG-CD-OE1	-5.31	106.19	118.40
1	A	14	TRP	CH2-CZ2-CE2	-5.26	110.66	117.50
1	A	132	ASN	CB-CG-ND2	5.25	124.28	116.40
1	A	97	HIS	N-CA-CB	5.24	117.92	110.06
1	A	4	GLU	CG-CD-OE1	-5.23	106.36	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	CB-CA-C	5.22	120.66	111.20
1	A	4	GLU	N-CA-C	-5.22	104.65	111.02
1	A	44	ASP	CB-CA-C	-5.21	102.13	110.79
1	A	21	VAL	CA-CB-CG1	5.21	119.25	110.40
1	A	96	LYS	CA-C-N	5.19	127.49	120.38
1	A	96	LYS	C-N-CA	5.19	127.49	120.38
1	A	94	ALA	N-CA-CB	5.19	117.59	110.07
1	A	128	GLN	N-CA-C	5.17	117.32	111.11
1	A	100	PRO	N-CA-C	5.17	119.20	111.14
1	A	20	ASP	N-CA-CB	5.15	120.97	111.96
1	A	104	LEU	N-CA-C	-5.13	105.12	111.33
1	A	138	PHE	N-CA-C	-5.11	105.71	111.28
1	A	122	ASP	CB-CA-C	5.11	120.07	110.63
1	A	83	GLU	CG-CD-OE1	-5.10	106.67	118.40
1	A	142	ILE	CA-CB-CG2	-5.08	101.86	110.50
1	A	101	ILE	CA-CB-CG2	-5.07	101.88	110.50
1	A	85	GLU	CA-C-O	5.04	125.83	120.24
1	A	69	LEU	N-CA-CB	-5.03	102.51	110.06
1	A	52	GLU	CG-CD-OE1	-5.03	106.83	118.40
1	A	46	PHE	CA-C-N	5.03	128.36	120.82
1	A	46	PHE	C-N-CA	5.03	128.36	120.82
1	A	140	LYS	O-C-N	5.01	128.26	122.20

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	140	5
2	A	1	0	0	0	0
3	A	43	0	30	6	0
All	All	1260	0	1272	142	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 56.

