Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 06:28 PM GMT

PDB ID	:	1AZU
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

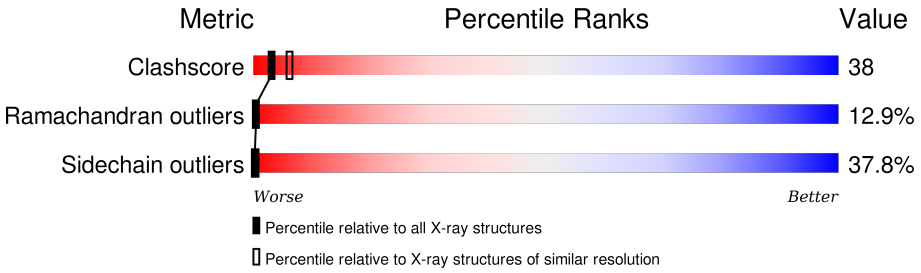
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	128	15% 31% 34% 18%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	126	930	584	152	185	9	0	0	1

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

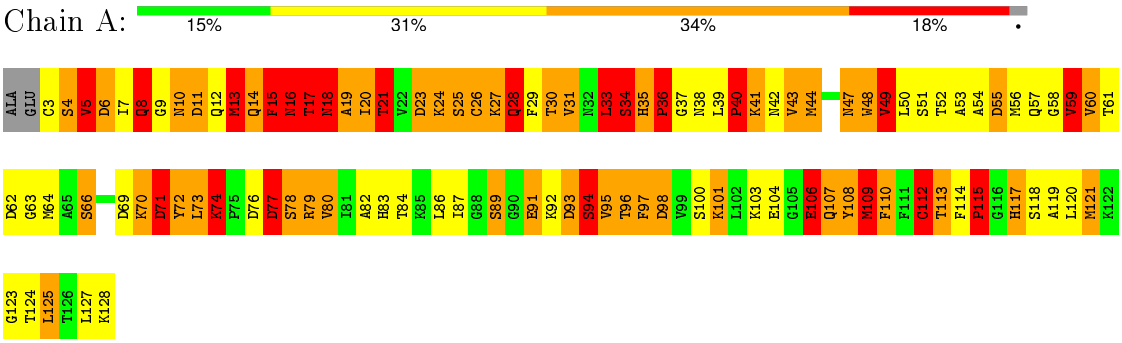
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: AZURIN

Chain A:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Sour
Space group	P 21 21 21	Deposi
Cell constants a, b, c, α, β, γ	58.85Å 78.98Å 108.47Å 90.00° 90.00° 90.00°	Deposi
Resolution (Å)	(Not available) – 2.70	Deposi
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70)	Deposi
R_{merge}	(Not available)	Deposi
R_{sym}	(Not available)	Deposi
Refinement program	HENDRICKSON-KONNERT LEAST-SQUARES REFINEMENT	Deposi
R, R_{free}	0.350 , (Not available)	Deposi
Estimated twinning fraction	No twinning to report.	Xtria
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	2.34	18/947 (1.9%)	3.38	157/1282 (12.2%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	34	SER	CB-OG	40.69	1.95	1.42
1	A	25	SER	CB-OG	18.12	1.65	1.42
1	A	4	SER	CB-OG	17.21	1.64	1.42
1	A	109	MET	CG-SD	11.12	2.10	1.81
1	A	24	LYS	CB-CG	9.86	1.79	1.52
1	A	79	ARG	CZ-NH1	8.00	1.43	1.33
1	A	48	TRP	NE1-CE2	-7.28	1.28	1.37
1	A	58	GLY	N-CA	-6.56	1.36	1.46
1	A	37	GLY	N-CA	6.19	1.55	1.46
1	A	104	GLU	CD-OE2	-6.15	1.18	1.25
1	A	44	MET	SD-CE	6.03	2.11	1.77
1	A	101	LYS	CD-CE	5.83	1.65	1.51
1	A	89	SER	CB-OG	5.75	1.49	1.42
1	A	108	TYR	CD1-CE1	5.45	1.47	1.39
1	A	61	THR	CB-OG1	5.35	1.53	1.43
1	A	41	LYS	CE-NZ	5.30	1.62	1.49
1	A	106	GLU	CG-CD	5.24	1.59	1.51
1	A	24	LYS	CD-CE	5.02	1.63	1.51

