



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:19 AM EDT

PDB ID : 1I3E / pdb_00001i3e
Title : HUMAN AZIDO-MET HEMOGLOBIN BART'S (GAMMA4)
Authors : Kidd, R.D.; Baker, H.M.; Mathews, A.J.; Brittain, T.; Baker, E.N.
Deposited on : 2001-02-15
Resolution : 1.86 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) : 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

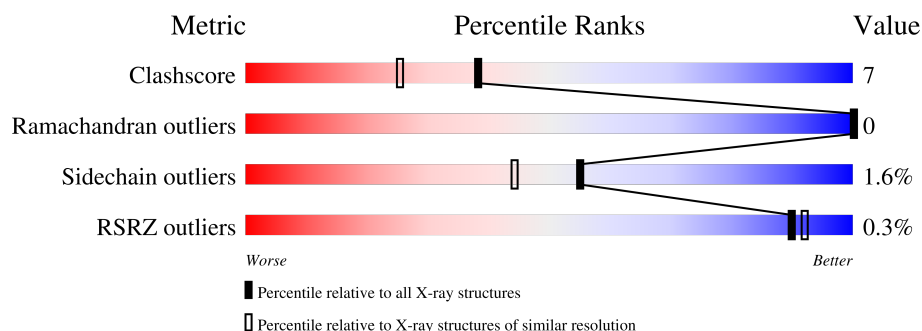
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.86 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	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	146	
1	B	146	

2 Entry composition [i](#)

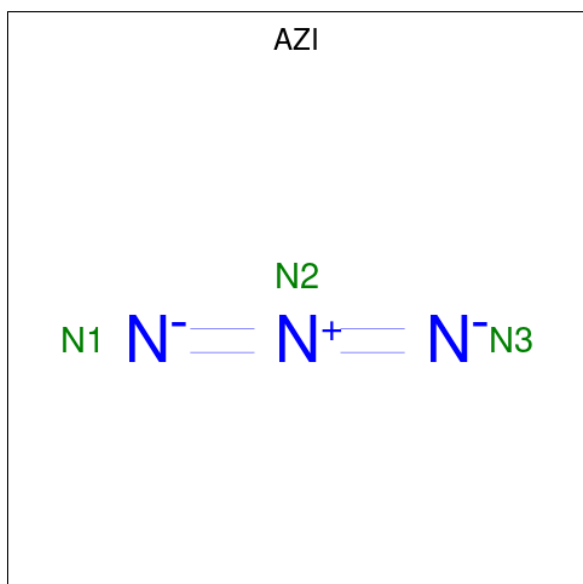
There are 4 unique types of molecules in this entry. The entry contains 2596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEMOGLOBIN GAMMA CHAINS.

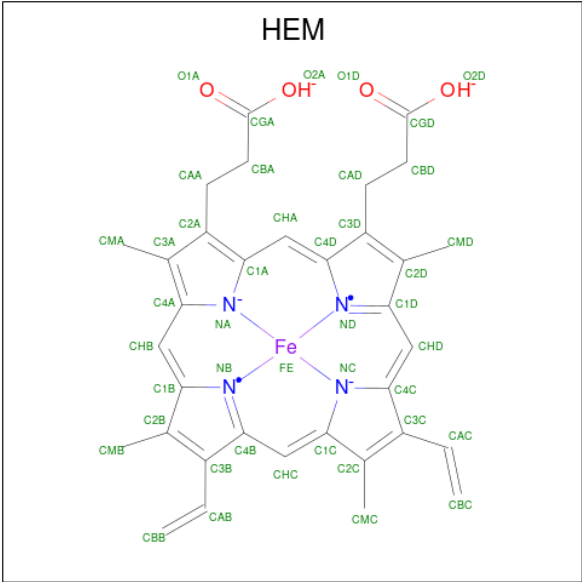
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	3	0	0
			1131	724	193	211	3			
1	B	146	Total	C	N	O	S	12	0	0
			1131	724	193	211	3			

- Molecule 2 is AZIDE ION (CCD ID: AZI) (formula: N₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	N	0	0
			3	3		
2	B	1	Total	N	0	0
			3	3		

- 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	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

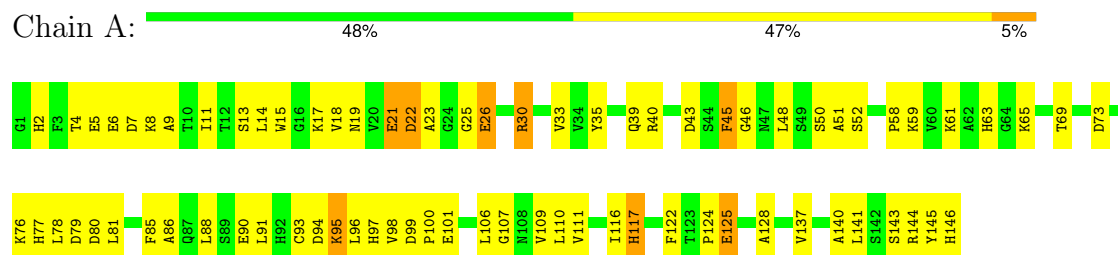
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		
4	B	108	Total	O	0	0
			108	108		

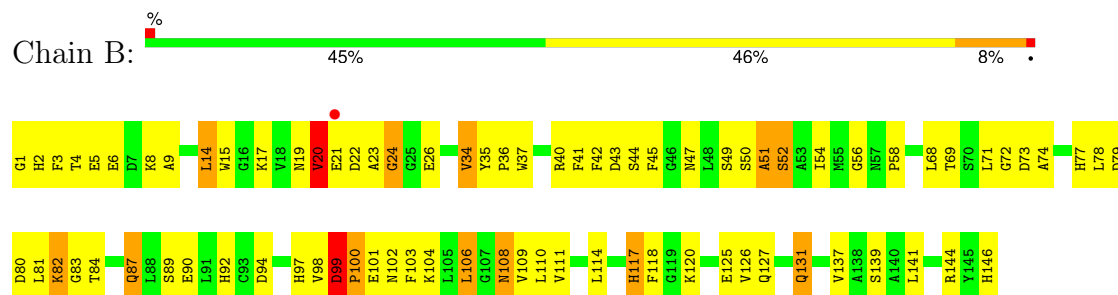
3 Residue-property plots [i](#)

