WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 1, 2023 – 04:04 PM JST

PDB ID	:	5WU3
Title	:	Crystal structure of human Tut1 bound with MgUTP, form II
Authors	:	Yamashita, S.; Tomita, K.
Deposited on	:	2016-12-16
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:

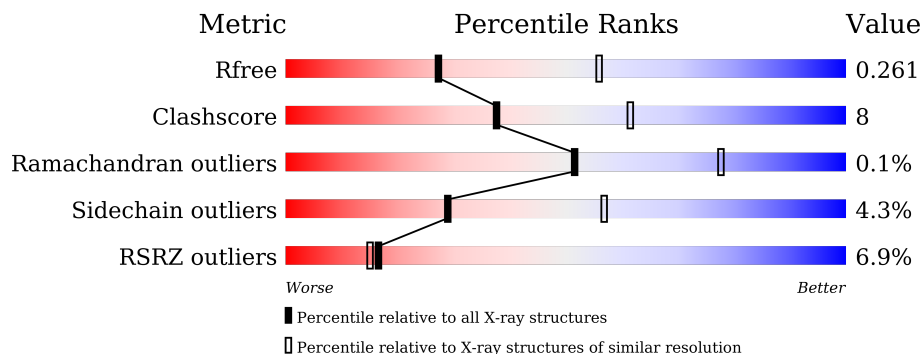|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	Percentile Ranks	Value
Rfree		0.261
Clashscore		8
Ramachandran outliers		0.1%
Sidechain outliers		4.3%
RSRZ outliers		6.9%

Worse   Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	6% 68% 15% • 16%
1	B	573	6% 69% 14% • 15%

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 7599 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	484	Total	C	N	O	S	0	0	0
			3759	2380	686	681	12			
1	B	485	Total	C	N	O	S	0	0	0
			3768	2385	687	684	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 URIDINE 5'-TRIPHOSPHATE (three-letter code: UTP) (formula: $C_9H_{15}N_2O_{15}P_3$).
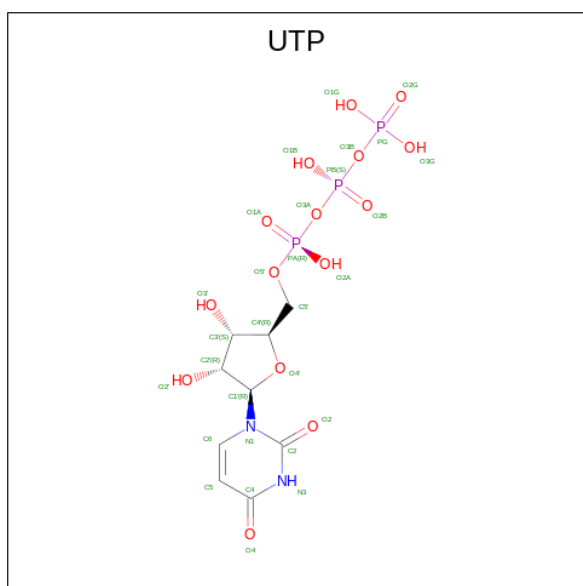
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
2	B	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
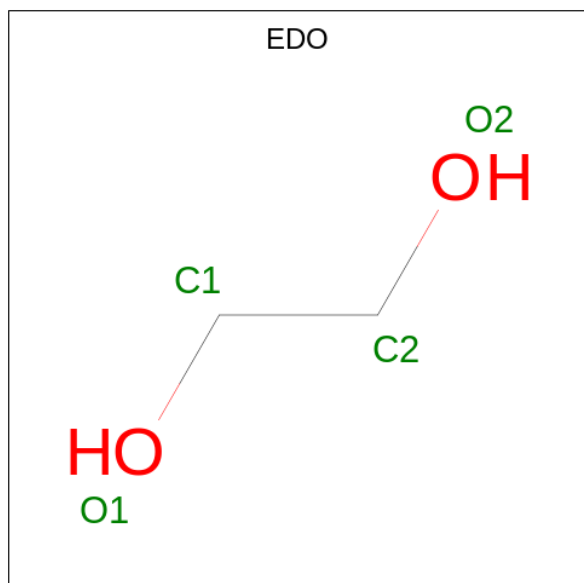
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total C O 4 2 2			0	0
5	B	1	Total C O 4 2 2			0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total O 1 1		0	0
6	B	1	Total O 1 1		0	0

