Full wwPDB X-ray Structure Validation Report (i)

Mar 13, 2024 – 06:54 PM JST

PDB ID	:	5WU2
Title	:	Crystal structure of human Tut1 bound with BaUTP, form I
Authors	:	Yamashita, S.; Tomita, K.
Deposited on	:	2016-12-16
Resolution	:	2.95 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 (i) 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 (i)) were used in the production of this report:

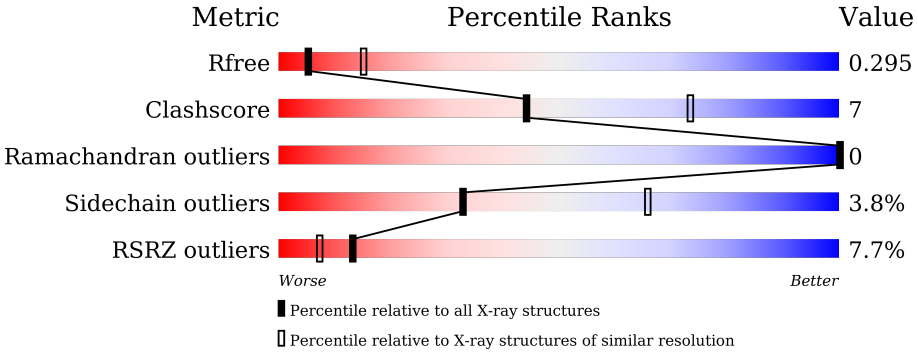
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	5% 69% 15% • 16%
1	B	573	8% 67% 16% • 16%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7584 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
			Total	C	N	O	S			
1	A	484	3761	2380	686	681	14	0	0	0
1	B	484	3761	2380	686	681	14	0	0	0

There are 366 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	415	ALA	CYS	engineered mutation	UNP Q9H6E5
A	501	ALA	CYS	engineered mutation	UNP Q9H6E5
A	504	SER	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
A	?	-	ASP	deletion	UNP Q9H6E5
A	?	-	GLY	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	?	-	GLY	deletion	UNP Q9H6E5
A	?	-	GLU	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	?	-	ASP	deletion	UNP Q9H6E5
B	?	-	SER	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	?	-	SER	deletion	UNP Q9H6E5
B	?	-	LEU	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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	conflict	UNP Q9H6E5
B	415	ALA	CYS	conflict	UNP Q9H6E5
B	501	ALA	CYS	conflict	UNP Q9H6E5
B	504	SER	CYS	conflict	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
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	LYS	deletion	UNP Q9H6E5
B	?	-	ASN	deletion	UNP Q9H6E5
B	?	-	CYS	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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
B	?	-	PRO	deletion	UNP Q9H6E5
B	?	-	GLY	deletion	UNP Q9H6E5
B	?	-	GLN	deletion	UNP Q9H6E5
B	?	-	PRO	deletion	UNP Q9H6E5

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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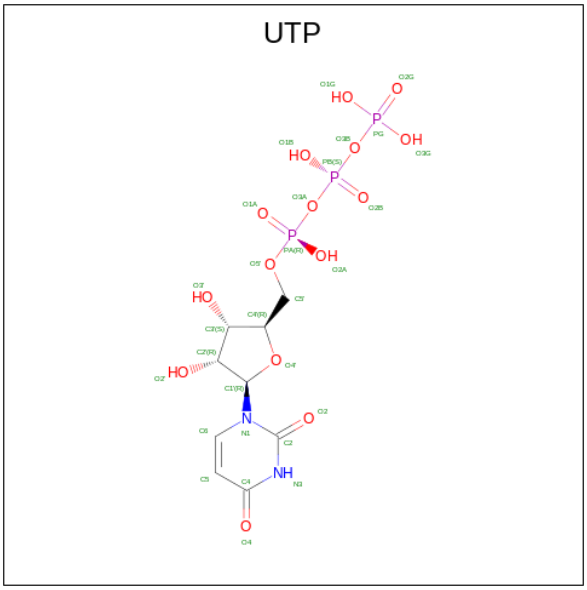
Chain	Residue	Modelled	Actual	Comment	Reference
B	878	HIS	-	expression tag	UNP Q9H6E5
B	879	HIS	-	expression tag	UNP Q9H6E5
B	880	HIS	-	expression tag	UNP Q9H6E5
B	881	HIS	-	expression tag	UNP Q9H6E5
B	882	HIS	-	expression tag	UNP Q9H6E5

- 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 BARIUM ION (three-letter code: BA) (formula: Ba).