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: HEMOGLOBIN GAMMA CHAINS



• Molecule 1: HEMOGLOBIN GAMMA CHAINS



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.54Å 81.62Å 53.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.86 20.00 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.1 (20.00-1.86) 98.1 (20.00-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 1.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.184 , 0.220 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2596	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, AZI

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	3.03	106/1157 (9.2%)	1.77	15/1565 (1.0%)
1	B	3.23	113/1157 (9.8%)	1.93	30/1565 (1.9%)
All	All	3.13	219/2314 (9.5%)	1.85	45/3130 (1.4%)

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	B	0	1

All (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	HIS	CE1-NE2	23.68	1.56	1.32
1	B	20	VAL	C-N	-20.25	1.09	1.33
1	B	21	GLU	C-O	16.68	1.43	1.24
1	B	80	ASP	CA-CB	-14.78	1.42	1.53
1	B	20	VAL	C-O	13.98	1.40	1.24
1	A	117	HIS	CD2-NE2	13.48	1.52	1.37
1	A	30	ARG	NE-CZ	12.96	1.47	1.33
1	B	52	SER	CA-CB	12.20	1.72	1.53
1	B	87	GLN	CD-NE2	-11.59	1.08	1.33
1	A	94	ASP	N-CA	11.47	1.60	1.46
1	B	94	ASP	N-CA	11.36	1.61	1.46
1	A	77	HIS	CD2-NE2	10.77	1.49	1.37
1	A	143	SER	C-N	-10.60	1.19	1.33
1	A	97	HIS	ND1-CE1	10.45	1.43	1.32
1	B	20	VAL	N-CA	10.45	1.58	1.46
1	A	6	GLU	CD-OE2	10.42	1.45	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	94	ASP	C-N	10.40	1.47	1.33
1	B	8	LYS	CA-C	-9.99	1.39	1.52
1	A	146	HIS	CE1-NE2	9.96	1.42	1.32
1	B	4	THR	CA-C	-9.73	1.39	1.53
1	A	4	THR	C-N	9.64	1.47	1.34
1	B	117	HIS	ND1-CE1	-9.57	1.23	1.32
1	B	43	ASP	CB-CG	-9.46	1.28	1.52
1	A	99	ASP	CA-C	-9.39	1.42	1.53
1	B	43	ASP	N-CA	9.34	1.58	1.46
1	A	51	ALA	CA-CB	9.30	1.67	1.53
1	B	101	GLU	CD-OE2	9.29	1.43	1.25
1	A	26	GLU	CD-OE2	-9.26	1.07	1.25
1	B	146	HIS	CG-ND1	9.23	1.48	1.38
1	A	52	SER	CA-CB	9.20	1.68	1.53
1	B	97	HIS	CG-CD2	-9.11	1.25	1.35
1	B	77	HIS	ND1-CE1	9.09	1.41	1.32
1	B	144	ARG	CZ-NH1	9.05	1.45	1.32
1	A	144	ARG	CZ-NH2	8.97	1.45	1.33
1	B	5	GLU	CA-CB	8.91	1.68	1.53
1	B	2	HIS	ND1-CE1	8.75	1.41	1.32
1	A	17	LYS	C-N	-8.62	1.18	1.33
1	A	18	VAL	CA-CB	8.61	1.65	1.54
1	A	43	ASP	N-CA	8.51	1.57	1.46
1	B	22	ASP	C-O	8.48	1.33	1.24
1	B	14	LEU	CA-C	-8.38	1.41	1.52
1	A	43	ASP	CG-OD2	8.28	1.41	1.25
1	B	47	ASN	CA-C	8.15	1.63	1.52
1	B	82	LYS	CD-CE	8.14	1.76	1.52
1	A	21	GLU	CG-CD	-8.09	1.31	1.52
1	B	14	LEU	C-N	8.08	1.45	1.34
1	A	140	ALA	C-O	8.07	1.33	1.24
1	A	22	ASP	C-N	8.07	1.44	1.33
1	A	26	GLU	CG-CD	8.06	1.72	1.52
1	B	98	VAL	CA-CB	8.00	1.64	1.54
1	B	117	HIS	CD2-NE2	8.00	1.46	1.37
1	B	137	VAL	CA-C	7.97	1.62	1.52
1	B	114	LEU	C-N	7.92	1.44	1.33
1	B	131	GLN	CD-NE2	-7.90	1.16	1.33
1	A	143	SER	CA-CB	7.89	1.65	1.53
1	A	77	HIS	ND1-CE1	7.83	1.40	1.32
1	B	21	GLU	N-CA	-7.82	1.37	1.46
1	B	44	SER	CA-CB	-7.66	1.39	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	ASP	N-CA	7.64	1.55	1.46
1	A	117	HIS	CG-CD2	7.64	1.44	1.35
1	A	4	THR	CA-C	-7.59	1.42	1.53
1	B	21	GLU	CA-CB	-7.55	1.41	1.53
1	A	19	ASN	CA-CB	-7.47	1.43	1.53
1	A	6	GLU	CA-C	7.45	1.62	1.52
1	A	43	ASP	CA-C	-7.43	1.42	1.52
1	B	15	TRP	CD2-CE3	-7.41	1.28	1.40
1	B	45	PHE	N-CA	7.40	1.55	1.46
1	A	78	LEU	C-N	7.36	1.44	1.33
1	B	146	HIS	CE1-NE2	7.36	1.40	1.32
1	B	139	SER	N-CA	7.34	1.55	1.46
1	A	144	ARG	NE-CZ	-7.33	1.25	1.33
1	B	19	ASN	C-N	-7.33	1.24	1.33
1	B	94	ASP	C-O	-7.32	1.14	1.24
1	B	43	ASP	CG-OD2	7.32	1.39	1.25
1	B	111	VAL	CA-C	7.30	1.62	1.52
1	A	76	LYS	CG-CD	7.28	1.74	1.52
1	A	128	ALA	CA-CB	7.27	1.64	1.53
1	B	35	TYR	CA-C	-7.24	1.43	1.52
1	B	99	ASP	CA-C	-7.24	1.44	1.53
1	B	108	ASN	CG-ND2	7.18	1.48	1.33
1	A	144	ARG	CA-C	-7.17	1.42	1.52
1	A	13	SER	C-O	7.16	1.32	1.24
1	B	84	THR	N-CA	-7.16	1.37	1.46
1	B	41	PHE	C-N	-7.03	1.23	1.33
1	A	25	GLY	CA-C	-7.02	1.43	1.52
1	A	6	GLU	CD-OE1	-6.99	1.12	1.25
1	B	80	ASP	CG-OD1	6.99	1.38	1.25
1	B	45	PHE	C-N	-6.97	1.23	1.33
1	B	2	HIS	CD2-NE2	6.96	1.45	1.37
1	B	89	SER	N-CA	6.94	1.54	1.46
1	B	22	ASP	C-N	-6.94	1.24	1.33
1	A	144	ARG	N-CA	6.93	1.55	1.46
1	A	101	GLU	CA-C	6.91	1.62	1.52
1	B	42	PHE	CA-C	6.86	1.61	1.52
1	A	21	GLU	C-O	6.85	1.32	1.24
1	B	2	HIS	C-O	6.84	1.32	1.23