3 Residue-property plots ⓘ

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: Speckle targeted PIP5K1A-regulated poly(A) polymerase

• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.79Å 85.11Å 93.76Å 90.00° 99.56° 90.00°	Depositor
Resolution (Å)	19.93 – 2.70	Depositor
	46.51 – 2.70	EDS
% Data completeness	99.2 (19.93-2.70)	Depositor
(in resolution range)	99.2 (46.51-2.70)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.229 , 0.257	Depositor
	0.233 , 0.261	DCC
R_{free} test set	1691 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 45.0	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7599	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: UTP, CL, MG, EDO

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	0.31	0/3842	0.47	1/5221 (0.0%)
1	B	0.27	0/3851	0.45	0/5233
All	All	0.29	0/7693	0.46	1/10454 (0.0%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	329	THR	C-N-CD	5.88	140.76	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	SER	Peptide
1	B	385	SER	Peptide

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	3759	0	3779	64	0
1	B	3768	0	3785	51	0
2	A	29	0	11	1	0
2	B	29	0	11	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	6	3	0
5	B	4	0	6	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	7599	0	7598	117	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 8.

All (117) 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	0.99
1:A:330:PRO:HG2	1:A:331:LYS:H	1.32	0.91
2:B:1001:UTP:O2B	2:B:1001:UTP:H5'2	1.85	0.76
2:B:1001:UTP:O1B	5:B:1004:EDO:O2	2.03	0.74
1:A:329:THR:O	1:A:333:GLU:HG2	1.90	0.72
1:A:394:ARG:HB3	1:A:477:ARG:HH22	1.56	0.69
1:A:193:GLU:HG3	1:B:613:LEU:HB3	1.77	0.66
1:B:188:GLN:O	1:B:192:THR:OG1	2.15	0.62
1:B:210:PHE:HE2	1:B:396:LEU:HB3	1.66	0.61
1:A:774:VAL:HA	1:A:814:LEU:HD13	1.83	0.61
1:A:834:ALA:HB1	1:A:843:LEU:HD11	1.82	0.60
1:A:330:PRO:HG2	1:A:331:LYS:N	2.10	0.60
1:A:210:PHE:HE2	1:A:396:LEU:HB3	1.67	0.60
1:A:582:ARG:HG2	1:A:583:SER:H	1.67	0.60
1:A:148:GLN:HA	1:A:151:LYS:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:PHE:HE1	1:B:385:SER:HA	1.66	0.59
1:B:834:ALA:HB1	1:B:843:LEU:HD11	1.84	0.59
1:A:332:GLU:OE2	1:B:783:ARG:NH2	2.36	0.58
1:A:220:PHE:HE1	1:A:385:SER:HA	1.68	0.58
1:A:368:VAL:HG21	1:A:381:ASP:HB3	1.86	0.57
1:B:522:VAL:HG13	1:B:536:LEU:HD13	1.87	0.57