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

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

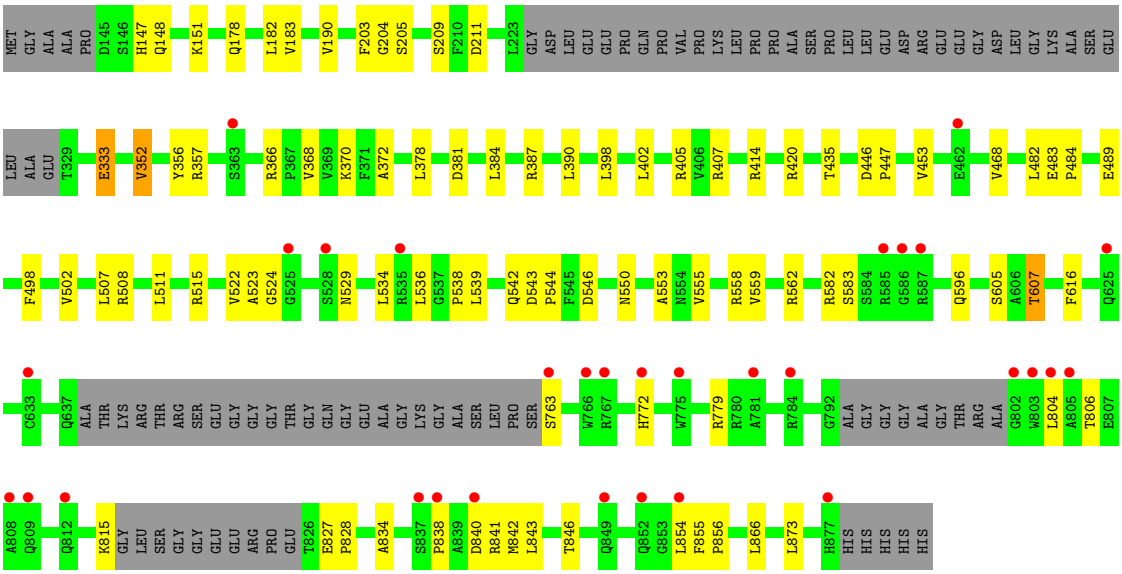
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	A	1	1	1	0	0
			Total	Cl		
4	B	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

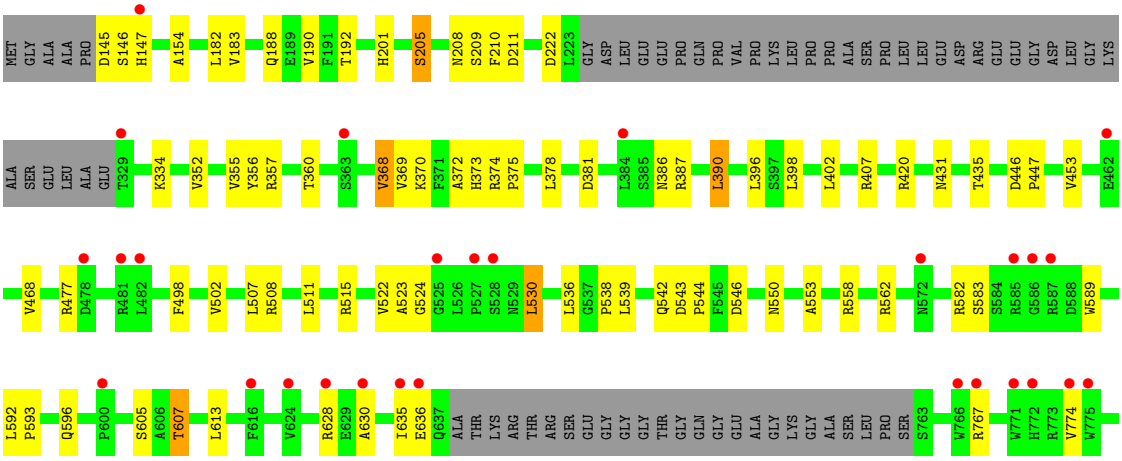
• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase

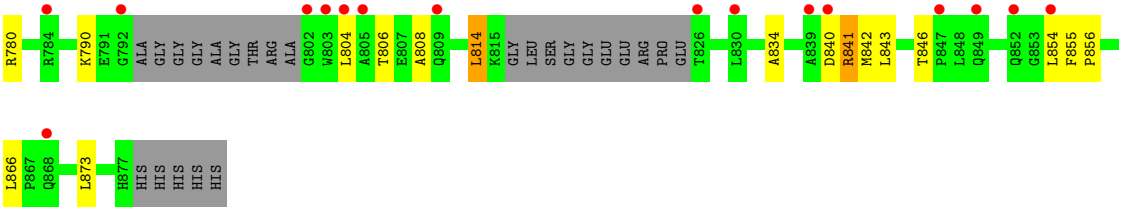
Chain A:



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

Chain B:




R780
R784
K790
E791
G792
ALA
GLY
GLY
GLY
ALA
GLY
THR
ARG
ALA
G802
W803
L804
A805
T806
E807
A808
Q809
L814
K815
GLY
LEU
SER
GLY
GLY
GLU
GLU
ARG
PRO
GLU
T826
L830
A834
A839
D840
R841
M842
L843
T846
P847
L848
Q849
Q852
G853
L854
F855
P856
L866
P867
Q868
L873
H877
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	77.33Å 88.40Å 184.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.95 49.20 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.94-2.95) 99.9 (49.20-2.95)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.246 , 0.294 0.251 , 0.295	Depositor DCC
R_{free} test set	1372 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7584	wwPDB-VP
Average B, all atoms (Å^2)	68.0	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 51.88 % 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 5.2651e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: UTP, BA, 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	0.24	0/3844	0.43	0/5223
1	B	0.24	0/3844	0.42	0/5223
All	All	0.24	0/7688	0.42	0/10446

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3761	0	3779	45	0
1	B	3761	0	3779	57	0
2	A	29	0	11	1	0
2	B	29	0	11	1	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
All	All	7584	0	7580	100	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 7.