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ASP	CB-CG-OD1	18.56	135.00	118.30
1	A	91	GLU	OE1-CD-OE2	15.28	141.64	123.30
1	A	35	HIS	C-N-CD	-14.74	88.18	120.60
1	A	71	ASP	CB-CG-OD1	13.65	130.59	118.30
1	A	76	ASP	CB-CG-OD1	12.35	129.41	118.30
1	A	110	PHE	CB-CG-CD1	-12.11	112.32	120.80
1	A	117	HIS	CA-CB-CG	11.98	133.97	113.60
1	A	55	ASP	CB-CG-OD1	11.95	129.06	118.30
1	A	72	TYR	CB-CG-CD1	11.76	128.06	121.00
1	A	59	VAL	CA-C-O	-11.67	95.60	120.10
1	A	59	VAL	CA-C-N	11.39	142.25	117.20
1	A	72	TYR	CB-CG-CD2	-11.14	114.32	121.00
1	A	63	GLY	O-C-N	-10.71	105.56	122.70
1	A	110	PHE	CE1-CZ-CE2	10.61	139.10	120.00
1	A	26	CYS	O-C-N	-10.40	106.06	122.70
1	A	3	CYS	O-C-N	-10.23	106.33	122.70
1	A	95	VAL	CA-CB-CG1	10.07	126.00	110.90
1	A	95	VAL	CA-CB-CG2	-9.54	96.58	110.90
1	A	59	VAL	CB-CA-C	9.46	129.37	111.40
1	A	69	ASP	CB-CG-OD2	9.39	126.75	118.30
1	A	72	TYR	O-C-N	-9.26	107.88	122.70
1	A	107	GLN	O-C-N	9.22	137.45	122.70
1	A	26	CYS	CA-CB-SG	9.14	130.45	114.00
1	A	110	PHE	CZ-CE2-CD2	-9.07	109.22	120.10
1	A	78	SER	CA-C-O	8.90	138.78	120.10
1	A	18	ASN	CA-CB-CG	8.85	132.87	113.40
1	A	121	MET	CB-CG-SD	8.82	138.86	112.40
1	A	66	SER	O-C-N	-8.75	108.33	123.20
1	A	104	GLU	OE1-CD-OE2	8.73	133.78	123.30
1	A	109	MET	CG-SD-CE	-8.68	86.32	100.20
1	A	58	GLY	O-C-N	8.61	136.47	122.70
1	A	114	PHE	CB-CG-CD2	8.60	126.82	120.80
1	A	110	PHE	CD1-CE1-CZ	-8.53	109.87	120.10
1	A	6	ASP	CB-CG-OD1	8.45	125.91	118.30
1	A	125	LEU	CA-CB-CG	8.30	134.40	115.30
1	A	36	PRO	N-CA-CB	-8.11	93.57	103.30
1	A	30	THR	CA-CB-CG2	8.04	123.65	112.40
1	A	18	ASN	CB-CA-C	7.95	126.31	110.40
1	A	76	ASP	OD1-CG-OD2	-7.92	108.25	123.30
1	A	23	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	79	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	A	53	ALA	CA-C-O	7.74	136.35	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	ASP	CA-C-N	-7.73	100.20	117.20
1	A	44	MET	CG-SD-CE	-7.72	87.84	100.20
1	A	115	PRO	N-CA-CB	-7.64	94.13	103.30
1	A	83	HIS	CA-CB-CG	7.61	126.54	113.60
1	A	53	ALA	O-C-N	-7.54	110.64	122.70
1	A	13	MET	CA-CB-CG	-7.48	100.58	113.30
1	A	55	ASP	OD1-CG-OD2	-7.46	109.13	123.30
1	A	3	CYS	C-N-CA	-7.45	103.08	121.70
1	A	78	SER	O-C-N	-7.44	110.79	122.70
1	A	77	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	98	ASP	CB-CG-OD2	7.39	124.95	118.30
1	A	96	THR	OG1-CB-CG2	-7.30	93.22	110.00
1	A	20	ILE	CA-C-N	-7.26	101.23	117.20
1	A	104	GLU	CA-CB-CG	7.20	129.24	113.40
1	A	91	GLU	CG-CD-OE1	-7.17	103.95	118.30
1	A	17	THR	CA-CB-CG2	7.12	122.37	112.40
1	A	17	THR	N-CA-C	-7.11	91.81	111.00
1	A	15	PHE	CB-CG-CD1	-7.03	115.88	120.80
1	A	93	ASP	OD1-CG-OD2	-7.03	109.95	123.30
1	A	41	LYS	CA-CB-CG	7.02	128.85	113.40
1	A	62	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	79	ARG	NH1-CZ-NH2	-6.91	111.80	119.40
1	A	73	LEU	CB-CG-CD2	-6.79	99.47	111.00
1	A	29	PHE	O-C-N	6.78	133.55	122.70
1	A	8	GLN	C-N-CA	-6.75	108.12	122.30
1	A	76	ASP	CB-CA-C	-6.70	96.99	110.40
1	A	59	VAL	CA-CB-CG1	6.66	120.89	110.90
1	A	5	VAL	CA-C-N	-6.63	102.61	117.20
1	A	94	SER	O-C-N	6.62	133.29	122.70
1	A	30	THR	CA-CB-OG1	-6.61	95.12	109.00
1	A	44	MET	CA-C-N	6.58	129.36	116.20
1	A	20	ILE	CA-CB-CG1	6.54	123.44	111.00
1	A	41	LYS	O-C-N	-6.52	112.27	122.70
1	A	70	LYS	CA-CB-CG	6.51	127.73	113.40
1	A	15	PHE	CB-CG-CD2	6.50	125.35	120.80
1	A	3	CYS	CB-CA-C	-6.49	97.43	110.40
