



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:13 AM UTC

PDB ID : 2LH6 / pdb_00002lh6
Title : X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI.
STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESO-
LUTION OF 2.0 ANGSTROMS (RUSSIAN)
Authors : Vainshtein, B.K.; Harutyunyan, E.H.; Kuranova, I.P.; Borisov, V.V.; Sosfenov,
N.I.; Pavlovsky, A.G.; Grebenko, A.I.; Konareva, N.V.
Deposited on : 1982-04-23
Resolution : 2.00 Å(reported)

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

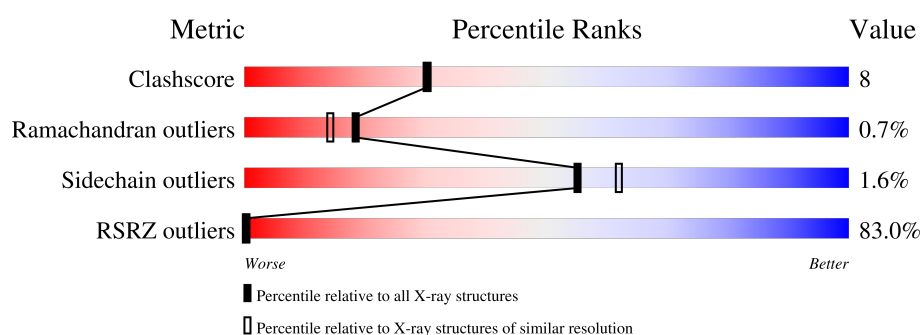
1 Overall quality at a glance

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	83% 70% 25% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NIO	A	155	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1297 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.

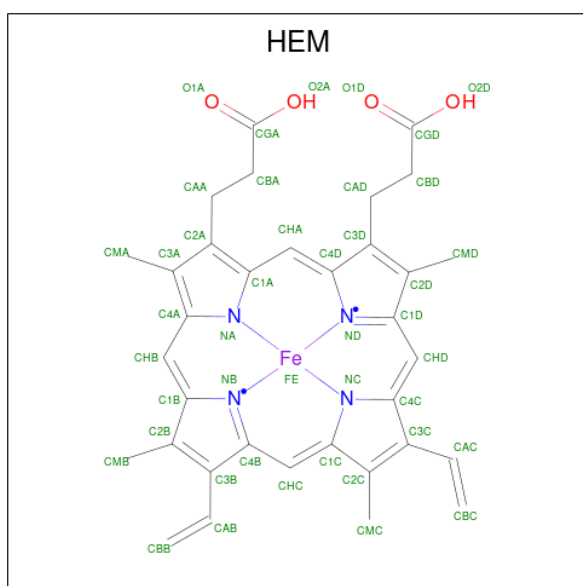
- Molecule 1 is a protein called LEGHEMOGLOBIN A (NICOTINATE MET).

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

There are 2 discrepancies between the modelled and reference sequences:

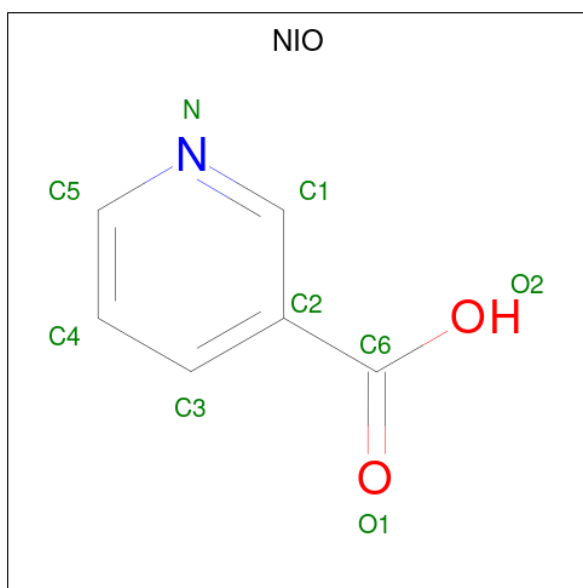
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLU	GLN	conflict	UNP P02240
A	150	ASP	ASN	conflict	UNP P02240

- 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 NICOTINIC ACID (CCD ID: NIO) (formula: $C_6H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		

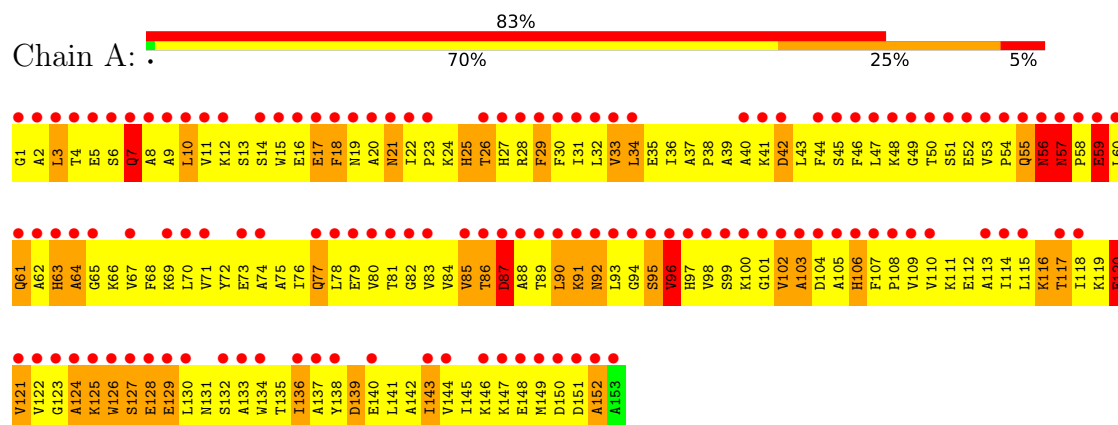
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	65	Total	O	0	0
			65	65		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 A (NICOTINATE MET)



4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	92.92Å 38.64Å 52.36Å 90.00° 90.00° 99.60°	Depositor
Resolution (Å)	(Not available) – 2.00 45.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 92.3 (45.81-2.00)	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) 0.447 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 93.5	EDS
L-test for twinning ¹	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	1297	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 11.51% 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

