



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:42 PM UTC

PDB ID : 1AZU / pdb_00001azu
Title : STRUCTURAL FEATURES OF AZURIN AT 2.7 ANGSTROMS RESOLUTION
Authors : Adman, E.T.; Sieker, L.C.; Jensen, L.H.
Deposited on : 1980-08-04
Resolution : 2.70 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
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

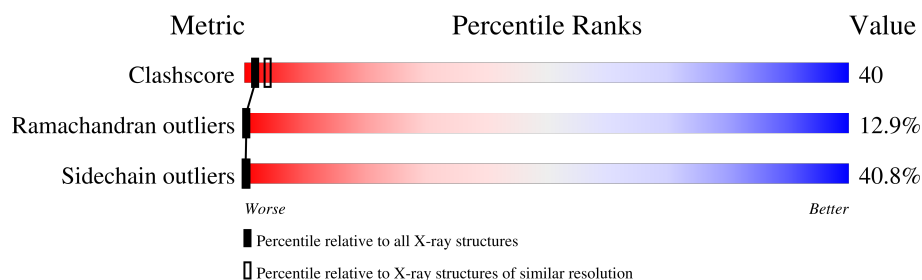
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	128	40% 36% 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 931 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 AZURIN.

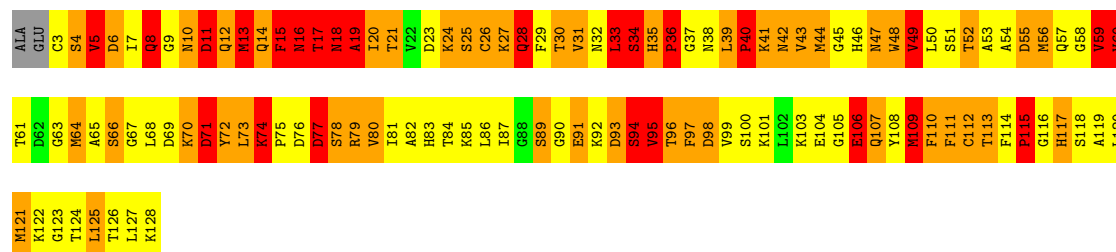
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	126	Total	C	N	O	S	0	0	1
			930	584	152	185	9			

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		

Note EDS was not executed.

Chain A: 40% 36% 20%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Deposition
Cell constants a, b, c, α , β , γ	58.85Å 78.98Å 108.47Å 90.00° 90.00° 90.00°	Deposition
Resolution (Å)	(Not available) – 2.70	Deposition
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Deposition
R_{merge}	(Not available)	Deposition
R_{sym}	(Not available)	Deposition
Refinement program	HENDRICKSON-KONNERT LEAST-SQUARES REFINEMENT	Deposition
R, R_{free}	0.350 , (Not available)	Deposition
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	931	wwPDB
Average B, all atoms (Å ²)	0.0	wwPDB

5 Model quality

5.1 Standard geometry

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

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	2.38	30/947 (3.2%)	4.23	259/1282 (20.2%)

