



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:35 PM UTC

PDB ID : 1LH3 / pdb_00001lh3
Title : X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI. STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESOLUTION 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

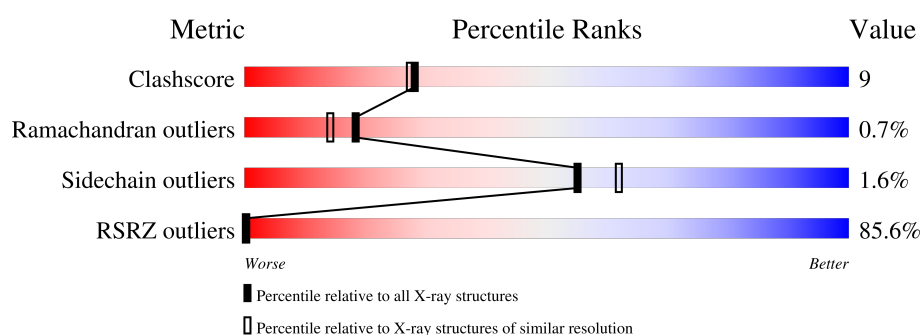
1 Overall quality at a glance

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	86% 67% 24% 5%

2 Entry composition [i](#)

There are 4 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.

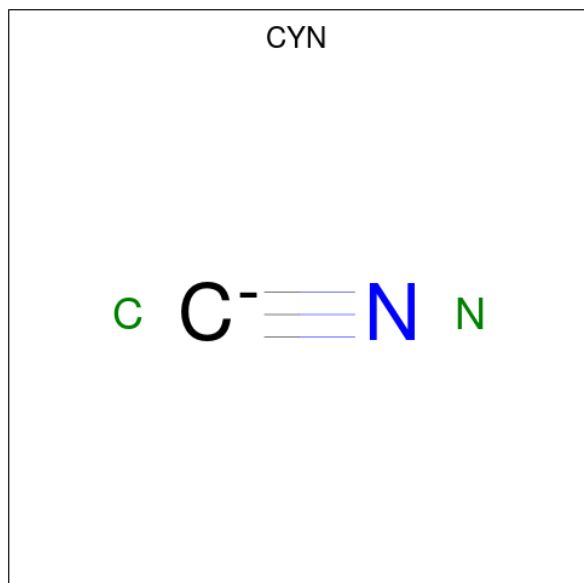
- Molecule 1 is a protein called LEGHEMOGLOBIN (CYANO MET).

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

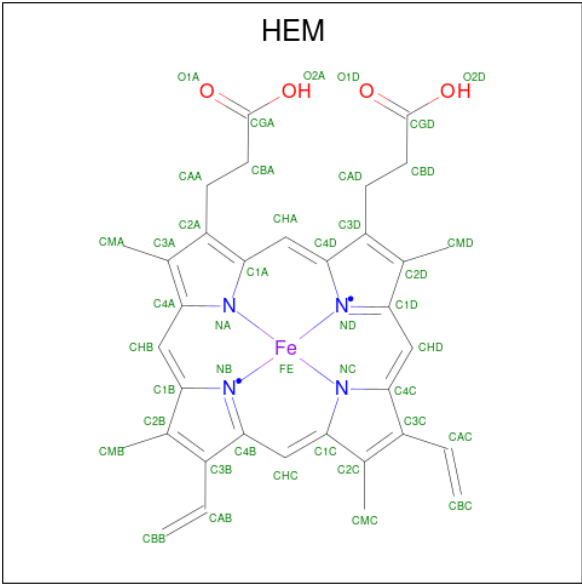
- Molecule 2 is CYANIDE ION (CCD ID: CYN) (formula: CN).



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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

C₃₄H₃₂FeN₄O₄).



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

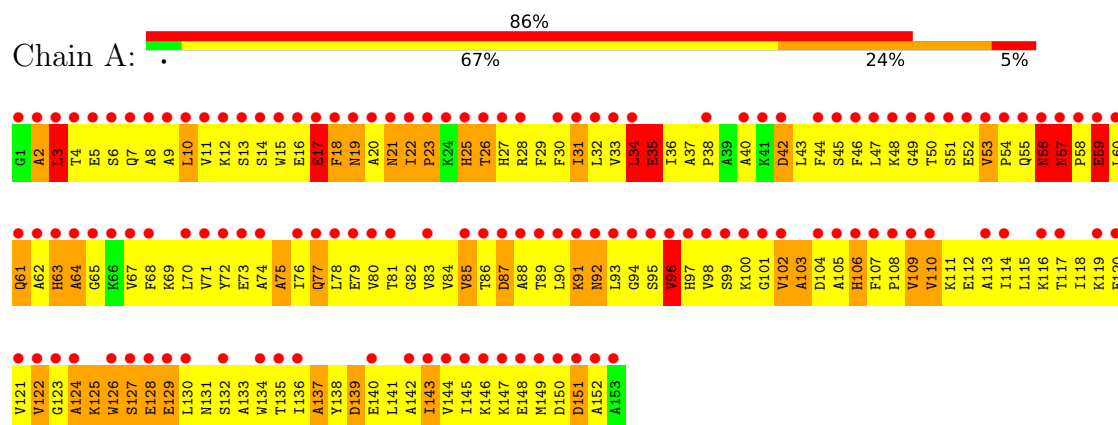
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		

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 (CYANO MET)



4 Data and refinement statistics

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	93.19Å 38.41Å 52.07Å 90.00° 90.00° 98.90°	Depositor
Resolution (Å)	(Not available) – 2.00 46.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 92.5 (46.03-2.00)	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) 0.440 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 109.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	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)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.59% 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: CYN, 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	4.44	315/1214 (25.9%)	2.92	142/1648 (8.6%)

