



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:08 PM UTC

PDB ID : 1LH2 / pdb_00001lh2
Title : X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI. STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESOLUTION OF 2.0 ANGSTROMS (RUSSIAN)
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Deposited on : 1982-04-23
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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

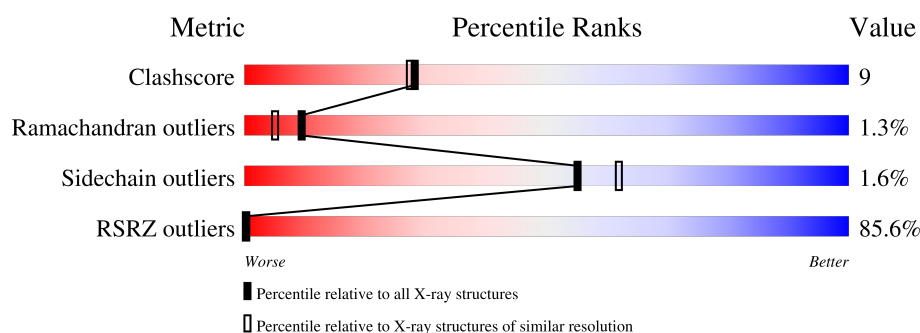
1 Overall quality at a glance

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)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	153	86% 66%29%

2 Entry composition [i](#)

There are 3 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.

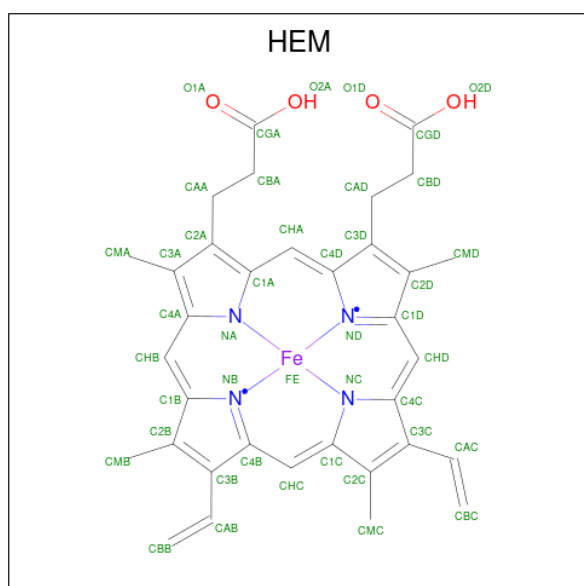
- Molecule 1 is a protein called LEGHEMOGLOBIN (AQUO MET).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	36	1	0
			1180	761	193	225	1			

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 PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

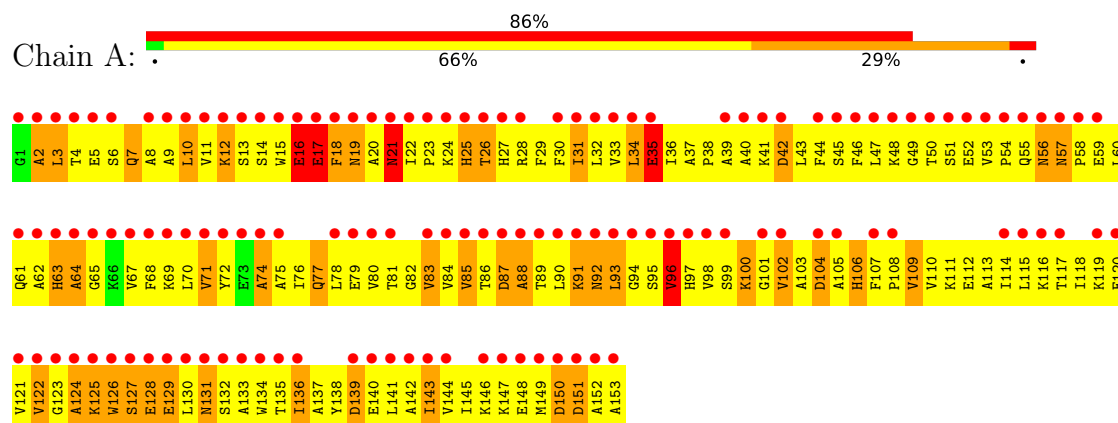
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total 68	O 68	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 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.

• Molecule 1: LEGHEMOGLOBIN (AQUO MET)



4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	93.22Å 38.26Å 52.01Å 90.00° 90.00° 98.80°	Depositor
Resolution (Å)	(Not available) – 2.00 46.06 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 95.8 (46.06-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.445 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 111.7	EDS
L-test for twinning ¹	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.65	EDS
Total number of atoms	1291	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	4.53	327/1214 (26.9%)	3.00	163/1648 (9.9%)