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	1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	SER	CB-OG	26.50	1.95	1.42
1	A	44	MET	SD-CE	12.82	2.11	1.79
1	A	37	GLY	N-CA	12.30	1.55	1.44
1	A	25	SER	CB-OG	11.83	1.65	1.42
1	A	109	MET	CG-SD	11.72	2.10	1.80
1	A	4	SER	CB-OG	11.24	1.64	1.42
1	A	24	LYS	CB-CG	8.91	1.79	1.52
1	A	48	TRP	NE1-CE2	-8.52	1.28	1.37
1	A	79	ARG	CZ-NH1	7.64	1.43	1.32
1	A	45	GLY	N-CA	6.82	1.52	1.44
1	A	66	SER	C-O	6.50	1.31	1.24
1	A	61	THR	CB-OG1	6.37	1.53	1.43
1	A	66	SER	N-CA	6.37	1.54	1.46
1	A	58	GLY	N-CA	-6.32	1.36	1.45
1	A	59	VAL	N-CA	6.31	1.53	1.46
1	A	18	ASN	N-CA	6.28	1.54	1.46
1	A	47	ASN	N-CA	-6.16	1.38	1.45
1	A	126	THR	N-CA	6.13	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	SER	N-CA	6.08	1.53	1.45
1	A	64	MET	N-CA	6.08	1.54	1.46
1	A	49	VAL	N-CA	6.04	1.53	1.46
1	A	10	ASN	CG-ND2	5.52	1.44	1.33
1	A	41	LYS	N-CA	5.43	1.52	1.46
1	A	81	ILE	N-CA	5.42	1.51	1.46
1	A	70	LYS	N-CA	5.40	1.53	1.46
1	A	36	PRO	C-O	5.36	1.30	1.24
1	A	122	LYS	N-CA	5.09	1.52	1.45
1	A	89	SER	C-O	5.09	1.30	1.24
1	A	28	GLN	CD-OE1	5.08	1.33	1.23
1	A	68	LEU	CA-CB	5.08	1.62	1.53