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 (315) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	HIS	ND1-CE1	18.07	1.50	1.32
1	A	27	HIS	CE1-NE2	15.29	1.47	1.32
1	A	27	HIS	CG-ND1	13.38	1.52	1.38
1	A	106	HIS	CD2-NE2	12.88	1.52	1.37
1	A	133	ALA	CA-C	12.29	1.69	1.52
1	A	88	ALA	N-CA	12.23	1.61	1.46
1	A	94	GLY	CA-C	12.06	1.65	1.52
1	A	85	VAL	CA-C	12.03	1.66	1.53
1	A	63	HIS	CA-C	11.91	1.68	1.52
1	A	65	GLY	C-O	11.47	1.37	1.23
1	A	137	ALA	CA-C	11.29	1.68	1.52
1	A	11	VAL	N-CA	11.20	1.59	1.46
1	A	61	GLN	C-O	11.01	1.37	1.24
1	A	98	VAL	CA-C	10.96	1.66	1.52
1	A	111	LYS	N-CA	10.95	1.59	1.46
1	A	52	GLU	N-CA	10.94	1.58	1.45
1	A	106	HIS	CB-CG	10.85	1.65	1.50
1	A	102	VAL	N-CA	10.76	1.59	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	PRO	C-N	10.73	1.46	1.33
1	A	95	SER	N-CA	10.71	1.59	1.46
1	A	53	VAL	CA-CB	10.71	1.68	1.54
1	A	99	SER	N-CA	10.52	1.59	1.46
1	A	145	ILE	N-CA	10.52	1.59	1.46
1	A	110	VAL	CA-C	10.48	1.67	1.52
1	A	143	ILE	CA-CB	10.27	1.67	1.54
1	A	71	VAL	N-CA	10.25	1.58	1.46
1	A	15	TRP	C-O	10.23	1.37	1.24
1	A	97	HIS	CG-CD2	-10.14	1.24	1.35
1	A	67	VAL	CA-C	10.14	1.65	1.52
1	A	109	VAL	CA-CB	10.10	1.65	1.54
1	A	91	LYS	CA-C	10.09	1.65	1.52
1	A	124	ALA	N-CA	10.02	1.59	1.46
1	A	107	PHE	N-CA	9.99	1.56	1.46
1	A	63	HIS	CE1-NE2	9.98	1.42	1.32
1	A	121	VAL	CA-C	9.98	1.65	1.52
1	A	136	ILE	CA-CB	9.97	1.66	1.54
1	A	30	PHE	N-CA	9.95	1.58	1.46
1	A	113	ALA	CA-CB	9.94	1.69	1.53
1	A	18	PHE	N-CA	9.93	1.58	1.46
1	A	122	VAL	N-CA	9.89	1.58	1.46
1	A	124	ALA	C-O	9.87	1.36	1.24
1	A	72	TYR	C-O	9.84	1.35	1.24
1	A	45	SER	N-CA	9.78	1.58	1.46
1	A	86	THR	N-CA	9.75	1.58	1.46
1	A	84	VAL	N-CA	9.72	1.58	1.46
1	A	144	VAL	CA-C	9.71	1.65	1.52
1	A	131	ASN	CA-C	-9.58	1.40	1.52
1	A	130	LEU	N-CA	9.54	1.58	1.46
1	A	25	HIS	ND1-CE1	9.51	1.42	1.32
1	A	115	LEU	N-CA	9.39	1.57	1.46
1	A	152	ALA	C-O	9.36	1.36	1.24
1	A	138	TYR	CZ-OH	9.30	1.57	1.38
1	A	52	GLU	C-N	9.29	1.43	1.33
1	A	77	GLN	CA-CB	9.25	1.67	1.53
1	A	83	VAL	N-CA	9.20	1.57	1.46
1	A	101	GLY	CA-C	9.20	1.64	1.51
1	A	149	MET	C-O	9.20	1.35	1.24
1	A	103	ALA	CA-C	9.18	1.64	1.52
1	A	74	ALA	CA-C	9.08	1.64	1.52
1	A	55	GLN	C-O	9.07	1.35	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	ALA	C-O	9.06	1.34	1.24
1	A	136	ILE	N-CA	-9.05	1.35	1.46
1	A	75	ALA	N-CA	9.00	1.57	1.46
1	A	81	THR	N-CA	-9.00	1.34	1.46
1	A	12	LYS	CA-C	-8.95	1.41	1.52
1	A	141	LEU	CB-CG	8.94	1.71	1.53
1	A	152	ALA	N-CA	8.89	1.57	1.46
1	A	104	ASP	N-CA	8.86	1.57	1.46
1	A	10	LEU	CA-C	8.81	1.64	1.52
1	A	87	ASP	CA-C	8.81	1.66	1.53
1	A	151	ASP	CA-C	8.78	1.64	1.52
1	A	120	GLU	CA-CB	8.72	1.67	1.53
1	A	148	GLU	N-CA	8.72	1.57	1.46
1	A	80	VAL	CA-CB	8.64	1.64	1.54
1	A	51	SER	CA-C	8.61	1.64	1.52
1	A	43	LEU	CA-CB	8.61	1.67	1.53
1	A	77	GLN	N-CA	-8.60	1.35	1.46
1	A	68	PHE	C-O	8.54	1.34	1.24
1	A	78	LEU	CA-C	8.54	1.63	1.52
1	A	20	ALA	N-CA	-8.52	1.34	1.46
1	A	81	THR	CA-CB	8.48	1.66	1.53
1	A	76	ILE	C-O	8.43	1.34	1.24
1	A	75	ALA	C-O	8.33	1.33	1.24
1	A	45	SER	CA-C	-8.27	1.41	1.52
1	A	99	SER	C-O	8.25	1.34	1.24
1	A	47	LEU	CA-C	8.20	1.63	1.52
1	A	17	GLU	CA-C	8.19	1.63	1.52
1	A	9	ALA	N-CA	-8.16	1.36	1.46
1	A	97	HIS	CA-CB	8.15	1.66	1.53
1	A	68	PHE	N-CA	8.13	1.56	1.46
1	A	132[A]	SER	CA-CB	8.12	1.66	1.53
1	A	132[B]	SER	CA-CB	8.12	1.66	1.53
1	A	132[C]	SER	CA-CB	8.12	1.66	1.53
1	A	46	PHE	N-CA	-8.10	1.35	1.46
1	A	147	LYS	CA-CB	8.07	1.65	1.53
1	A	142	ALA	CA-C	-8.06	1.41	1.52
1	A	114	ILE	CA-C	8.00	1.64	1.52
1	A	148	GLU	C-O	8.00	1.34	1.24
1	A	129	GLU	CA-C	7.98	1.63	1.52
1	A	60	LEU	CA-C	7.92	1.63	1.52
1	A	60	LEU	C-N	-7.90	1.23	1.33
1	A	49	GLY	C-N	7.89	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	LYS	C-O	7.86	1.33	1.24
1	A	37	ALA	CA-C	7.78	1.62	1.52
1	A	149	MET	N-CA	7.74	1.56	1.46
1	A	80	VAL	CA-C	-7.74	1.43	1.52
1	A	123	GLY	CA-C	7.73	1.64	1.51
1	A	78	LEU	C-N	-7.63	1.23	1.33
1	A	134	TRP	N-CA	7.62	1.56	1.46
1	A	96	VAL	C-O	7.62	1.33	1.24
1	A	2	ALA	C-N	-7.60	1.23	1.33
1	A	147	LYS	N-CA	-7.59	1.37	1.46
1	A	50	THR	CA-CB	7.53	1.64	1.53
1	A	127	SER	C-O	7.49	1.33	1.23
1	A	131	ASN	C-N	7.47	1.43	1.33
1	A	54	PRO	CA-C	7.43	1.61	1.52
1	A	100	LYS	C-N	-7.34	1.23	1.33
1	A	42	ASP	C-N	7.28	1.44	1.33
1	A	92	ASN	C-N	7.27	1.43	1.33
1	A	4	THR	C-O	7.27	1.33	1.23
1	A	79	GLU	C-O	7.25	1.32	1.24
1	A	126	TRP	CA-C	7.25	1.61	1.52
1	A	16	GLU	C-O	7.23	1.32	1.24
1	A	13	SER	N-CA	-7.23	1.37	1.46
1	A	45	SER	C-O	7.20	1.33	1.24
1	A	148	GLU	CA-C	7.20	1.62	1.52
1	A	48	LYS	N-CA	7.16	1.55	1.46
1	A	119	LYS	CA-C	-7.13	1.43	1.52
1	A	125	LYS	CA-C	-7.12	1.43	1.52
1	A	11	VAL	CA-CB	-7.11	1.45	1.54
1	A	127	SER	N-CA	7.09	1.55	1.45
1	A	43	LEU	C-N	-7.04	1.23	1.33
1	A	64	ALA	N-CA	7.00	1.55	1.46
1	A	14	SER	CA-C	6.99	1.62	1.52
1	A	71	VAL	CA-C	6.99	1.61	1.52
1	A	147	LYS	CA-C	6.97	1.61	1.52
1	A	115	LEU	CA-C	-6.97	1.43	1.52
1	A	18	PHE	C-O	6.96	1.32	1.24
1	A	64	ALA	C-O	6.94	1.32	1.24
1	A	145	ILE	C-O	6.93	1.32	1.24
1	A	12	LYS	C-O	6.93	1.32	1.24
1	A	15	TRP	CD2-CE2	6.93	1.53	1.41
1	A	17	GLU	C-N	-6.91	1.24	1.33
1	A	138	TYR	CB-CG	6.91	1.66	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	ASN	C-O	6.89	1.32	1.24
1	A	150	ASP	C-O	6.89	1.32	1.24
1	A	63	HIS	CG-ND1	-6.88	1.30	1.38
1	A	76	ILE	CA-C	-6.88	1.43	1.52
1	A	136	ILE	C-N	-6.82	1.24	1.34
1	A	58	PRO	C-O	6.82	1.32	1.24
1	A	140	GLU	CA-C	6.80	1.61	1.52
1	A	44	PHE	CA-C	6.79	1.61	1.52
1	A	90	LEU	CA-CB	6.78	1.64	1.53
1	A	30	PHE	CA-CB	6.77	1.64	1.53
1	A	2	ALA	CA-CB	6.75	1.64	1.53
1	A	74	ALA	C-N	-6.75	1.25	1.33
1	A	82	GLY	CA-C	6.74	1.61	1.51
1	A	140	GLU	CA-CB	6.72	1.64	1.53
1	A	138	TYR	CA-C	-6.72	1.44	1.52
1	A	29	PHE	C-N	6.72	1.43	1.34
1	A	68	PHE	CA-CB	-6.71	1.42	1.53
1	A	40	ALA	CA-CB	6.71	1.66	1.53
1	A	6	SER	CA-C	6.69	1.61	1.52
1	A	18	PHE	CB-CG	6.69	1.66	1.50
1	A	142	ALA	C-O	6.68	1.32	1.24
1	A	64	ALA	CA-C	6.67	1.61	1.52
1	A	56	ASN	C-O	6.66	1.31	1.23
1	A	52	GLU	C-O	6.64	1.32	1.23
1	A	62	ALA	C-O	6.63	1.32	1.24
1	A	97	HIS	C-N	-6.60	1.25	1.33
1	A	142	ALA	C-N	6.58	1.42	1.33
1	A	71	VAL	C-O	6.53	1.31	1.24
1	A	117	THR	CA-C	6.53	1.61	1.52
1	A	95	SER	CB-OG	6.52	1.55	1.42
1	A	130	LEU	CB-CG	6.48	1.66	1.53
1	A	121	VAL	CA-CB	-6.45	1.47	1.54
1	A	89	THR	C-O	6.42	1.31	1.24
1	A	93	LEU	CA-CB	6.37	1.63	1.53
1	A	88	ALA	C-N	-6.36	1.25	1.33
1	A	127	SER	CA-C	-6.36	1.44	1.52
1	A	138	TYR	N-CA	6.35	1.53	1.46
1	A	59	GLU	N-CA	-6.35	1.38	1.46
1	A	61	GLN	N-CA	6.35	1.54	1.46
1	A	128	GLU	N-CA	-6.34	1.38	1.46
1	A	44	PHE	CB-CG	6.34	1.65	1.50
1	A	72	TYR	N-CA	6.33	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	8	ALA	CA-C	-6.28	1.44	1.52
1	A	19	ASN	CA-C	-6.28	1.44	1.52
1	A	150	ASP	CA-CB	6.28	1.63	1.53
1	A	139	ASP	CA-CB	6.27	1.63	1.53
1	A	22	ILE	C-N	-6.27	1.26	1.34
1	A	54	PRO	C-O	6.27	1.31	1.23
1	A	71	VAL	C-N	-6.26	1.25	1.33
1	A	79	GLU	CA-CB	-6.24	1.43	1.53
1	A	28	ARG	CA-C	-6.23	1.45	1.52
1	A	95	SER	C-N	-6.22	1.26	1.34
1	A	42	ASP	C-O	6.17	1.31	1.24
1	A	70	LEU	N-CA	-6.13	1.39	1.46
1	A	67	VAL	C-N	-6.13	1.25	1.34
1	A	137	ALA	N-CA	6.12	1.53	1.46
1	A	11	VAL	C-O	6.11	1.31	1.24
1	A	60	LEU	C-O	6.10	1.31	1.24
1	A	76	ILE	C-N	6.09	1.42	1.33
1	A	13	SER	CA-CB	6.09	1.62	1.53
1	A	118	ILE	N-CA	6.08	1.54	1.46
1	A	8	ALA	N-CA	6.05	1.53	1.46
1	A	98	VAL	CA-CB	-6.05	1.47	1.54
1	A	73	GLU	CA-CB	6.05	1.63	1.53
1	A	146	LYS	CA-C	-6.04	1.44	1.52
1	A	7	GLN	N-CA	6.03	1.53	1.46
1	A	122	VAL	C-O	6.03	1.31	1.24
1	A	29	PHE	CA-C	6.02	1.60	1.52
1	A	150	ASP	N-CA	-6.01	1.39	1.46
1	A	131	ASN	C-O	5.96	1.31	1.24
1	A	104	ASP	C-O	5.95	1.31	1.24
1	A	46	PHE	C-O	-5.94	1.16	1.24
1	A	59	GLU	C-N	-5.94	1.26	1.33
1	A	73	GLU	C-O	5.94	1.31	1.24
1	A	91	LYS	C-N	-5.94	1.25	1.34
1	A	55	GLN	CA-CB	-5.92	1.44	1.53
1	A	112	GLU	CG-CD	5.91	1.66	1.52
1	A	27	HIS	ND1-CE1	5.90	1.38	1.32
1	A	3	LEU	CA-CB	5.90	1.63	1.53
1	A	128	GLU	CA-CB	5.90	1.62	1.53
1	A	6	SER	C-N	-5.89	1.25	1.33
1	A	20	ALA	CA-CB	5.89	1.63	1.53
1	A	54	PRO	C-N	-5.89	1.25	1.33
1	A	78	LEU	N-CA	5.88	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	PRO	C-N	-5.87	1.26	1.33
1	A	79	GLU	N-CA	5.87	1.53	1.46
1	A	80	VAL	C-O	5.87	1.30	1.24
1	A	126	TRP	C-N	-5.86	1.25	1.33
1	A	14	SER	N-CA	5.85	1.53	1.46
1	A	105	ALA	CA-C	-5.85	1.44	1.52
1	A	116	LYS	N-CA	-5.85	1.39	1.46
1	A	135	THR	CA-C	-5.81	1.45	1.52
1	A	58	PRO	CA-C	-5.80	1.43	1.52
1	A	10	LEU	CB-CG	5.79	1.65	1.53
1	A	32	LEU	CA-CB	5.79	1.62	1.53
1	A	6	SER	N-CA	-5.76	1.39	1.46
1	A	75	ALA	CA-CB	-5.74	1.44	1.53
1	A	120	GLU	C-N	-5.73	1.26	1.33
1	A	15	TRP	N-CA	5.73	1.53	1.46
1	A	38	PRO	N-CA	5.69	1.55	1.47
1	A	49	GLY	CA-C	-5.65	1.44	1.52
1	A	7	GLN	CA-C	5.62	1.60	1.52
1	A	121	VAL	CB-CG2	5.62	1.71	1.52
1	A	96	VAL	C-N	5.61	1.41	1.34
1	A	92	ASN	N-CA	5.61	1.53	1.46
1	A	119	LYS	C-N	5.61	1.41	1.33
1	A	106	HIS	N-CA	-5.61	1.39	1.46
1	A	62	ALA	CA-C	-5.59	1.45	1.52
1	A	46	PHE	CB-CG	5.59	1.63	1.50
1	A	149	MET	CA-C	-5.58	1.45	1.52
1	A	50	THR	C-N	-5.57	1.26	1.33
1	A	32	LEU	CA-C	-5.57	1.45	1.52
1	A	22	ILE	CA-CB	5.56	1.56	1.54
1	A	27	HIS	C-N	5.56	1.41	1.33
1	A	132[A]	SER	N-CA	-5.55	1.39	1.46
1	A	132[B]	SER	N-CA	-5.55	1.39	1.46
1	A	132[C]	SER	N-CA	-5.55	1.39	1.46
1	A	120	GLU	CG-CD	5.54	1.66	1.52
1	A	13	SER	CA-C	5.53	1.59	1.52
1	A	15	TRP	CD1-NE1	5.52	1.49	1.37
1	A	106	HIS	C-O	-5.51	1.17	1.24
1	A	83	VAL	C-N	5.51	1.40	1.33
1	A	29	PHE	N-CA	-5.49	1.40	1.46
1	A	21	ASN	CA-CB	-5.48	1.48	1.53
1	A	5	GLU	CA-CB	5.47	1.62	1.53
1	A	34	LEU	C-N	5.46	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	ALA	N-CA	5.46	1.53	1.46
1	A	69	LYS	CA-C	-5.46	1.45	1.52
1	A	144	VAL	C-N	-5.46	1.26	1.33
1	A	36	ILE	CB-CG1	5.43	1.64	1.53
1	A	134	TRP	C-O	5.42	1.31	1.24
1	A	126	TRP	N-CA	-5.42	1.39	1.46
1	A	152	ALA	CA-CB	-5.40	1.44	1.53
1	A	5	GLU	CA-C	-5.40	1.45	1.52
1	A	14	SER	C-N	-5.40	1.26	1.33
1	A	113	ALA	C-O	-5.40	1.17	1.24
1	A	28	ARG	CA-CB	5.37	1.61	1.53
1	A	18	PHE	CA-C	5.36	1.59	1.52
1	A	27	HIS	CD2-NE2	5.36	1.43	1.37
1	A	151	ASP	C-N	-5.36	1.25	1.33
1	A	106	HIS	CA-CB	5.36	1.61	1.53
1	A	147	LYS	C-N	-5.31	1.26	1.33
1	A	9	ALA	CA-CB	5.31	1.61	1.53
1	A	141	LEU	CA-C	5.31	1.59	1.52
1	A	52	GLU	CA-CB	-5.29	1.45	1.53
1	A	15	TRP	NE1-CE2	-5.29	1.31	1.37
1	A	93	LEU	C-N	-5.27	1.26	1.33
1	A	95	SER	C-O	5.25	1.30	1.24
1	A	70	LEU	CA-C	5.24	1.59	1.52
1	A	117	THR	C-O	-5.24	1.18	1.24
1	A	63	HIS	CD2-NE2	-5.23	1.32	1.37
1	A	111	LYS	CA-C	-5.20	1.46	1.52
1	A	93	LEU	CB-CG	-5.17	1.43	1.53
1	A	18	PHE	CA-CB	-5.16	1.45	1.53
1	A	19	ASN	C-O	5.14	1.30	1.24
1	A	34	LEU	N-CA	5.12	1.53	1.46
1	A	19	ASN	N-CA	5.12	1.52	1.46
1	A	144	VAL	CB-CG2	5.11	1.69	1.52
1	A	126	TRP	CZ2-CH2	5.10	1.47	1.37
1	A	5	GLU	N-CA	-5.09	1.40	1.46
1	A	126	TRP	C-O	5.09	1.29	1.23
1	A	26	THR	C-N	-5.08	1.26	1.33
1	A	112	GLU	CA-C	-5.08	1.45	1.52
1	A	140	GLU	CB-CG	5.06	1.67	1.52
1	A	63	HIS	ND1-CE1	5.06	1.37	1.32
1	A	25	HIS	CE1-NE2	5.06	1.37	1.32
1	A	10	LEU	C-N	-5.04	1.27	1.33
1	A	141	LEU	C-O	5.04	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	65	GLY	N-CA	5.03	1.52	1.45
1	A	7	GLN	C-O	5.01	1.30	1.24
1	A	89	THR	N-CA	-5.00	1.40	1.46