All (100) 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	2.17	0.78
1:B:562:ARG:HE	1:B:607:THR:HB	1.47	0.78
1:A:562:ARG:HE	1:A:607:THR:HB	1.52	0.75
1:B:453:VAL:HB	1:B:515:ARG:HA	1.79	0.63
1:A:414:ARG:NH2	1:A:435:THR:OG1	2.31	0.62
1:A:453:VAL:HB	1:A:515:ARG:HA	1.81	0.60
1:B:843:LEU:HD23	1:B:866:LEU:HD13	1.82	0.60
1:A:550:ASN:HB3	1:A:553:ALA:HB2	1.84	0.60
1:A:605:SER:HB2	1:A:846:THR:HG22	1.84	0.60
1:A:209:SER:O	1:A:407:ARG:NH1	2.35	0.60
1:B:188:GLN:HE21	1:B:192:THR:HG23	1.65	0.60
1:A:582:ARG:HG2	1:A:583:SER:H	1.67	0.59
1:B:420:ARG:NH2	1:B:596:GLN:O	2.37	0.57
1:A:370:LYS:HG2	1:A:381:ASP:OD2	2.04	0.56
1:B:804:LEU:HG	1:B:873:LEU:HD21	1.87	0.56
1:B:453:VAL:HG21	1:B:544:PRO:HB3	1.88	0.56
1:B:605:SER:HB2	1:B:846:THR:HG22	1.87	0.56
1:A:178:GLN:NE2	1:B:375:PRO:O	2.35	0.56
1:B:498:PHE:O	1:B:502:VAL:HG22	2.06	0.55
1:B:530:LEU:HD23	1:B:530:LEU:H	1.71	0.55
1:B:834:ALA:HB1	1:B:843:LEU:HD11	1.88	0.55
1:B:613:LEU:HG	1:B:841:ARG:HH11	1.71	0.55
1:B:628:ARG:HE	1:B:635:ILE:HG12	1.73	0.54
1:A:148:GLN:HA	1:A:151:LYS:HE2	1.88	0.54
1:B:370:LYS:HG2	1:B:381:ASP:OD2	2.08	0.54
1:B:613:LEU:HG	1:B:841:ARG:NH1	2.23	0.53
1:B:357:ARG:HB2	1:B:372:ALA:HB3	1.90	0.53
1:B:154:ALA:HB2	1:B:592:LEU:HD11	1.91	0.52
1:B:582:ARG:HG2	1:B:583:SER:H	1.74	0.52
1:A:507:LEU:HG	1:A:539:LEU:HD13	1.91	0.52
1:A:357:ARG:HB2	1:A:372:ALA:HB3	1.91	0.52
1:A:772:HIS:CE1	1:A:815:LYS:HD2	2.45	0.51
1:B:210:PHE:HE2	1:B:396:LEU:HB3	1.75	0.51
1:A:508:ARG:HG2	1:A:538:PRO:HA	1.91	0.51
1:A:555:VAL:HG13	1:A:559:VAL:HB	1.91	0.51
1:B:636:GLU:OE1	1:B:767:ARG:NH2	2.43	0.51
1:A:190:VAL:HG21	1:A:352:VAL:HB	1.93	0.51
1:A:834:ALA:HB1	1:A:843:LEU:HD11	1.92	0.50
1:A:204:GLY:HA2	2:A:1001:UTP:O3'	2.12	0.50
1:A:420:ARG:NH2	1:A:596:GLN:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:NH1	1:A:489:GLU:O	2.42	0.50
1:A:508:ARG:HE	1:A:840:ASP:HB2	1.77	0.50
1:B:507:LEU:HD13	1:B:539:LEU:HD13	1.93	0.49
1:B:550:ASN:HB3	1:B:553:ALA:HB2	1.94	0.49
1:A:387:ARG:HB3	1:A:468:VAL:HG11	1.94	0.49
1:B:511:LEU:HD11	1:B:542:GLN:HB2	1.94	0.48
1:A:511:LEU:HD11	1:A:542:GLN:HB2	1.94	0.48
1:B:431:ASN:ND2	2:B:1001:UTP:O1G	2.46	0.48
1:A:182:LEU:HD23	1:B:182:LEU:HD23	1.95	0.47
1:B:368:VAL:HG21	1:B:381:ASP:HB3	1.96	0.47
1:B:396:LEU:HD13	1:B:435:THR:HG21	1.95	0.47
1:B:630:ALA:HA	1:B:808:ALA:HA	1.97	0.47
1:A:804:LEU:HG	1:A:873:LEU:HD21	1.95	0.47
1:A:843:LEU:HD23	1:A:866:LEU:HD13	1.96	0.47
1:B:190:VAL:HG21	1:B:352:VAL:HB	1.96	0.47
1:B:209:SER:HB2	1:B:407:ARG:HH11	1.79	0.47
1:B:183:VAL:HG21	1:B:378:LEU:HD12	1.97	0.47
1:A:522:VAL:HG13	1:A:536:LEU:HD13	1.98	0.46
1:B:387:ARG:HB3	1:B:468:VAL:HG11	1.98	0.46
1:A:446:ASP:HB3	1:A:447:PRO:HD3	1.97	0.46
1:B:592:LEU:HB2	1:B:593:PRO:HD3	1.97	0.46
1:A:523:ALA:HA	1:A:524:GLY:HA2	1.45	0.45
1:B:446:ASP:HB3	1:B:447:PRO:HD3	1.97	0.45
1:B:774:VAL:HA	1:B:814:LEU:HD13	1.97	0.45
1:A:453:VAL:HG21	1:A:544:PRO:HB3	1.96	0.45
1:B:373:HIS:CE1	1:B:375:PRO:HD2	2.52	0.45
1:B:188:GLN:NE2	1:B:192:THR:HG23	2.32	0.45
1:B:522:VAL:HG13	1:B:536:LEU:HD13	1.98	0.45
1:B:589:TRP:H	1:B:592:LEU:HD12	1.82	0.45
1:A:498:PHE:O	1:A:502:VAL:HG22	2.17	0.44
1:A:205:SER:O	1:A:211:ASP:HB3	2.16	0.44
1:B:205:SER:O	1:B:211:ASP:HB3	2.16	0.44
1:B:543:ASP:HB3	1:B:546:ASP:O	2.18	0.44
1:A:582:ARG:HG2	1:A:583:SER:N	2.33	0.44
1:B:558:ARG:HG2	1:B:842:MET:HE1	2.00	0.44
1:A:183:VAL:HG21	1:A:378:LEU:HD12	2.00	0.44
1:A:398:LEU:O	1:A:402:LEU:HG	2.18	0.43
1:B:201:HIS:HB3	1:B:390:LEU:HD11	2.01	0.43
1:B:374:ARG:HB3	1:B:375:PRO:HD3	2.01	0.43
1:B:790:LYS:NZ	1:B:790:LYS:HB2	2.32	0.43
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ARG:HG2	1:A:842:MET:HE1	2.01	0.43
1:A:827:GLU:HA	1:A:828:PRO:HD3	1.91	0.43
1:A:402:LEU:HD21	1:A:482:LEU:HD12	2.01	0.43
1:A:543:ASP:HB3	1:A:546:ASP:O	2.20	0.42
1:B:508:ARG:HE	1:B:840:ASP:HB2	1.85	0.42
1:B:855:PHE:N	1:B:856:PRO:HD2	2.34	0.42
1:B:523:ALA:HA	1:B:524:GLY:HA2	1.49	0.42
1:B:222:ASP:CG	1:B:387:ARG:HH22	2.23	0.42
1:A:333:GLU:HA	1:A:333:GLU:OE2	2.20	0.41
1:B:210:PHE:CE2	1:B:396:LEU:HB3	2.55	0.41
1:A:483:GLU:HA	1:A:484:PRO:HD3	1.88	0.41
1:A:855:PHE:N	1:A:856:PRO:HD2	2.35	0.41
1:A:203:PHE:HB3	1:A:390:LEU:HD12	2.02	0.41
1:A:763:SER:HB3	1:A:838:PRO:HD3	2.01	0.41
1:B:208:ASN:O	1:B:209:SER:OG	2.33	0.41
1:B:356:TYR:CD2	1:B:357:ARG:HG3	2.56	0.41
1:B:398:LEU:O	1:B:402:LEU:HG	2.21	0.41
1:B:508:ARG:HG2	1:B:538:PRO:HA	2.03	0.40
1:B:360:THR:HG22	1:B:369:VAL:HG22	2.03	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	474/573 (83%)	451 (95%)	23 (5%)	0	100	100
1	B	474/573 (83%)	451 (95%)	23 (5%)	0	100	100
All	All	948/1146 (83%)	902 (95%)	46 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	409/469 (87%)	395 (97%)	14 (3%)	37	69
1	B	409/469 (87%)	392 (96%)	17 (4%)	30	63
All	All	818/938 (87%)	787 (96%)	31 (4%)	33	66