5.1 Standard geometry

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

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	4.67	339/1214 (27.9%)	2.83	123/1648 (7.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (339) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	HIS	ND1-CE1	17.54	1.50	1.32
1	A	27	HIS	CE1-NE2	16.08	1.48	1.32
1	A	63	HIS	ND1-CE1	15.55	1.48	1.32
1	A	27	HIS	CG-ND1	13.62	1.53	1.38
1	A	109	VAL	CA-CB	12.97	1.69	1.54
1	A	111	LYS	N-CA	12.60	1.61	1.46
1	A	85	VAL	CA-C	12.39	1.67	1.53
1	A	106	HIS	CD2-NE2	12.27	1.51	1.37
1	A	94	GLY	CA-C	12.24	1.65	1.52
1	A	88	ALA	N-CA	11.81	1.60	1.46
1	A	133	ALA	CA-C	11.69	1.67	1.52
1	A	134	TRP	N-CA	11.65	1.61	1.46
1	A	104	ASP	N-CA	11.53	1.60	1.46
1	A	144	VAL	CA-C	11.42	1.66	1.52
1	A	95	SER	N-CA	11.38	1.60	1.46
1	A	72	TYR	C-O	11.35	1.37	1.24
1	A	106	HIS	CB-CG	11.34	1.66	1.50
1	A	124	ALA	N-CA	11.23	1.61	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	ILE	N-CA	11.09	1.59	1.46
1	A	65	GLY	C-O	10.89	1.36	1.23
1	A	11	VAL	N-CA	10.80	1.59	1.46
1	A	99	SER	N-CA	10.79	1.59	1.46
1	A	67	VAL	CA-C	10.77	1.66	1.52
1	A	143	ILE	CA-CB	10.76	1.68	1.54
1	A	25	HIS	ND1-CE1	10.73	1.43	1.32
1	A	136	ILE	CA-CB	10.69	1.67	1.54
1	A	102	VAL	N-CA	10.56	1.58	1.46
1	A	75	ALA	N-CA	10.51	1.59	1.46
1	A	10	LEU	CA-C	10.41	1.66	1.52
1	A	86	THR	N-CA	10.36	1.59	1.46
1	A	123	GLY	CA-C	10.36	1.66	1.51
1	A	61	GLN	C-O	10.32	1.36	1.24
1	A	103	ALA	CA-C	10.26	1.65	1.52
1	A	18	PHE	N-CA	10.18	1.58	1.46
1	A	53	VAL	CA-CB	10.07	1.67	1.54
1	A	110	VAL	CA-C	10.03	1.66	1.52
1	A	74	ALA	CA-C	10.01	1.65	1.52
1	A	99	SER	C-O	9.92	1.35	1.24
1	A	98	VAL	CA-C	9.88	1.65	1.52
1	A	51	SER	CA-C	9.87	1.65	1.52
1	A	107	PHE	N-CA	9.84	1.55	1.46
1	A	108	PRO	C-N	9.82	1.45	1.33
1	A	68	PHE	C-O	9.77	1.36	1.24
1	A	52	GLU	N-CA	9.73	1.58	1.45
1	A	45	SER	N-CA	9.63	1.58	1.46
1	A	124	ALA	C-O	9.61	1.36	1.24
1	A	122	VAL	N-CA	9.60	1.59	1.46
1	A	63	HIS	CA-C	9.60	1.65	1.52
1	A	15	TRP	C-O	9.56	1.36	1.24
1	A	97	HIS	CG-CD2	-9.56	1.25	1.35
1	A	141	LEU	N-CA	9.55	1.58	1.46
1	A	75	ALA	C-O	9.49	1.35	1.24
1	A	17	GLU	CA-C	9.48	1.65	1.52
1	A	97	HIS	CA-CB	9.45	1.68	1.53
1	A	149	MET	C-O	9.45	1.35	1.24
1	A	101	GLY	CA-C	9.39	1.64	1.51
1	A	130	LEU	N-CA	9.36	1.57	1.46
1	A	138	TYR	N-CA	9.33	1.57	1.46
1	A	14	SER	CA-C	9.23	1.65	1.52
1	A	113	ALA	CA-CB	9.22	1.67	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	LEU	CA-CB	9.14	1.68	1.53
1	A	79	GLU	C-O	9.13	1.34	1.24
1	A	68	PHE	N-CA	9.12	1.57	1.46
1	A	25	HIS	CE1-NE2	9.06	1.41	1.32
1	A	115	LEU	N-CA	9.05	1.57	1.46
1	A	60	LEU	CA-C	9.03	1.64	1.52
1	A	64	ALA	N-CA	9.00	1.57	1.46
1	A	81	THR	CA-CB	8.97	1.66	1.54
1	A	137	ALA	CA-C	8.96	1.64	1.52
1	A	132[A]	SER	CA-CB	8.94	1.67	1.53
1	A	132[B]	SER	CA-CB	8.94	1.67	1.53
1	A	132[C]	SER	CA-CB	8.94	1.67	1.53
1	A	131	ASN	CA-C	-8.93	1.41	1.52
1	A	121	VAL	CA-C	8.92	1.63	1.52
1	A	84	VAL	N-CA	8.91	1.56	1.46
1	A	87	ASP	CA-C	8.91	1.66	1.53
1	A	78	LEU	CA-C	8.89	1.64	1.52
1	A	13	SER	N-CA	-8.80	1.35	1.46
1	A	120	GLU	CA-CB	8.76	1.67	1.53
1	A	7	GLN	N-CA	8.73	1.56	1.46
1	A	61	GLN	N-CA	8.72	1.57	1.46
1	A	76	ILE	C-O	8.68	1.34	1.24
1	A	129	GLU	CA-C	8.67	1.64	1.52
1	A	83	VAL	N-CA	8.63	1.56	1.46
1	A	55	GLN	C-O	8.61	1.35	1.24
1	A	12	LYS	CA-C	-8.58	1.41	1.52
1	A	152	ALA	C-O	8.56	1.35	1.24
1	A	52	GLU	C-N	8.54	1.43	1.33
1	A	97	HIS	C-N	-8.53	1.23	1.33
1	A	54	PRO	CA-C	8.50	1.62	1.52
1	A	114	ILE	CA-C	8.46	1.63	1.52
1	A	79	GLU	N-CA	8.46	1.56	1.46
1	A	54	PRO	C-N	-8.45	1.22	1.33
1	A	91	LYS	CA-C	8.43	1.63	1.52
1	A	11	VAL	CA-CB	-8.38	1.43	1.54
1	A	37	ALA	CA-C	8.35	1.62	1.52
1	A	142	ALA	CA-C	-8.35	1.41	1.52
1	A	29	PHE	N-CA	-8.33	1.36	1.46
1	A	146	LYS	CA-C	-8.27	1.42	1.52
1	A	8	ALA	C-O	8.26	1.34	1.24
1	A	140	GLU	CA-C	8.26	1.63	1.52
1	A	149	MET	N-CA	8.25	1.56	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	GLU	N-CA	-8.23	1.36	1.46
1	A	138	TYR	CZ-OH	8.23	1.55	1.38
1	A	69	LYS	C-O	8.20	1.33	1.24
1	A	127	SER	C-O	8.13	1.34	1.23