1	A	86	ALA	C-O	-6.83	1.16	1.24
1	A	19	ASN	CA-C	6.81	1.61	1.53
1	B	125	GLU	CD-OE2	-6.77	1.12	1.25
1	A	15	TRP	CD2-CE2	6.76	1.52	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	109	VAL	CA-C	6.73	1.61	1.52
1	A	86	ALA	CA-C	6.68	1.61	1.52
1	A	69	THR	N-CA	6.67	1.54	1.46
1	B	56	GLY	CA-C	6.59	1.62	1.51
1	B	34	VAL	C-N	-6.54	1.24	1.33
1	A	106	LEU	CA-C	-6.50	1.44	1.52
1	B	71	LEU	C-O	-6.49	1.16	1.24
1	A	117	HIS	ND1-CE1	-6.46	1.26	1.32
1	B	73	ASP	CA-CB	6.42	1.64	1.53
1	B	72	GLY	N-CA	-6.41	1.37	1.45
1	A	63	HIS	CD2-NE2	6.40	1.44	1.37
1	B	23	ALA	N-CA	6.39	1.54	1.46
1	B	19	ASN	CA-C	6.38	1.60	1.52
1	B	4	THR	C-O	6.36	1.32	1.23
1	A	137	VAL	CA-CB	6.31	1.62	1.54
1	B	110	LEU	N-CA	6.29	1.53	1.46
1	B	24	GLY	N-CA	6.28	1.53	1.45
1	A	45	PHE	CA-C	6.27	1.61	1.52
1	A	146	HIS	CD2-NE2	-6.24	1.30	1.37
1	B	90	GLU	CA-CB	6.23	1.63	1.53
1	B	8	LYS	CA-CB	6.20	1.62	1.53
1	A	8	LYS	CG-CD	6.18	1.71	1.52
1	A	98	VAL	CA-CB	6.15	1.61	1.54
1	A	90	GLU	CD-OE2	6.15	1.37	1.25
1	A	21	GLU	N-CA	6.14	1.53	1.46
1	A	23	ALA	C-O	-6.12	1.17	1.24
1	B	78	LEU	C-O	6.11	1.31	1.24
1	B	100	PRO	CA-CB	6.11	1.62	1.53
1	A	48	LEU	N-CA	-6.07	1.39	1.46
1	B	35	TYR	CA-CB	6.04	1.60	1.53
1	B	69	THR	C-N	6.03	1.41	1.33
1	A	2	HIS	CE1-NE2	6.03	1.38	1.32
1	B	77	HIS	CG-CD2	-6.02	1.29	1.35
1	A	80	ASP	CA-CB	-5.97	1.48	1.53
1	A	46	GLY	N-CA	5.96	1.54	1.45
1	A	122	PHE	C-O	5.96	1.30	1.23
1	B	44	SER	C-O	-5.90	1.16	1.24
1	B	97	HIS	CA-C	5.90	1.60	1.53
1	A	95	LYS	CG-CD	5.89	1.70	1.52
1	B	92	HIS	ND1-CE1	5.88	1.38	1.32
1	B	6	GLU	C-N	-5.87	1.26	1.33
1	B	44	SER	CA-C	5.85	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	106	LEU	C-N	-5.84	1.26	1.33
1	B	9	ALA	CA-C	5.84	1.60	1.52
1	A	33	VAL	N-CA	-5.79	1.39	1.46
1	A	78	LEU	N-CA	5.78	1.53	1.46
1	A	40	ARG	NE-CZ	5.77	1.39	1.33
1	B	131	GLN	CA-C	-5.75	1.45	1.52
1	A	143	SER	C-O	5.73	1.30	1.24
1	B	54	ILE	N-CA	5.73	1.53	1.46
1	B	79	ASP	N-CA	5.72	1.53	1.46
1	A	5	GLU	CA-CB	5.72	1.62	1.53
1	A	5	GLU	C-O	-5.70	1.16	1.24
1	B	131	GLN	CD-OE1	5.69	1.34	1.23
1	B	117	HIS	CE1-NE2	5.68	1.38	1.32
1	B	51	ALA	C-N	5.62	1.41	1.33
1	A	39	GLN	CA-CB	5.60	1.63	1.53
1	A	128	ALA	N-CA	-5.60	1.39	1.46
1	A	107	GLY	CA-C	-5.60	1.45	1.52
1	B	49	SER	CA-CB	5.59	1.62	1.53
1	B	17	LYS	N-CA	-5.56	1.39	1.46
1	A	111	VAL	CA-CB	5.55	1.61	1.54
1	A	15	TRP	C-O	5.55	1.31	1.24
1	B	109	VAL	CA-CB	5.55	1.61	1.54
1	B	97	HIS	CE1-NE2	5.54	1.38	1.32
1	B	77	HIS	N-CA	-5.54	1.38	1.46
1	A	97	HIS	CG-ND1	5.49	1.44	1.38
1	B	3	PHE	N-CA	5.48	1.52	1.46
1	A	144	ARG	CZ-NH1	5.47	1.40	1.32
1	B	144	ARG	C-N	-5.45	1.25	1.33
1	B	87	GLN	CD-OE1	5.44	1.33	1.23
1	A	9	ALA	C-N	5.42	1.40	1.33
1	A	22	ASP	CA-CB	5.42	1.62	1.53
1	B	40	ARG	CA-C	5.40	1.60	1.52
1	B	81	LEU	C-O	-5.40	1.17	1.24
1	A	96	LEU	C-O	5.40	1.31	1.24
1	A	124	PRO	N-CD	5.39	1.55	1.47
1	B	111	VAL	C-N	-5.39	1.26	1.33
1	A	30	ARG	CZ-NH1	-5.37	1.25	1.32
1	B	58	PRO	N-CA	5.37	1.54	1.47
1	A	11	ILE	N-CA	5.34	1.52	1.46
1	B	1	GLY	C-N	5.33	1.40	1.33
1	B	117	HIS	CG-ND1	-5.33	1.32	1.38
1	B	24	GLY	CA-C	-5.31	1.46	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	GLU	CD-OE2	-5.29	1.15	1.25
1	A	88	LEU	CB-CG	5.29	1.64	1.53
1	A	61	LYS	CG-CD	5.27	1.68	1.52
1	B	6	GLU	CD-OE2	5.26	1.35	1.25
1	B	22	ASP	CB-CG	5.26	1.65	1.52
1	A	35	TYR	CA-CB	5.26	1.59	1.53
1	A	125	GLU	C-O	5.23	1.30	1.24
1	B	102	ASN	CB-CG	5.21	1.65	1.52
1	A	110	LEU	N-CA	5.20	1.52	1.46
1	B	52	SER	CA-C	-5.20	1.46	1.52
1	B	37	TRP	NE1-CE2	5.20	1.43	1.37
1	B	117	HIS	CA-CB	-5.19	1.45	1.53
1	A	79	ASP	CG-OD1	5.18	1.35	1.25
1	A	50	SER	C-N	5.18	1.40	1.33
1	A	85	PHE	CA-C	-5.16	1.45	1.52
1	A	14	LEU	CA-C	-5.15	1.46	1.52
1	A	46	GLY	CA-C	5.15	1.59	1.51
1	A	22	ASP	CA-C	-5.14	1.46	1.53
1	A	50	SER	CA-C	-5.13	1.46	1.52
1	B	58	PRO	C-O	5.12	1.30	1.24
1	A	6	GLU	C-N	-5.12	1.27	1.33
1	B	83	GLY	C-O	5.11	1.29	1.23
1	B	114	LEU	CA-C	-5.09	1.45	1.52
1	A	81	LEU	C-N	5.09	1.40	1.33
1	B	74	ALA	CA-CB	-5.07	1.45	1.53
1	A	77	HIS	CG-CD2	-5.06	1.30	1.35
1	A	141	LEU	CG-CD2	5.06	1.69	1.52
1	A	69	THR	C-O	5.05	1.30	1.24
1	A	144	ARG	CD-NE	5.05	1.53	1.46
1	B	84	THR	CA-C	5.04	1.59	1.52
1	A	116	ILE	C-O	5.03	1.29	1.24
1	A	93	CYS	CA-C	5.03	1.59	1.53
1	B	50	SER	N-CA	-5.02	1.39	1.45
1	A	73	ASP	C-O	-5.02	1.18	1.24
1	A	22	ASP	N-CA	5.00	1.52	1.46