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ILE	CB-CA-C	-10.16	104.05	113.70
1	A	110	VAL	O-C-N	-9.91	111.86	121.87
1	A	54	PRO	N-CA-CB	9.86	111.93	103.25
1	A	131	ASN	CA-CB-CG	-9.51	103.09	112.60
1	A	19	ASN	CA-CB-CG	-9.43	103.17	112.60
1	A	56	ASN	CA-CB-CG	-9.07	103.53	112.60
1	A	92	ASN	CA-CB-CG	-8.97	103.63	112.60
1	A	12	LYS	O-C-N	8.89	131.69	122.09
1	A	48	LYS	CB-CA-C	-8.82	97.47	110.16
1	A	131	ASN	O-C-N	8.80	132.18	122.15
1	A	49	GLY	N-CA-C	-8.62	103.04	114.25
1	A	21	ASN	CA-CB-CG	-8.55	104.05	112.60
1	A	27	HIS	N-CA-C	-8.50	101.52	112.23
1	A	45	SER	O-C-N	8.49	132.15	122.22
1	A	71	VAL	N-CA-C	8.48	119.27	110.62
1	A	61	GLN	O-C-N	8.47	131.81	122.15
1	A	133	ALA	O-C-N	-8.44	113.17	122.12
1	A	65	GLY	O-C-N	8.37	130.31	122.19
1	A	87	ASP	CA-CB-CG	-7.89	104.71	112.60
1	A	15	TRP	CG-CD2-CE3	-7.81	126.09	133.90
1	A	76	ILE	O-C-N	7.80	132.14	121.84
1	A	8	ALA	O-C-N	7.73	130.97	122.15
1	A	63	HIS	CA-CB-CG	-7.68	106.12	113.80
1	A	128	GLU	O-C-N	7.65	130.36	122.09
1	A	102	VAL	CA-C-O	-7.64	112.14	120.85
1	A	22	ILE	N-CA-CB	7.58	115.60	110.52
1	A	139	ASP	CA-CB-CG	-7.36	105.24	112.60
1	A	142	ALA	O-C-N	7.36	131.32	122.27
1	A	108	PRO	N-CA-C	-7.34	104.69	113.86
1	A	33	VAL	N-CA-C	7.26	117.35	110.30
1	A	33	VAL	CB-CA-C	-7.26	102.74	111.81
1	A	80	VAL	CA-CB-CG2	-7.25	98.07	110.40
1	A	78	LEU	N-CA-C	7.17	119.17	111.36
1	A	63	HIS	CE1-NE2-CD2	-7.16	101.84	109.00
1	A	104	ASP	CA-CB-CG	-7.14	105.46	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLY	CA-C-O	-7.11	111.87	119.55
1	A	49	GLY	O-C-N	7.11	130.04	122.65
1	A	77	GLN	O-C-N	-7.11	114.58	122.12
1	A	15	TRP	CE2-CD2-CE3	7.04	125.84	118.80
1	A	113	ALA	N-CA-C	-6.99	103.71	111.82
1	A	36	ILE	N-CA-C	-6.93	102.15	111.44
1	A	121	VAL	O-C-N	-6.83	115.11	121.94
1	A	80	VAL	O-C-N	6.80	129.21	121.94
1	A	106	HIS	ND1-CE1-NE2	-6.79	101.61	108.40
1	A	99	SER	O-C-N	6.78	129.93	122.20
1	A	67	VAL	N-CA-C	6.73	117.42	110.36
1	A	106	HIS	CA-C-N	6.69	129.41	120.58
1	A	106	HIS	C-N-CA	6.69	129.41	120.58
1	A	71	VAL	CA-C-O	6.68	127.90	120.95
1	A	31	ILE	CB-CA-C	-6.66	103.03	112.22
1	A	83	VAL	CA-C-O	-6.63	114.91	121.67
1	A	91	LYS	CA-C-O	6.61	127.43	120.42
1	A	83	VAL	N-CA-C	6.55	118.36	108.80
1	A	97	HIS	ND1-CE1-NE2	-6.53	101.87	108.40
1	A	112	GLU	CA-C-O	-6.51	112.75	120.10
1	A	89	THR	N-CA-CB	-6.45	100.64	110.12
1	A	51	SER	CA-C-O	6.40	127.53	119.78
1	A	119	LYS	O-C-N	6.37	130.10	122.27
1	A	129	GLU	O-C-N	-6.36	115.38	122.12
1	A	122	VAL	O-C-N	6.30	129.62	122.18
1	A	85	VAL	O-C-N	-6.29	115.82	122.68
1	A	138	TYR	O-C-N	6.25	128.84	122.09
1	A	54	PRO	CA-C-O	6.24	128.41	121.36
1	A	4	THR	CA-CB-OG1	-6.23	100.25	109.60
1	A	57	ASN	CB-CA-C	6.22	116.97	109.31
1	A	88	ALA	N-CA-C	6.21	118.05	111.28
1	A	15	TRP	CD2-CE3-CZ3	-6.21	110.53	118.60
1	A	106	HIS	CG-CD2-NE2	6.20	113.40	107.20
1	A	91	LYS	N-CA-C	6.20	118.11	111.36
1	A	23	PRO	N-CA-CB	6.16	110.05	103.52
1	A	149	MET	O-C-N	6.15	130.23	122.23
1	A	151	ASP	N-CA-C	6.15	118.78	111.71
1	A	42	ASP	O-C-N	6.15	130.38	122.39
1	A	93	LEU	N-CA-C	6.14	117.64	111.07
1	A	104	ASP	CB-CA-C	-6.12	99.31	110.63
1	A	134	TRP	CG-CD1-NE1	-6.10	102.27	110.20
1	A	126	TRP	CE2-CD2-CE3	6.10	124.90	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	TYR	CA-C-O	-6.07	114.45	120.70
1	A	84	VAL	CA-C-O	-6.05	113.99	120.59
1	A	115	LEU	O-C-N	6.03	129.03	122.15
1	A	69	LYS	O-C-N	5.93	128.40	122.12
1	A	102	VAL	N-CA-C	5.91	116.69	108.89
1	A	15	TRP	O-C-N	5.89	130.23	122.33
1	A	21	ASN	N-CA-C	5.89	120.02	108.18
1	A	92	ASN	O-C-N	5.89	129.51	122.27
1	A	15	TRP	CA-C-N	-5.87	111.95	120.29
1	A	15	TRP	C-N-CA	-5.87	111.95	120.29
1	A	97	HIS	CA-C-N	-5.87	113.16	120.56
1	A	97	HIS	C-N-CA	-5.87	113.16	120.56
1	A	127	SER	O-C-N	5.83	130.30	122.96
1	A	108	PRO	N-CA-CB	5.82	109.10	103.51
1	A	87	ASP	N-CA-C	5.82	118.72	109.65
1	A	64	ALA	N-CA-C	5.81	118.40	111.71
1	A	42	ASP	CA-C-O	-5.77	112.51	119.49
1	A	85	VAL	N-CA-C	5.76	116.68	107.98
1	A	27	HIS	ND1-CE1-NE2	-5.74	102.66	108.40
1	A	29	PHE	CA-C-O	-5.74	114.76	121.07
1	A	124	ALA	CB-CA-C	-5.70	97.73	110.21
1	A	76	ILE	CB-CA-C	-5.61	104.72	112.24
1	A	34	LEU	N-CA-C	-5.60	105.71	112.54
1	A	35	GLU	CB-CG-CD	-5.59	103.09	112.60
1	A	112	GLU	O-C-N	5.58	128.75	122.22
1	A	108	PRO	CA-C-O	-5.57	111.20	119.00
1	A	30	PHE	N-CA-C	5.55	118.10	111.71
1	A	28	ARG	O-C-N	5.55	127.78	122.07
1	A	61	GLN	N-CA-C	5.49	117.35	111.36
1	A	35	GLU	N-CA-C	5.49	117.34	111.36
1	A	126	TRP	CD2-CE2-CZ2	-5.49	116.92	122.40
1	A	58	PRO	O-C-N	5.46	129.97	122.38
1	A	76	ILE	CA-C-N	-5.45	112.98	120.28
1	A	76	ILE	C-N-CA	-5.45	112.98	120.28
1	A	3	LEU	N-CA-CB	5.44	119.69	110.49
1	A	145	ILE	N-CA-C	5.44	116.22	110.72
1	A	29	PHE	CD1-CG-CD2	5.44	126.76	118.60
1	A	84	VAL	CB-CA-C	-5.43	103.53	110.98
1	A	74	ALA	N-CA-C	5.42	116.87	111.07
1	A	14	SER	CA-C-O	5.40	126.18	119.97
1	A	78	LEU	CA-C-O	5.36	126.10	120.42
1	A	119	LYS	CA-C-O	-5.35	113.82	119.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	LYS	CA-C-O	-5.34	114.76	120.42
1	A	77	GLN	CB-CA-C	5.34	119.65	110.79
1	A	19	ASN	N-CA-CB	-5.29	101.53	110.41
1	A	54	PRO	CA-N-CD	-5.27	104.62	112.00
1	A	114	ILE	CB-CA-C	-5.26	105.19	112.24
1	A	27	HIS	ND1-CG-CD2	5.26	111.36	106.10
1	A	53	VAL	CA-CB-CG1	5.25	119.32	110.40
1	A	68	PHE	O-C-N	5.23	128.70	122.27
1	A	117	THR	N-CA-CB	5.23	117.76	109.82
1	A	89	THR	N-CA-C	5.19	116.94	111.28
1	A	105	ALA	N-CA-C	-5.18	106.93	113.20
1	A	107	PHE	N-CA-CB	5.17	119.34	110.34
1	A	151	ASP	O-C-N	-5.14	116.21	122.22
1	A	125	LYS	N-CA-C	-5.12	106.98	113.18
1	A	117	THR	O-C-N	-5.11	116.61	122.08
1	A	131	ASN	CA-C-O	-5.10	115.01	120.42
1	A	144	VAL	O-C-N	-5.09	116.58	121.83
1	A	91	LYS	O-C-N	-5.08	116.36	122.15
1	A	44	PHE	CA-CB-CG	5.06	118.86	113.80
1	A	53	VAL	CA-CB-CG2	-5.04	101.83	110.40
1	A	115	LEU	CA-C-O	-5.02	115.10	120.42
1	A	98	VAL	N-CA-C	5.00	115.22	110.42
1	A	147	LYS	O-C-N	-5.00	116.92	122.07