1:A:329:THR:HA	1:A:332:GLU:HG3	1.86	0.56
1:B:804:LEU:HG	1:B:873:LEU:HD21	1.88	0.55
1:B:394:ARG:HB3	1:B:477:ARG:HH22	1.71	0.55
1:B:502:VAL:HG12	1:B:505:TRP:CZ3	2.41	0.54
1:B:368:VAL:HG21	1:B:381:ASP:HB3	1.88	0.54
1:A:786:GLN:O	1:A:790:LYS:HG2	2.08	0.54
1:A:414:ARG:NH1	1:A:418:GLN:OE1	2.41	0.54
2:B:1001:UTP:O1B	5:B:1004:EDO:C2	2.56	0.53
1:B:774:VAL:HA	1:B:814:LEU:HD13	1.90	0.53
1:B:183:VAL:HG21	1:B:378:LEU:HD12	1.91	0.53
1:A:420:ARG:NH2	1:A:596:GLN:O	2.42	0.52
1:B:453:VAL:HG21	1:B:544:PRO:HB3	1.92	0.52
1:A:329:THR:N	1:A:330:PRO:CD	2.73	0.52
1:B:605:SER:HB2	1:B:846:THR:HG22	1.91	0.52
1:A:502:VAL:HG12	1:A:505:TRP:CZ3	2.45	0.52
1:A:183:VAL:HG21	1:A:378:LEU:HD12	1.93	0.51
1:A:414:ARG:NH1	1:A:431:ASN:HD21	2.09	0.51
1:A:628:ARG:HE	1:A:635:ILE:HG12	1.76	0.51
1:A:605:SER:HB2	1:A:846:THR:HG22	1.91	0.51
1:A:453:VAL:HG21	1:A:544:PRO:HB3	1.93	0.51
1:B:453:VAL:HB	1:B:515:ARG:HA	1.93	0.50
1:A:357:ARG:O	1:A:371:PHE:HA	2.11	0.50
1:A:562:ARG:HE	1:A:607:THR:HB	1.77	0.49
1:B:428:LEU:HA	1:B:559:VAL:HG11	1.93	0.49
1:B:582:ARG:HG2	1:B:583:SER:H	1.77	0.49
1:A:210:PHE:HB2	5:A:1004:EDO:H11	1.93	0.49
1:A:330:PRO:CG	1:A:331:LYS:H	2.10	0.49
2:A:1001:UTP:O2B	5:A:1004:EDO:H12	2.13	0.49
1:A:555:VAL:HG13	1:A:559:VAL:HB	1.94	0.48
1:B:420:ARG:NH2	1:B:596:GLN:O	2.46	0.48
1:A:374:ARG:HB3	1:A:375:PRO:HD3	1.96	0.48
1:B:427:PRO:O	1:B:555:VAL:HA	2.14	0.48
1:A:330:PRO:CG	1:A:331:LYS:N	2.73	0.48
1:A:522:VAL:HG13	1:A:536:LEU:HD13	1.95	0.48
1:B:613:LEU:HG	1:B:841:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:HA	1:A:559:VAL:HG11	1.95	0.47
1:A:523:ALA:HA	1:A:524:GLY:HA2	1.42	0.47
1:A:827:GLU:N	1:A:827:GLU:OE1	2.48	0.47
1:B:613:LEU:HG	1:B:841:ARG:HH11	1.79	0.46
1:A:414:ARG:NH1	1:A:431:ASN:ND2	2.64	0.46
1:A:431:ASN:HB3	5:A:1004:EDO:H21	1.98	0.46
1:B:357:ARG:O	1:B:371:PHE:HA	2.16	0.46
1:A:498:PHE:O	1:A:502:VAL:HG22	2.16	0.46
1:B:374:ARG:HB3	1:B:375:PRO:HD3	1.98	0.45
1:A:630:ALA:HA	1:A:808:ALA:HA	1.97	0.45
1:B:827:GLU:OE1	1:B:827:GLU:N	2.49	0.45
1:A:405:ARG:NH1	1:A:489:GLU:O	2.42	0.45
1:B:523:ALA:HA	1:B:524:GLY:HA2	1.43	0.45
1:B:366:ARG:NH1	1:B:366:ARG:HB2	2.31	0.44
1:B:452:THR:HG22	1:B:517:GLY:HA3	1.99	0.44
1:B:630:ALA:HA	1:B:808:ALA:HA	2.00	0.44
1:B:785:LEU:HD11	1:B:813:GLU:HG3	1.98	0.44
1:A:187:MET:HE3	1:A:191:PHE:HE2	1.82	0.44