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	0	13

All (327) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	HIS	ND1-CE1	17.42	1.50	1.32
1	A	27	HIS	CE1-NE2	17.17	1.49	1.32
1	A	109	VAL	CA-CB	13.63	1.69	1.54
1	A	27	HIS	CG-ND1	13.02	1.52	1.38
1	A	106	HIS	CD2-NE2	12.78	1.51	1.37
1	A	111	LYS	N-CA	12.17	1.60	1.46
1	A	133	ALA	CA-C	11.78	1.67	1.52
1	A	143	ILE	CA-CB	11.68	1.69	1.54
1	A	106	HIS	CB-CG	11.53	1.66	1.50
1	A	63	HIS	CA-C	11.51	1.68	1.52
1	A	63	HIS	CE1-NE2	11.49	1.44	1.32
1	A	88	ALA	N-CA	11.44	1.60	1.46
1	A	94	GLY	CA-C	11.24	1.64	1.52
1	A	85	VAL	CA-C	11.10	1.65	1.52
1	A	99	SER	N-CA	11.08	1.60	1.46
1	A	95	SER	N-CA	11.01	1.59	1.46
1	A	53	VAL	CA-CB	10.97	1.68	1.54
1	A	72	TYR	C-O	10.91	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	VAL	CA-C	10.88	1.66	1.52
1	A	136	ILE	CA-CB	10.84	1.67	1.54
1	A	45	SER	N-CA	10.71	1.59	1.46
1	A	97	HIS	CG-CD2	-10.62	1.24	1.35
1	A	137	ALA	CA-C	10.62	1.66	1.52
1	A	144	VAL	CA-C	10.53	1.66	1.52
1	A	25	HIS	ND1-CE1	10.52	1.43	1.32
1	A	134	TRP	N-CA	10.48	1.59	1.46
1	A	11	VAL	N-CA	10.30	1.58	1.46
1	A	124	ALA	N-CA	10.22	1.59	1.46
1	A	52	GLU	C-N	10.20	1.44	1.33
1	A	110	VAL	CA-C	10.18	1.67	1.52
1	A	145	ILE	N-CA	10.15	1.58	1.46
1	A	108	PRO	C-N	10.15	1.46	1.33
1	A	102	VAL	N-CA	10.12	1.58	1.46
1	A	18	PHE	N-CA	10.08	1.58	1.46
1	A	86	THR	N-CA	10.03	1.58	1.46
1	A	121	VAL	CA-C	9.94	1.65	1.52
1	A	51	SER	CA-C	9.94	1.64	1.52
1	A	65	GLY	C-O	9.92	1.35	1.23
1	A	123	GLY	CA-C	9.83	1.65	1.51
1	A	97	HIS	CA-CB	9.78	1.68	1.53
1	A	71	VAL	N-CA	9.67	1.58	1.46
1	A	15	TRP	C-O	9.58	1.35	1.24
1	A	98	VAL	CA-C	9.53	1.64	1.52
1	A	97	HIS	C-N	-9.49	1.22	1.33
1	A	130	LEU	N-CA	9.46	1.58	1.46
1	A	87	ASP	CA-C	9.46	1.67	1.53
1	A	61	GLN	C-O	9.45	1.35	1.24
1	A	122	VAL	N-CA	9.45	1.58	1.46
1	A	76	ILE	C-O	9.43	1.34	1.24
1	A	149	MET	C-O	9.42	1.35	1.24
1	A	10	LEU	CA-C	9.36	1.64	1.52
1	A	103	ALA	CA-C	9.30	1.64	1.52
1	A	74	ALA	CA-C	9.29	1.64	1.52
1	A	52	GLU	N-CA	9.27	1.56	1.45
1	A	107	PHE	N-CA	9.25	1.56	1.46
1	A	84	VAL	N-CA	9.24	1.57	1.46
1	A	75	ALA	C-O	9.21	1.34	1.24
1	A	152	ALA	N-CA	9.19	1.58	1.46
1	A	68	PHE	C-O	9.12	1.35	1.24
1	A	152	ALA	C-O	9.08	1.36	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	ALA	C-O	9.04	1.35	1.24
1	A	78	LEU	CA-C	8.99	1.64	1.52
1	A	81	THR	CA-CB	8.95	1.67	1.53
1	A	81	THR	N-CA	-8.88	1.34	1.46
1	A	92	ASN	C-O	8.85	1.35	1.24
1	A	75	ALA	N-CA	8.83	1.57	1.46
1	A	90	LEU	CA-CB	8.82	1.68	1.53
1	A	113	ALA	CA-CB	8.77	1.67	1.53
1	A	136	ILE	N-CA	-8.74	1.36	1.46
1	A	101	GLY	CA-C	8.73	1.63	1.51
1	A	114	ILE	CA-C	8.64	1.64	1.52
1	A	120	GLU	CA-CB	8.62	1.67	1.53
1	A	68	PHE	N-CA	8.56	1.57	1.46
1	A	141	LEU	N-CA	8.55	1.57	1.46
1	A	104	ASP	N-CA	8.54	1.57	1.46
1	A	131	ASN	C-N	8.51	1.45	1.33
1	A	115	LEU	CA-C	-8.51	1.41	1.52
1	A	148	GLU	N-CA	8.47	1.57	1.46
1	A	64	ALA	N-CA	8.44	1.56	1.46
1	A	30	PHE	CA-CB	8.44	1.67	1.53
1	A	29	PHE	N-CA	-8.42	1.36	1.46
1	A	2	ALA	C-N	-8.41	1.22	1.33
1	A	46	PHE	N-CA	-8.39	1.35	1.46
1	A	129	GLU	CA-C	8.38	1.64	1.52
1	A	127	SER	C-O	8.34	1.34	1.23
1	A	17	GLU	CA-C	8.32	1.63	1.52
1	A	36	ILE	C-N	8.29	1.40	1.33
1	A	91	LYS	CA-C	8.29	1.63	1.52
1	A	7	GLN	N-CA	8.28	1.56	1.46
1	A	13	SER	CA-CB	8.25	1.66	1.53
1	A	12	LYS	CA-C	-8.22	1.42	1.52
1	A	145	ILE	CA-CB	-8.22	1.43	1.54
1	A	132[A]	SER	CA-CB	8.18	1.66	1.53
1	A	132[B]	SER	CA-CB	8.18	1.66	1.53
1	A	132[C]	SER	CA-CB	8.18	1.66	1.53
1	A	26	THR	C-N	-8.16	1.22	1.34
1	A	54	PRO	C-N	-8.11	1.22	1.33
1	A	70	LEU	N-CA	-8.10	1.36	1.46
1	A	8	ALA	N-CA	8.08	1.56	1.46
1	A	20	ALA	N-CA	-8.05	1.35	1.46
1	A	54	PRO	CA-C	8.03	1.61	1.52
1	A	13	SER	N-CA	-8.03	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	GLN	C-O	8.01	1.34	1.24
1	A	99	SER	C-O	8.00	1.34	1.24
1	A	142	ALA	CA-C	-7.97	1.41	1.52