All (259) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	VAL	CA-C-O	-22.93	95.60	121.05
1	A	35	HIS	CA-C-N	20.52	145.48	119.84
1	A	35	HIS	C-N-CA	20.52	145.48	119.84
1	A	18	ASN	CA-CB-CG	20.27	132.87	112.60
1	A	117	HIS	CA-CB-CG	20.17	133.97	113.80
1	A	63	GLY	O-C-N	-15.15	105.56	122.68
1	A	76	ASP	CA-CB-CG	13.54	126.14	112.60
1	A	59	VAL	CB-CA-C	13.25	129.37	112.02
1	A	81	ILE	N-CA-C	-12.84	101.51	113.71
1	A	83	HIS	CA-CB-CG	12.74	126.54	113.80
1	A	3	CYS	CA-C-N	-12.57	103.08	122.81
1	A	3	CYS	C-N-CA	-12.57	103.08	122.81
1	A	114	PHE	CA-C-N	12.45	135.41	119.84
1	A	114	PHE	C-N-CA	12.45	135.41	119.84
1	A	26	CYS	O-C-N	-12.43	106.06	122.59
1	A	97	PHE	CA-CB-CG	12.35	126.14	113.80
1	A	69	ASP	CA-CB-CG	12.18	124.78	112.60
1	A	78	SER	CA-C-O	12.14	138.78	122.51
1	A	107	GLN	O-C-N	12.08	137.45	123.31
1	A	66	SER	O-C-N	-11.98	108.33	122.11
1	A	18	ASN	CB-CA-C	11.56	126.31	111.40
1	A	80	VAL	CA-C-O	11.40	133.44	120.67
1	A	53	ALA	CA-C-O	11.08	136.35	120.51
1	A	72	TYR	O-C-N	-11.06	107.88	122.59
1	A	63	GLY	CA-C-O	10.77	132.21	119.50
1	A	33	LEU	CA-C-N	-10.66	108.09	122.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LEU	C-N-CA	-10.66	108.09	122.16
1	A	110	PHE	CE1-CZ-CE2	10.61	139.10	120.00
1	A	58	GLY	O-C-N	10.59	136.47	122.70
1	A	3	CYS	O-C-N	-10.42	106.33	123.00
1	A	100	SER	CA-C-N	10.18	137.02	120.63
1	A	100	SER	C-N-CA	10.18	137.02	120.63
1	A	66	SER	CA-C-O	10.16	132.29	120.92
1	A	18	ASN	OD1-CG-ND2	-10.14	112.46	122.60
1	A	59	VAL	N-CA-C	-10.01	101.12	110.53
1	A	55	ASP	CA-C-O	-9.84	108.29	119.81
1	A	30	THR	CA-CB-OG1	-9.65	95.12	109.60
1	A	121	MET	O-C-N	-9.59	112.47	122.64
1	A	81	ILE	CB-CA-C	9.31	119.38	110.63
1	A	39	LEU	CA-C-N	9.29	131.46	119.84
1	A	39	LEU	C-N-CA	9.29	131.46	119.84
1	A	36	PRO	N-CA-CB	-9.22	93.57	103.25
1	A	78	SER	O-C-N	-9.19	110.79	122.83
1	A	95	VAL	CA-CB-CG1	9.18	126.00	110.40
1	A	117	HIS	N-CA-C	-9.03	102.82	112.93
1	A	53	ALA	O-C-N	-8.98	110.64	122.59
1	A	17	THR	CA-CB-OG1	-8.98	96.13	109.60
1	A	35	HIS	C-N-CD	-8.98	88.18	125.00
1	A	100	SER	N-CA-C	-8.96	100.47	111.40
1	A	17	THR	N-CA-C	-8.92	91.81	110.80
1	A	44	MET	CA-C-N	-8.89	111.75	122.15
1	A	44	MET	C-N-CA	-8.89	111.75	122.15
1	A	36	PRO	CA-C-N	-8.88	112.03	122.77
1	A	36	PRO	C-N-CA	-8.88	112.03	122.77
1	A	29	PHE	O-C-N	8.86	133.55	123.27
1	A	94	SER	O-C-N	8.81	133.29	123.33
1	A	10	ASN	CA-C-N	8.75	136.25	122.60
1	A	10	ASN	C-N-CA	8.75	136.25	122.60
1	A	15	PHE	CA-CB-CG	8.73	122.53	113.80
1	A	121	MET	CB-CG-SD	8.72	138.86	112.70
1	A	18	ASN	N-CA-C	-8.69	99.64	111.55
1	A	115	PRO	N-CA-CB	-8.69	94.13	103.25
1	A	123	GLY	CA-C-N	-8.60	109.20	122.62
1	A	123	GLY	C-N-CA	-8.60	109.20	122.62