1	A	138	TYR	CA-C	-8.12	1.42	1.52
1	A	28	ARG	CA-C	-8.10	1.42	1.52
1	A	4	THR	C-O	8.09	1.34	1.23
1	A	78	LEU	C-N	-8.08	1.23	1.33
1	A	15	TRP	N-CA	8.05	1.56	1.46
1	A	26	THR	C-N	-8.00	1.23	1.33
1	A	151	ASP	CA-C	7.95	1.63	1.52
1	A	6	SER	CA-C	7.95	1.63	1.52
1	A	71	VAL	N-CA	7.93	1.56	1.46
1	A	2	ALA	C-N	-7.93	1.22	1.33
1	A	3	LEU	CA-CB	7.91	1.66	1.53
1	A	15	TRP	NE1-CE2	-7.91	1.28	1.37
1	A	43	LEU	CA-CB	7.90	1.66	1.53
1	A	152	ALA	N-CA	7.89	1.56	1.46
1	A	145	ILE	CA-CB	-7.88	1.44	1.54
1	A	45	SER	CA-C	-7.79	1.42	1.52
1	A	77	GLN	N-CA	-7.78	1.36	1.46
1	A	9	ALA	CA-CB	7.76	1.66	1.53
1	A	92	ASN	C-O	7.75	1.33	1.24
1	A	147	LYS	N-CA	-7.74	1.37	1.46
1	A	80	VAL	CA-C	-7.74	1.42	1.52
1	A	27	HIS	CD2-NE2	7.72	1.46	1.37
1	A	143	ILE	N-CA	-7.72	1.37	1.46
1	A	62	ALA	C-O	7.68	1.33	1.24
1	A	148	GLU	CA-C	7.65	1.63	1.52
1	A	100	LYS	C-N	-7.62	1.23	1.33
1	A	67	VAL	C-N	-7.62	1.23	1.34
1	A	17	GLU	C-N	-7.61	1.24	1.33
1	A	40	ALA	CA-CB	7.61	1.67	1.53
1	A	9	ALA	N-CA	-7.56	1.36	1.46
1	A	18	PHE	C-O	7.55	1.32	1.24
1	A	119	LYS	C-N	7.50	1.44	1.33
1	A	132[A]	SER	N-CA	-7.49	1.37	1.46
1	A	132[B]	SER	N-CA	-7.49	1.37	1.46
1	A	132[C]	SER	N-CA	-7.49	1.37	1.46
1	A	49	GLY	C-N	7.49	1.43	1.33
1	A	48	LYS	N-CA	7.43	1.55	1.46
1	A	76	ILE	CA-C	-7.40	1.43	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	LYS	CA-C	-7.40	1.42	1.52
1	A	50	THR	C-N	-7.39	1.23	1.33
1	A	95	SER	CB-OG	7.38	1.56	1.42
1	A	55	GLN	N-CA	7.38	1.55	1.46
1	A	118	ILE	N-CA	7.37	1.55	1.46
1	A	20	ALA	N-CA	-7.36	1.36	1.46
1	A	138	TYR	CB-CG	7.36	1.67	1.51
1	A	30	PHE	CA-CB	7.30	1.65	1.53
1	A	135	THR	CA-C	-7.28	1.43	1.52
1	A	128	GLU	N-CA	-7.28	1.37	1.46
1	A	69	LYS	CA-C	-7.26	1.43	1.52
1	A	147	LYS	CA-CB	7.25	1.64	1.53
1	A	98	VAL	CA-CB	-7.25	1.45	1.54
1	A	13	SER	CA-CB	7.24	1.64	1.53
1	A	46	PHE	N-CA	-7.24	1.36	1.46
1	A	147	LYS	CA-C	7.24	1.62	1.52
1	A	22	ILE	CA-C	7.24	1.60	1.52
1	A	27	HIS	ND1-CE1	7.24	1.39	1.32
1	A	70	LEU	CA-C	7.20	1.62	1.52
1	A	38	PRO	C-N	-7.19	1.24	1.33
1	A	95	SER	C-N	-7.19	1.25	1.33
1	A	19	ASN	CA-C	-7.19	1.42	1.52
1	A	126	TRP	N-CA	-7.16	1.37	1.46
1	A	10	LEU	C-N	-7.12	1.25	1.33
1	A	77	GLN	CA-CB	7.11	1.64	1.53
1	A	81	THR	N-CA	-7.10	1.36	1.45
1	A	105	ALA	CA-C	-7.08	1.43	1.52
1	A	148	GLU	N-CA	7.08	1.55	1.46
1	A	82	GLY	CA-C	7.07	1.61	1.51
1	A	149	MET	CA-C	-7.07	1.43	1.52
1	A	126	TRP	C-N	-7.07	1.23	1.33
1	A	70	LEU	N-CA	-7.04	1.37	1.46
1	A	45	SER	C-O	7.04	1.32	1.24
1	A	115	LEU	CA-C	-7.03	1.43	1.52
1	A	119	LYS	CA-C	-7.01	1.43	1.52
1	A	139	ASP	CA-CB	6.99	1.64	1.53
1	A	28	ARG	CA-CB	6.96	1.64	1.53
1	A	64	ALA	CA-C	6.95	1.61	1.52
1	A	32	LEU	CA-CB	6.94	1.64	1.53
1	A	74	ALA	C-N	-6.94	1.24	1.33
1	A	8	ALA	N-CA	6.94	1.55	1.46
1	A	73	GLU	C-O	6.93	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	HIS	CB-CG	6.92	1.59	1.50
1	A	8	ALA	CA-C	-6.89	1.43	1.52
1	A	12	LYS	C-O	6.89	1.32	1.24
1	A	144	VAL	C-N	-6.88	1.25	1.33
1	A	15	TRP	CD2-CE2	6.88	1.53	1.41
1	A	27	HIS	C-N	6.87	1.43	1.33
1	A	92	ASN	N-CA	6.86	1.54	1.46
1	A	42	ASP	C-O	6.81	1.32	1.24
1	A	73	GLU	CA-CB	6.81	1.64	1.53
1	A	126	TRP	CA-C	6.80	1.61	1.52
1	A	148	GLU	C-O	6.75	1.32	1.24
1	A	28	ARG	CZ-NH1	6.75	1.42	1.32
1	A	52	GLU	CA-CB	-6.74	1.43	1.53
1	A	93	LEU	C-N	-6.74	1.25	1.33
1	A	58	PRO	CA-C	-6.73	1.41	1.52
1	A	42	ASP	C-N	6.72	1.43	1.34
1	A	95	SER	C-O	6.72	1.31	1.24
1	A	7	GLN	CA-C	6.67	1.61	1.52
1	A	112	GLU	C-N	6.64	1.42	1.33
1	A	93	LEU	CA-CB	6.63	1.63	1.53
1	A	131	ASN	C-O	6.63	1.31	1.24
1	A	96	VAL	C-O	6.62	1.32	1.24
1	A	139	ASP	N-CA	-6.60	1.38	1.46
1	A	30	PHE	N-CA	6.59	1.54	1.46
1	A	39	ALA	C-O	6.55	1.32	1.24
1	A	38	PRO	N-CA	6.55	1.56	1.47
1	A	127	SER	CA-C	-6.53	1.44	1.52
1	A	29	PHE	C-N	6.52	1.42	1.34
1	A	63	HIS	C-N	-6.52	1.25	1.33
1	A	150	ASP	N-CA	-6.49	1.38	1.46
1	A	19	ASN	C-O	6.48	1.32	1.24
1	A	30	PHE	C-N	-6.48	1.25	1.33
1	A	130	LEU	CB-CG	6.47	1.66	1.53
1	A	142	ALA	C-O	6.45	1.32	1.24
1	A	43	LEU	C-N	-6.44	1.23	1.33
1	A	97	HIS	CE1-NE2	6.43	1.39	1.32
1	A	6	SER	CA-CB	6.39	1.63	1.53