1	A	14	SER	CA-C	7.92	1.63	1.52
1	A	50	THR	CA-CB	7.91	1.65	1.53
1	A	56	ASN	C-N	-7.91	1.22	1.33
1	A	4	THR	C-O	7.87	1.34	1.23
1	A	138	TYR	N-CA	7.83	1.55	1.46
1	A	80	VAL	CA-CB	7.82	1.63	1.54
1	A	48	LYS	N-CA	7.80	1.56	1.46
1	A	69	LYS	CA-C	-7.80	1.43	1.52
1	A	131	ASN	CA-C	-7.74	1.42	1.52
1	A	136	ILE	C-N	-7.69	1.23	1.33
1	A	80	VAL	CA-C	-7.67	1.43	1.52
1	A	59	GLU	N-CA	-7.66	1.37	1.46
1	A	64	ALA	C-O	7.65	1.33	1.24
1	A	15	TRP	CD2-CE2	7.60	1.54	1.41
1	A	137	ALA	N-CA	7.59	1.55	1.46
1	A	11	VAL	CA-CB	-7.57	1.44	1.54
1	A	45	SER	CA-C	-7.57	1.42	1.52
1	A	68	PHE	CA-CB	-7.55	1.40	1.53
1	A	126	TRP	CA-C	7.54	1.62	1.52
1	A	95	SER	C-N	-7.54	1.24	1.33
1	A	100	LYS	C-N	-7.52	1.23	1.33
1	A	141	LEU	CB-CG	7.52	1.68	1.53
1	A	91	LYS	C-N	-7.49	1.23	1.34
1	A	83	VAL	N-CA	7.47	1.55	1.46
1	A	71	VAL	C-N	-7.47	1.24	1.33
1	A	43	LEU	CA-CB	7.44	1.66	1.53
1	A	27	HIS	C-N	7.44	1.43	1.33
1	A	135	THR	C-N	7.43	1.43	1.33
1	A	146	LYS	CA-C	-7.42	1.42	1.52
1	A	79	GLU	C-O	7.42	1.33	1.24
1	A	79	GLU	CA-CB	-7.41	1.41	1.53
1	A	147	LYS	C-N	-7.40	1.23	1.33
1	A	72	TYR	N-CA	7.37	1.55	1.46
1	A	118	ILE	N-CA	7.35	1.55	1.46
1	A	30	PHE	N-CA	7.31	1.55	1.46
1	A	60	LEU	CA-C	7.27	1.62	1.52
1	A	64	ALA	CA-C	7.26	1.62	1.52
1	A	38	PRO	C-N	-7.25	1.24	1.33
1	A	138	TYR	CB-CG	7.24	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ILE	C-O	7.22	1.32	1.24
1	A	149	MET	N-CA	7.18	1.55	1.46
1	A	142	ALA	C-N	7.17	1.43	1.33
1	A	150	ASP	CA-CB	7.16	1.64	1.53
1	A	19	ASN	CA-C	-7.15	1.42	1.52
1	A	37	ALA	N-CA	7.15	1.53	1.46
1	A	34	LEU	N-CA	7.15	1.55	1.46
1	A	132[A]	SER	N-CA	-7.13	1.37	1.46
1	A	132[B]	SER	N-CA	-7.13	1.37	1.46
1	A	132[C]	SER	N-CA	-7.13	1.37	1.46
1	A	115	LEU	N-CA	7.12	1.55	1.46
1	A	28	ARG	CA-C	-7.10	1.43	1.52
1	A	151	ASP	CA-C	7.09	1.62	1.52
1	A	77	GLN	N-CA	-7.08	1.37	1.46
1	A	63	HIS	CD2-NE2	-7.07	1.30	1.37
1	A	148	GLU	CA-C	7.07	1.62	1.52
1	A	18	PHE	C-O	7.06	1.32	1.24
1	A	140	GLU	CA-C	7.05	1.61	1.52
1	A	134	TRP	C-O	7.04	1.32	1.24
1	A	69	LYS	C-O	7.03	1.32	1.24
1	A	76	ILE	CA-C	-7.03	1.44	1.52
1	A	61	GLN	N-CA	7.02	1.54	1.46
1	A	147	LYS	CA-CB	7.02	1.64	1.53
1	A	8	ALA	C-O	7.01	1.32	1.24
1	A	40	ALA	CA-CB	7.00	1.65	1.53
1	A	117	THR	CA-C	6.98	1.61	1.52
1	A	105	ALA	CA-C	-6.97	1.43	1.52
1	A	33	VAL	CA-CB	6.96	1.62	1.54
1	A	47	LEU	CA-C	6.96	1.61	1.52
1	A	55	GLN	N-CA	6.93	1.55	1.46
1	A	77	GLN	CA-CB	6.91	1.64	1.53
1	A	17	GLU	C-N	-6.90	1.25	1.33
1	A	44	PHE	CB-CG	6.88	1.66	1.50
1	A	2	ALA	CA-CB	6.86	1.65	1.53
1	A	119	LYS	CA-C	-6.84	1.43	1.52
1	A	71	VAL	CA-C	6.83	1.61	1.52
1	A	144	VAL	C-N	-6.80	1.25	1.33
1	A	15	TRP	N-CA	6.78	1.54	1.46
1	A	70	LEU	CA-C	6.75	1.61	1.52
1	A	16	GLU	CA-CB	6.75	1.64	1.53
1	A	74	ALA	C-N	-6.74	1.25	1.33
1	A	125	LYS	CA-C	-6.74	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLU	N-CA	-6.71	1.38	1.46
1	A	78	LEU	C-N	-6.70	1.24	1.33
1	A	138	TYR	CA-C	-6.70	1.44	1.52
1	A	95	SER	CB-OG	6.68	1.55	1.42
1	A	59	GLU	C-N	-6.68	1.25	1.33
1	A	88	ALA	C-N	-6.65	1.25	1.33
1	A	57	ASN	C-O	6.61	1.32	1.24
1	A	9	ALA	N-CA	-6.61	1.37	1.46
1	A	79	GLU	N-CA	6.60	1.54	1.46
1	A	96	VAL	C-O	6.59	1.32	1.24
1	A	147	LYS	CA-C	6.58	1.61	1.52
1	A	55	GLN	CA-CB	-6.58	1.43	1.53
1	A	139	ASP	CA-CB	6.58	1.63	1.53
1	A	28	ARG	CA-CB	6.54	1.63	1.53
1	A	130	LEU	CB-CG	6.52	1.66	1.53
1	A	129	GLU	C-N	-6.52	1.24	1.33
1	A	65	GLY	N-CA	6.48	1.53	1.45
1	A	138	TYR	CZ-OH	6.47	1.51	1.38
1	A	9	ALA	CA-CB	6.46	1.64	1.53
1	A	23	PRO	N-CA	6.43	1.56	1.47
1	A	25	HIS	CE1-NE2	6.41	1.39	1.32
1	A	127	SER	CA-C	-6.39	1.44	1.52
1	A	18	PHE	CA-CB	-6.37	1.43	1.53
1	A	142	ALA	C-O	6.37	1.32	1.24
1	A	52	GLU	CA-CB	-6.34	1.43	1.53
1	A	42	ASP	C-O	6.32	1.32	1.24
1	A	147	LYS	N-CA	-6.32	1.38	1.46
1	A	49	GLY	CA-C	-6.32	1.43	1.51
1	A	93	LEU	C-N	-6.23	1.25	1.33
1	A	106	HIS	CA-CB	6.20	1.63	1.53
1	A	6	SER	CA-C	6.19	1.61	1.52