1:A:582:ARG:HG3	1:A:589:TRP:CZ2	2.52	0.44
1:A:329:THR:HA	1:A:332:GLU:HB2	1.99	0.44
1:B:436:LEU:HD12	1:B:436:LEU:HA	1.83	0.44
1:A:583:SER:OG	1:A:587:ARG:HB2	2.18	0.44
1:B:555:VAL:HG13	1:B:559:VAL:HB	1.99	0.44
1:B:507:LEU:HD13	1:B:539:LEU:HD13	2.00	0.44
1:A:398:LEU:O	1:A:402:LEU:HG	2.17	0.43
1:B:205:SER:O	1:B:211:ASP:HB3	2.18	0.43
1:A:622:ALA:O	1:A:626:VAL:HG23	2.18	0.43
1:B:498:PHE:O	1:B:502:VAL:HG22	2.18	0.43
1:B:839:ALA:HA	1:B:840:ASP:HA	1.79	0.43
1:A:427:PRO:O	1:A:555:VAL:HA	2.19	0.43
1:A:452:THR:HG22	1:A:517:GLY:HA3	2.00	0.43
1:B:155:GLU:O	1:B:582:ARG:NH2	2.52	0.43
1:B:774:VAL:HG12	1:B:778:ARG:NH1	2.33	0.43
1:A:329:THR:N	1:A:330:PRO:HD2	2.34	0.42
1:A:368:VAL:CG2	1:A:381:ASP:HB3	2.49	0.42
1:A:582:ARG:HG2	1:A:583:SER:N	2.33	0.42
1:A:543:ASP:HB3	1:A:546:ASP:O	2.19	0.42
1:A:872:HIS:O	1:A:876:GLU:HG3	2.20	0.42
1:B:804:LEU:HD23	1:B:804:LEU:HA	1.94	0.42
1:B:459:LYS:HD3	1:B:459:LYS:HA	1.79	0.42
1:A:343:LEU:O	1:A:347:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASP:HB3	1:B:406:VAL:HG23	2.00	0.42
1:B:210:PHE:CE2	1:B:396:LEU:HB3	2.51	0.42
1:B:511:LEU:HD11	1:B:542:GLN:HB2	2.01	0.42
1:A:217:LEU:O	1:A:380:GLY:HA3	2.19	0.41
1:A:145:ASP:C	1:A:147:HIS:H	2.24	0.41
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.86	0.41
1:A:804:LEU:HD23	1:A:804:LEU:HA	1.90	0.41
1:B:558:ARG:HH11	1:B:610:PRO:HG2	1.84	0.41
1:B:778:ARG:HH21	1:B:807:GLU:HG3	1.85	0.41
1:A:835:SER:O	1:A:843:LEU:HD12	2.20	0.41
1:A:373:HIS:CE1	1:A:375:PRO:HD2	2.56	0.41
1:B:190:VAL:HG21	1:B:352:VAL:HB	2.02	0.41
1:B:515:ARG:NH2	1:B:544:PRO:O	2.53	0.41
1:B:855:PHE:N	1:B:856:PRO:HD2	2.36	0.41
1:A:210:PHE:CE2	1:A:396:LEU:HB3	2.51	0.41
1:B:604:LEU:HD11	1:B:860:HIS:CE1	2.56	0.41
1:A:530:LEU:H	1:A:530:LEU:HD23	1.86	0.41
1:B:405:ARG:NH1	1:B:489:GLU:O	2.47	0.41
1:A:803:TRP:HE3	1:A:804:LEU:H	1.70	0.40
1:A:867:PRO:O	1:A:871:ARG: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	474/573 (83%)	455 (96%)	18 (4%)	1 (0%)	47	73
1	B	475/573 (83%)	453 (95%)	22 (5%)	0	100	100
All	All	949/1146 (83%)	908 (96%)	40 (4%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	330	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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/467 (87%)	390 (96%)	17 (4%)	30	58
1	B	408/467 (87%)	390 (96%)	18 (4%)	28	56
All	All	815/934 (87%)	780 (96%)	35 (4%)	29	57