1	A	150	ASP	CA-CB	6.38	1.63	1.53
1	A	18	PHE	CB-CG	6.38	1.65	1.50
1	A	50	THR	CA-CB	6.35	1.64	1.53
1	A	52	GLU	C-O	6.32	1.32	1.23
1	A	152	ALA	CA-CB	-6.32	1.42	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	TRP	C-O	6.30	1.32	1.24
1	A	117	THR	CA-C	6.29	1.60	1.52
1	A	66	LYS	CA-CB	6.29	1.63	1.53
1	A	58	PRO	C-O	6.27	1.31	1.24
1	A	32	LEU	CA-C	-6.24	1.44	1.52
1	A	65	GLY	N-CA	6.23	1.53	1.45
1	A	56	ASN	C-N	-6.21	1.23	1.33
1	A	66	LYS	N-CA	-6.21	1.38	1.46
1	A	59	GLU	CA-CB	6.21	1.62	1.53
1	A	44	PHE	CA-C	6.21	1.60	1.52
1	A	136	ILE	N-CA	-6.20	1.39	1.46
1	A	106	HIS	N-CA	-6.19	1.38	1.46
1	A	79	GLU	CA-CB	-6.18	1.43	1.53
1	A	11	VAL	C-O	6.17	1.31	1.24
1	A	112	GLU	CG-CD	6.17	1.67	1.52
1	A	71	VAL	CA-C	6.16	1.61	1.52
1	A	116	LYS	N-CA	-6.16	1.38	1.46
1	A	16	GLU	C-O	6.13	1.31	1.24
1	A	141	LEU	CB-CG	6.13	1.65	1.53
1	A	145	ILE	C-O	6.12	1.31	1.24
1	A	6	SER	C-N	-6.11	1.25	1.33
1	A	44	PHE	CB-CG	6.10	1.64	1.50
1	A	89	THR	C-O	6.09	1.31	1.24
1	A	47	LEU	CA-C	6.08	1.60	1.52
1	A	151	ASP	C-N	-6.03	1.24	1.33
1	A	96	VAL	C-N	6.02	1.41	1.33
1	A	55	GLN	CA-CB	-6.00	1.44	1.53
1	A	68	PHE	CA-CB	-6.00	1.43	1.53
1	A	137	ALA	N-CA	5.99	1.53	1.46
1	A	142	ALA	C-N	5.98	1.41	1.33
1	A	117	THR	CB-OG1	5.97	1.53	1.43
1	A	62	ALA	CA-CB	5.96	1.62	1.53
1	A	71	VAL	C-O	5.96	1.31	1.24
1	A	72	TYR	N-CA	5.96	1.53	1.46
1	A	63	HIS	CG-ND1	-5.96	1.31	1.38
1	A	113	ALA	C-O	-5.95	1.17	1.24
1	A	62	ALA	CA-C	-5.93	1.45	1.52
1	A	10	LEU	CB-CG	5.91	1.65	1.53
1	A	140	GLU	CA-CB	5.88	1.62	1.53
1	A	34	LEU	N-CA	5.88	1.54	1.46
1	A	18	PHE	CA-CB	-5.88	1.44	1.53
1	A	57	ASN	C-O	5.85	1.32	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	47	LEU	CA-CB	5.85	1.62	1.53
1	A	88	ALA	C-N	-5.82	1.26	1.33
1	A	55	GLN	C-N	5.81	1.41	1.33
1	A	31	ILE	CA-CB	-5.80	1.47	1.54
1	A	6	SER	N-CA	-5.80	1.39	1.46
1	A	65	GLY	CA-C	-5.80	1.45	1.52
1	A	55	GLN	CD-OE1	5.79	1.34	1.23
1	A	117	THR	C-O	-5.78	1.17	1.24
1	A	106	HIS	C-O	-5.77	1.17	1.24
1	A	136	ILE	C-N	-5.76	1.26	1.33
1	A	5	GLU	CA-C	-5.75	1.44	1.52
1	A	104	ASP	C-O	5.72	1.31	1.24
1	A	138	TYR	C-O	5.71	1.30	1.24
1	A	56	ASN	C-O	5.71	1.30	1.23
1	A	131	ASN	C-N	5.71	1.41	1.33
1	A	16	GLU	CA-CB	5.70	1.62	1.53
1	A	71	VAL	C-N	-5.68	1.26	1.33
1	A	20	ALA	CA-CB	5.67	1.63	1.53
1	A	60	LEU	C-N	-5.65	1.26	1.33
1	A	128	GLU	CA-CB	5.65	1.62	1.53
1	A	114	ILE	CB-CG1	5.65	1.64	1.53
1	A	46	PHE	CB-CG	5.64	1.63	1.50
1	A	3	LEU	CA-C	5.62	1.60	1.52
1	A	53	VAL	CA-C	-5.61	1.47	1.52
1	A	63	HIS	CE1-NE2	5.59	1.38	1.32
1	A	60	LEU	N-CA	5.58	1.53	1.46
1	A	5	GLU	CA-CB	5.56	1.62	1.53
1	A	85	VAL	C-N	-5.55	1.25	1.33
1	A	106	HIS	CA-CB	5.55	1.62	1.53
1	A	114	ILE	CA-CB	-5.52	1.47	1.54
1	A	15	TRP	CD1-NE1	5.52	1.49	1.37
1	A	136	ILE	CA-C	5.50	1.59	1.52
1	A	24	LYS	CA-C	-5.47	1.45	1.52
1	A	59	GLU	CA-C	5.47	1.59	1.52
1	A	75	ALA	CA-CB	-5.46	1.44	1.53
1	A	106	HIS	CA-C	5.44	1.60	1.52
1	A	2	ALA	CA-CB	5.44	1.62	1.53
1	A	111	LYS	CB-CG	5.43	1.68	1.52
1	A	47	LEU	CB-CG	5.41	1.64	1.53
1	A	120	GLU	CG-CD	5.39	1.65	1.52
1	A	86	THR	CA-CB	-5.37	1.46	1.52
1	A	135	THR	C-N	5.34	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	PHE	CA-C	5.33	1.59	1.52
1	A	7	GLN	C-O	5.32	1.30	1.24
1	A	120	GLU	N-CA	-5.32	1.39	1.46
1	A	39	ALA	C-N	5.26	1.40	1.33
1	A	13	SER	CA-C	5.26	1.59	1.52
1	A	130	LEU	CA-CB	-5.25	1.45	1.53
1	A	23	PRO	N-CA	5.24	1.54	1.47
1	A	63	HIS	N-CA	-5.23	1.40	1.46
1	A	46	PHE	C-O	-5.23	1.17	1.24
1	A	81	THR	C-O	-5.23	1.17	1.23
1	A	88	ALA	C-O	5.22	1.30	1.24
1	A	80	VAL	C-O	5.22	1.30	1.24
1	A	111	LYS	CD-CE	5.21	1.68	1.52
1	A	37	ALA	CA-CB	-5.20	1.47	1.53
1	A	58	PRO	N-CD	5.19	1.55	1.47
1	A	29	PHE	CA-C	5.17	1.59	1.52
1	A	27	HIS	CA-CB	-5.16	1.45	1.53
1	A	77	GLN	CG-CD	5.15	1.65	1.52
1	A	35	GLU	CD-OE2	5.14	1.35	1.25
1	A	49	GLY	CA-C	-5.13	1.45	1.51
1	A	7	GLN	CA-CB	-5.09	1.45	1.53
1	A	148	GLU	CD-OE2	5.08	1.35	1.25
1	A	14	SER	C-N	-5.08	1.26	1.34
1	A	23	PRO	C-N	5.04	1.41	1.33
1	A	82	GLY	C-N	5.04	1.40	1.33
1	A	25	HIS	CA-CB	5.03	1.61	1.53
1	A	54	PRO	C-O	5.02	1.29	1.23