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	VAL	CA-C-O	-11.53	108.95	121.17
1	B	21	GLU	CB-CA-C	-9.20	96.29	110.92
1	A	117	HIS	CG-CD2-NE2	-8.72	98.48	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	NE-CZ-NH2	-8.12	111.89	119.20
1	B	87	GLN	OE1-CD-NE2	7.72	130.32	122.60
1	A	117	HIS	CB-CG-CD2	-7.15	121.90	131.20
1	B	43	ASP	CB-CG-OD1	7.06	134.63	118.40
1	B	35	TYR	CA-C-N	6.93	127.50	119.47
1	B	35	TYR	C-N-CA	6.93	127.50	119.47
1	B	99	ASP	CA-C-N	6.73	126.68	119.28
1	B	99	ASP	C-N-CA	6.73	126.68	119.28
1	B	137	VAL	N-CA-C	-6.71	104.22	110.53
1	A	117	HIS	ND1-CG-CD2	6.60	112.70	106.10
1	B	21	GLU	N-CA-CB	6.60	119.86	109.82
1	B	20	VAL	N-CA-C	-6.36	104.31	110.42
1	B	114	LEU	CA-C-O	6.05	126.93	119.97
1	B	22	ASP	CA-C-O	-6.04	114.48	120.70
1	B	34	VAL	CA-C-O	-6.03	113.74	120.25
1	B	103	PHE	N-CA-C	-6.01	104.81	111.36
1	B	80	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	97	HIS	CE1-NE2-CD2	5.97	114.97	109.00
1	B	43	ASP	OD1-CG-OD2	-5.94	108.65	122.90
1	A	98	VAL	CB-CA-C	-5.89	103.49	111.15
1	B	20	VAL	CA-C-N	5.83	128.89	120.79
1	B	20	VAL	C-N-CA	5.83	128.89	120.79
1	A	97	HIS	ND1-CE1-NE2	-5.73	102.67	108.40
1	B	146	HIS	CA-C-O	-5.73	103.82	121.00
1	B	126	VAL	N-CA-C	-5.64	104.86	110.62
1	A	117	HIS	ND1-CE1-NE2	-5.64	102.76	108.40
1	B	97	HIS	CB-CA-C	-5.54	104.03	111.89
1	A	86	ALA	O-C-N	5.50	127.81	122.09
1	A	43	ASP	N-CA-CB	-5.47	101.80	110.28
1	B	117	HIS	CG-CD2-NE2	-5.34	101.86	107.20
1	A	99	ASP	CA-C-N	5.24	125.55	119.47
1	A	99	ASP	C-N-CA	5.24	125.55	119.47
1	B	89	SER	N-CA-C	-5.22	105.67	111.36
1	B	111	VAL	O-C-N	5.21	126.93	121.87
1	A	17	LYS	CA-C-O	-5.20	113.26	119.35
1	A	143	SER	CA-C-O	-5.13	115.09	120.63
1	B	100	PRO	CB-CA-C	-5.11	104.25	112.21
1	A	17	LYS	N-CA-C	-5.07	106.78	113.17
1	B	43	ASP	N-CA-CB	-5.05	102.45	110.28
1	A	30	ARG	NH1-CZ-NH2	5.05	125.86	119.30
1	B	77	HIS	ND1-CG-CD2	5.03	111.13	106.10
1	B	111	VAL	CA-C-O	-5.01	115.74	120.95

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	20	VAL	Mainchain

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	1131	0	1128	10	0
1	B	1131	0	1127	24	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	43	0	30	0	0
3	B	43	0	30	2	0
4	A	134	0	0	2	0
4	B	108	0	0	6	0
All	All	2596	0	2315	32	0

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 7.