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	178	GLN
1	A	331	LYS
1	A	334	LYS
1	A	352	VAL
1	A	355	VAL
1	A	368	VAL
1	A	414	ARG
1	A	436	LEU
1	A	507	LEU
1	A	530	LEU
1	A	535	ARG
1	A	604	LEU
1	A	803	TRP
1	A	806	THR
1	A	841	ARG
1	A	854	LEU
1	B	147	HIS
1	B	178	GLN
1	B	192	THR
1	B	216	ASP
1	B	334	LYS
1	B	352	VAL

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Mol	Chain	Res	Type
1	B	355	VAL
1	B	368	VAL
1	B	414	ARG
1	B	436	LEU
1	B	477	ARG
1	B	530	LEU
1	B	535	ARG
1	B	604	LEU
1	B	803	TRP
1	B	806	THR
1	B	841	ARG
1	B	854	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	UTP	B	1001	3	22,30,30	1.57	7 (31%)	27,47,47	1.21	2 (7%)
2	UTP	A	1001	3	22,30,30	0.99	1 (4%)	27,47,47	1.38	3 (11%)
5	EDO	B	1004	-	3,3,3	0.48	0	2,2,2	0.16	0
5	EDO	A	1004	-	3,3,3	0.48	0	2,2,2	0.14	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
2	UTP	B	1001	3	-	0/20/38/38	0/2/2/2
2	UTP	A	1001	3	-	7/20/38/38	0/2/2/2
5	EDO	B	1004	-	-	1/1/1/1	-
5	EDO	A	1004	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	UTP	C4-N3	3.03	1.38	1.33
2	B	1001	UTP	C2'-C1'	-2.88	1.49	1.53
2	B	1001	UTP	C2-N3	-2.47	1.33	1.38
2	B	1001	UTP	O4'-C4'	-2.30	1.39	1.45
2	B	1001	UTP	PA-O2A	-2.22	1.44	1.55
2	B	1001	UTP	PG-O3G	-2.22	1.46	1.54
2	B	1001	UTP	O4-C4	-2.04	1.19	1.24
2	B	1001	UTP	O3'-C3'	-2.02	1.38	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	UTP	PB-O3B-PG	-4.12	118.70	132.83
2	A	1001	UTP	PB-O3A-PA	-3.14	122.07	132.83
2	B	1001	UTP	PB-O3B-PG	-2.77	123.33	132.83
2	A	1001	UTP	C3'-C2'-C1'	2.42	104.62	100.98
2	B	1001	UTP	O1B-PB-O2B	2.05	122.39	112.24

There are no chirality outliers.
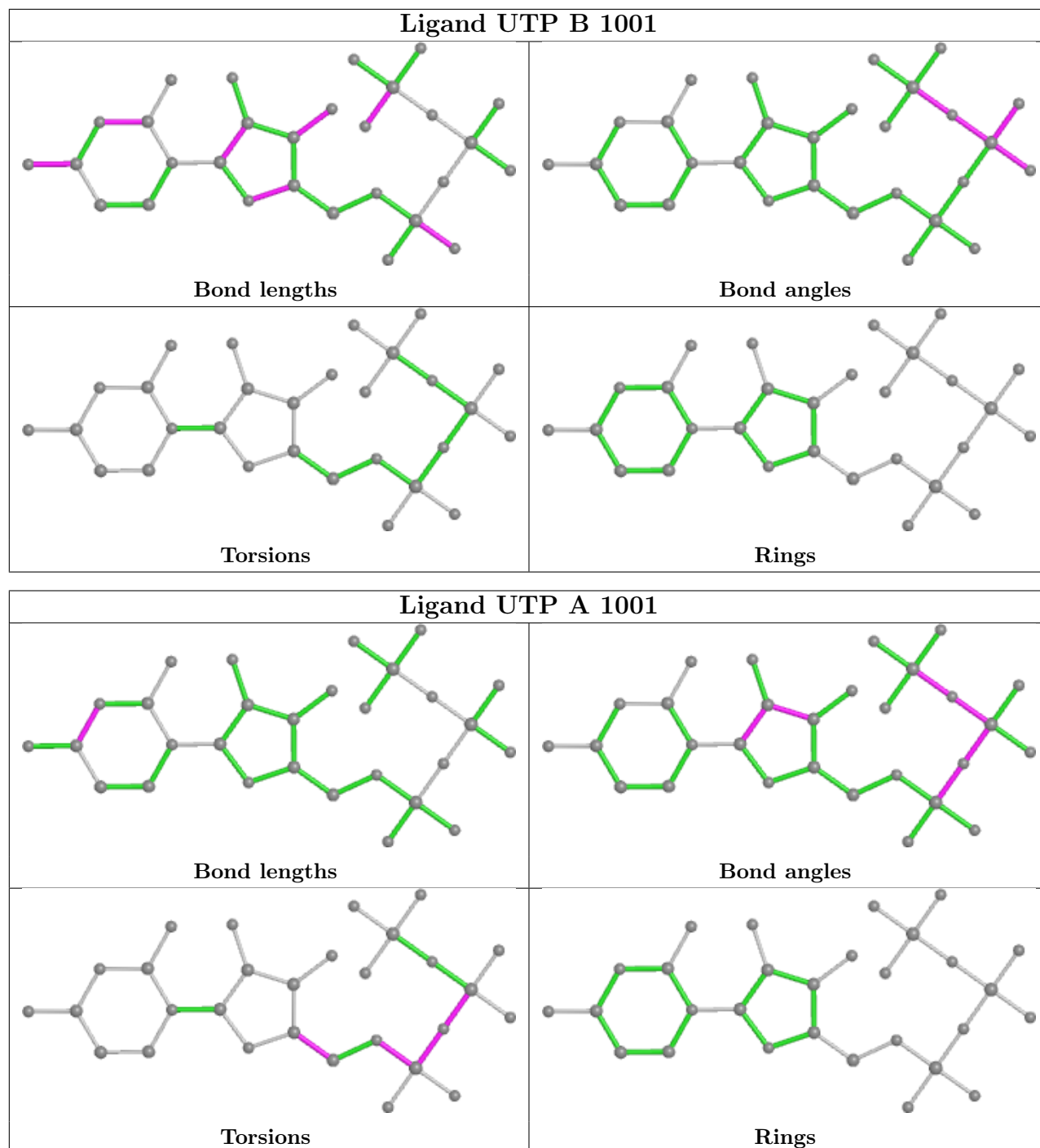
All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	UTP	PB-O3A-PA-O5'
2	A	1001	UTP	C5'-O5'-PA-O2A
2	A	1001	UTP	C3'-C4'-C5'-O5'
2	A	1001	UTP	O4'-C4'-C5'-O5'
2	A	1001	UTP	C5'-O5'-PA-O3A
2	A	1001	UTP	C5'-O5'-PA-O1A
5	A	1004	EDO	O1-C1-C2-O2
2	A	1001	UTP	PA-O3A-PB-O2B
5	B	1004	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	UTP	3	0
2	A	1001	UTP	1	0
5	B	1004	EDO	2	0
5	A	1004	EDO	3	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 then 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.