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ASN	CA-CB-CG	-9.91	102.69	112.60
1	A	131	ASN	O-C-N	9.84	132.55	122.12
1	A	19	ASN	CA-CB-CG	-9.74	102.86	112.60
1	A	21	ASN	CA-CB-CG	-9.39	103.21	112.60
1	A	54	PRO	N-CA-CB	9.34	111.47	103.25
1	A	108	PRO	N-CA-CB	9.22	112.36	103.51
1	A	49	GLY	N-CA-C	-8.90	104.49	115.08
1	A	76	ILE	O-C-N	8.57	130.66	121.83
1	A	107	PHE	CA-CB-CG	-8.49	105.31	113.80
1	A	83	VAL	N-CA-C	8.43	121.10	108.80
1	A	65	GLY	O-C-N	8.40	130.25	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ILE	CB-CA-C	-8.34	100.71	112.22
1	A	63	HIS	CE1-NE2-CD2	-8.34	100.66	109.00
1	A	138	TYR	O-C-N	8.30	131.06	122.09
1	A	99	SER	O-C-N	8.16	130.76	122.12
1	A	112	GLU	CA-C-O	-7.98	111.96	120.42
1	A	44	PHE	CA-CB-CG	7.94	121.74	113.80
1	A	45	SER	O-C-N	7.83	130.42	122.12
1	A	142	ALA	O-C-N	7.82	131.89	122.27
1	A	12	LYS	O-C-N	7.75	130.98	122.15
1	A	135	THR	O-C-N	7.70	130.41	122.09
1	A	149	MET	O-C-N	7.70	130.93	122.15
1	A	146	LYS	O-C-N	7.59	130.80	122.15
1	A	104	ASP	CA-CB-CG	-7.48	105.12	112.60
1	A	63	HIS	CG-CD2-NE2	7.39	114.59	107.20
1	A	15	TRP	CG-CD2-CE3	-7.36	126.55	133.90
1	A	72	TYR	O-C-N	7.34	129.63	122.07
1	A	48	LYS	CB-CA-C	-7.27	98.57	109.90
1	A	69	LYS	O-C-N	7.21	130.37	122.15
1	A	49	GLY	CA-C-O	-7.16	111.82	119.27
1	A	119	LYS	O-C-N	7.16	130.31	122.15
1	A	44	PHE	CA-C-N	7.12	130.13	120.38
1	A	44	PHE	C-N-CA	7.12	130.13	120.38
1	A	61	GLN	O-C-N	7.07	130.21	122.15
1	A	8	ALA	O-C-N	6.99	131.70	122.33
1	A	119	LYS	CA-C-O	-6.97	113.03	120.42
1	A	102	VAL	N-CA-C	6.95	118.07	108.89
1	A	106	HIS	CG-CD2-NE2	6.91	114.11	107.20
1	A	62	ALA	O-C-N	6.73	129.36	122.09
1	A	23	PRO	N-CA-CB	6.73	110.66	103.39
1	A	131	ASN	CA-CB-CG	-6.65	105.95	112.60
1	A	97	HIS	ND1-CE1-NE2	-6.63	101.77	108.40
1	A	67	VAL	N-CA-C	6.51	116.67	110.42
1	A	108	PRO	CA-C-O	-6.50	109.91	119.00
1	A	98	VAL	N-CA-C	6.47	117.25	110.72
1	A	53	VAL	CA-C-N	6.46	126.49	119.90
1	A	53	VAL	C-N-CA	6.46	126.49	119.90
1	A	87	ASP	CA-CB-CG	-6.39	106.21	112.60
1	A	145	ILE	O-C-N	6.31	128.33	121.83
1	A	115	LEU	O-C-N	6.30	130.02	122.27
1	A	35	GLU	CB-CG-CD	-6.28	101.93	112.60
1	A	36	ILE	N-CA-C	-6.23	104.78	110.82
1	A	112	GLU	O-C-N	6.19	129.20	122.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	VAL	CB-CA-C	-6.14	103.98	112.02
1	A	83	VAL	CB-CA-C	-6.12	101.77	110.82
1	A	58	PRO	O-C-N	6.07	130.46	122.27
1	A	135	THR	CA-C-O	-6.05	114.46	120.70
1	A	109	VAL	N-CA-CB	6.05	117.48	110.65
1	A	103	ALA	CA-C-N	6.04	128.97	120.28
1	A	103	ALA	C-N-CA	6.04	128.97	120.28
1	A	71	VAL	N-CA-C	6.04	118.64	111.09
1	A	116	LYS	CA-C-O	-6.01	114.05	120.42
1	A	22	ILE	N-CA-C	5.99	121.82	108.88
1	A	92	ASN	O-C-N	5.91	129.13	122.22
1	A	29	PHE	CA-C-O	-5.87	114.66	120.82
1	A	78	LEU	CA-C-O	5.85	126.75	120.55
1	A	84	VAL	N-CA-C	5.83	116.19	107.51
1	A	19	ASN	O-C-N	5.81	130.22	122.43
1	A	91	LYS	N-CA-C	5.81	117.69	111.36
1	A	102	VAL	CA-C-O	-5.74	114.31	120.85
1	A	127	SER	O-C-N	5.74	130.61	123.15
1	A	79	GLU	O-C-N	5.71	128.66	122.15
1	A	32	LEU	N-CA-C	-5.69	105.22	111.82
1	A	15	TRP	CD2-CE3-CZ3	-5.66	111.25	118.60
1	A	85	VAL	N-CA-C	5.66	115.70	108.12
1	A	28	ARG	O-C-N	5.65	128.59	122.15
1	A	29	PHE	CD1-CG-CD2	5.63	127.05	118.60
1	A	95	SER	N-CA-C	5.63	117.22	111.14
1	A	139	ASP	O-C-N	5.57	127.81	122.07
1	A	4	THR	N-CA-C	-5.53	103.39	110.53
1	A	27	HIS	CB-CG-CD2	-5.53	124.02	131.20
1	A	118	ILE	CB-CA-C	-5.51	103.33	112.26
1	A	14	SER	CA-C-O	5.51	126.31	119.97
1	A	111	LYS	CB-CA-C	-5.51	102.19	110.90
1	A	15	TRP	CE2-CD2-CE3	5.49	124.29	118.80
1	A	41	LYS	N-CA-C	5.49	117.26	111.28
1	A	74	ALA	N-CA-C	5.48	117.25	111.28
1	A	15	TRP	O-C-N	5.48	129.00	122.27
1	A	25	HIS	CA-C-O	-5.45	114.64	120.42
1	A	133	ALA	O-C-N	-5.44	116.46	122.07
1	A	92	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	144	VAL	O-C-N	-5.43	116.59	121.91
1	A	11	VAL	N-CA-C	5.43	116.20	110.72
1	A	145	ILE	N-CA-C	5.41	116.19	110.72
1	A	134	TRP	O-C-N	5.40	128.91	122.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	THR	N-CA-CB	-5.37	102.23	110.01
1	A	83	VAL	CA-C-O	-5.31	116.25	121.67
1	A	138	TYR	CA-C-O	-5.28	115.26	120.70
1	A	56	ASN	CB-CA-C	-5.27	99.74	111.77
1	A	27	HIS	ND1-CE1-NE2	-5.27	103.13	108.40
1	A	144	VAL	N-CA-C	5.26	115.47	110.42
1	A	89	THR	O-C-N	5.25	127.47	122.07
1	A	125	LYS	N-CA-C	-5.25	106.65	113.16
1	A	126	TRP	CE2-CD2-CE3	5.25	124.05	118.80
1	A	110	VAL	O-C-N	-5.24	116.58	121.87
1	A	80	VAL	O-C-N	5.24	128.75	121.84
1	A	108	PRO	O-C-N	5.23	129.41	122.30
1	A	21	ASN	N-CA-C	5.23	119.12	109.24
1	A	38	PRO	N-CA-C	5.20	121.50	113.75
1	A	102	VAL	CB-CA-C	-5.20	104.39	111.15
1	A	131	ASN	CA-C-O	-5.18	115.06	120.55
1	A	151	ASP	CA-C-O	5.16	125.71	119.31
1	A	49	GLY	O-C-N	5.16	128.81	122.46
1	A	104	ASP	O-C-N	5.15	128.25	122.22
1	A	88	ALA	O-C-N	5.15	127.58	122.12
1	A	67	VAL	CA-C-O	5.13	126.60	121.17
1	A	71	VAL	CA-C-O	5.13	126.01	120.47
1	A	85	VAL	O-C-N	-5.12	116.90	122.64
1	A	134	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	A	51	SER	CA-C-O	5.09	125.94	119.78
1	A	4	THR	O-C-N	5.08	128.90	122.65
1	A	42	ASP	O-C-N	5.08	128.99	122.39
1	A	27	HIS	ND1-CG-CD2	5.06	111.16	106.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	GLU	Sidechain
1	A	17	GLU	Sidechain
1	A	42	ASP	Sidechain
1	A	55	GLN	Sidechain
1	A	56	ASN	Sidechain
1	A	57	ASN	Sidechain
1	A	59	GLU	Sidechain
1	A	61	GLN	Sidechain
1	A	7	GLN	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
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	19	19
2	A	43	0	30	2	0
3	A	9	0	4	2	0
4	A	65	0	0	0	4
All	All	1297	0	1234	20	21