1	A	49	GLY	C-N	6.19	1.41	1.33
1	A	22	ILE	C-N	-6.17	1.26	1.34
1	A	71	VAL	C-O	6.15	1.31	1.24
1	A	92	ASN	C-N	6.12	1.42	1.33
1	A	10	LEU	CB-CG	6.11	1.65	1.53
1	A	37	ALA	CA-C	6.11	1.61	1.52
1	A	143	ILE	N-CA	-6.10	1.39	1.46
1	A	12	LYS	C-O	6.07	1.31	1.24
1	A	16	GLU	C-O	6.05	1.31	1.24
1	A	78	LEU	N-CA	6.04	1.53	1.46
1	A	67	VAL	C-N	-6.03	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	LEU	CA-C	6.01	1.60	1.52
1	A	42	ASP	C-N	5.98	1.42	1.33
1	A	138	TYR	C-N	5.98	1.41	1.33
1	A	58	PRO	CA-C	-5.98	1.42	1.52
1	A	140	GLU	CA-CB	5.97	1.62	1.53
1	A	146	LYS	CA-CB	5.97	1.63	1.53
1	A	5	GLU	CA-CB	5.96	1.63	1.53
1	A	82	GLY	CA-C	5.92	1.60	1.51
1	A	50	THR	C-N	-5.91	1.25	1.33
1	A	117	THR	CA-CB	5.89	1.62	1.53
1	A	108	PRO	N-CD	-5.86	1.39	1.47
1	A	13	SER	CB-OG	-5.85	1.30	1.42
1	A	46	PHE	CB-CG	5.85	1.64	1.50
1	A	89	THR	C-O	5.84	1.30	1.24
1	A	127	SER	N-CA	5.83	1.53	1.45
1	A	18	PHE	CB-CG	5.82	1.64	1.50
1	A	120	GLU	N-CA	-5.80	1.39	1.46
1	A	52	GLU	C-O	5.79	1.31	1.23
1	A	5	GLU	N-CA	-5.78	1.39	1.46
1	A	122	VAL	C-O	5.78	1.31	1.24
1	A	67	VAL	N-CA	5.76	1.53	1.46
1	A	104	ASP	C-O	5.76	1.31	1.24
1	A	152	ALA	CA-CB	-5.76	1.43	1.53
1	A	27	HIS	CD2-NE2	5.76	1.44	1.37
1	A	95	SER	C-O	5.75	1.30	1.24
1	A	137	ALA	CA-CB	-5.75	1.44	1.53
1	A	148	GLU	C-O	5.73	1.31	1.24
1	A	98	VAL	CA-CB	-5.73	1.47	1.54
1	A	31	ILE	CA-CB	-5.72	1.47	1.54
1	A	121	VAL	CB-CG2	5.71	1.71	1.52
1	A	31	ILE	C-N	5.68	1.41	1.34
1	A	149	MET	CA-C	-5.68	1.45	1.52
1	A	60	LEU	C-O	5.67	1.30	1.24
1	A	5	GLU	CA-C	-5.67	1.45	1.52
1	A	113	ALA	C-O	-5.67	1.17	1.24
1	A	8	ALA	CA-C	-5.64	1.45	1.52
1	A	29	PHE	CA-C	5.64	1.60	1.52
1	A	23	PRO	C-N	5.64	1.41	1.33
1	A	6	SER	CA-CB	5.61	1.62	1.53
1	A	32	LEU	CA-C	-5.61	1.45	1.52
1	A	112	GLU	CG-CD	5.61	1.66	1.52
1	A	40	ALA	C-N	-5.59	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	PRO	C-O	5.58	1.30	1.23
1	A	29	PHE	C-N	5.58	1.41	1.34
1	A	117	THR	C-O	-5.56	1.17	1.24
1	A	151	ASP	C-N	-5.54	1.25	1.33
1	A	99	SER	CA-C	-5.53	1.45	1.52
1	A	47	LEU	CB-CG	5.51	1.64	1.53
1	A	11	VAL	C-O	5.51	1.30	1.24
1	A	114	ILE	CB-CG1	5.49	1.64	1.53
1	A	116	LYS	N-CA	-5.48	1.39	1.46
1	A	45	SER	CB-OG	5.48	1.53	1.42
1	A	139	ASP	N-CA	-5.47	1.39	1.46
1	A	112	GLU	CA-C	-5.46	1.45	1.52
1	A	69	LYS	CA-CB	5.46	1.61	1.53
1	A	28	ARG	CZ-NH1	5.45	1.40	1.32
1	A	35	GLU	CD-OE2	5.44	1.35	1.25
1	A	6	SER	C-N	-5.42	1.26	1.33
1	A	14	SER	N-CA	5.39	1.53	1.46
1	A	92	ASN	CB-CG	5.39	1.65	1.52
1	A	45	SER	C-O	5.39	1.30	1.24
1	A	44	PHE	CA-C	5.37	1.59	1.52
1	A	11	VAL	CB-CG1	5.36	1.70	1.52
1	A	20	ALA	CA-CB	5.35	1.62	1.53
1	A	15	TRP	NE1-CE2	-5.31	1.31	1.37
1	A	3	LEU	CA-CB	5.30	1.62	1.53
1	A	58	PRO	C-O	5.28	1.30	1.24
1	A	27	HIS	CA-CB	-5.28	1.44	1.53
1	A	114	ILE	N-CA	5.25	1.52	1.46
1	A	15	TRP	CD1-NE1	5.24	1.48	1.37
1	A	96	VAL	C-N	5.24	1.41	1.33
1	A	10	LEU	C-N	-5.24	1.27	1.33
1	A	36	ILE	CA-CB	5.24	1.61	1.54
1	A	28	ARG	N-CA	5.22	1.52	1.46
1	A	120	GLU	CG-CD	5.22	1.65	1.52
1	A	13	SER	CA-C	5.21	1.59	1.52
1	A	136	ILE	CA-C	5.21	1.59	1.52
1	A	14	SER	C-N	-5.20	1.26	1.33
1	A	27	HIS	ND1-CE1	5.18	1.37	1.32
1	A	38	PRO	N-CA	5.17	1.54	1.47
1	A	62	ALA	C-O	5.17	1.30	1.24
1	A	84	VAL	C-O	-5.16	1.18	1.24
1	A	106	HIS	CA-C	5.15	1.59	1.52
1	A	126	TRP	C-N	-5.15	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLU	CA-C	5.15	1.59	1.52
1	A	20	ALA	C-O	-5.13	1.17	1.24
1	A	75	ALA	CA-CB	-5.12	1.45	1.53
1	A	18	PHE	CA-C	5.07	1.59	1.52
1	A	15	TRP	CZ3-CH2	5.07	1.53	1.40
1	A	120	GLU	C-O	-5.05	1.18	1.24
1	A	111	LYS	CB-CG	5.04	1.67	1.52
1	A	126	TRP	NE1-CE2	-5.04	1.31	1.37
1	A	131	ASN	C-O	5.04	1.30	1.24
1	A	138	TYR	C-O	5.04	1.29	1.24
1	A	56	ASN	C-O	5.04	1.29	1.23
1	A	120	GLU	C-N	-5.03	1.27	1.33
1	A	39	ALA	C-N	5.03	1.40	1.33
1	A	93	LEU	CA-C	-5.02	1.46	1.52
1	A	85	VAL	C-N	-5.01	1.26	1.33

