



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 10:11 AM UTC

PDB ID : 5WU1 / pdb_00005wu1
Title : Crystal structure of apo human Tut1, form I
Authors : Yamashita, S.; Tomita, K.
Deposited on : 2016-12-16
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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)	:	2.0
EDS	:	3.0
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

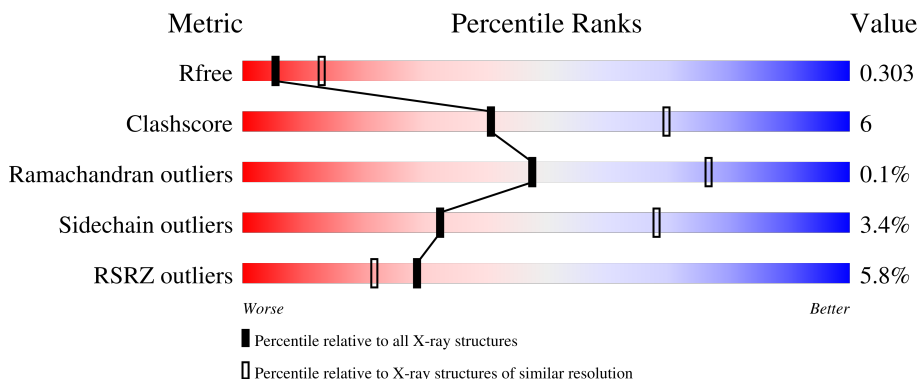
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	573	 5% 71% 14% • 14%
1	B	573	 5% 66% 17% • 16%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7569 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 Speckle targeted PIP5K1A-regulated poly(A) polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3808	2407	698	691	12			
1	B	484	Total	C	N	O	S	0	0	0
			3759	2380	686	681	12			

There are 370 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	140	MET	-	initiating methionine	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	CYS	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	PHE	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	372	ALA	CYS	engineered mutation	UNP Q9H6E5
A	399	ALA	CYS	engineered mutation	UNP Q9H6E5
A	415	ALA	CYS	engineered mutation	UNP Q9H6E5
A	501	ALA	CYS	engineered mutation	UNP Q9H6E5
A	504	SER	CYS	engineered mutation	UNP Q9H6E5
A	574	ALA	CYS	engineered mutation	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	LYS	deletion	UNP Q9H6E5
A	?	-	ARG	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	LYS	deletion	UNP Q9H6E5
A	?	-	VAL	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	LYS	deletion	UNP Q9H6E5
A	?	-	ASN	deletion	UNP Q9H6E5
A	?	-	CYS	deletion	UNP Q9H6E5
A	?	-	CYS	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	LYS	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	CYS	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	ARG	deletion	UNP Q9H6E5
A	?	-	VAL	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	MET	deletion	UNP Q9H6E5
A	?	-	VAL	deletion	UNP Q9H6E5
A	?	-	ILE	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	VAL	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	MET	deletion	UNP Q9H6E5
A	?	-	VAL	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	TRP	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	MET	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	LYS	deletion	UNP Q9H6E5
A	?	-	HIS	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	?	-	HIS	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	ARG	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
A	?	-	LYS	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	HIS	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	GLN	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	TRP	deletion	UNP Q9H6E5
A	?	-	SER	deletion	UNP Q9H6E5
A	875	LEU	-	expression tag	UNP Q9H6E5
A	876	GLU	-	expression tag	UNP Q9H6E5
A	877	HIS	-	expression tag	UNP Q9H6E5
A	878	HIS	-	expression tag	UNP Q9H6E5
A	879	HIS	-	expression tag	UNP Q9H6E5
A	880	HIS	-	expression tag	UNP Q9H6E5
A	881	HIS	-	expression tag	UNP Q9H6E5
A	882	HIS	-	expression tag	UNP Q9H6E5
B	140	MET	-	initiating methionine	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	CYS	deletion	UNP Q9H6E5
B	?	-	THR	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	PHE	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	THR	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	THR	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	THR	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	372	ALA	CYS	engineered mutation	UNP Q9H6E5
B	399	ALA	CYS	engineered mutation	UNP Q9H6E5
B	415	ALA	CYS	engineered mutation	UNP Q9H6E5
B	501	ALA	CYS	engineered mutation	UNP Q9H6E5
B	504	SER	CYS	engineered mutation	UNP Q9H6E5
B	574	ALA	CYS	engineered mutation	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	THR	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	LYS	deletion	UNP Q9H6E5
B	?	-	ARG	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	LYS	deletion	UNP Q9H6E5
B	?	-	VAL	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	LYS	deletion	UNP Q9H6E5
B	?	-	ASN	deletion	UNP Q9H6E5
B	?	-	CYS	deletion	UNP Q9H6E5
B	?	-	CYS	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	LYS	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	CYS	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	ARG	deletion	UNP Q9H6E5
B	?	-	VAL	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	MET	deletion	UNP Q9H6E5
B	?	-	VAL	deletion	UNP Q9H6E5
B	?	-	ILE	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	VAL	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	MET	deletion	UNP Q9H6E5
B	?	-	VAL	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	TRP	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	MET	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	THR	deletion	UNP Q9H6E5
B	?	-	THR	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	LYS	deletion	UNP Q9H6E5
B	?	-	HIS	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	HIS	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	ARG	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	LYS	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	HIS	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	ALA	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	GLU	deletion	UNP Q9H6E5
B	?	-	TRP	deletion	UNP Q9H6E5