1	A	111	PHE	CA-CB-CG	8.55	122.35	113.80
1	A	10	ASN	OD1-CG-ND2	-8.44	114.16	122.60
1	A	5	VAL	CB-CA-C	8.34	123.22	110.55
1	A	28	GLN	CG-CD-NE2	8.33	128.90	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	THR	CA-C-N	-8.28	107.89	122.62
1	A	17	THR	C-N-CA	-8.28	107.89	122.62
1	A	91	GLU	O-C-N	8.27	132.45	122.20
1	A	104	GLU	CB-CG-CD	8.26	126.64	112.60
1	A	121	MET	CA-C-O	8.24	131.80	121.58
1	A	32	ASN	CA-C-N	-8.22	110.40	122.65
1	A	32	ASN	C-N-CA	-8.22	110.40	122.65
1	A	29	PHE	CA-C-N	-8.21	108.25	122.37
1	A	29	PHE	C-N-CA	-8.21	108.25	122.37
1	A	30	THR	CA-C-N	8.18	134.34	123.06
1	A	30	THR	C-N-CA	8.18	134.34	123.06
1	A	64	MET	N-CA-C	-8.17	103.10	113.23
1	A	33	LEU	CA-C-O	-8.16	111.75	120.80
1	A	95	VAL	CA-CB-CG2	-8.13	96.58	110.40
1	A	16	ASN	CA-CB-CG	8.05	120.65	112.60
1	A	96	THR	OG1-CB-CG2	-8.04	93.22	109.30
1	A	32	ASN	CA-CB-CG	7.97	120.57	112.60
1	A	70	LYS	CA-C-N	7.97	136.76	121.54
1	A	70	LYS	C-N-CA	7.97	136.76	121.54
1	A	95	VAL	CA-C-O	-7.93	111.95	120.36
1	A	63	GLY	CA-C-N	-7.89	107.78	121.66
1	A	63	GLY	C-N-CA	-7.89	107.78	121.66
1	A	104	GLU	CA-C-N	-7.89	111.75	122.63
1	A	104	GLU	C-N-CA	-7.89	111.75	122.63
1	A	91	GLU	OE1-CD-OE2	7.81	141.64	122.90
1	A	30	THR	CA-CB-CG2	7.74	123.65	110.50
1	A	44	MET	O-C-N	-7.69	112.36	122.59
1	A	85	LYS	CA-C-N	-7.69	110.53	121.99
1	A	85	LYS	C-N-CA	-7.69	110.53	121.99
1	A	20	ILE	CA-CB-CG1	7.67	123.44	110.40
1	A	10	ASN	CA-CB-CG	-7.67	104.93	112.60
1	A	14	GLN	CA-C-N	7.59	135.25	122.20
1	A	14	GLN	C-N-CA	7.59	135.25	122.20
1	A	104	GLU	CA-CB-CG	7.57	129.24	114.10
1	A	126	THR	CB-CA-C	7.57	123.34	109.71
1	A	6	ASP	CA-C-O	7.49	130.58	120.47
1	A	5	VAL	CA-C-O	7.46	129.50	121.67
1	A	41	LYS	CA-CB-CG	7.37	128.85	114.10
1	A	35	HIS	CB-CG-ND1	-7.37	111.65	122.70
1	A	41	LYS	O-C-N	-7.31	112.27	122.06
1	A	74	LYS	CG-CD-CE	7.28	128.03	111.30
1	A	96	THR	CA-CB-OG1	7.25	120.47	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ASP	CB-CG-OD1	7.22	135.00	118.40
1	A	35	HIS	CA-CB-CG	-7.21	106.59	113.80
1	A	47	ASN	OD1-CG-ND2	-7.20	115.40	122.60
1	A	42	ASN	O-C-N	7.15	129.56	122.19
1	A	119	ALA	CA-C-N	7.14	134.22	121.66
1	A	119	ALA	C-N-CA	7.14	134.22	121.66
1	A	77	ASP	CA-CB-CG	-7.13	105.47	112.60
1	A	18	ASN	CB-CG-ND2	7.11	127.07	116.40
1	A	94	SER	CA-CB-OG	-7.08	96.94	111.10
1	A	73	LEU	CB-CA-C	7.07	120.95	110.62
1	A	112	CYS	CB-CA-C	7.03	121.83	110.16
1	A	41	LYS	CA-C-O	7.02	129.20	119.80
1	A	55	ASP	N-CA-C	-7.01	103.74	112.72
1	A	17	THR	CA-CB-CG2	6.99	122.37	110.50
1	A	26	CYS	CA-CB-SG	6.98	130.45	114.40
1	A	10	ASN	CB-CG-ND2	6.93	126.80	116.40
1	A	72	TYR	CA-C-N	6.92	132.47	122.44
1	A	72	TYR	C-N-CA	6.92	132.47	122.44
1	A	17	THR	N-CA-CB	6.91	122.16	110.49