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	VAL	Mainchain
1	A	151	ASP	Sidechain
1	A	17	GLU	Sidechain
1	A	19	ASN	Sidechain
1	A	35	GLU	Sidechain
1	A	42	ASP	Sidechain
1	A	56	ASN	Sidechain
1	A	57	ASN	Sidechain
1	A	59	GLU	Sidechain
1	A	61	GLN	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	2	0	0	0	0
3	A	43	0	30	2	0
4	A	66	0	0	0	4
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:77:GLN:NE2	1:A:85:VAL:H	1.98	0.61
1:A:31:ILE:O	1:A:35:GLU:HG3	2.01	0.60
1:A:21:ASN:C	1:A:21:ASN:HD22	2.12	0.57
1:A:92:ASN:O	1:A:96:VAL:HG12	2.05	0.57
1:A:87:ASP:O	1:A:91:LYS:HG3	2.04	0.57
1:A:106:HIS:O	1:A:109:VAL:HB	2.06	0.56
1:A:21:ASN:C	1:A:21:ASN:ND2	2.67	0.53
1:A:26:THR:HB	1:A:64:ALA:HB3	1.90	0.52
1:A:18:PHE:CE1	1:A:25:HIS:HB3	2.45	0.51
1:A:34:LEU:HD22	1:A:53:VAL:HG21	1.92	0.50
1:A:17:GLU:OE2	1:A:122:VAL:HG12	2.15	0.47
1:A:75:ALA:HB2	1:A:137:ALA:HB2	1.97	0.47
1:A:2:ALA:O	1:A:3:LEU:HB2	2.14	0.47
1:A:22:ILE:HB	1:A:23:PRO:HD3	1.97	0.46
1:A:63:HIS:HE1	3:A:155:HEM:CHA	2.29	0.45
1:A:139:ASP:O	1:A:143:ILE:HG13	2.16	0.45
1:A:103:ALA:O	1:A:106:HIS:HB2	2.20	0.42
1:A:57:ASN:OD1	1:A:59:GLU:HB2	2.20	0.42
1:A:102:VAL:HG13	3:A:155:HEM:HAC	2.01	0.41
1:A:34:LEU:HD22	1:A:53:VAL:CG2	2.51	0.41
1:A:75:ALA:HB2	1:A:137:ALA:CB	2.51	0.41