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASN	CA-CB-CG	-9.71	102.89	112.60
1	A	19	ASN	CA-CB-CG	-9.60	103.00	112.60
1	A	49	GLY	N-CA-C	-9.46	103.43	114.69
1	A	139	ASP	CA-CB-CG	-9.29	103.31	112.60
1	A	108	PRO	N-CA-C	-9.25	102.29	113.86
1	A	69	LYS	O-C-N	9.20	132.03	122.09
1	A	31	ILE	CB-CA-C	-9.06	99.90	112.14
1	A	87	ASP	CA-CB-CG	-8.86	103.74	112.60
1	A	135	THR	CA-C-O	-8.79	111.65	120.70
1	A	76	ILE	O-C-N	8.68	130.93	121.90
1	A	91	LYS	CA-C-O	8.51	129.56	120.55
1	A	145	ILE	N-CA-C	8.48	119.29	110.72
1	A	36	ILE	N-CA-C	-8.44	101.80	111.00
1	A	102	VAL	CA-C-O	-8.42	111.19	120.71
1	A	107	PHE	CA-CB-CG	-8.33	105.47	113.80
1	A	56	ASN	CA-CB-CG	-8.30	104.30	112.60
1	A	15	TRP	CG-CD2-CE3	-8.23	125.67	133.90
1	A	97	HIS	ND1-CE1-NE2	-8.07	100.33	108.40
1	A	121	VAL	CA-C-O	-8.06	112.62	121.17
1	A	71	VAL	CA-C-O	8.04	129.31	120.95
1	A	104	ASP	CA-CB-CG	-7.91	104.69	112.60
1	A	15	TRP	CE2-CD2-CE3	7.74	126.54	118.80
1	A	131	ASN	CA-C-O	-7.65	112.44	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	144	VAL	O-C-N	-7.60	114.00	121.83
1	A	41	LYS	N-CA-C	7.58	119.54	111.28
1	A	80	VAL	O-C-N	7.51	129.72	121.90
1	A	65	GLY	O-C-N	7.44	129.32	122.18
1	A	54	PRO	N-CA-CB	7.37	109.51	103.32
1	A	62	ALA	O-C-N	7.34	129.64	122.07
1	A	57	ASN	CA-CB-CG	-7.31	105.29	112.60
1	A	131	ASN	O-C-N	7.25	129.81	122.12
1	A	109	VAL	N-CA-CB	7.23	118.50	110.62
1	A	61	GLN	O-C-N	7.03	130.16	122.15
1	A	106	HIS	CG-CD2-NE2	7.02	114.22	107.20
1	A	136	ILE	N-CA-C	-7.02	103.68	110.42
1	A	146	LYS	N-CA-C	-6.95	103.72	111.71
1	A	22	ILE	O-C-N	-6.91	116.00	120.42
1	A	48	LYS	CB-CA-C	-6.85	100.53	110.06
1	A	49	GLY	O-C-N	6.85	130.39	122.65
1	A	23	PRO	N-CA-CB	6.83	110.76	103.52
1	A	72	TYR	N-CA-CB	-6.80	100.12	110.12
1	A	27	HIS	ND1-CG-CD2	6.76	112.86	106.10
1	A	28	ARG	O-C-N	6.76	129.03	122.07
1	A	127	SER	O-C-N	6.75	131.46	122.96
1	A	129	GLU	CA-C-O	6.74	127.75	120.20
1	A	92	ASN	CA-CB-CG	-6.69	105.91	112.60
1	A	92	ASN	O-C-N	6.68	130.49	122.27
1	A	135	THR	O-C-N	6.67	129.30	122.09
1	A	35	GLU	CB-CG-CD	-6.67	101.26	112.60
1	A	89	THR	N-CA-CB	-6.64	100.36	110.12
1	A	76	ILE	CA-C-N	-6.64	110.72	120.28
1	A	76	ILE	C-N-CA	-6.64	110.72	120.28
1	A	138	TYR	O-C-N	6.63	129.26	122.09
1	A	71	VAL	N-CA-C	6.61	117.36	110.62
1	A	78	LEU	CA-C-O	6.60	127.55	120.55
1	A	146	LYS	O-C-N	6.58	129.93	122.22
1	A	54	PRO	CA-C-O	6.57	128.78	121.43
1	A	26	THR	CA-C-O	6.47	127.28	120.42
1	A	99	SER	O-C-N	6.41	129.72	122.22
1	A	83	VAL	N-CA-C	6.41	118.16	108.80
1	A	74	ALA	CA-C-O	6.40	127.33	120.55
1	A	4	THR	N-CA-C	-6.38	102.30	110.53
1	A	20	ALA	N-CA-C	-6.38	105.36	113.01
1	A	3	LEU	N-CA-CB	6.33	121.19	110.49
1	A	51	SER	CA-C-O	6.33	126.95	119.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	THR	N-CA-C	6.33	118.18	111.28
1	A	110	VAL	O-C-N	-6.32	114.65	121.80
1	A	12	LYS	O-C-N	6.29	128.88	122.09
1	A	31	ILE	CA-C-O	-6.26	114.44	120.95
1	A	4	THR	CA-CB-OG1	-6.24	100.24	109.60
1	A	149	MET	O-C-N	6.20	130.29	122.23
1	A	67	VAL	N-CA-C	6.17	116.34	110.42
1	A	122	VAL	CA-CB-CG1	-6.15	99.94	110.40
1	A	29	PHE	CD1-CG-CD2	6.14	127.81	118.60
1	A	38	PRO	N-CA-C	6.13	122.70	113.81
1	A	15	TRP	CB-CG-CD1	6.11	136.06	126.90
1	A	115	LEU	O-C-N	6.09	129.09	122.15
1	A	78	LEU	N-CA-C	6.08	117.91	111.28
1	A	128	GLU	O-C-N	6.06	128.54	122.12
1	A	58	PRO	O-C-N	6.05	130.53	122.30
1	A	126	TRP	CE2-CD2-CE3	6.03	124.83	118.80
1	A	30	PHE	N-CA-CB	6.02	119.61	110.28
1	A	138	TYR	CA-C-O	-6.02	114.50	120.70
1	A	142	ALA	O-C-N	6.01	130.39	122.33
1	A	63	HIS	ND1-CG-CD2	5.99	112.08	106.10
1	A	129	GLU	O-C-N	-5.98	115.39	122.20
1	A	49	GLY	CA-C-O	-5.95	112.91	119.27
1	A	153	ALA	N-CA-CB	-5.94	101.49	110.40
1	A	126	TRP	CD2-CE2-CZ2	-5.93	116.47	122.40
1	A	15	TRP	CA-C-N	-5.90	111.91	120.29
1	A	15	TRP	C-N-CA	-5.90	111.91	120.29
1	A	131	ASN	CA-CB-CG	-5.88	106.72	112.60
1	A	35	GLU	N-CA-C	5.86	118.62	111.82
1	A	105	ALA	N-CA-C	-5.83	106.13	113.18
1	A	93	LEU	CB-CA-C	-5.77	101.21	110.79
1	A	64	ALA	N-CA-C	5.74	117.54	111.28
1	A	9	ALA	N-CA-C	-5.73	105.17	111.82
1	A	42	ASP	O-C-N	5.71	130.02	122.43
1	A	15	TRP	CD2-CE3-CZ3	-5.70	111.19	118.60
1	A	92	ASN	OD1-CG-ND2	-5.70	116.91	122.60
1	A	117	THR	O-C-N	-5.69	116.21	122.07
1	A	134	TRP	O-C-N	5.69	129.27	122.27
1	A	52	GLU	CB-CG-CD	-5.68	102.94	112.60
1	A	80	VAL	CA-CB-CG2	-5.68	100.74	110.40
1	A	72	TYR	N-CA-C	5.68	117.47	111.28
1	A	35	GLU	CB-CA-C	-5.66	99.80	110.67
1	A	114	ILE	CB-CA-C	-5.66	104.41	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	GLN	CB-CA-C	5.66	121.09	110.63
1	A	124	ALA	O-C-N	5.64	130.25	122.46
1	A	87	ASP	N-CA-C	5.61	118.41	109.65
1	A	32	LEU	N-CA-C	-5.61	105.32	111.82
1	A	112	GLU	CA-C-O	-5.59	113.54	119.97
1	A	118	ILE	CB-CA-C	-5.59	103.49	112.16
1	A	5	GLU	N-CA-C	-5.55	105.33	111.71
1	A	67	VAL	CA-C-O	5.55	127.06	121.17
1	A	72	TYR	O-C-N	5.54	127.99	122.12
1	A	147	LYS	CA-C-O	5.50	126.60	120.82
1	A	144	VAL	CA-C-O	5.48	126.66	120.85
1	A	146	LYS	N-CA-CB	-5.46	101.81	110.22
1	A	121	VAL	O-C-N	-5.46	116.56	121.91
1	A	21	ASN	N-CA-C	5.45	119.13	108.18
1	A	137	ALA	N-CA-C	5.44	117.21	111.28
1	A	117	THR	CA-CB-OG1	5.43	117.75	109.60
1	A	24	LYS	N-CA-C	5.42	117.05	111.03
1	A	99	SER	CA-C-N	-5.41	113.99	122.65
1	A	99	SER	C-N-CA	-5.41	113.99	122.65
1	A	117	THR	N-CA-CB	5.40	117.84	110.01
1	A	52	GLU	CA-C-O	-5.40	115.03	121.56
1	A	17	GLU	O-C-N	-5.35	116.45	122.12
1	A	83	VAL	O-C-N	-5.29	117.19	123.00
1	A	40	ALA	CA-C-O	5.28	125.91	119.05
1	A	83	VAL	CA-C-O	-5.28	116.29	121.67
1	A	130	LEU	N-CA-C	5.26	118.16	111.69
1	A	21	ASN	CB-CG-OD1	-5.26	110.28	120.80
1	A	145	ILE	O-C-N	5.24	127.23	121.83
1	A	95	SER	N-CA-C	5.24	116.67	111.07
1	A	106	HIS	ND1-CE1-NE2	-5.23	103.17	108.40
1	A	104	ASP	CB-CA-C	-5.23	100.32	110.46
1	A	77	GLN	N-CA-CB	-5.22	102.17	110.22
1	A	61	GLN	N-CA-C	5.22	117.05	111.36
1	A	146	LYS	CA-C-O	-5.22	114.20	120.10
1	A	27	HIS	N-CA-C	-5.22	105.77	111.82
1	A	120	GLU	N-CA-CB	5.21	117.63	110.07
1	A	81	THR	CA-CB-CG2	5.21	119.35	110.50
1	A	60	LEU	CA-C-O	5.21	126.07	120.55
1	A	133	ALA	O-C-N	-5.17	116.74	122.07
1	A	90	LEU	N-CA-C	-5.17	105.83	111.82
1	A	45	SER	O-C-N	5.16	127.59	122.12
1	A	115	LEU	N-CA-CB	5.16	117.80	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	VAL	CA-C-O	-5.15	114.91	120.47
1	A	148	GLU	N-CA-C	5.14	118.81	112.54
1	A	85	VAL	N-CA-C	5.11	116.10	108.54
1	A	113	ALA	CA-C-O	-5.10	115.02	120.42
1	A	116	LYS	CA-C-O	-5.08	114.13	119.97
1	A	3	LEU	CD1-CG-CD2	-5.08	99.64	110.80
1	A	21	ASN	CB-CG-ND2	5.07	124.01	116.40
1	A	134	TRP	CG-CD1-NE1	-5.07	103.61	110.20
1	A	33	VAL	CA-C-N	5.06	129.16	120.72
1	A	33	VAL	C-N-CA	5.06	129.16	120.72
1	A	126	TRP	NE1-CE2-CD2	5.05	113.97	107.40
1	A	16	GLU	OE1-CD-OE2	-5.03	110.82	122.90
1	A	67	VAL	O-C-N	-5.01	117.00	121.91
1	A	84	VAL	CB-CA-C	-5.00	104.12	110.98