1	A	59	VAL	N-CA-CB	-6.91	101.73	110.57
1	A	4	SER	N-CA-C	-6.89	98.70	109.72
1	A	70	LYS	CA-CB-CG	6.82	127.73	114.10
1	A	47	ASN	CB-CA-C	-6.81	97.99	109.50
1	A	8	GLN	CA-C-N	-6.78	108.12	121.41
1	A	8	GLN	C-N-CA	-6.78	108.12	121.41
1	A	5	VAL	N-CA-CB	-6.76	101.08	112.44
1	A	13	MET	CA-CB-CG	-6.76	100.58	114.10
1	A	37	GLY	CA-C-O	-6.75	111.43	122.56
1	A	76	ASP	CB-CA-C	-6.75	96.99	110.42
1	A	120	LEU	N-CA-C	-6.74	104.88	113.23
1	A	73	LEU	N-CA-CB	-6.73	100.41	110.90
1	A	46	HIS	CA-C-N	6.72	134.06	122.64
1	A	46	HIS	C-N-CA	6.72	134.06	122.64
1	A	74	LYS	CA-CB-CG	6.70	127.49	114.10
1	A	99	VAL	CA-C-N	6.69	131.88	120.71
1	A	99	VAL	C-N-CA	6.69	131.88	120.71
1	A	117	HIS	CB-CG-CD2	6.69	139.89	131.20
1	A	3	CYS	CB-CA-C	-6.67	97.43	110.10
1	A	109	MET	CG-SD-CE	-6.63	86.32	100.90
1	A	85	LYS	N-CA-C	-6.51	99.68	108.86
1	A	94	SER	CA-C-O	-6.51	113.70	120.99
1	A	19	ALA	CA-C-N	6.48	133.07	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ALA	C-N-CA	6.48	133.07	122.64
1	A	20	ILE	CA-C-O	6.46	129.69	121.48
1	A	49	VAL	O-C-N	6.44	130.03	122.69
1	A	106	GLU	CA-C-O	6.43	128.98	121.46
1	A	83	HIS	O-C-N	6.39	131.07	123.27
1	A	11	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	84	THR	N-CA-C	-6.31	97.37	110.80
1	A	52	THR	CA-CB-OG1	-6.29	100.17	109.60
1	A	91	GLU	CG-CD-OE1	-6.28	103.95	118.40
1	A	3	CYS	CA-C-O	6.23	131.40	120.80
1	A	40	PRO	N-CA-CB	-6.23	96.71	103.25
1	A	30	THR	CB-CA-C	6.20	121.97	109.38
1	A	32	ASN	OD1-CG-ND2	-6.20	116.40	122.60
1	A	16	ASN	N-CA-C	-6.17	97.65	110.80
1	A	59	VAL	CA-CB-CG1	6.17	120.89	110.40
1	A	35	HIS	ND1-CE1-NE2	6.15	114.55	108.40
1	A	79	ARG	CA-C-N	6.13	131.46	122.94
1	A	79	ARG	C-N-CA	6.13	131.46	122.94
1	A	76	ASP	OD1-CG-OD2	-6.10	108.25	122.90
1	A	45	GLY	CA-C-N	-6.07	113.39	122.74
1	A	45	GLY	C-N-CA	-6.07	113.39	122.74
1	A	42	ASN	OD1-CG-ND2	6.07	128.67	122.60
1	A	103	LYS	CA-CB-CG	6.03	126.16	114.10
1	A	115	PRO	N-CA-C	6.00	124.83	112.47
1	A	110	PHE	CZ-CE2-CD2	-5.99	109.22	120.00
1	A	93	ASP	CA-CB-CG	-5.99	106.61	112.60
1	A	71	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	44	MET	CG-SD-CE	-5.93	87.84	100.90
1	A	61	THR	CA-CB-OG1	-5.93	100.71	109.60
1	A	71	ASP	CA-C-N	5.93	132.86	121.54
1	A	71	ASP	C-N-CA	5.93	132.86	121.54
1	A	104	GLU	N-CA-CB	5.92	120.75	110.81
1	A	5	VAL	N-CA-C	-5.91	99.20	108.95
1	A	60	VAL	CA-CB-CG2	5.88	120.39	110.40
1	A	57	GLN	CA-CB-CG	-5.88	102.35	114.10
1	A	35	HIS	CB-CG-CD2	5.84	138.79	131.20
1	A	49	VAL	CA-CB-CG1	5.82	120.30	110.40
1	A	98	ASP	N-CA-C	-5.81	103.26	110.41
1	A	49	VAL	CB-CA-C	5.80	120.07	111.31
1	A	30	THR	O-C-N	5.79	130.33	123.33
1	A	60	VAL	CA-C-O	-5.78	113.56	120.78