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 8.

All (20) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:HA	1:A:152:ALA:HB1	1.77	0.65
1:A:21:ASN:C	1:A:21:ASN:HD22	2.08	0.61
1:A:77:GLN:NE2	1:A:85:VAL:H	1.99	0.60
1:A:26:THR:HB	1:A:64:ALA:HB3	1.83	0.60
1:A:102:VAL:HG13	2:A:154:HEM:HAC	1.90	0.53
1:A:18:PHE:CE1	1:A:25:HIS:HB3	2.44	0.52
1:A:86:THR:HA	1:A:90:LEU:HD12	1.91	0.51
1:A:92:ASN:O	1:A:96:VAL:HG12	2.11	0.50
1:A:63:HIS:HB3	3:A:155:NIO:O1	2.12	0.50
1:A:21:ASN:C	1:A:21:ASN:ND2	2.71	0.49
1:A:103:ALA:O	1:A:106:HIS:HB2	2.13	0.48
1:A:29:PHE:O	1:A:33:VAL:HG23	2.14	0.47
1:A:116:LYS:O	1:A:120:GLU:HG3	2.15	0.47
1:A:87:ASP:O	1:A:91:LYS:HG3	2.15	0.46
1:A:139:ASP:O	1:A:143:ILE:HG13	2.18	0.44
2:A:154:HEM:C1A	3:A:155:NIO:H1	2.55	0.42
1:A:117:THR:O	1:A:121:VAL:HG23	2.19	0.42
1:A:1:GLY:HA3	1:A:7:GLN:HE22	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:OD1	1:A:59:GLU:HB2	2.20	0.41

All (21) 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]	1.04	1.16
1:A:124:ALA:CB	1:A:129:GLU:N[2_555]	1.16	1.04
1:A:124:ALA:O	1:A:127:SER:CA[2_555]	1.27	0.93
1:A:124:ALA:O	1:A:127:SER:CB[2_555]	1.29	0.91
1:A:124:ALA:O	1:A:127:SER:C[2_555]	1.37	0.83
1:A:56:ASN:OD1	4:A:171:HOH:O[1_565]	1.41	0.79
1:A:124:ALA:C	1:A:127:SER:CB[2_555]	1.45	0.75
1:A:125:LYS:CA	1:A:127:SER:OG[2_555]	1.63	0.57
4:A:217:HOH:O	4:A:217:HOH:O[2_555]	1.64	0.56
1:A:125:LYS:CA	1:A:127:SER:CB[2_555]	1.69	0.51
1:A:10:LEU:CD1	1:A:125:LYS:CD[2_555]	1.73	0.47
1:A:125:LYS:N	1:A:127:SER:CB[2_555]	1.73	0.47
1:A:124:ALA:O	1:A:128:GLU:N[2_555]	1.75	0.45
1:A:124:ALA:O	1:A:127:SER:OG[2_555]	1.77	0.43
4:A:190:HOH:O	4:A:217:HOH:O[2_555]	1.81	0.39
1:A:125:LYS:C	1:A:127:SER:CB[2_555]	1.95	0.25
1:A:124:ALA:CB	1:A:128:GLU:C[2_555]	1.98	0.22
1:A:124:ALA:C	1:A:127:SER:OG[2_555]	2.00	0.20
1:A:125:LYS:N	1:A:127:SER:OG[2_555]	2.03	0.17
1:A:127:SER:CA	4:A:159:HOH:O[2_555]	2.11	0.09
1:A:10:LEU:CD1	1:A:125:LYS:CG[2_555]	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	153/153 (100%)	149 (97%)	3 (2%)	1 (1%)	18	14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	25	HIS
1	A	56	ASN
1	A	61	GLN
1	A	77	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NIO	A	155	2	9,9,9	3.17	7 (77%)	11,11,11	3.12	8 (72%)
2	HEM	A	154	1,3	50,50,50	4.44	34 (68%)	67,82,82	2.23	24 (35%)

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	NIO	A	155	2	-	0/4/4/4	0/1/1/1
2	HEM	A	154	1,3	-	4/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	FE-NB	10.08	2.25	1.94
2	A	154	HEM	FE-ND	10.00	2.25	1.94
2	A	154	HEM	C1B-C2B	7.60	1.59	1.44
2	A	154	HEM	C1D-C2D	7.41	1.59	1.44
2	A	154	HEM	C4D-C3D	7.01	1.56	1.45
2	A	154	HEM	C3B-C4B	7.01	1.58	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	CAB-C3B	6.95	1.65	1.47
2	A	154	HEM	CHD-C4C	6.78	1.51	1.38
2	A	154	HEM	FE-NA	6.29	2.15	1.95
2	A	154	HEM	CBD-CGD	6.27	1.65	1.50
3	A	155	NIO	C1-C2	-5.96	1.29	1.39
2	A	154	HEM	CHB-C4A	5.88	1.52	1.39
2	A	154	HEM	CHC-C1C	5.80	1.49	1.38
2	A	154	HEM	CAD-C3D	5.19	1.64	1.51
2	A	154	HEM	CMC-C2C	4.96	1.60	1.50
2	A	154	HEM	C3C-C2C	4.90	1.47	1.37
2	A	154	HEM	CMD-C2D	4.80	1.60	1.50
2	A	154	HEM	C1A-NA	4.78	1.48	1.39
2	A	154	HEM	CMB-C2B	4.76	1.60	1.50
2	A	154	HEM	CHA-C1A	4.69	1.49	1.39
2	A	154	HEM	C1C-NC	4.36	1.47	1.39
2	A	154	HEM	CAA-C2A	4.28	1.62	1.51
2	A	154	HEM	C2A-C3A	4.01	1.49	1.38
2	A	154	HEM	O2A-CGA	-3.93	1.17	1.30
2	A	154	HEM	CAC-C3C	3.73	1.57	1.47
3	A	155	NIO	O1-C6	-3.37	1.13	1.22
2	A	154	HEM	CBA-CGA	3.27	1.58	1.50
2	A	154	HEM	CMA-C3A	3.25	1.57	1.50
3	A	155	NIO	C2-C6	3.04	1.55	1.49
3	A	155	NIO	C4-C3	3.03	1.44	1.38
3	A	155	NIO	C1-N	3.01	1.40	1.34
3	A	155	NIO	C4-C5	-2.92	1.29	1.37
3	A	155	NIO	O2-C6	-2.68	1.22	1.30
2	A	154	HEM	C4B-NB	2.68	1.44	1.38
2	A	154	HEM	CBD-CAD	-2.59	1.43	1.51
2	A	154	HEM	C4D-ND	2.59	1.44	1.40
2	A	154	HEM	C4A-C3A	2.41	1.48	1.43
2	A	154	HEM	C4A-NA	2.35	1.44	1.39
2	A	154	HEM	C4C-NC	2.31	1.44	1.39
2	A	154	HEM	CBA-CAA	-2.27	1.44	1.51
2	A	154	HEM	CBB-CAB	2.13	1.40	1.30