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ASP	Sidechain
1	A	150	ASP	Sidechain
1	A	151	ASP	Sidechain
1	A	16	GLU	Sidechain
1	A	17	GLU	Sidechain
1	A	19	ASN	Sidechain
1	A	21	ASN	Sidechain
1	A	35	GLU	Sidechain
1	A	42	ASP	Sidechain
1	A	57	ASN	Sidechain
1	A	7	GLN	Sidechain
1	A	83	VAL	Mainchain
1	A	87	ASP	Sidechain

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	1180	0	1200	21	18
2	A	43	0	30	3	0
3	A	68	0	0	0	5
All	All	1291	0	1230	21	20

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 (21) 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:92:ASN:O	1:A:96:VAL:HG12	1.94	0.67
1:A:31:ILE:O	1:A:35:GLU:HG3	2.02	0.59
1:A:21:ASN:C	1:A:21:ASN:HD22	2.13	0.56
1:A:21:ASN:C	1:A:21:ASN:ND2	2.64	0.56
1:A:77:GLN:NE2	1:A:85:VAL:H	2.03	0.56
1:A:139:ASP:O	1:A:143:ILE:HG13	2.06	0.55
1:A:17:GLU:OE2	1:A:122:VAL:HG12	2.12	0.50
1:A:106:HIS:O	1:A:109:VAL:HB	2.12	0.49
1:A:18:PHE:CE1	1:A:25:HIS:HB3	2.48	0.49
1:A:63:HIS:HE1	2:A:154:HEM:C4D	2.31	0.47
1:A:126:TRP:CZ2	1:A:131:ASN:HB2	2.48	0.47
1:A:100:LYS:HG3	2:A:154:HEM:HAD2	1.97	0.47
1:A:88:ALA:O	1:A:91:LYS:HB2	2.17	0.45
1:A:102:VAL:HG13	2:A:154:HEM:HAC	1.99	0.45
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.50	0.44
1:A:71:VAL:O	1:A:74:ALA:HB3	2.17	0.43
1:A:26:THR:HB	1:A:64:ALA:HB3	1.99	0.43
1:A:18:PHE:O	1:A:25:HIS:HD2	2.03	0.41
1:A:143:ILE:HD13	1:A:143:ILE:HG21	1.88	0.41
1:A:12:LYS:HE3	1:A:16:GLU:OE2	2.21	0.40

All (20) 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:126:TRP:O	1:A:126:TRP:O[2_555]	1.19	1.01
3:A:219:HOH:O	3:A:219:HOH:O[2_555]	1.21	0.99
1:A:124:ALA:CB	1:A:129:GLU:N[2_555]	1.39	0.81
1:A:124:ALA:O	1:A:127:SER:C[2_555]	1.47	0.73
1:A:124:ALA:O	1:A:127:SER:CB[2_555]	1.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ALA:O	1:A:127:SER:CA[2_555]	1.54	0.66
1:A:124:ALA:O	1:A:128:GLU:N[2_555]	1.67	0.53
1:A:125:LYS:CA	1:A:127:SER:OG[2_555]	1.71	0.49
1:A:125:LYS:CA	1:A:127:SER:CB[2_555]	1.74	0.46
1:A:124:ALA:C	1:A:127:SER:CB[2_555]	1.77	0.43
1:A:124:ALA:O	1:A:127:SER:OG[2_555]	1.82	0.38
1:A:125:LYS:C	1:A:127:SER:CB[2_555]	1.86	0.34
1:A:10:LEU:CD1	1:A:125:LYS:CD[2_555]	1.97	0.23
1:A:56:ASN:OD1	3:A:171:HOH:O[1_565]	1.97	0.23
1:A:125:LYS:N	1:A:127:SER:CB[2_555]	2.00	0.20
3:A:192:HOH:O	3:A:219:HOH:O[2_555]	2.12	0.08
1:A:124:ALA:C	1:A:127:SER:OG[2_555]	2.13	0.07
1:A:56:ASN:N	3:A:171:HOH:O[1_565]	2.17	0.03
1:A:124:ALA:CB	1:A:128:GLU:C[2_555]	2.17	0.03
1:A:127:SER:CA	3:A:159:HOH:O[2_555]	2.19	0.01

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	153/153 (100%)	148 (97%)	3 (2%)	2 (1%)	9 5

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ALA
1	A	3	LEU

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	127/125 (102%)	125 (98%)	2 (2%)	55 62

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU
1	A	96	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	25	HIS
1	A	27	HIS
1	A	56	ASN
1	A	61	GLN
1	A	63	HIS
1	A	77	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	HEM	A	154	1,3	50,50,50	4.31	35 (70%)	67,82,82	2.27	26 (38%)