1	A	4	SER	CA-C-N	-6.46	102.99	117.20
1	A	86	LEU	CB-CG-CD2	-6.45	100.03	111.00
1	A	63	GLY	CA-C-O	6.45	132.21	120.60
1	A	74	LYS	CA-CB-CG	6.41	127.49	113.40
1	A	121	MET	O-C-N	-6.39	112.47	122.70
1	A	108	TYR	CB-CG-CD1	-6.39	117.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	44	MET	O-C-N	-6.38	112.36	123.20
1	A	80	VAL	CA-C-O	6.35	133.44	120.10
1	A	60	VAL	CA-CB-CG2	6.33	120.39	110.90
1	A	49	VAL	CA-CB-CG1	6.26	120.30	110.90
1	A	20	ILE	CG1-CB-CG2	-6.26	97.63	111.40
1	A	71	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	17	THR	N-CA-CB	6.24	122.16	110.30
1	A	5	VAL	CB-CA-C	6.22	123.22	111.40
1	A	47	ASN	CB-CA-C	-6.21	97.99	110.40
1	A	120	LEU	CB-CG-CD1	-6.16	100.54	111.00
1	A	17	THR	CA-CB-OG1	-6.13	96.13	109.00
1	A	100	SER	C-N-CA	6.13	137.02	121.70
1	A	21	THR	CA-CB-CG2	-6.10	103.86	112.40
1	A	91	GLU	O-C-N	6.10	132.45	122.70
1	A	77	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	70	LYS	C-N-CA	6.02	136.76	121.70
1	A	106	GLU	OE1-CD-OE2	5.92	130.41	123.30
1	A	10	ASN	C-N-CA	5.82	136.25	121.70
1	A	66	SER	CA-C-O	5.81	132.29	120.10
1	A	103	LYS	CA-CB-CG	5.80	126.16	113.40
1	A	76	ASP	CA-CB-CG	5.79	126.14	113.40
1	A	43	VAL	CA-CB-CG1	5.78	119.57	110.90
1	A	27	LYS	CA-C-N	5.76	129.88	117.20
1	A	112	CYS	CB-CA-C	5.72	121.83	110.40
1	A	31	VAL	CA-CB-CG1	5.71	119.47	110.90
1	A	89	SER	CB-CA-C	-5.69	99.28	110.10
1	A	73	LEU	CB-CA-C	5.66	120.95	110.20
1	A	74	LYS	N-CA-CB	-5.66	100.42	110.60
1	A	104	GLU	N-CA-CB	5.64	120.75	110.60
1	A	55	ASP	CA-C-O	-5.62	108.29	120.10
1	A	35	HIS	C-N-CA	5.59	145.48	122.00
1	A	121	MET	CA-C-O	5.57	131.80	120.10
1	A	63	GLY	C-N-CA	-5.57	107.78	121.70
1	A	69	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	A	6	ASP	OD1-CG-OD2	-5.53	112.80	123.30
1	A	17	THR	C-N-CA	-5.52	107.89	121.70
1	A	66	SER	N-CA-CB	-5.50	102.25	110.50
1	A	48	TRP	NE1-CE2-CZ2	-5.48	124.37	130.40
1	A	29	PHE	CB-CG-CD1	-5.48	116.97	120.80
1	A	96	THR	CA-CB-OG1	5.46	120.47	109.00
1	A	33	LEU	C-N-CA	-5.45	108.09	121.70
1	A	107	GLN	CA-C-N	-5.44	105.24	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	GLN	C-N-CA	5.42	135.25	121.70
1	A	80	VAL	CA-C-N	-5.41	105.30	117.20
1	A	115	PRO	CA-N-CD	-5.38	103.96	111.50
1	A	29	PHE	C-N-CA	-5.38	108.25	121.70
1	A	3	CYS	CA-C-O	5.38	131.40	120.10
1	A	74	LYS	CG-CD-CE	5.38	128.03	111.90
1	A	29	PHE	CB-CG-CD2	5.36	124.56	120.80
1	A	16	ASN	N-CA-CB	5.36	120.25	110.60
1	A	40	PRO	N-CA-CB	-5.36	96.71	102.60
1	A	79	ARG	CA-CB-CG	5.33	125.14	113.40
1	A	94	SER	CA-CB-OG	-5.28	96.94	111.20
1	A	5	VAL	CA-CB-CG1	5.27	118.81	110.90
1	A	83	HIS	O-C-N	5.23	131.07	122.70
1	A	79	ARG	CB-CG-CD	-5.20	98.07	111.60
1	A	69	ASP	CA-CB-CG	5.17	124.78	113.40
1	A	44	MET	CB-CA-C	5.14	120.69	110.40
1	A	58	GLY	CA-C-N	-5.11	105.95	117.20
1	A	114	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	A	97	PHE	CA-CB-CG	5.10	126.14	113.90
1	A	37	GLY	CA-C-O	-5.10	111.43	120.60
1	A	9	GLY	CA-C-O	-5.09	111.44	120.60
1	A	28	GLN	CG-CD-NE2	5.08	128.90	116.70
1	A	28	GLN	CG-CD-OE1	-5.08	111.44	121.60
1	A	30	THR	C-N-CA	5.06	134.34	121.70
1	A	84	THR	N-CA-C	-5.05	97.37	111.00
1	A	16	ASN	CA-C-N	-5.04	106.11	117.20
1	A	104	GLU	C-N-CA	-5.03	111.75	122.30
1	A	44	MET	C-N-CA	-5.02	111.75	122.30
1	A	57	GLN	CA-CB-CG	-5.02	102.35	113.40
1	A	119	ALA	C-N-CA	5.01	134.22	121.70
1	A	123	GLY	C-N-CA	-5.00	109.20	121.70