1	A	16	ASN	N-CA-CB	5.77	120.25	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	ARG	NH1-CZ-NH2	-5.77	111.80	119.30
1	A	79	ARG	CB-CG-CD	-5.75	98.07	111.30
1	A	115	PRO	CA-N-CD	-5.74	103.96	112.00
1	A	55	ASP	OD1-CG-OD2	-5.74	109.13	122.90
1	A	9	GLY	O-C-N	5.73	130.15	122.70
1	A	16	ASN	CA-C-O	5.71	128.67	120.51
1	A	48	TRP	CD2-CE2-CZ2	5.70	128.10	122.40
1	A	104	GLU	O-C-N	5.66	130.26	123.36
1	A	110	PHE	CD1-CE1-CZ	-5.63	109.87	120.00
1	A	89	SER	CA-CB-OG	-5.62	99.87	111.10
1	A	71	ASP	O-C-N	-5.60	115.14	122.59
1	A	89	SER	CB-CA-C	-5.60	99.28	110.42
1	A	74	LYS	N-CA-CB	-5.59	100.42	110.37
1	A	11	ASP	N-CA-C	-5.55	105.72	112.88
1	A	94	SER	N-CA-C	5.54	117.69	108.99
1	A	37	GLY	O-C-N	5.53	129.65	123.12
1	A	79	ARG	CA-CB-CG	5.52	125.14	114.10
1	A	80	VAL	N-CA-C	-5.51	100.25	108.46
1	A	110	PHE	CA-CB-CG	5.51	119.31	113.80
1	A	121	MET	CB-CA-C	-5.48	103.24	111.73
1	A	112	CYS	N-CA-C	-5.46	99.50	108.41
1	A	125	LEU	CA-C-O	-5.44	114.46	120.33
1	A	27	LYS	CA-C-O	-5.43	112.74	120.51
1	A	57	GLN	O-C-N	-5.43	115.27	122.33
1	A	75	PRO	CA-C-N	5.42	131.90	121.54
1	A	75	PRO	C-N-CA	5.42	131.90	121.54
1	A	48	TRP	O-C-N	-5.42	115.77	122.82
1	A	93	ASP	OD1-CG-OD2	-5.40	109.95	122.90
1	A	43	VAL	CA-CB-CG1	5.39	119.57	110.40
1	A	12	GLN	CA-C-N	5.39	131.83	121.54
1	A	12	GLN	C-N-CA	5.39	131.83	121.54
1	A	117	HIS	CA-C-O	-5.39	112.96	119.59
1	A	104	GLU	N-CA-C	-5.38	99.17	108.69
1	A	84	THR	CA-C-N	-5.37	113.88	122.53
1	A	84	THR	C-N-CA	-5.37	113.88	122.53
1	A	106	GLU	N-CA-C	-5.37	101.37	109.85
1	A	4	SER	O-C-N	5.36	130.16	123.19
1	A	103	LYS	CA-C-O	-5.36	113.71	120.84
1	A	36	PRO	N-CA-C	5.34	123.47	112.47
1	A	31	VAL	CA-CB-CG1	5.34	119.47	110.40
1	A	71	ASP	CB-CG-OD1	5.30	130.59	118.40
1	A	24	LYS	N-CA-C	-5.28	105.98	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	GLY	CA-C-O	-5.25	111.44	120.57
1	A	65	ALA	CA-C-O	-5.25	115.30	121.07
1	A	42	ASN	CA-C-N	5.25	131.41	121.97
1	A	42	ASN	C-N-CA	5.25	131.41	121.97
1	A	27	LYS	N-CA-C	5.23	121.93	110.80
1	A	84	THR	O-C-N	-5.21	115.66	122.59
1	A	96	THR	CB-CA-C	5.19	120.12	111.51
1	A	125	LEU	CA-CB-CG	5.17	134.40	116.30
1	A	65	ALA	O-C-N	5.17	127.61	122.08
1	A	44	MET	CB-CA-C	5.16	120.69	110.42
1	A	105	GLY	O-C-N	5.14	127.86	122.51
1	A	116	GLY	CA-C-N	-5.14	114.12	122.65
1	A	116	GLY	C-N-CA	-5.14	114.12	122.65
1	A	109	MET	CA-C-N	-5.11	113.88	123.03
1	A	109	MET	C-N-CA	-5.11	113.88	123.03
1	A	12	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	48	TRP	CA-C-N	-5.05	114.51	122.64
1	A	48	TRP	C-N-CA	-5.05	114.51	122.64
1	A	67	GLY	CA-C-N	-5.01	111.96	121.54
1	A	67	GLY	C-N-CA	-5.01	111.96	121.54
1	A	112	CYS	O-C-N	5.01	129.09	123.27
1	A	106	GLU	CB-CA-C	5.01	119.38	109.66
1	A	90	GLY	N-CA-C	-5.00	108.74	114.69