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
2	HEM	A	154	1,3	-	3/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	FE-NB	13.15	2.35	1.94
2	A	154	HEM	C1D-C2D	8.26	1.61	1.44
2	A	154	HEM	CAB-C3B	6.77	1.65	1.47
2	A	154	HEM	CBD-CGD	6.70	1.66	1.50
2	A	154	HEM	C4D-C3D	6.62	1.56	1.45
2	A	154	HEM	FE-ND	6.49	2.14	1.94
2	A	154	HEM	C3B-C4B	6.36	1.57	1.44
2	A	154	HEM	CHB-C4A	6.27	1.53	1.39
2	A	154	HEM	CHD-C4C	6.25	1.50	1.38
2	A	154	HEM	C1B-C2B	5.53	1.55	1.44
2	A	154	HEM	CMD-C2D	5.33	1.61	1.50
2	A	154	HEM	C3C-C2C	5.18	1.47	1.37
2	A	154	HEM	CAD-C3D	4.91	1.64	1.51
2	A	154	HEM	FE-NA	4.83	2.11	1.95
2	A	154	HEM	CMC-C2C	4.44	1.59	1.50
2	A	154	HEM	CHA-C1A	4.43	1.49	1.39
2	A	154	HEM	CMB-C2B	4.11	1.59	1.50
2	A	154	HEM	CHC-C1C	4.03	1.46	1.38
2	A	154	HEM	C1A-NA	3.97	1.47	1.39
2	A	154	HEM	CAC-C3C	3.86	1.57	1.47
2	A	154	HEM	C4D-ND	3.74	1.46	1.40
2	A	154	HEM	O2A-CGA	-3.73	1.18	1.30
2	A	154	HEM	C1C-NC	3.54	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	CBA-CGA	3.50	1.58	1.50
2	A	154	HEM	C4A-NA	3.47	1.46	1.39
2	A	154	HEM	CAA-C2A	3.46	1.60	1.51
2	A	154	HEM	C2A-C3A	3.19	1.47	1.38
2	A	154	HEM	CMA-C3A	3.04	1.57	1.50
2	A	154	HEM	O2D-CGD	-3.02	1.20	1.30
2	A	154	HEM	O1D-CGD	2.53	1.30	1.22
2	A	154	HEM	CBD-CAD	-2.31	1.43	1.51
2	A	154	HEM	FE-NC	2.28	2.02	1.95
2	A	154	HEM	C4A-C3A	2.25	1.48	1.43
2	A	154	HEM	CBB-CAB	2.09	1.40	1.30
2	A	154	HEM	CBA-CAA	-2.08	1.44	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	C4C-NC-C1C	4.74	113.55	105.82
2	A	154	HEM	C3B-C4B-NB	4.52	112.71	109.47
2	A	154	HEM	C4B-C3B-C2B	-4.34	103.29	107.28
2	A	154	HEM	CHD-C1D-ND	-4.31	119.79	124.42
2	A	154	HEM	CMA-C3A-C4A	-4.11	119.15	125.42
2	A	154	HEM	C3A-C4A-NA	-4.11	103.56	110.14
2	A	154	HEM	C4A-NA-C1A	4.06	112.45	105.82
2	A	154	HEM	C2A-C1A-NA	-4.02	105.69	110.15
2	A	154	HEM	CHD-C4C-NC	3.80	128.59	124.45
2	A	154	HEM	C4C-C3C-C2C	3.66	109.99	106.81
2	A	154	HEM	CHB-C4A-NA	3.64	130.47	123.86
2	A	154	HEM	O2A-CGA-O1A	-3.36	114.68	123.33
2	A	154	HEM	O2D-CGD-O1D	-3.36	114.68	123.33
2	A	154	HEM	CHC-C1C-NC	3.27	128.02	124.45
2	A	154	HEM	CBA-CAA-C2A	-3.24	103.58	112.53
2	A	154	HEM	CHA-C1A-NA	2.97	129.25	123.86
2	A	154	HEM	C4A-C3A-C2A	2.94	110.18	106.82
2	A	154	HEM	CHB-C1B-NB	-2.87	120.81	124.37
2	A	154	HEM	CMD-C2D-C1D	2.75	129.33	125.03
2	A	154	HEM	C3D-C4D-ND	2.59	113.02	110.17
2	A	154	HEM	C2C-C1C-NC	-2.47	105.07	109.64
2	A	154	HEM	CMA-C3A-C2A	2.36	130.62	125.62
2	A	154	HEM	CHC-C4B-NB	-2.23	122.02	124.42
2	A	154	HEM	CHD-C1D-C2D	2.21	128.51	125.03
2	A	154	HEM	CAA-CBA-CGA	-2.04	108.26	113.67
2	A	154	HEM	C4D-ND-C1D	-2.03	102.81	105.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

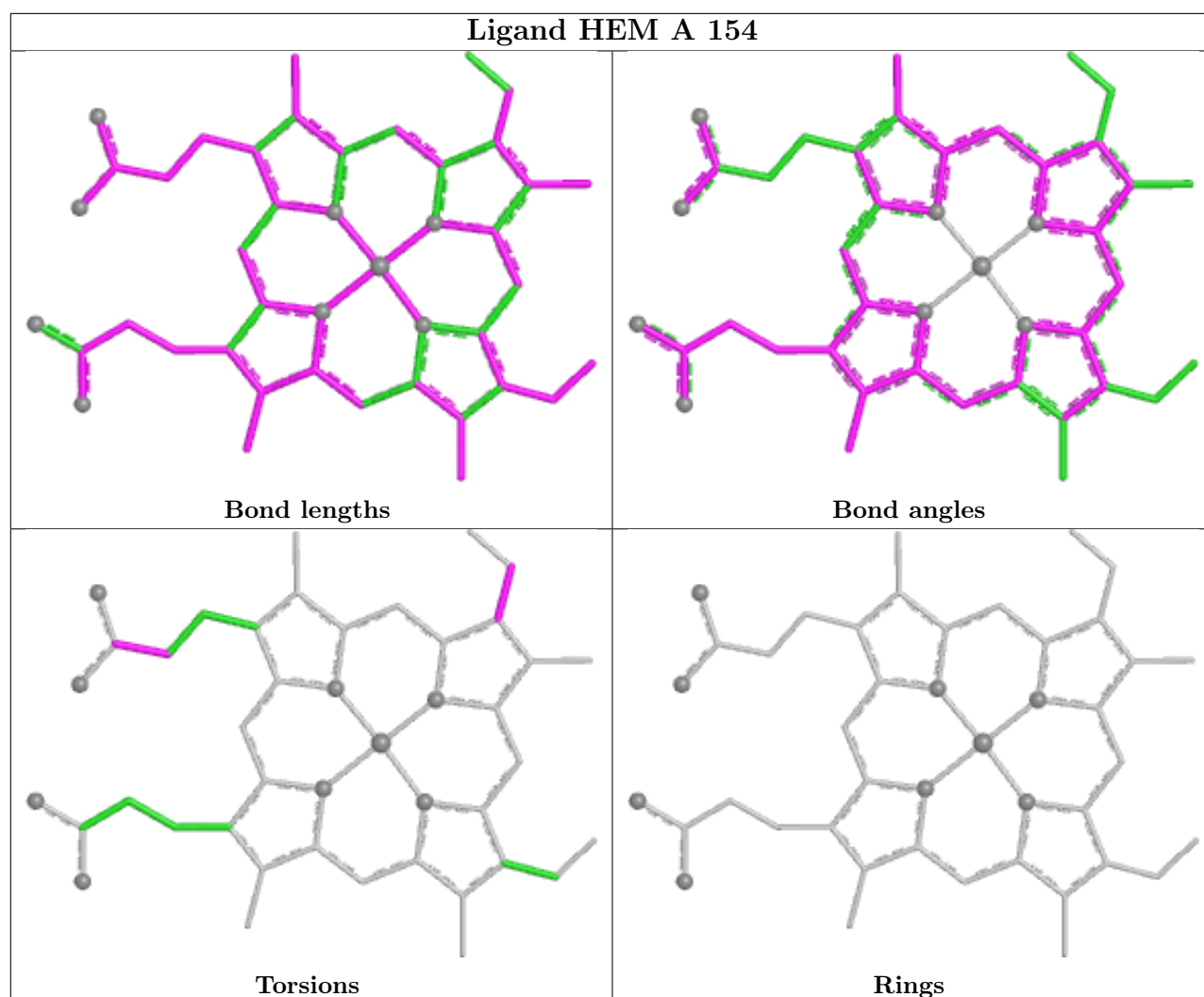
Mol	Chain	Res	Type	Atoms
2	A	154	HEM	C2C-C3C-CAC-CBC
2	A	154	HEM	C4C-C3C-CAC-CBC
2	A	154	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	HEM	3	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	153/153 (100%)	3.71	131 (85%) 0 0	6, 16, 38, 52	20 (13%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	ALA	10.0
1	A	88	ALA	9.2
1	A	2	ALA	9.1
1	A	50	THR	8.5
1	A	151	ASP	8.4
1	A	45	SER	8.3
1	A	48	LYS	8.1
1	A	1	GLY	8.0
1	A	153	ALA	7.9
1	A	150	ASP	7.3
1	A	58	PRO	7.0
1	A	126	TRP	6.7
1	A	86	THR	6.5
1	A	49	GLY	6.2
1	A	83	VAL	6.1
1	A	144	VAL	6.1
1	A	3	LEU	5.9
1	A	5	GLU	5.6
1	A	6	SER	5.5
1	A	42	ASP	5.5
1	A	90	LEU	5.4
1	A	99	SER	5.4
1	A	127	SER	5.3
1	A	54	PRO	5.3
1	A	123	GLY	5.3
1	A	91	LYS	5.3
1	A	143	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	9	ALA	5.1
1	A	147	LYS	5.1
1	A	53	VAL	5.1
1	A	95	SER	5.1
1	A	130	LEU	5.1
1	A	136	ILE	5.0
1	A	51	SER	4.9
1	A	4	THR	4.9
1	A	149	MET	4.9
1	A	117	THR	4.8
1	A	132[A]	SER	4.8
1	A	12	LYS	4.7
1	A	98	VAL	4.6
1	A	128	GLU	4.4
1	A	14	SER	4.4
1	A	23	PRO	4.4
1	A	20	ALA	4.4
1	A	67	VAL	4.4
1	A	93	LEU	4.4
1	A	89	THR	4.4
1	A	146	LYS	4.3
1	A	87	ASP	4.3
1	A	81	THR	4.3
1	A	15	TRP	4.2
1	A	148	GLU	4.2
1	A	92	ASN	4.1
1	A	10	LEU	4.1
1	A	11	VAL	4.1
1	A	78	LEU	4.1
1	A	56	ASN	4.0
1	A	107	PHE	4.0
1	A	121	VAL	4.0
1	A	39	ALA	4.0
1	A	13	SER	3.8
1	A	41	LYS	3.8
1	A	44	PHE	3.7
1	A	27	HIS	3.7
1	A	52	GLU	3.7
1	A	55	GLN	3.6
1	A	16	GLU	3.6
1	A	96	VAL	3.6
1	A	46	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	32	LEU	3.6
1	A	21	ASN	3.5
1	A	34	LEU	3.5
1	A	142	ALA	3.4
1	A	85	VAL	3.4
1	A	94	GLY	3.4
1	A	61	GLN	3.4
1	A	79	GLU	3.3
1	A	59	GLU	3.3
1	A	47	LEU	3.3
1	A	133	ALA	3.2
1	A	26	THR	3.2
1	A	31	ILE	3.2
1	A	66	LYS	3.2
1	A	114	ILE	3.1
1	A	24	LYS	3.1
1	A	72	TYR	3.1
1	A	101	GLY	3.1
1	A	104	ASP	3.1
1	A	131	ASN	3.1
1	A	73	GLU	3.0
1	A	22	ILE	3.0
1	A	64	ALA	3.0
1	A	35	GLU	3.0
1	A	120	GLU	3.0
1	A	18	PHE	3.0
1	A	129	GLU	3.0
1	A	105	ALA	2.9
1	A	140	GLU	2.8
1	A	80	VAL	2.8
1	A	19	ASN	2.8
1	A	102	VAL	2.8
1	A	119	LYS	2.8
1	A	65	GLY	2.7
1	A	97	HIS	2.7
1	A	25	HIS	2.7
1	A	84	VAL	2.6
1	A	40	ALA	2.5
1	A	75	ALA	2.5
1	A	17	GLU	2.5
1	A	68	PHE	2.5
1	A	134	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	116	LYS	2.5
1	A	115	LEU	2.5
1	A	139	ASP	2.4
1	A	8	ALA	2.4
1	A	74	ALA	2.3
1	A	141	LEU	2.2
1	A	108	PRO	2.2
1	A	124	ALA	2.2
1	A	28	ARG	2.2
1	A	125	LYS	2.2
1	A	30	PHE	2.2
1	A	71	VAL	2.1
1	A	62	ALA	2.1
1	A	70	LEU	2.1
1	A	122	VAL	2.1
1	A	57	ASN	2.1
1	A	135	THR	2.1
1	A	69	LYS	2.0
1	A	33	VAL	2.0
1	A	63	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