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 (i)

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	68	0
2	A	1	0	0	1	0
All	All	931	0	872	68	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 38.

All (68) 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:CB	1:A:4:SER:OG	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:SD	1:A:44:MET:CE	2.11	1.38
1:A:34:SER:OG	1:A:34:SER:CB	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:CE	1:A:109:MET:CG	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:49:VAL:HG11	1:A:73:LEU:HD13	1.81	0.63
1:A:4:SER:HG	1:A:4:SER:CB	2.08	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LYS:CD	1:A:24:LYS:CB	2.75	0.59
1:A:24:LYS:CG	1:A:24:LYS:CA	2.76	0.59
1:A:4:SER:CA	1:A:4:SER:OG	2.49	0.57
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:12:GLN:O	1:A:13:MET:HB2	2.08	0.53
1:A:24:LYS:HG2	1:A:127:LEU:HD21	1.91	0.53
1:A:59:VAL:HG21	1:A:80:VAL:CG2	2.39	0.52
1:A:70:LYS:O	1:A:71:ASP:HB2	2.09	0.52
1:A:7:ILE:HD11	1:A:31:VAL:HG13	1.91	0.52
1:A:25:SER:HG	1:A:25:SER:CB	2.09	0.52
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:15:PHE:CD1	1:A:121:MET:HB3	2.51	0.46
1:A:18:ASN:HD22	1:A:18:ASN:H	1.62	0.46
1:A:106:GLU:HB3	1:A:108:TYR:CE2	2.51	0.45
1:A:38:ASN:C	1:A:39:LEU:HD22	2.36	0.45
1:A:109:MET:CE	1:A:109:MET:HG2	2.46	0.44
1:A:20:ILE:CG2	1:A:21:THR:N	2.80	0.44
1:A:39:LEU:HD12	1:A:43:VAL:HG11	1.99	0.44
1:A:16:ASN:C	1:A:17:THR:OG1	2.47	0.44
1:A:28:GLN:HB3	1:A:97:PHE:O	2.18	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: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:93:ASP:CG	1:A:94:SER:H	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	98/110 (89%)	61 (62%)	37 (38%)	0 0

All (37) 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	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	66	SER
1	A	71	ASP
1	A	74	LYS
1	A	77	ASP
1	A	78	SER
1	A	94	SER
1	A	96	THR
1	A	106	GLU
1	A	107	GLN

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Mol	Chain	Res	Type
1	A	109	MET
1	A	112	CYS
1	A	113	THR
1	A	115	PRO
1	A	117	HIS
1	A	118	SER
1	A	125	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	16	ASN
1	A	18	ASN
1	A	32	ASN
1	A	35	HIS
1	A	42	ASN
1	A	47	ASN
1	A	107	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 carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.