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	59	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	930	0	872	72	0
2	A	1	0	0	1	0
All	All	931	0	872	72	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 40.

All (72) 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:24:LYS:CG	1:A:24:LYS:CB	1.79	1.58
1:A:4:SER:OG	1:A:4:SER:CB	1.64	1.45
1:A:25:SER:OG	1:A:25:SER:CB	1.65	1.42
1:A:109:MET:CG	1:A:109:MET:SD	2.10	1.39
1:A:44:MET:CE	1:A:44:MET:SD	2.11	1.38
1:A:34:SER:CB	1:A:34:SER:OG	1.95	1.14
1:A:34:SER:OG	1:A:92:LYS:CG	1.96	1.14
1:A:16:ASN:O	1:A:17:THR:OG1	1.84	0.95
1:A:43:VAL:O	1:A:44:MET:HG2	1.66	0.94
1:A:97:PHE:HD1	1:A:98:ASP:O	1.48	0.93
1:A:24:LYS:HE3	1:A:128:LYS:CA	2.04	0.88
1:A:112:CYS:HG	2:A:129:CU:CU	0.87	0.87
1:A:97:PHE:CD1	1:A:98:ASP:O	2.34	0.78
1:A:38:ASN:O	1:A:39:LEU:HD22	1.85	0.77
1:A:49:VAL:HG21	1:A:73:LEU:HD11	1.67	0.76
1:A:35:HIS:N	1:A:36:PRO:HD3	1.95	0.75
1:A:98:ASP:HB3	1:A:101:LYS:HG3	1.69	0.74
1:A:47:ASN:HB2	1:A:112:CYS:HA	1.73	0.70
1:A:109:MET:CG	1:A:109:MET:CE	2.71	0.68
1:A:7:ILE:HG13	1:A:33:LEU:HD23	1.77	0.66
1:A:44:MET:CE	1:A:44:MET:CG	2.73	0.66
1:A:25:SER:CB	1:A:25:SER:HG	2.09	0.63
1:A:49:VAL:HG11	1:A:73:LEU:HD13	1.81	0.63
1:A:59:VAL:HG21	1:A:80:VAL:HG22	1.84	0.60
1:A:11:ASP:OD2	1:A:39:LEU:HD23	2.02	0.60
1:A:24:LYS:CB	1:A:24:LYS:CD	2.75	0.59
1:A:24:LYS:CG	1:A:24:LYS:CA	2.76	0.59
1:A:4:SER:CB	1:A:4:SER:HG	2.08	0.57
1:A:4:SER:OG	1:A:4:SER:CA	2.49	0.57
1:A:34:SER:HG	1:A:92:LYS:CG	2.16	0.56
1:A:8:GLN:HG3	1:A:16:ASN:HD21	1.71	0.54
1:A:20:ILE:HG12	1:A:110:PHE:CE1	2.43	0.54
1:A:49:VAL:HG11	1:A:73:LEU:CD1	2.38	0.54
1:A:40:PRO:HB2	1:A:42:ASN:ND2	2.22	0.54
1:A:24:LYS:HG2	1:A:127:LEU:HD21	1.91	0.53
1:A:12:GLN:O	1:A:13:MET:HB2	2.08	0.52
1:A:59:VAL:HG21	1:A:80:VAL:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HD11	1:A:31:VAL:HG13	1.91	0.52
1:A:70:LYS:O	1:A:71:ASP:HB2	2.09	0.51
1:A:16:ASN:C	1:A:17:THR:OG1	2.47	0.50
1:A:38:ASN:C	1:A:39:LEU:HD22	2.36	0.50
1:A:47:ASN:HD22	1:A:113:THR:H	1.60	0.49
1:A:5:VAL:HG21	1:A:20:ILE:HD12	1.94	0.49
1:A:19:ALA:HA	1:A:124:THR:H	1.79	0.48
1:A:31:VAL:HG11	1:A:48:TRP:CE3	2.48	0.47
1:A:87:ILE:HB	1:A:91:GLU:HB2	1.94	0.47
1:A:25:SER:OG	1:A:25:SER:CA	2.55	0.47
1:A:64:MET:SD	1:A:115:PRO:HA	2.55	0.47
1:A:15:PHE:CE1	1:A:121:MET:HB3	2.50	0.47
1:A:20:ILE:HG22	1:A:21:THR:N	2.30	0.46
1:A:93:ASP:CG	1:A:94:SER:H	2.22	0.46
1:A:15:PHE:CD1	1:A:121:MET:HB3	2.51	0.46
1:A:18:ASN:H	1:A:18:ASN:HD22	1.62	0.46
1:A:11:ASP:O	1:A:44:MET:HE3	2.15	0.46
1:A:106:GLU:HB3	1:A:108:TYR:CE2	2.51	0.45
1:A:20:ILE:CG2	1:A:21:THR:N	2.80	0.44
1:A:109:MET:CE	1:A:109:MET:HG2	2.46	0.44
1:A:28:GLN:HB3	1:A:97:PHE:O	2.18	0.44
1:A:39:LEU:HD12	1:A:43:VAL:HG11	1.99	0.44
1:A:82:ALA:HB1	1:A:95:VAL:HG11	1.99	0.44
1:A:49:VAL:HG23	1:A:80:VAL:HG13	2.01	0.43
1:A:93:ASP:CG	1:A:94:SER:N	2.77	0.43
1:A:56:MET:HE3	1:A:111:PHE:CD1	2.53	0.43
1:A:52:THR:HG22	1:A:108:TYR:CD1	2.54	0.42
1:A:13:MET:HG3	1:A:44:MET:SD	2.59	0.42
1:A:24:LYS:CE	1:A:128:LYS:CA	2.87	0.41
1:A:8:GLN:HG3	1:A:16:ASN:ND2	2.35	0.41
1:A:39:LEU:HA	1:A:40:PRO:HD2	1.41	0.41
1:A:20:ILE:HG12	1:A:110:PHE:HE1	1.85	0.41
1:A:52:THR:HG22	1:A:108:TYR:CE1	2.56	0.41
1:A:49:VAL:HA	1:A:82:ALA:O	2.21	0.40
1:A:51:SER:OG	1:A:55:ASP:HB2	2.22	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	124/128 (97%)	86 (69%)	22 (18%)	16 (13%)	0 0