All (142) 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:145:LYS:HZ2	1:A:148:GLU:CD	1.65	1.03
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:HD12	1:A:2:LEU:H	1.26	0.98
1:A:104:LEU:CD1	1:A:142:ILE:HD12	1.94	0.97
1:A:145:LYS:NZ	1:A:148:GLU:CD	2.24	0.95
1:A:42:LYS:HZ3	1:A:98:LYS:HB2	1.36	0.90
1:A:145:LYS:NZ	1:A:148:GLU:OE1	2.08	0.87
1:A:49:LEU:C	1:A:50:LYS:HE2	2.00	0.86
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: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:12:HIS:NE2	1:A:16:LYS:NZ	2.32	0.78
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:145:LYS:NZ	1:A:148:GLU:OE2	2.20	0.74
1:A:82:HIS:CE1	1:A:137:LEU:HD21	2.22	0.74
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:HA	1:A:4:GLU:OE1	1.87	0.72
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:HBD1	3:A:155:HEM:CMD	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:147:LYS:O	1:A:148:GLU:C	2.42	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:48:HIS:C	1:A:50:LYS:HE3	2.26	0.61
1:A:99:ILE:N	1:A:99:ILE:HD13	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:13:VAL:HG21	1:A:123:PHE:CD2	2.36	0.60
1:A:44:ASP:OD1	1:A:47:LYS:HE2	2.02	0.60
3:A:155:HEM:CMC	3:A:155:HEM:HBC2	2.33	0.58
1:A:78:LYS:HZ1	1:A:85:GLU:CD	2.00	0.56
1:A:131:MET:O	1:A:135:LEU:HG	2.05	0.56
1:A:145:LYS:O	1:A:149:LEU:HD12	2.06	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:98:LYS:C	1:A:99:ILE:HD13	2.32	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
1:A:145:LYS:O	1:A:149:LEU:CD1	2.57	0.53
1:A:42:LYS:HZ3	1:A:98:LYS:CB	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:52:GLU:O	1:A:56:LYS:HG3	2.11	0.50
1:A:61:LEU:O	1:A:62:LYS:C	2.54	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:HA	1:A:109:GLU:OE2	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:100:PRO:C	1:A:102:LYS:N	2.67	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: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: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:99:ILE:O	1:A:99:ILE:HG22	2.13	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:14:TRP:O	1:A:17:VAL:HB	2.17	0.45
1:A:36:HIS:HA	1:A:38:GLU:OE2	2.17	0.45
1:A:129:GLY:O	1:A:130:ALA:C	2.60	0.44
1:A:72:LEU:O	1:A:76:LEU:HG	2.17	0.44
1:A:103:TYR:HA	1:A:106:PHE:HB2	1.99	0.44
1:A:78:LYS:NZ	1:A:85:GLU:CD	2.70	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:51:THR:HG1	1:A:54:GLU:HG3	1.80	0.43
1:A:76:LEU:C	1:A:78:LYS:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:LYS:NZ	1:A:105:GLU:OE2	2.42	0.42
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:62:LYS:O	1:A:63:LYS:C	2.62	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:71:ALA:O	1:A:75:ILE:HG13	2.21	0.41
1:A:103:TYR:O	1:A:107:ILE:N	2.44	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:105:GLU:O	1:A:106:PHE:C	2.63	0.41
1:A:43:PHE:CZ	3:A:155:HEM:CHD	3.04	0.41
1:A:50:LYS:HE2	1:A:50:LYS:N	2.36	0.40
1:A:102:LYS:HA	1:A:102:LYS:HD2	1.76	0.40
1:A:48:HIS:O	1:A:50:LYS:CE	2.60	0.40
1:A:85:GLU:H	1:A:85:GLU:HG2	1.71	0.40
1:A:109:GLU:C	1:A:111:ILE:N	2.76	0.40
1:A:14:TRP:HE1	1:A:73:GLY:HA3	1.87	0.40
1:A:75:ILE:HG23	1:A:82:HIS:HB3	2.04	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 ⓘ

5.3.1 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	151/153 (99%)	115 (76%)	31 (20%)	5 (3%)	3 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 ⓘ

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%)	100 (80%)	25 (20%)	1 0

All (25) 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	18	GLU
1	A	20	ASP
1	A	42	LYS
1	A	45	ARG
1	A	61	LEU
1	A	69	LEU
1	A	82	HIS
1	A	83	GLU
1	A	85	GLU

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Mol	Chain	Res	Type
1	A	86	LEU
1	A	99	ILE
1	A	104	LEU
1	A	105	GLU
1	A	107	ILE
1	A	109	GLU
1	A	111	ILE
1	A	115	LEU
1	A	117	SER
1	A	122	ASP
1	A	137	LEU
1	A	142	ILE
1	A	145	LYS

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	8	GLN
1	A	82	HIS
1	A	91	GLN
1	A	119	HIS

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 oligosaccharides 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	2,1	50,50,50	2.83	24 (48%)	67,82,82	3.46	30 (44%)