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	C3B-C4B-NB	5.85	113.67	109.47
3	A	155	NIO	C5-N-C1	5.38	126.28	116.85
3	A	155	NIO	C4-C3-C2	4.53	124.82	120.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	154	HEM	C4A-NA-C1A	4.38	112.96	105.82
2	A	154	HEM	CHC-C1C-NC	4.28	129.12	124.45
2	A	154	HEM	CHD-C4C-NC	4.12	128.94	124.45
2	A	154	HEM	C3A-C4A-NA	-4.04	103.67	110.14
2	A	154	HEM	CMA-C3A-C4A	-3.95	119.40	125.42
2	A	154	HEM	C4C-NC-C1C	3.94	112.24	105.82
2	A	154	HEM	C4B-C3B-C2B	-3.87	103.72	107.28
2	A	154	HEM	C2A-C1A-NA	-3.77	105.97	110.15
3	A	155	NIO	O2-C6-C2	3.66	124.22	114.84
3	A	155	NIO	O2-C6-O1	-3.61	115.59	123.35
2	A	154	HEM	C4C-C3C-C2C	3.53	109.87	106.81
2	A	154	HEM	O2A-CGA-O1A	-3.44	114.48	123.33
2	A	154	HEM	C4A-C3A-C2A	3.37	110.67	106.82
3	A	155	NIO	C3-C2-C6	3.15	126.61	120.37
2	A	154	HEM	O2D-CGD-O1D	-3.04	115.51	123.33
2	A	154	HEM	O2D-CGD-CBD	2.99	123.44	114.00
2	A	154	HEM	CHD-C1D-ND	-2.94	121.26	124.42
2	A	154	HEM	CHC-C4B-NB	-2.89	121.31	124.42
2	A	154	HEM	CHB-C4A-NA	2.87	129.06	123.86
2	A	154	HEM	CHA-C1A-NA	2.77	128.88	123.86
3	A	155	NIO	C3-C2-C1	-2.64	114.67	117.61
2	A	154	HEM	CHB-C1B-NB	-2.63	121.12	124.37
2	A	154	HEM	C3D-C4D-ND	2.51	112.93	110.17
3	A	155	NIO	C4-C5-N	-2.45	115.73	122.61
3	A	155	NIO	C2-C1-N	-2.44	119.87	123.50
2	A	154	HEM	CAD-CBD-CGD	-2.29	107.59	113.67
2	A	154	HEM	CAD-C3D-C4D	2.19	128.51	124.70
2	A	154	HEM	C2C-C1C-NC	-2.15	105.66	109.64
2	A	154	HEM	CMA-C3A-C2A	2.02	129.91	125.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

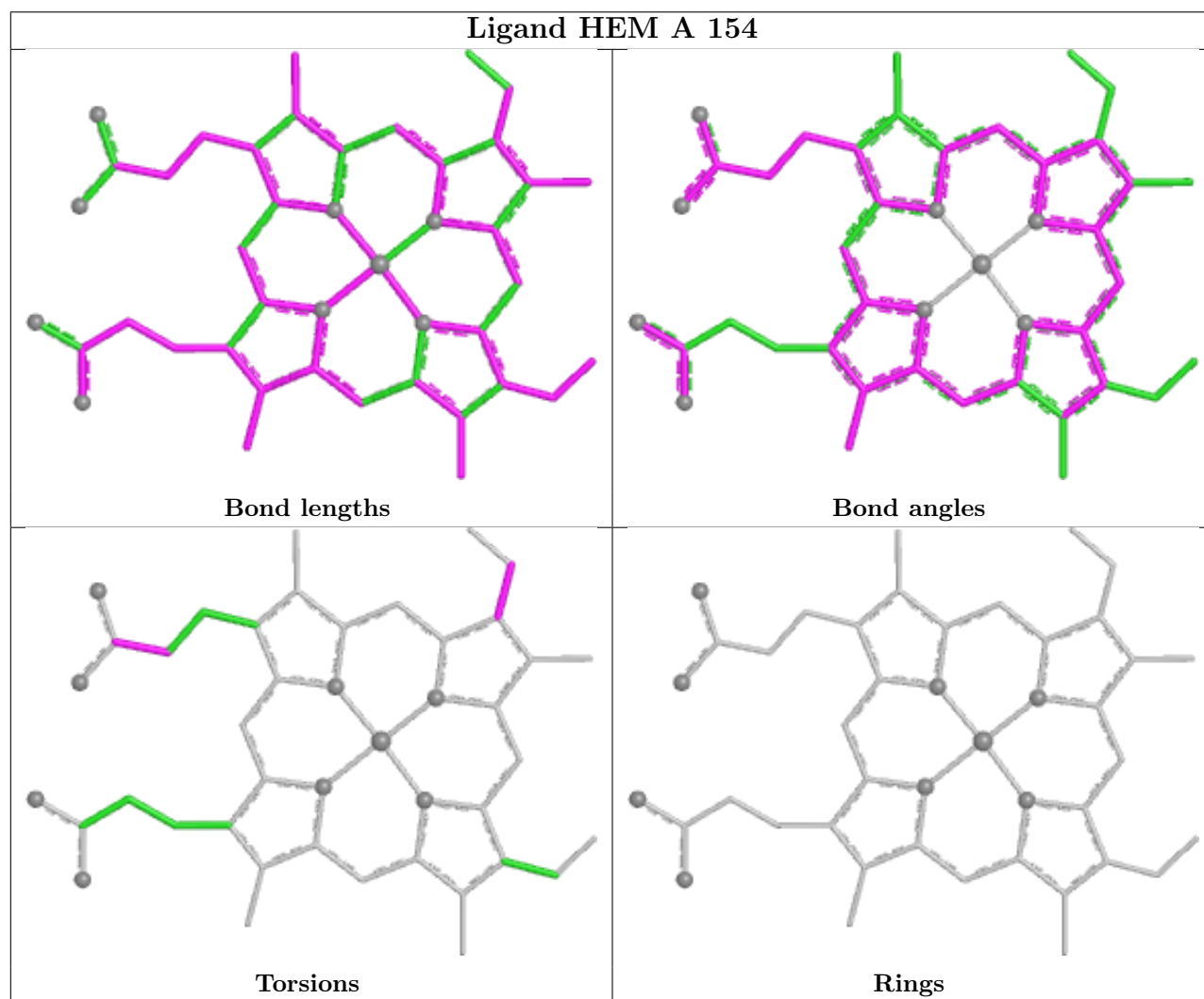
Mol	Chain	Res	Type	Atoms
2	A	154	HEM	C2C-C3C-CAC-CBC
2	A	154	HEM	C4C-C3C-CAC-CBC
2	A	154	HEM	CAD-CBD-CGD-O2D
2	A	154	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	NIO	2	0
2	A	154	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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%)	3.54	127 (83%) 0 0	6, 16, 38, 55	19 (12%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	ALA	16.7
1	A	1	GLY	12.7
1	A	151	ASP	12.3
1	A	88	ALA	9.2
1	A	45	SER	7.4
1	A	92	ASN	6.8
1	A	3	LEU	6.5
1	A	2	ALA	6.4
1	A	126	TRP	6.1
1	A	150	ASP	6.0
1	A	90	LEU	5.9
1	A	9	ALA	5.7
1	A	86	THR	5.6
1	A	128	GLU	5.5
1	A	48	LYS	5.5
1	A	148	GLU	5.3
1	A	49	GLY	5.3
1	A	100	LYS	5.2
1	A	143	ILE	5.0
1	A	130	LEU	4.9
1	A	12	LYS	4.9
1	A	153	ALA	4.9
1	A	144	VAL	4.8
1	A	50	THR	4.8
1	A	44	PHE	4.6
1	A	16	GLU	4.6
1	A	98	VAL	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	96	VAL	4.5
1	A	59	GLU	4.5
1	A	15	TRP	4.5
1	A	58	PRO	4.5
1	A	136	ILE	4.4
1	A	99	SER	4.4
1	A	42	ASP	4.4
1	A	4	THR	4.3
1	A	47	LEU	4.3
1	A	133	ALA	4.3
1	A	79	GLU	4.3
1	A	34	LEU	4.2
1	A	55	GLN	4.2
1	A	85	VAL	4.2
1	A	123	GLY	4.2
1	A	95	SER	4.2
1	A	132[A]	SER	4.2
1	A	62	ALA	4.2
1	A	107	PHE	4.2
1	A	31	ILE	4.1
1	A	10	LEU	4.1
1	A	21	ASN	4.1
1	A	41	LYS	4.0
1	A	102	VAL	4.0
1	A	147	LYS	4.0
1	A	60	LEU	3.9
1	A	20	ALA	3.9
1	A	89	THR	3.9
1	A	78	LEU	3.8
1	A	26	THR	3.7
1	A	74	ALA	3.7
1	A	110	VAL	3.7
1	A	27	HIS	3.7
1	A	23	PRO	3.6
1	A	5	GLU	3.6
1	A	105	ALA	3.6
1	A	146	LYS	3.6
1	A	122	VAL	3.5
1	A	56	ASN	3.5
1	A	94	GLY	3.5
1	A	114	ILE	3.4
1	A	93	LEU	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	54	PRO	3.4
1	A	108	PRO	3.4
1	A	149	MET	3.3
1	A	46	PHE	3.3
1	A	64	ALA	3.3
1	A	61	GLN	3.3
1	A	117	THR	3.2
1	A	57	ASN	3.2
1	A	11	VAL	3.2
1	A	51	SER	3.2
1	A	104	ASP	3.1
1	A	18	PHE	3.1
1	A	53	VAL	3.1
1	A	32	LEU	3.1
1	A	8	ALA	3.1
1	A	67	VAL	3.1
1	A	115	LEU	3.1
1	A	33	VAL	3.0
1	A	109	VAL	3.0
1	A	127	SER	3.0
1	A	29	PHE	3.0
1	A	121	VAL	3.0
1	A	77	GLN	2.9
1	A	28	ARG	2.9
1	A	69	LYS	2.9
1	A	40	ALA	2.9
1	A	6	SER	2.8
1	A	134	TRP	2.7
1	A	91	LYS	2.7
1	A	101	GLY	2.7
1	A	52	GLU	2.7
1	A	22	ILE	2.7
1	A	19	ASN	2.6
1	A	87	ASP	2.6
1	A	73	GLU	2.6
1	A	137	ALA	2.6
1	A	113	ALA	2.6
1	A	124	ALA	2.6
1	A	63	HIS	2.5
1	A	71	VAL	2.5
1	A	80	VAL	2.5
1	A	140	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	118	ILE	2.5
1	A	7	GLN	2.5
1	A	30	PHE	2.5
1	A	97	HIS	2.4
1	A	138	TYR	2.3
1	A	125	LYS	2.3
1	A	81	THR	2.3
1	A	65	GLY	2.3
1	A	106	HIS	2.2
1	A	14	SER	2.2
1	A	82	GLY	2.2
1	A	17	GLU	2.2
1	A	70	LEU	2.2
1	A	129	GLU	2.1
1	A	83	VAL	2.1
1	A	103	ALA	2.1