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]	1.03	1.17
1:A:124:ALA:CB	1:A:129:GLU:N[2_555]	1.20	1.00
1:A:124:ALA:O	1:A:127:SER:CB[2_555]	1.23	0.97
4:A:218:HOH:O	4:A:218:HOH:O[2_555]	1.34	0.86
1:A:124:ALA:O	1:A:127:SER:CA[2_555]	1.36	0.84
1:A:124:ALA:C	1:A:127:SER:CB[2_555]	1.42	0.78
1:A:124:ALA:O	1:A:127:SER:C[2_555]	1.46	0.74
1:A:124:ALA:O	1:A:128:GLU:N[2_555]	1.64	0.56
1:A:125:LYS:CA	1:A:127:SER:OG[2_555]	1.68	0.52
1:A:125:LYS:CA	1:A:127:SER:CB[2_555]	1.79	0.41
1:A:125:LYS:N	1:A:127:SER:CB[2_555]	1.82	0.38
1:A:10:LEU:CD1	1:A:125:LYS:CD[2_555]	1.83	0.37
1:A:56:ASN:OD1	4:A:171:HOH:O[1_565]	1.86	0.34
1:A:124:ALA:O	1:A:127:SER:OG[2_555]	1.86	0.34
1:A:124:ALA:CB	1:A:128:GLU:C[2_555]	2.02	0.18
1:A:125:LYS:C	1:A:127:SER:CB[2_555]	2.02	0.18
4:A:192:HOH:O	4:A:218:HOH:O[2_555]	2.07	0.13
1:A:56:ASN:N	4:A:171:HOH:O[1_565]	2.13	0.07
1:A:124:ALA:C	1:A:127:SER:OG[2_555]	2.17	0.03
1:A:125:LYS:N	1:A:127:SER:OG[2_555]	2.17	0.03