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	HIS
1	A	333	GLU
1	A	352	VAL
1	A	356	TYR
1	A	366	ARG
1	A	368	VAL
1	A	529	ASN
1	A	534	LEU
1	A	607	THR
1	A	616	PHE
1	A	779	ARG
1	A	806	THR
1	A	841	ARG
1	A	854	LEU
1	B	145	ASP
1	B	146	SER
1	B	147	HIS
1	B	205	SER
1	B	334	LYS
1	B	355	VAL
1	B	368	VAL
1	B	386	ASN
1	B	390	LEU
1	B	477	ARG
1	B	530	LEU
1	B	607	THR
1	B	780	ARG

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Mol	Chain	Res	Type
1	B	806	THR
1	B	814	LEU
1	B	841	ARG
1	B	854	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	ASN
1	B	386	ASN
1	B	458	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	A	1001	3	22,30,30	0.99	1 (4%)	27,47,47	1.25	3 (11%)
2	UTP	B	1001	3	22,30,30	1.01	1 (4%)	27,47,47	1.32	3 (11%)

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	A	1001	3	-	5/20/38/38	0/2/2/2
2	UTP	B	1001	3	-	5/20/38/38	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	UTP	C4-N3	3.12	1.38	1.33
2	A	1001	UTP	C4-N3	3.07	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	UTP	PB-O3A-PA	-3.26	121.64	132.83
2	B	1001	UTP	PB-O3B-PG	-3.15	122.03	132.83
2	B	1001	UTP	PB-O3A-PA	-3.13	122.07	132.83
2	B	1001	UTP	C3'-C2'-C1'	2.97	105.45	100.98
2	A	1001	UTP	C3'-C2'-C1'	2.84	105.25	100.98
2	A	1001	UTP	PB-O3B-PG	-2.35	124.77	132.83