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](#)

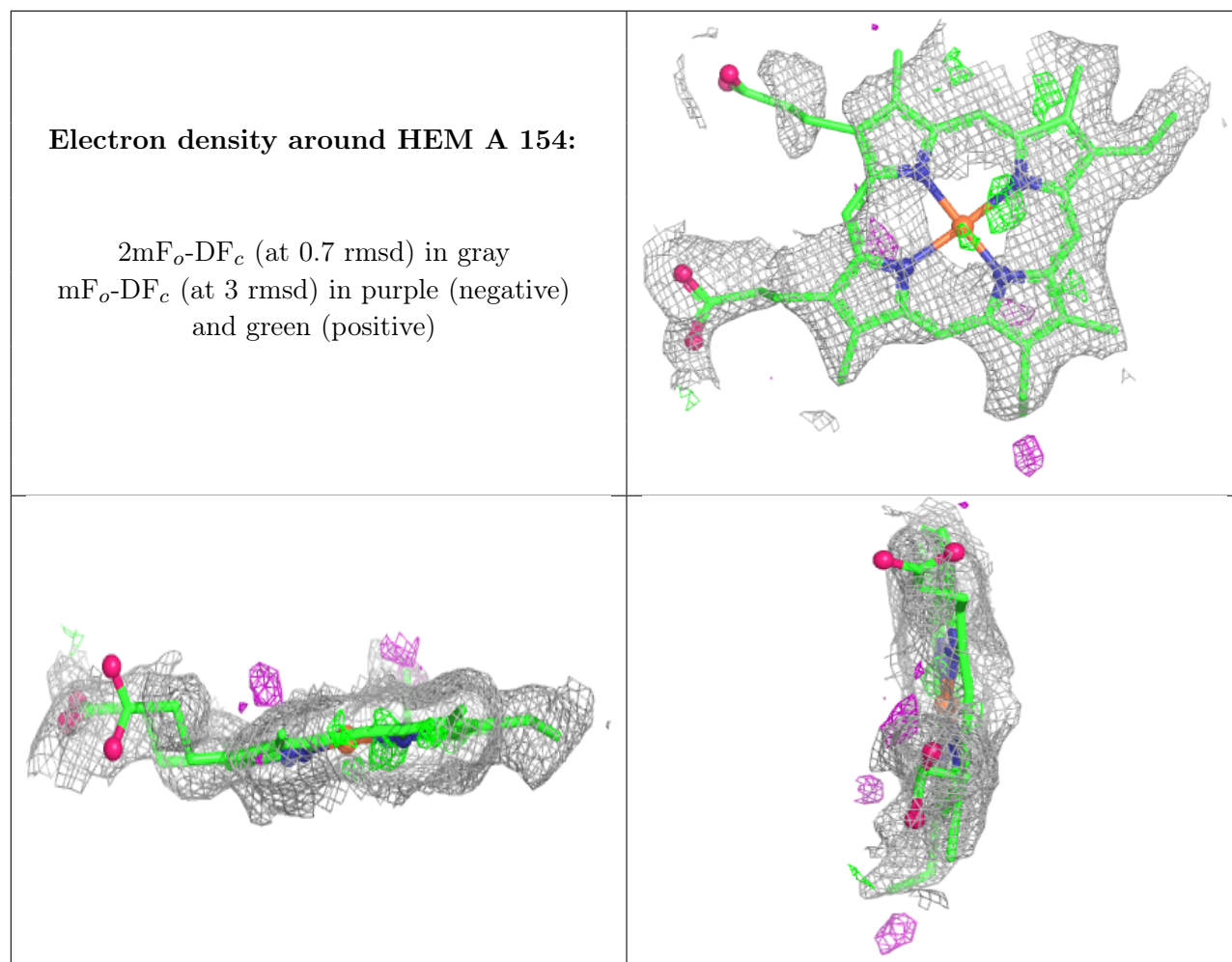
There are no oligosaccharides in this entry.

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
3	NIO	A	155	9/9	0.71	0.15	7,12,19,21	0
2	HEM	A	154	43/43	0.85	0.19	0,17,44,50	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.