All (32) 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:B:82:LYS:CD	1:B:82:LYS:CE	1.76	1.57
1:B:82:LYS:CD	1:B:82:LYS:NZ	2.43	0.79
1:B:131:GLN:HG3	4:B:277:HOH:O	1.91	0.71
1:B:20:VAL:HG13	1:B:68:LEU:HB3	1.77	0.65
1:B:106:LEU:C	1:B:106:LEU:HD23	2.23	0.64
1:B:106:LEU:HD23	1:B:106:LEU:O	2.01	0.61
1:A:30:ARG:HD3	1:B:127:GLN:OE1	2.03	0.57
1:A:22:ASP:O	1:A:26:GLU:HG3	2.06	0.56
1:B:82:LYS:CE	1:B:82:LYS:CG	2.77	0.55
1:A:100:PRO:HG3	1:A:145:TYR:CD2	2.42	0.54
1:B:131:GLN:NE2	4:B:277:HOH:O	2.35	0.52
1:A:45:PHE:HA	1:A:59:LYS:HD3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:OE1	1:A:117:HIS:NE2	2.44	0.51
1:B:99:ASP:OD2	1:B:99:ASP:N	2.45	0.48
1:B:117:HIS:HB2	4:B:433:HOH:O	2.14	0.47
1:B:82:LYS:CD	1:B:82:LYS:HZ3	2.26	0.46
1:B:131:GLN:CG	4:B:277:HOH:O	2.54	0.45
1:A:91:LEU:HD12	1:A:95:LYS:HD3	1.98	0.45
1:A:125:GLU:HG3	1:B:51:ALA:CB	2.47	0.44
1:B:108:ASN:ND2	4:B:439:HOH:O	2.50	0.44
1:A:21:GLU:OE2	1:A:65:LYS:HE3	2.17	0.43
1:B:24:GLY:N	1:B:68:LEU:HD22	2.34	0.42
1:B:24:GLY:CA	1:B:68:LEU:HD22	2.49	0.42
1:B:34:VAL:C	1:B:36:PRO:HD3	2.45	0.42
1:B:99:ASP:HA	1:B:100:PRO:HD3	1.89	0.42
1:A:26:GLU:HG2	4:A:394:HOH:O	2.20	0.41
1:A:58:PRO:HD2	4:A:404:HOH:O	2.21	0.41
1:B:141:LEU:HD11	3:B:147:HEM:CAB	2.51	0.41
1:B:14:LEU:HD11	1:B:118:PHE:CG	2.56	0.41
1:B:104:LYS:HG3	4:B:371:HOH:O	2.20	0.41
1:B:141:LEU:CD1	3:B:147:HEM:HAB	2.51	0.40
1:B:106:LEU:C	1:B:106:LEU:CD2	2.93	0.40

There are no symmetry-related clashes.

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	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
1	B	144/146 (99%)	143 (99%)	1 (1%)	0	100	100
All	All	288/292 (99%)	285 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	122/122 (100%)	122 (100%)	0	100	100
1	B	122/122 (100%)	118 (97%)	4 (3%)	33	18
All	All	244/244 (100%)	240 (98%)	4 (2%)	55	44

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

Mol	Chain	Res	Type
1	B	52	SER
1	B	87	GLN
1	B	99	ASP
1	B	120	LYS

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	77	HIS
1	B	2	HIS
1	B	39	GLN
1	B	87	GLN
1	B	97	HIS
1	B	108	ASN
1	B	117	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	AZI	A	148	3	2,2,2	1.51	0	0,1,1	-	-
3	HEM	B	147	1,2	50,50,50	2.79	20 (40%)	67,82,82	1.57	12 (17%)
2	AZI	B	148	3	2,2,2	0.58	0	0,1,1	-	-
3	HEM	A	147	1,2	50,50,50	2.71	20 (40%)	67,82,82	2.06	20 (29%)

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	B	147	1,2	-	4/14/54/54	-
3	HEM	A	147	1,2	-	5/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	CMA-C3A	7.34	1.65	1.50
3	B	147	HEM	CBA-CGA	6.29	1.65	1.50
3	A	147	HEM	CBD-CGD	6.26	1.65	1.50
3	B	147	HEM	CBD-CGD	6.14	1.64	1.50
3	A	147	HEM	C4D-C3D	6.04	1.55	1.45
3	B	147	HEM	C1D-ND	5.63	1.49	1.38
3	A	147	HEM	CMA-C3A	5.55	1.62	1.50
3	B	147	HEM	O1A-CGA	-5.46	1.04	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	147	HEM	CHD-C1D	-5.20	1.27	1.39
3	A	147	HEM	C1C-NC	-5.11	1.30	1.39
3	B	147	HEM	O2D-CGD	-5.04	1.14	1.30
3	A	147	HEM	CMB-C2B	5.00	1.61	1.50
3	A	147	HEM	CBB-CAB	4.94	1.54	1.30
3	A	147	HEM	O2D-CGD	-4.86	1.14	1.30
3	A	147	HEM	CHC-C1C	4.55	1.47	1.38
3	A	147	HEM	C3B-C4B	4.02	1.52	1.44
3	B	147	HEM	CBB-CAB	3.92	1.49	1.30
3	B	147	HEM	C4D-C3D	3.81	1.51	1.45
3	B	147	HEM	C1D-C2D	3.78	1.52	1.44
3	B	147	HEM	CBC-CAC	3.68	1.48	1.30
3	A	147	HEM	C4D-ND	-3.51	1.34	1.40
3	A	147	HEM	CBC-CAC	3.49	1.47	1.30
3	A	147	HEM	CAB-C3B	3.36	1.56	1.47
3	A	147	HEM	C3B-C2B	-3.25	1.30	1.37
3	A	147	HEM	C1C-C2C	3.23	1.51	1.45
3	B	147	HEM	CMB-C2B	3.02	1.57	1.50
3	B	147	HEM	CAC-C3C	3.02	1.55	1.47
3	B	147	HEM	C1C-C2C	2.72	1.50	1.45
3	A	147	HEM	CBA-CAA	2.67	1.61	1.51
3	A	147	HEM	FE-ND	2.63	2.03	1.94
3	B	147	HEM	CHC-C1C	2.62	1.43	1.38
3	B	147	HEM	C4D-ND	-2.56	1.35	1.40
3	A	147	HEM	C1A-C2A	2.49	1.49	1.44
3	B	147	HEM	C1B-NB	2.36	1.44	1.40
3	B	147	HEM	C4B-NB	-2.31	1.34	1.38
3	B	147	HEM	CAB-C3B	2.24	1.53	1.47
3	A	147	HEM	C3C-C4C	2.15	1.49	1.46
3	B	147	HEM	C1A-C2A	2.06	1.48	1.44
3	A	147	HEM	C4B-NB	-2.05	1.34	1.38
3	A	147	HEM	CBA-CGA	2.05	1.55	1.50