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	-	6/14/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C3C-C2C	7.36	1.52	1.37
3	A	155	HEM	C4B-NB	5.91	1.50	1.38
3	A	155	HEM	CBC-CAC	5.80	1.58	1.30
3	A	155	HEM	C4A-NA	5.22	1.49	1.39
3	A	155	HEM	CHA-C4D	4.97	1.48	1.38
3	A	155	HEM	CHD-C4C	4.96	1.48	1.38
3	A	155	HEM	FE-ND	4.35	2.08	1.94
3	A	155	HEM	C1B-NB	4.18	1.47	1.40
3	A	155	HEM	CAC-C3C	-3.96	1.36	1.47
3	A	155	HEM	CAA-C2A	-3.96	1.41	1.51
3	A	155	HEM	CHA-C1A	3.57	1.47	1.39
3	A	155	HEM	C2A-C3A	3.40	1.47	1.38
3	A	155	HEM	FE-NC	3.25	2.05	1.95
3	A	155	HEM	C1C-C2C	-2.83	1.39	1.45
3	A	155	HEM	CBA-CAA	2.82	1.61	1.51
3	A	155	HEM	O2D-CGD	-2.76	1.21	1.30
3	A	155	HEM	CHC-C1C	2.68	1.43	1.38
3	A	155	HEM	C3D-C2D	2.53	1.42	1.36
3	A	155	HEM	C3B-C2B	2.49	1.42	1.37
3	A	155	HEM	CBB-CAB	-2.33	1.19	1.30
3	A	155	HEM	CBD-CGD	2.21	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C1A-NA	2.13	1.43	1.39
3	A	155	HEM	CBA-CGA	-2.10	1.45	1.50
3	A	155	HEM	CHB-C1B	2.04	1.42	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	155	HEM	CBD-CAD-C3D	-15.42	69.89	112.53
3	A	155	HEM	CAD-CBD-CGD	-10.35	86.22	113.67
3	A	155	HEM	CAA-CBA-CGA	-8.00	92.45	113.67
3	A	155	HEM	C4C-C3C-C2C	-6.75	100.97	106.81
3	A	155	HEM	C3B-C4B-NB	6.44	114.09	109.47
3	A	155	HEM	C2A-C1A-NA	5.44	116.19	110.15
3	A	155	HEM	CHC-C4B-NB	-5.23	118.79	124.42
3	A	155	HEM	C1B-NB-C4B	-4.90	99.40	105.21
3	A	155	HEM	C3D-C4D-ND	4.58	115.20	110.17
3	A	155	HEM	CBC-CAC-C3C	-4.21	106.47	127.53
3	A	155	HEM	C1A-C2A-C3A	-3.95	100.75	106.87
3	A	155	HEM	C4A-C3A-C2A	3.64	110.99	106.82
3	A	155	HEM	C4D-C3D-C2D	-3.22	102.20	106.89
3	A	155	HEM	C2D-C1D-ND	3.05	113.43	109.90
3	A	155	HEM	CAD-C3D-C2D	2.99	133.47	127.87
3	A	155	HEM	CBA-CAA-C2A	2.76	120.16	112.53
3	A	155	HEM	CAA-C2A-C3A	2.75	133.24	127.07
3	A	155	HEM	C3B-C2B-C1B	2.74	108.47	106.41
3	A	155	HEM	C2B-C1B-NB	2.65	112.89	109.84
3	A	155	HEM	C4A-NA-C1A	-2.57	101.63	105.82
3	A	155	HEM	CHA-C4D-C3D	-2.53	120.56	125.23
3	A	155	HEM	CHD-C1D-C2D	-2.50	121.08	125.03
3	A	155	HEM	C4B-C3B-C2B	-2.46	105.02	107.28
3	A	155	HEM	CMA-C3A-C4A	-2.39	121.78	125.42
3	A	155	HEM	CAC-C3C-C2C	2.35	136.09	128.43
3	A	155	HEM	C4D-ND-C1D	-2.32	102.45	105.21
3	A	155	HEM	CMB-C2B-C1B	-2.29	121.45	125.03
3	A	155	HEM	CHA-C1A-C2A	-2.28	120.31	125.30
3	A	155	HEM	CHB-C1B-NB	-2.09	121.78	124.37
3	A	155	HEM	C1C-CHC-C4B	2.08	130.45	126.02

There are no chirality outliers.