Ligand UTP B 1001

Bond lengths

Bond angles

Torsions

Rings

Ligand UTP A 1001

Bond lengths

Bond angles

Torsions

Rings

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 ⓘ

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(Å²)	Q<0.9
1	A	484/573 (84%)	0.47	32 (6%)	18	16	28, 57, 125, 181	0
1	B	485/573 (84%)	0.45	35 (7%)	15	13	31, 60, 125, 170	0
All	All	969/1146 (84%)	0.46	67 (6%)	16	15	28, 58, 125, 181	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	802	GLY	21.0
1	B	802	GLY	9.0
1	A	804	LEU	5.9
1	A	803	TRP	5.4
1	B	804	LEU	4.7
1	B	792	GLY	4.5
1	B	585	ARG	4.3
1	A	587	ARG	4.3
1	B	586	GLY	4.2
1	B	584	SER	4.1
1	A	854	LEU	4.1
1	B	525	GLY	3.9
1	A	425	SER	3.7
1	A	525	GLY	3.6
1	A	814	LEU	3.4
1	B	814	LEU	3.4
1	A	772	HIS	3.3
1	B	587	ARG	3.2
1	A	527	PRO	3.1
1	B	803	TRP	3.1
1	B	805	ALA	3.1
1	A	633	CYS	3.0
1	A	147	HIS	3.0
1	B	780	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	772	HIS	3.0
1	B	813	GLU	3.0
1	A	585	ARG	2.9
1	B	527	PRO	2.9
1	B	523	ALA	2.7
1	B	529	ASN	2.7
1	B	783	ARG	2.7
1	A	529	ASN	2.7
1	A	826	THR	2.7
1	B	329	THR	2.7
1	B	785	LEU	2.7
1	B	632	GLY	2.6
1	B	812	GLN	2.6
1	A	151	LYS	2.6
1	B	810	VAL	2.6
1	A	635	ILE	2.5
1	A	771	TRP	2.5
1	A	586	GLY	2.4
1	B	854	LEU	2.4
1	B	528	SER	2.4
1	B	331	LYS	2.4
1	B	524	GLY	2.3
1	B	425	SER	2.3
1	A	830	LEU	2.3
1	B	481	ARG	2.3
1	A	811	THR	2.3
1	B	630	ALA	2.3
1	B	147	HIS	2.2
1	B	526	LEU	2.2
1	A	523	ALA	2.2
1	A	766	TRP	2.2
1	A	522	VAL	2.2
1	B	146	SER	2.2
1	A	810	VAL	2.1
1	A	777	GLY	2.1
1	A	815	LYS	2.1
1	A	840	ASP	2.0
1	A	624	VAL	2.0
1	B	784	ARG	2.0
1	A	805	ALA	2.0
1	A	792	GLY	2.0
1	A	770	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	869	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	MG	B	1002	1/1	0.66	0.26	113,113,113,113	0
3	MG	A	1002	1/1	0.68	0.17	144,144,144,144	0
4	CL	B	1003	1/1	0.87	0.09	68,68,68,68	0
5	EDO	B	1004	4/4	0.88	0.28	58,60,64,67	0
5	EDO	A	1004	4/4	0.89	0.24	50,53,55,57	0
4	CL	A	1003	1/1	0.91	0.10	71,71,71,71	0
2	UTP	A	1001	29/29	0.94	0.17	28,46,166,260	0
2	UTP	B	1001	29/29	0.94	0.17	27,47,166,255	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.