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	UTP	C5'-O5'-PA-O1A
2	A	1001	UTP	C5'-O5'-PA-O2A
2	B	1001	UTP	C5'-O5'-PA-O1A
2	B	1001	UTP	C5'-O5'-PA-O2A
2	A	1001	UTP	C3'-C4'-C5'-O5'
2	B	1001	UTP	O4'-C4'-C5'-O5'
2	B	1001	UTP	C3'-C4'-C5'-O5'
2	A	1001	UTP	O4'-C4'-C5'-O5'
2	A	1001	UTP	C5'-O5'-PA-O3A
2	B	1001	UTP	C5'-O5'-PA-O3A

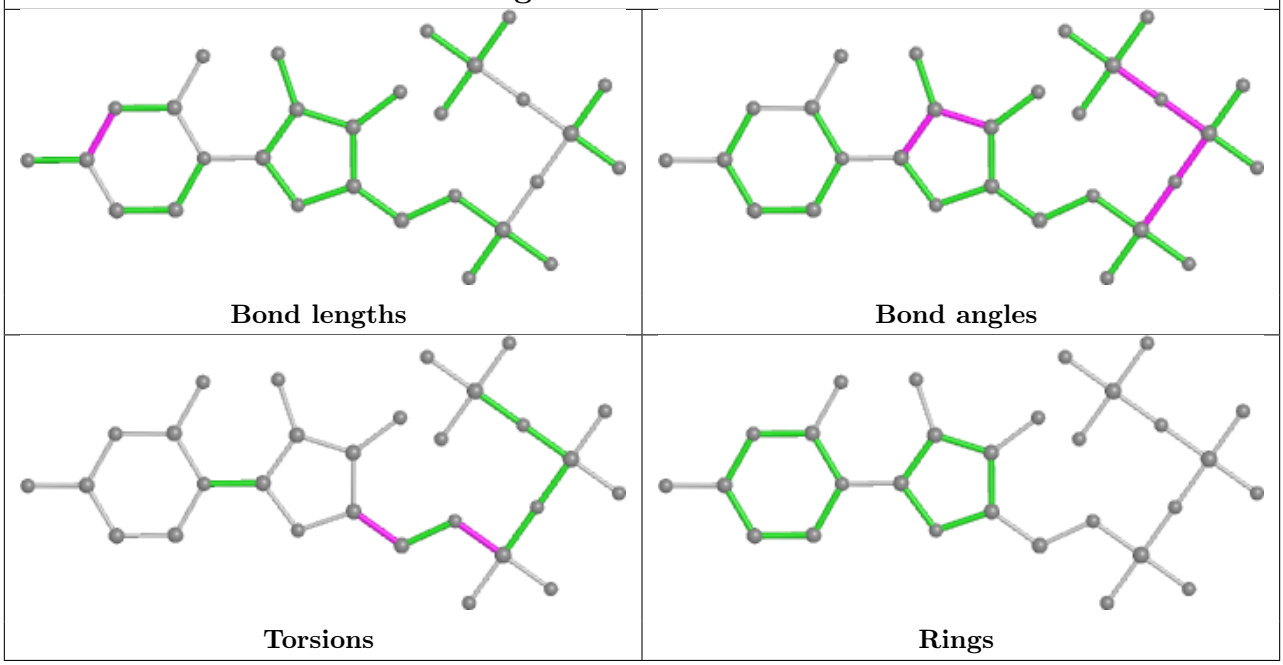
There are no ring outliers.

2 monomers are involved in 2 short contacts:

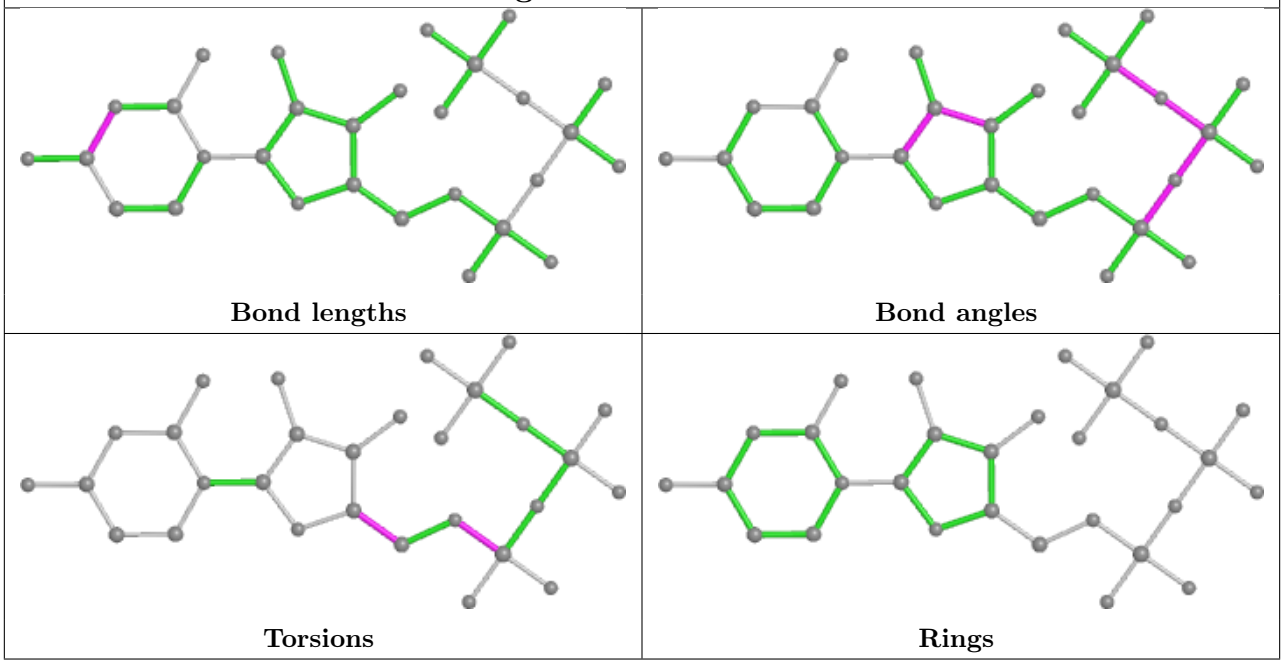
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	UTP	1	0
2	B	1001	UTP	1	0

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 A 1001



Ligand UTP B 1001



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	484/573 (84%)	0.59	31 (6%) 19 11	29, 61, 121, 178	0
1	B	484/573 (84%)	0.62	44 (9%) 9 5	30, 59, 122, 169	0
All	All	968/1146 (84%)	0.60	75 (7%) 13 7	29, 60, 122, 178	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	802	GLY	10.0
1	A	586	GLY	6.4
1	B	802	GLY	5.4
1	A	585	ARG	5.4
1	B	329	THR	5.3
1	A	528	SER	4.6
1	A	804	LEU	4.5
1	A	462	GLU	4.3
1	B	527	PRO	4.2
1	A	803	TRP	4.2
1	B	586	GLY	4.1
1	B	481	ARG	4.1
1	B	585	ARG	4.0
1	B	854	LEU	4.0
1	A	587	ARG	3.8
1	B	525	GLY	3.7
1	A	525	GLY	3.6
1	B	587	ARG	3.5
1	B	384	LEU	3.4
1	B	792	GLY	3.3
1	A	838	PRO	3.3
1	B	630	ALA	3.2
1	B	766	TRP	3.1
1	B	774	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	767	ARG	3.1
1	A	772	HIS	3.1
1	A	812	GLN	3.0
1	A	809	GLN	3.0
1	B	809	GLN	3.0
1	A	877	HIS	3.0
1	B	528	SER	2.9
1	A	805	ALA	2.8
1	B	482	LEU	2.8
1	A	849	GLN	2.8
1	B	635	ILE	2.8
1	A	763	SER	2.7
1	A	837	SER	2.7
1	B	804	LEU	2.7
1	A	808	ALA	2.7
1	B	767	ARG	2.6
1	B	636	GLU	2.6
1	B	868	GLN	2.6
1	B	805	ALA	2.6
1	B	849	GLN	2.6
1	A	625	GLN	2.5
1	B	840	ASP	2.5
1	A	781	ALA	2.5
1	A	766	TRP	2.4
1	B	803	TRP	2.4
1	A	852	GLN	2.4
1	B	572	ASN	2.4
1	B	839	ALA	2.4
1	B	616	PHE	2.4
1	B	624	VAL	2.4
1	A	633	CYS	2.4
1	B	826	THR	2.4
1	B	830	LEU	2.4
1	B	772	HIS	2.3
1	A	775	TRP	2.3
1	B	775	TRP	2.3
1	A	854	LEU	2.2
1	A	784	ARG	2.2
1	B	147	HIS	2.2
1	B	628	ARG	2.1
1	B	462	GLU	2.1
1	A	363	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	600	PRO	2.1
1	A	535	ARG	2.1
1	B	363	SER	2.0
1	B	852	GLN	2.0
1	B	847	PRO	2.0
1	A	840	ASP	2.0
1	B	771	TRP	2.0
1	B	478	ASP	2.0
1	B	784	ARG	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