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%)	148 (97%)	4 (3%)	1 (1%)	18 14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU

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	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 (4) such sidechains are listed below:

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

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	HEM	A	155	1,2	50,50,50	4.51	33 (66%)	67,82,82	2.31	24 (35%)
2	CYN	A	154	3	1,1,1	0.20	0	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	155	1,2	-	6/14/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	FE-NB	12.27	2.32	1.94
3	A	155	HEM	FE-ND	9.56	2.24	1.94
3	A	155	HEM	C1D-C2D	8.00	1.60	1.44
3	A	155	HEM	C4D-C3D	7.31	1.57	1.45
3	A	155	HEM	C3B-C4B	7.06	1.58	1.44
3	A	155	HEM	C1A-NA	6.72	1.52	1.39
3	A	155	HEM	CAB-C3B	6.55	1.64	1.47
3	A	155	HEM	CBD-CGD	6.54	1.65	1.50
3	A	155	HEM	CHB-C4A	6.38	1.53	1.39
3	A	155	HEM	CHD-C4C	6.12	1.50	1.38
3	A	155	HEM	FE-NA	5.89	2.14	1.95
3	A	155	HEM	CHC-C1C	5.86	1.49	1.38
3	A	155	HEM	C1B-C2B	5.83	1.56	1.44
3	A	155	HEM	CMD-C2D	5.39	1.61	1.50
3	A	155	HEM	C1C-NC	5.00	1.49	1.39
3	A	155	HEM	CHA-C1A	4.75	1.50	1.39
3	A	155	HEM	CMC-C2C	4.74	1.60	1.50
3	A	155	HEM	CAD-C3D	4.56	1.63	1.51
3	A	155	HEM	C3C-C2C	4.46	1.46	1.37
3	A	155	HEM	CMB-C2B	4.36	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	155	HEM	C2A-C3A	4.26	1.50	1.38
3	A	155	HEM	O1A-CGA	3.85	1.34	1.22
3	A	155	HEM	CAC-C3C	3.28	1.56	1.47
3	A	155	HEM	CBA-CGA	3.24	1.58	1.50
3	A	155	HEM	CMA-C3A	3.23	1.57	1.50
3	A	155	HEM	CAA-C2A	3.05	1.59	1.51
3	A	155	HEM	C4A-NA	2.58	1.44	1.39
3	A	155	HEM	O1D-CGD	2.58	1.30	1.22
3	A	155	HEM	C4D-ND	2.50	1.44	1.40
3	A	155	HEM	CBD-CAD	-2.43	1.43	1.51
3	A	155	HEM	CBB-CAB	2.34	1.41	1.30
3	A	155	HEM	C4B-NB	2.16	1.43	1.38
3	A	155	HEM	C4A-C3A	2.04	1.47	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	155	HEM	C2A-C1A-NA	-5.08	104.51	110.15
3	A	155	HEM	C4C-C3C-C2C	4.78	110.95	106.81
3	A	155	HEM	C4A-NA-C1A	4.73	113.54	105.82
3	A	155	HEM	C3A-C4A-NA	-4.73	102.56	110.14
3	A	155	HEM	CMA-C3A-C4A	-4.53	118.52	125.42
3	A	155	HEM	CAD-CBD-CGD	-4.13	102.72	113.67
3	A	155	HEM	C4C-NC-C1C	4.09	112.48	105.82
3	A	155	HEM	C4A-C3A-C2A	3.96	111.35	106.82
3	A	155	HEM	CHB-C4A-NA	3.90	130.94	123.86
3	A	155	HEM	CHC-C1C-NC	3.89	128.69	124.45
3	A	155	HEM	CHA-C1A-NA	3.85	130.84	123.86
3	A	155	HEM	CHD-C4C-NC	3.84	128.64	124.45
3	A	155	HEM	CAD-C3D-C4D	3.34	130.51	124.70
3	A	155	HEM	C3B-C4B-NB	3.33	111.86	109.47
3	A	155	HEM	O2D-CGD-O1D	-3.08	115.41	123.33
3	A	155	HEM	C4B-C3B-C2B	-2.97	104.55	107.28
3	A	155	HEM	CHD-C1D-ND	-2.85	121.35	124.42
3	A	155	HEM	CHB-C1B-NB	-2.73	120.99	124.37
3	A	155	HEM	CMD-C2D-C1D	2.67	129.20	125.03
3	A	155	HEM	CHA-C4D-ND	-2.35	121.46	124.37
3	A	155	HEM	C2C-C1C-NC	-2.20	105.57	109.64
3	A	155	HEM	CAD-C3D-C2D	-2.17	123.80	127.87
3	A	155	HEM	CMA-C3A-C2A	2.12	130.11	125.62
3	A	155	HEM	O2D-CGD-CBD	2.06	120.50	114.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