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	19	ALA
1	A	27	LYS
1	A	40	PRO
1	A	56	MET
1	A	71	ASP
1	A	115	PRO
1	A	60	VAL
1	A	72	TYR
1	A	77	ASP
1	A	13	MET
1	A	54	ALA
1	A	74	LYS
1	A	79	ARG
1	A	89	SER
1	A	36	PRO

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	98/110 (89%)	58 (59%)	40 (41%)	0 0

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	6	ASP
1	A	8	GLN
1	A	10	ASN
1	A	11	ASP
1	A	13	MET
1	A	14	GLN
1	A	15	PHE
1	A	16	ASN
1	A	17	THR
1	A	18	ASN
1	A	21	THR
1	A	23	ASP
1	A	26	CYS
1	A	28	GLN
1	A	30	THR
1	A	33	LEU
1	A	34	SER
1	A	36	PRO
1	A	41	LYS
1	A	49	VAL
1	A	50	LEU
1	A	59	VAL
1	A	60	VAL
1	A	66	SER
1	A	74	LYS
1	A	77	ASP
1	A	78	SER
1	A	86	LEU
1	A	94	SER
1	A	95	VAL
1	A	96	THR
1	A	106	GLU
1	A	107	GLN
1	A	109	MET

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Mol	Chain	Res	Type
1	A	113	THR
1	A	115	PRO
1	A	117	HIS
1	A	118	SER
1	A	125	LEU

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	8	GLN
1	A	16	ASN
1	A	18	ASN
1	A	28	GLN
1	A	32	ASN
1	A	42	ASN
1	A	47	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.