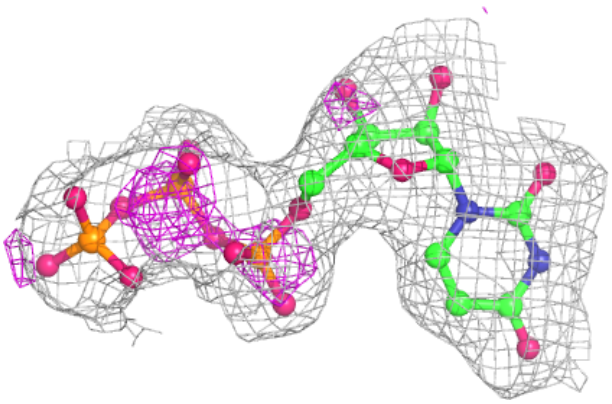
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

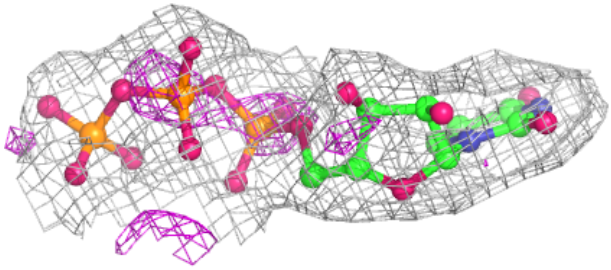
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	A	1003	1/1	0.86	0.17	70,70,70,70	0
4	CL	B	1003	1/1	0.90	0.14	67,67,67,67	0
2	UTP	A	1001	29/29	0.97	0.16	10,37,50,63	0
2	UTP	B	1001	29/29	0.97	0.16	26,37,50,73	0
3	BA	B	1002	1/1	0.98	0.23	64,64,64,64	0
3	BA	A	1002	1/1	0.99	0.13	51,51,51,51	0

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:

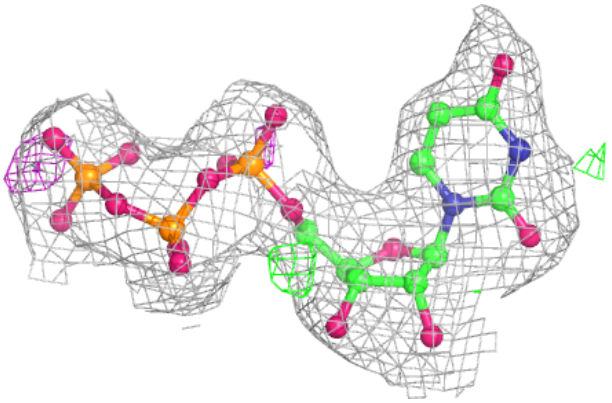
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

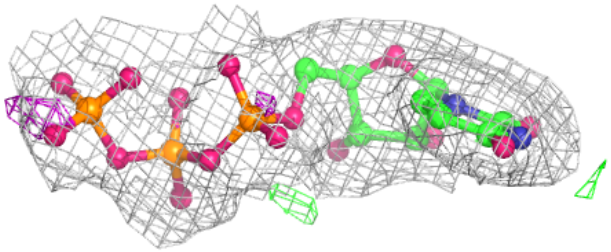


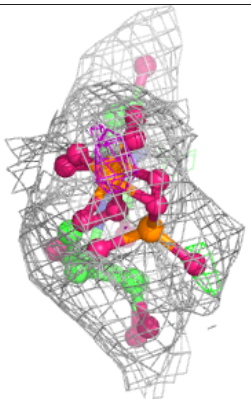


Electron density around UTP B 1001:

$2mF_o$-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.