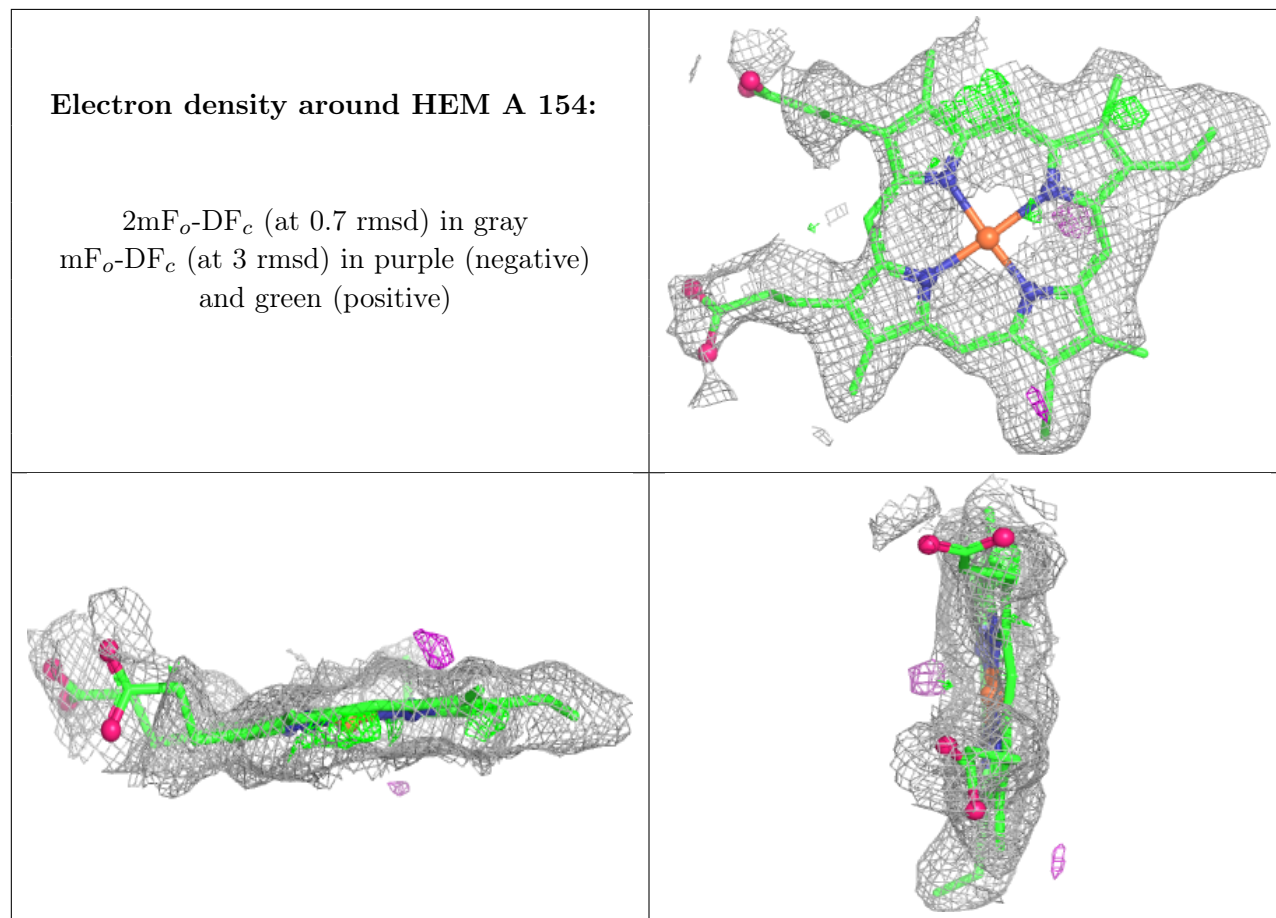
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	154	43/43	0.78	0.20	0,15,37,45	3

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.



6.5 Other polymers ⓘ

There are no such residues in this entry.