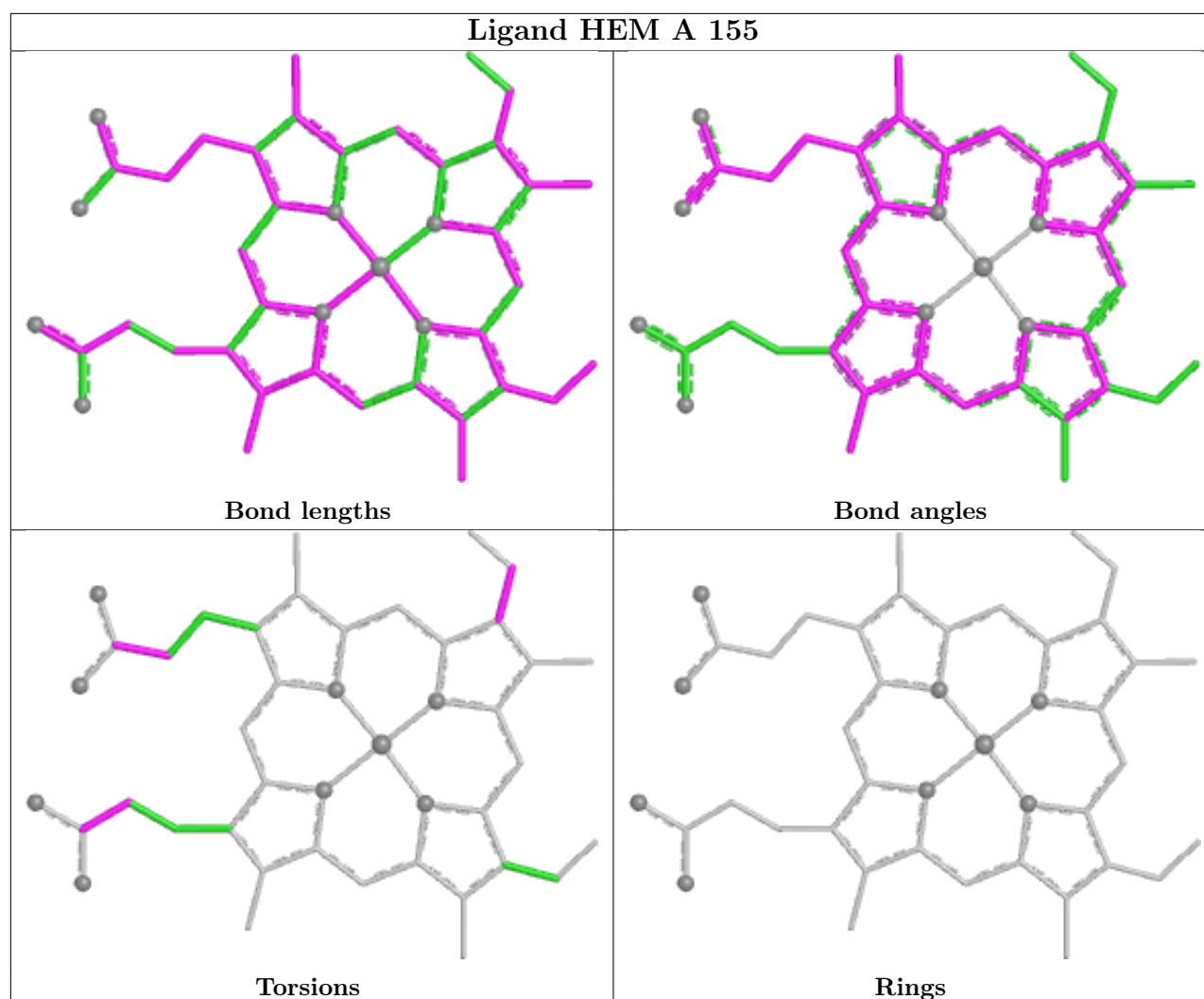
Mol	Chain	Res	Type	Atoms
3	A	155	HEM	C2C-C3C-CAC-CBC
3	A	155	HEM	C4C-C3C-CAC-CBC
3	A	155	HEM	CAA-CBA-CGA-O1A
3	A	155	HEM	CAA-CBA-CGA-O2A
3	A	155	HEM	CAD-CBD-CGD-O1D
3	A	155	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	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%)	3.74	131 (85%) 0 0	7, 17, 39, 54	19 (12%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	13.8
1	A	152	ALA	8.9
1	A	9	ALA	8.1
1	A	48	LYS	8.1
1	A	2	ALA	7.8
1	A	153	ALA	7.5
1	A	88	ALA	7.0
1	A	126	TRP	7.0
1	A	49	GLY	7.0
1	A	45	SER	6.9
1	A	83	VAL	6.8
1	A	123	GLY	6.7
1	A	50	THR	6.3
1	A	150	ASP	6.2
1	A	136	ILE	6.2
1	A	62	ALA	6.1
1	A	4	THR	5.8
1	A	128	GLU	5.7
1	A	58	PRO	5.7
1	A	142	ALA	5.7
1	A	92	ASN	5.7
1	A	3	LEU	5.6
1	A	86	THR	5.6
1	A	56	ASN	5.6
1	A	149	MET	5.6
1	A	151	ASP	5.6
1	A	90	LEU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	147	LYS	5.5
1	A	23	PRO	5.4
1	A	143	ILE	5.3
1	A	5	GLU	5.2
1	A	79	GLU	5.1
1	A	20	ALA	5.0
1	A	53	VAL	5.0
1	A	54	PRO	4.6
1	A	130	LEU	4.6
1	A	129	GLU	4.6
1	A	26	THR	4.5
1	A	6	SER	4.5
1	A	107	PHE	4.5
1	A	81	THR	4.4
1	A	96	VAL	4.4
1	A	15	TRP	4.3
1	A	10	LEU	4.2
1	A	78	LEU	4.2
1	A	51	SER	4.2
1	A	91	LYS	4.1
1	A	85	VAL	4.1
1	A	144	VAL	4.1
1	A	64	ALA	4.0
1	A	59	GLU	4.0
1	A	27	HIS	4.0
1	A	74	ALA	3.9
1	A	18	PHE	3.9
1	A	148	GLU	3.9
1	A	21	ASN	3.9
1	A	14	SER	3.9
1	A	146	LYS	3.8
1	A	55	GLN	3.8
1	A	57	ASN	3.8
1	A	67	VAL	3.8
1	A	94	GLY	3.8
1	A	44	PHE	3.8
1	A	95	SER	3.7
1	A	22	ILE	3.7
1	A	47	LEU	3.7
1	A	132[A]	SER	3.7
1	A	114	ILE	3.6
1	A	12	LYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	3.6
1	A	97	HIS	3.6
1	A	61	GLN	3.6
1	A	25	HIS	3.6
1	A	71	VAL	3.5
1	A	11	VAL	3.5
1	A	98	VAL	3.5
1	A	89	THR	3.5
1	A	42	ASP	3.4
1	A	119	LYS	3.4
1	A	117	THR	3.3
1	A	99	SER	3.3
1	A	127	SER	3.3
1	A	31	ILE	3.3
1	A	120	GLU	3.2
1	A	33	VAL	3.2
1	A	52	GLU	3.1
1	A	46	PHE	3.1
1	A	124	ALA	3.1
1	A	87	ASP	3.1
1	A	102	VAL	3.1
1	A	122	VAL	3.0
1	A	60	LEU	3.0
1	A	19	ASN	3.0
1	A	105	ALA	2.9
1	A	77	GLN	2.9
1	A	93	LEU	2.9
1	A	65	GLY	2.9
1	A	104	ASP	2.9
1	A	121	VAL	2.8
1	A	70	LEU	2.8
1	A	80	VAL	2.8
1	A	16	GLU	2.8
1	A	100	LYS	2.8
1	A	145	ILE	2.8
1	A	24	LYS	2.7
1	A	72	TYR	2.7
1	A	8	ALA	2.6
1	A	140	GLU	2.6
1	A	34	LEU	2.6
1	A	110	VAL	2.6
1	A	73	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	68	PHE	2.6
1	A	66	LYS	2.5
1	A	41	LYS	2.5
1	A	17	GLU	2.5
1	A	101	GLY	2.5
1	A	113	ALA	2.4
1	A	40	ALA	2.4
1	A	76	ILE	2.4
1	A	116	LYS	2.3
1	A	135	THR	2.3
1	A	30	PHE	2.3
1	A	13	SER	2.3
1	A	32	LEU	2.3
1	A	109	VAL	2.3
1	A	28	ARG	2.3
1	A	38	PRO	2.2
1	A	134	TRP	2.2
1	A	63	HIS	2.1
1	A	7	GLN	2.1
1	A	106	HIS	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](#)