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	147	HEM	C3C-C2C-C1C	-5.23	102.09	107.05
3	A	147	HEM	O2D-CGD-O1D	5.01	136.21	123.33
3	A	147	HEM	O1D-CGD-CBD	-4.91	107.50	123.09
3	A	147	HEM	CHC-C4B-NB	4.64	129.41	124.42
3	B	147	HEM	C3B-C4B-NB	4.16	112.46	109.47
3	B	147	HEM	C3C-C2C-C1C	-4.06	103.21	107.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	147	HEM	CHC-C1C-C2C	-3.98	117.22	125.49
3	A	147	HEM	C1C-CHC-C4B	-3.70	118.16	126.02
3	A	147	HEM	CHD-C4C-NC	3.67	128.44	124.45
3	A	147	HEM	C2D-C1D-ND	3.52	113.97	109.90
3	B	147	HEM	C1C-CHC-C4B	-3.20	119.21	126.02
3	A	147	HEM	CHD-C1D-C2D	-3.14	120.07	125.03
3	A	147	HEM	CHC-C1C-NC	3.02	127.75	124.45
3	A	147	HEM	C3B-C2B-C1B	2.98	108.65	106.41
3	B	147	HEM	C3D-C4D-ND	2.96	113.42	110.17
3	B	147	HEM	C4C-C3C-C2C	2.95	109.37	106.81
3	A	147	HEM	C2C-C1C-NC	2.92	115.04	109.64
3	B	147	HEM	O1D-CGD-CBD	-2.90	113.90	123.09
3	B	147	HEM	CHC-C1C-C2C	-2.89	119.48	125.49
3	A	147	HEM	CMD-C2D-C1D	2.81	129.43	125.03
3	B	147	HEM	CBD-CAD-C3D	-2.64	105.23	112.53
3	B	147	HEM	O2D-CGD-CBD	2.59	122.19	114.00
3	A	147	HEM	C1D-C2D-C3D	-2.56	104.29	106.98
3	A	147	HEM	C4A-C3A-C2A	2.55	109.73	106.82
3	A	147	HEM	CHA-C4D-ND	2.48	127.44	124.37
3	A	147	HEM	CMC-C2C-C1C	2.38	128.92	124.73
3	B	147	HEM	C2C-C1C-NC	2.22	113.73	109.64
3	B	147	HEM	CHC-C1C-NC	2.12	126.76	124.45
3	A	147	HEM	CHA-C4D-C3D	-2.08	121.39	125.23
3	A	147	HEM	CHD-C4C-C3C	-2.06	121.74	125.21
3	B	147	HEM	CHA-C4D-C3D	-2.03	121.48	125.23
3	A	147	HEM	CAA-C2A-C1A	2.02	128.88	124.94

There are no chirality outliers.

All (9) torsion outliers are listed below:

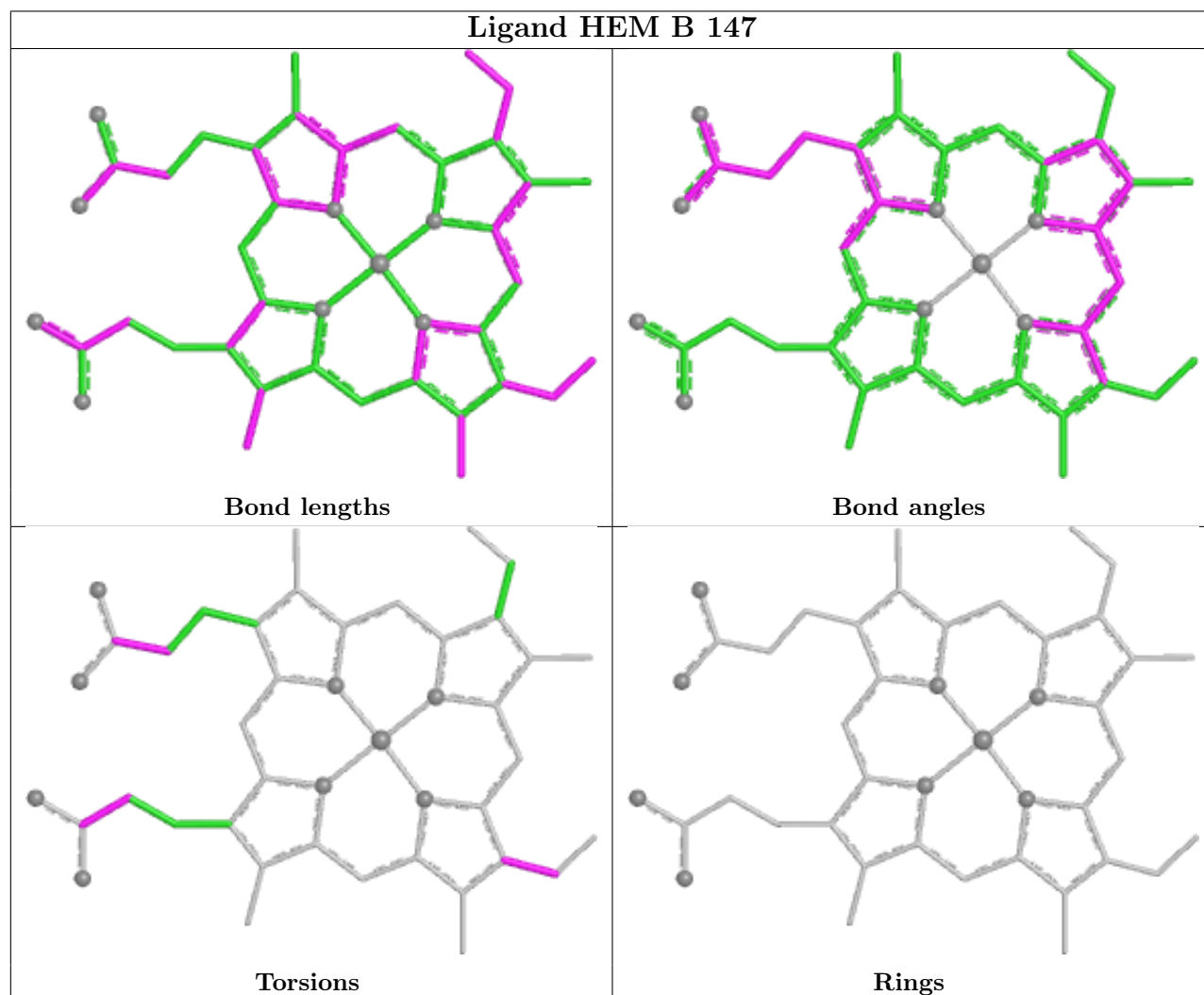
Mol	Chain	Res	Type	Atoms
3	A	147	HEM	C2C-C3C-CAC-CBC
3	B	147	HEM	C2B-C3B-CAB-CBB
3	A	147	HEM	CAD-CBD-CGD-O2D
3	A	147	HEM	CAD-CBD-CGD-O1D
3	A	147	HEM	C4C-C3C-CAC-CBC
3	B	147	HEM	C4B-C3B-CAB-CBB
3	A	147	HEM	CAA-CBA-CGA-O1A
3	B	147	HEM	CAD-CBD-CGD-O1D
3	B	147	HEM	CAA-CBA-CGA-O2A