Electron density around UTP A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
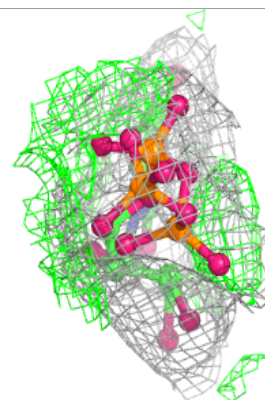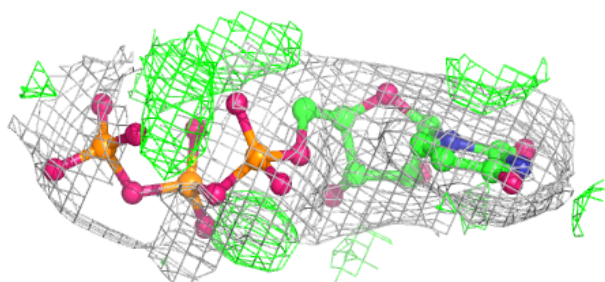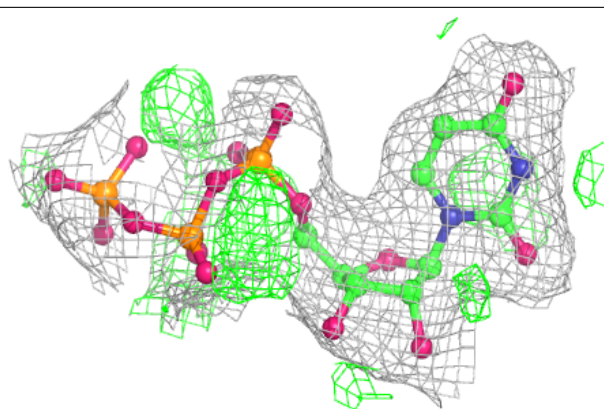
Electron density around UTP B 1001:

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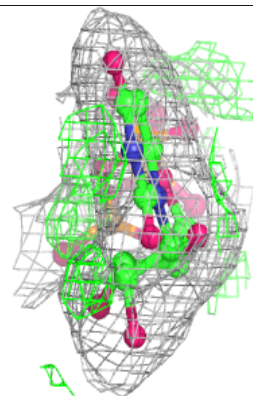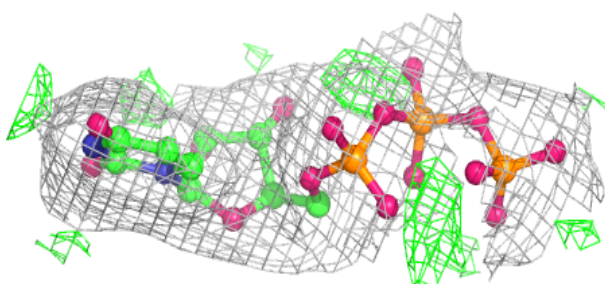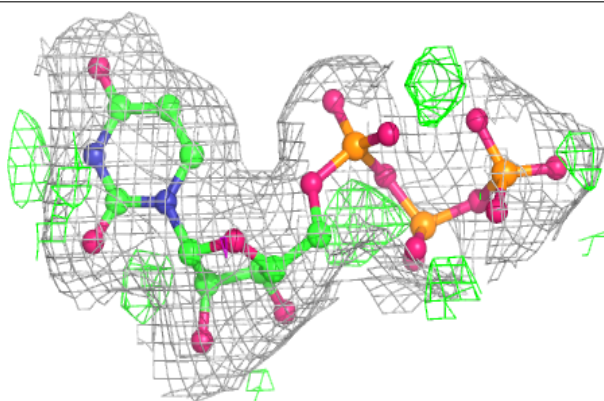
6.5 Other polymers (i)

There are no such residues in this entry.