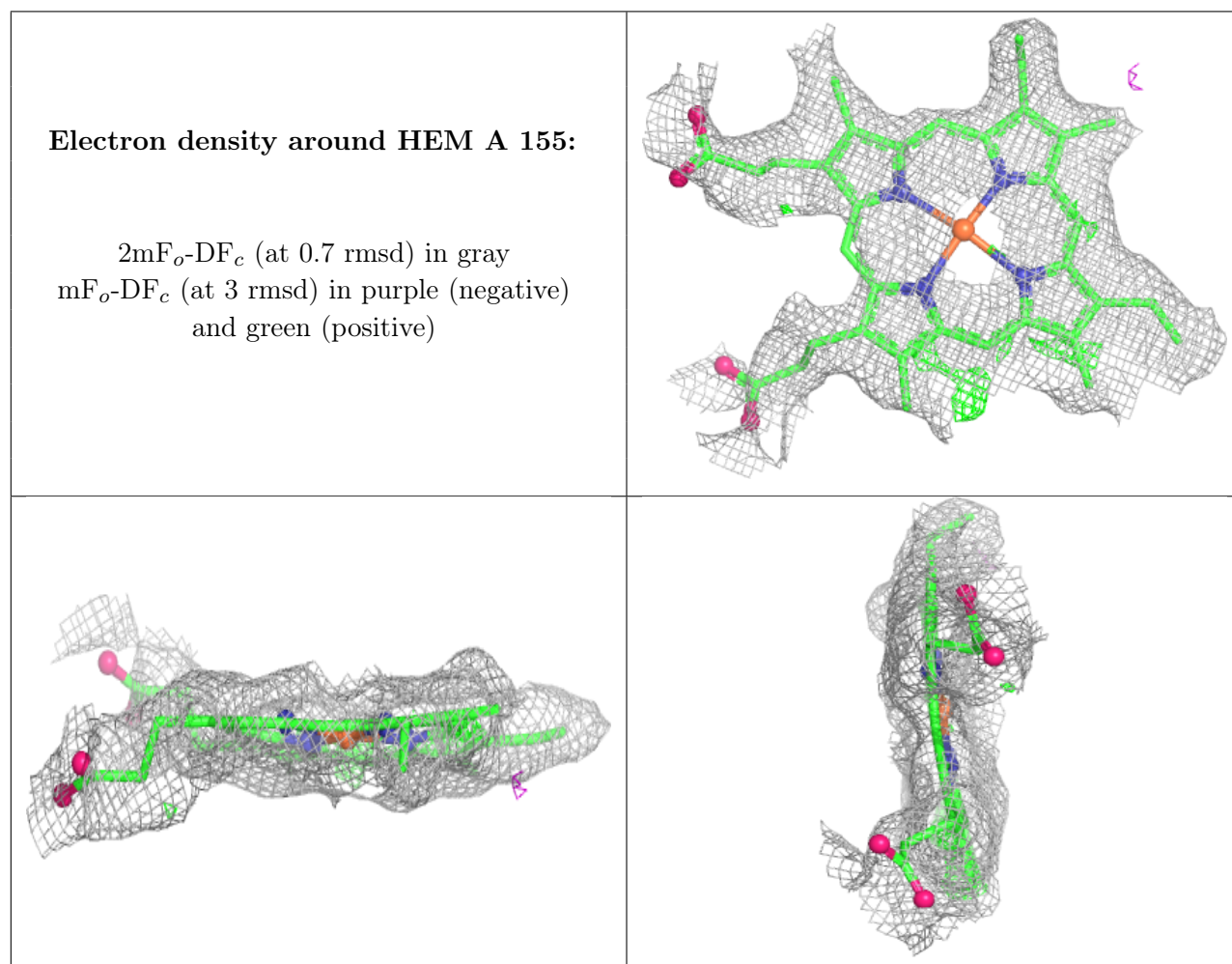
There are no oligosaccharides in this entry.

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	HEM	A	155	43/43	0.85	0.18	5,14,50,61	0
2	CYN	A	154	2/2	0.88	0.24	3,3,3,15	0

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 [i](#)

There are no such residues in this entry.