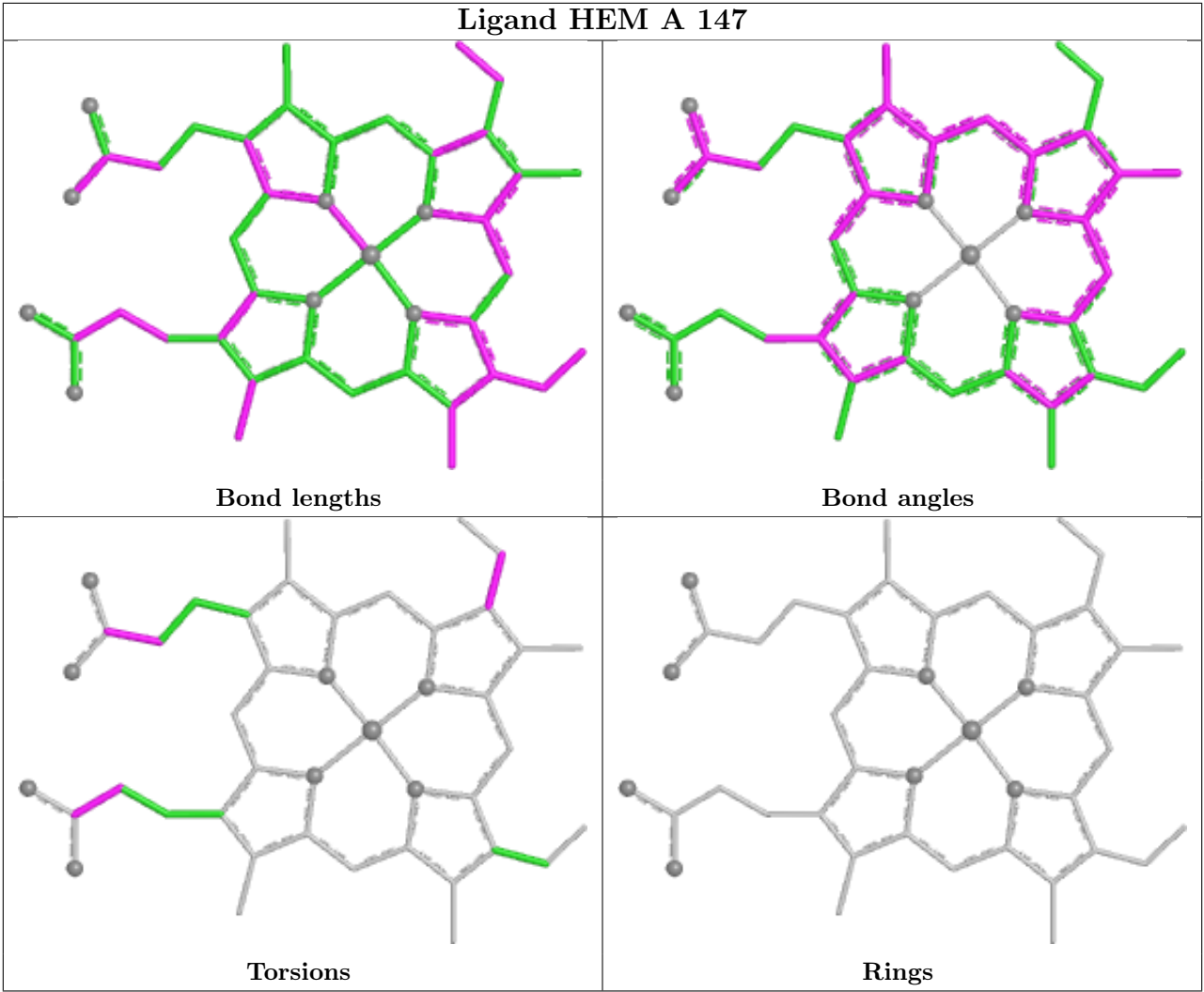
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	147	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	143:SER	C	144:ARG	N	1.19

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	17:LYS	C	18:VAL	N	1.18
1	B	20:VAL	C	21:GLU	N	1.09