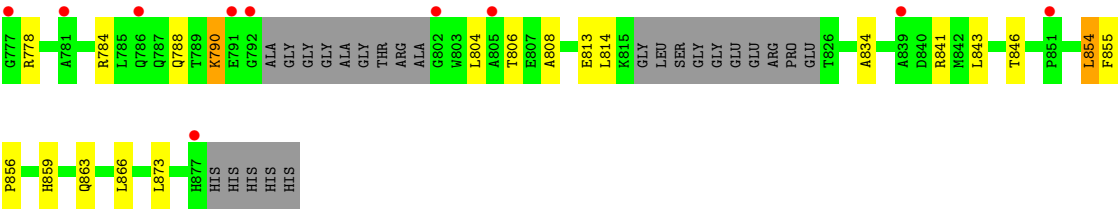
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q9H6E5
B	875	LEU	-	expression tag	UNP Q9H6E5
B	876	GLU	-	expression tag	UNP Q9H6E5
B	877	HIS	-	expression tag	UNP Q9H6E5
B	878	HIS	-	expression tag	UNP Q9H6E5
B	879	HIS	-	expression tag	UNP Q9H6E5
B	880	HIS	-	expression tag	UNP Q9H6E5
B	881	HIS	-	expression tag	UNP Q9H6E5
B	882	HIS	-	expression tag	UNP Q9H6E5

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.63Å 87.78Å 185.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.98-2.80) 99.4 (19.98-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.253 , 0.297 0.265 , 0.303	Depositor DCC
R_{free} test set	1592 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7569	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1620e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.30	0/3892	0.79	3/5289 (0.1%)
1	B	0.29	0/3842	0.78	5/5221 (0.1%)
All	All	0.29	0/7734	0.78	8/10510 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	446	ASP	CA-C-N	-10.49	109.58	120.38
1	A	446	ASP	C-N-CA	-10.49	109.58	120.38
1	B	446	ASP	CA-C-N	-10.46	109.60	120.38
1	B	446	ASP	C-N-CA	-10.46	109.60	120.38
1	B	460	ALA	CB-CA-C	-5.73	109.95	116.54

There are no chirality outliers.

There are no planarity outliers.

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	3808	0	3827	43	0
1	B	3759	0	3779	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7569	0	7606	98	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 6.

The worst 5 of 98 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:209:SER:O	1:B:407:ARG:NH1	1.95	1.00
1:A:209:SER:O	1:A:407:ARG:NH1	2.06	0.88
1:B:562:ARG:HE	1:B:607:THR:HB	1.54	0.72
1:A:605:SER:HB2	1:A:846:THR:HG22	1.71	0.71
1:A:453:VAL:HB	1:A:515:ARG:HA	1.77	0.66

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	485/573 (85%)	461 (95%)	23 (5%)	1 (0%)	43	72
1	B	474/573 (83%)	455 (96%)	19 (4%)	0	100	100
All	All	959/1146 (84%)	916 (96%)	42 (4%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	801	ALA

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	409/467 (88%)	395 (97%)	14 (3%)	32	68
1	B	407/467 (87%)	393 (97%)	14 (3%)	32	68
All	All	816/934 (87%)	788 (97%)	28 (3%)	32	68

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	145	ASP
1	B	854	LEU
1	B	331	LYS
1	B	790	LYS
1	B	192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	GLN
1	B	201	HIS
1	B	549	HIS
1	B	386	ASN
1	A	618	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are 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 [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	493/573 (86%)	0.41	27 (5%)	30 23	34, 69, 130, 198	0
1	B	484/573 (84%)	0.45	30 (6%)	26 20	30, 71, 127, 176	0
All	All	977/1146 (85%)	0.43	57 (5%)	29 22	30, 70, 129, 198	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	528	SER	5.4
1	B	792	GLY	5.3
1	B	527	PRO	4.8
1	B	529	ASN	4.2
1	B	781	ALA	4.0

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($\text{\AA}^2$)	Q<0.9
2	CL	A	1001	1/1	0.92	0.11	76,76,76,76	0
2	CL	B	1001	1/1	0.95	0.05	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.