All (6) torsion outliers are listed below:

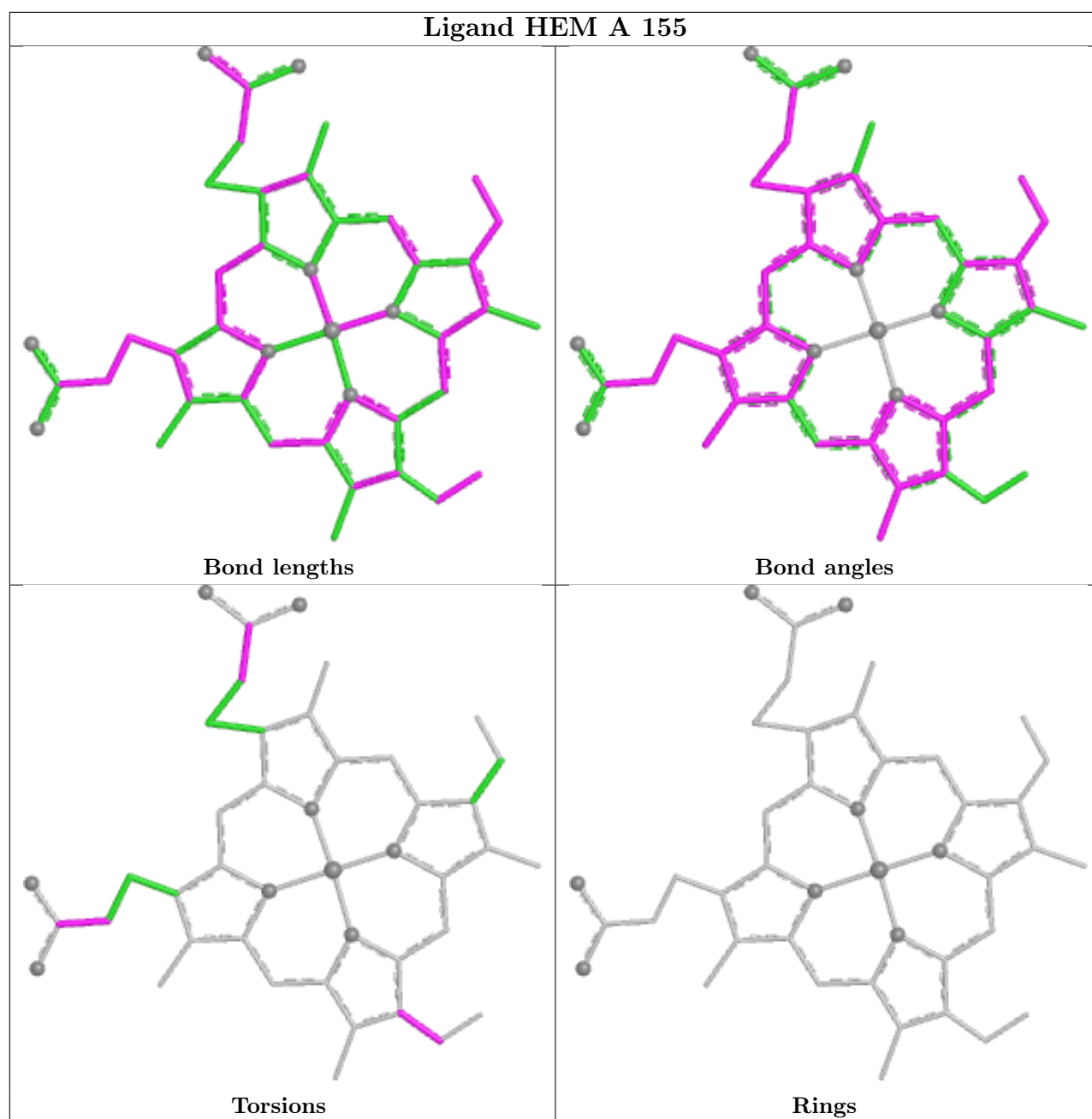
Mol	Chain	Res	Type	Atoms
3	A	155	HEM	C2B-C3B-CAB-CBB
3	A	155	HEM	C4B-C3B-CAB-CBB
3	A	155	HEM	CAA-CBA-CGA-O2A
3	A	155	HEM	CAD-CBD-CGD-O1D
3	A	155	HEM	CAA-CBA-CGA-O1A
3	A	155	HEM	CAD-CBD-CGD-O2D

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

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 than 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.



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.