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	146/146 (100%)	-0.51	0 100 100	9, 14, 20, 25	12 (8%)
1	B	146/146 (100%)	-0.36	1 (0%) 84 87	9, 16, 23, 29	16 (10%)
All	All	292/292 (100%)	-0.44	1 (0%) 90 92	9, 14, 22, 29	28 (9%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	GLU	3.1

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](#)

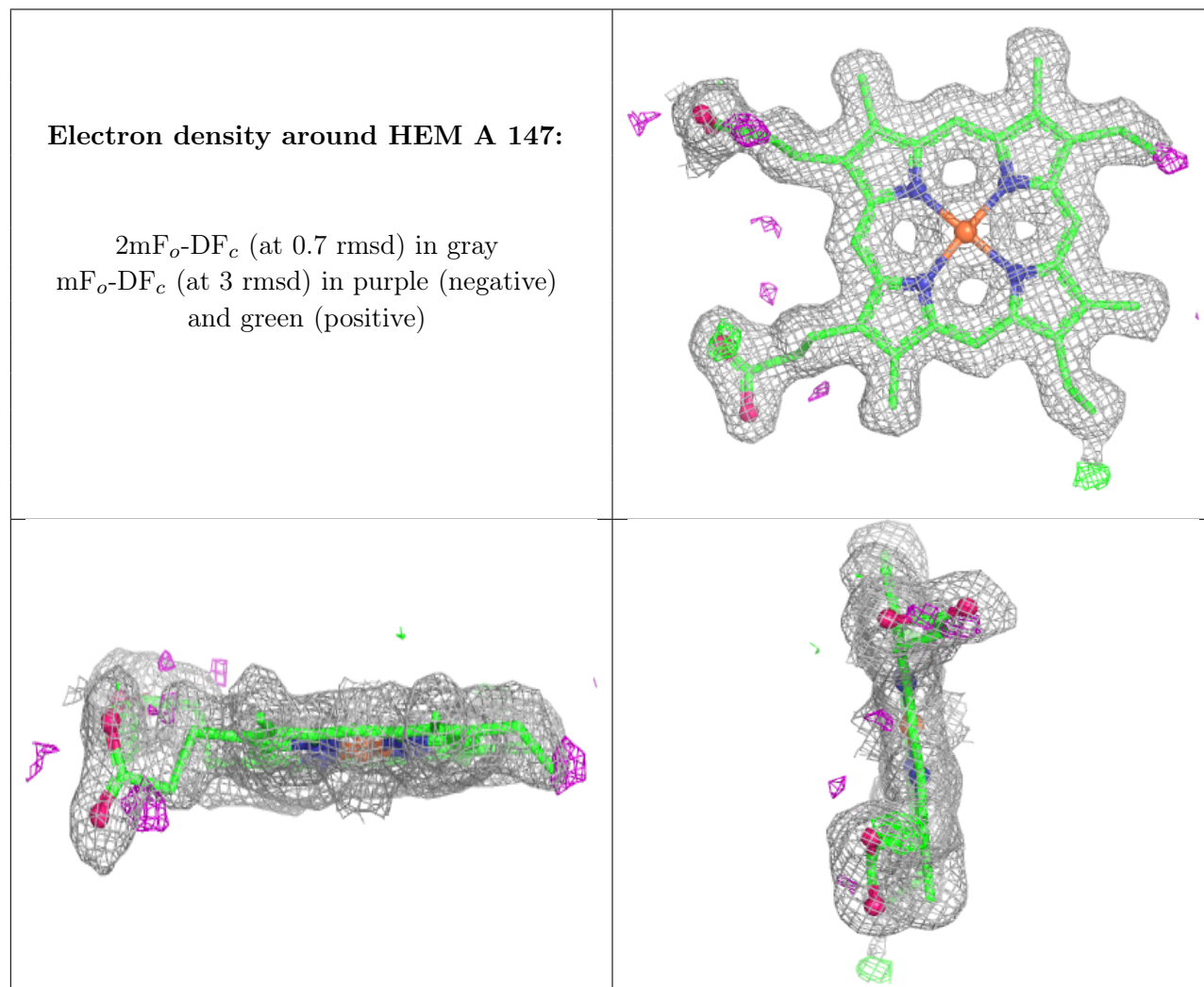
There are no oligosaccharides in this entry.

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.

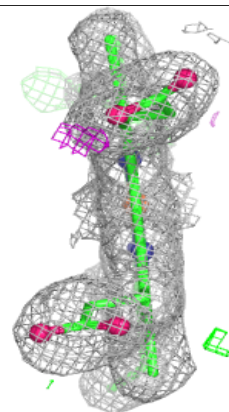
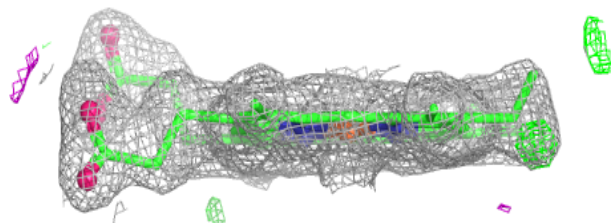
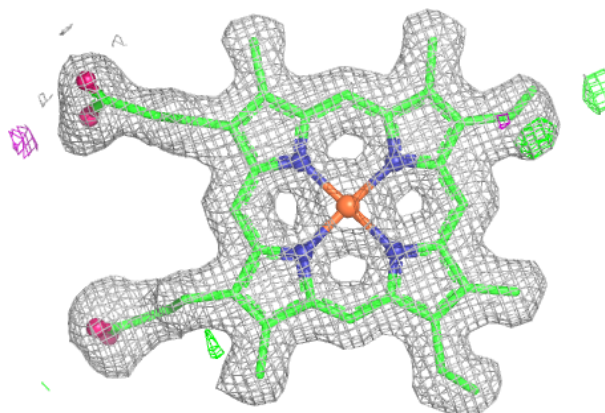
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	AZI	A	148	3/3	0.88	0.12	13,13,15,17	0
2	AZI	B	148	3/3	0.94	0.09	14,14,14,15	0
3	HEM	A	147	43/43	0.97	0.07	8,12,18,21	2
3	HEM	B	147	43/43	0.97	0.06	10,14,24,31	1

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



Electron density around HEM B 147:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.