Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 03:54 PM JST

PDB ID	:	5WU1
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 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 (1)) were used in the production of this report:

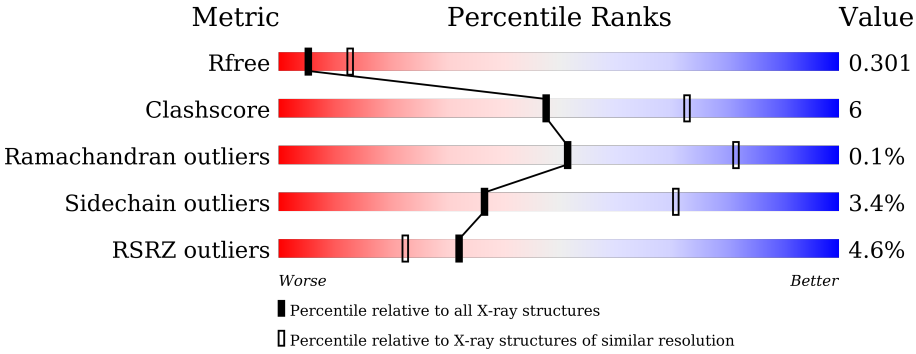
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	4% 72% 13% • 14%
1	B	573	4% 67% 16% • 16%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	493	3808	2407	698	691	12	0	0	0
1	B	484	3759	2380	686	681	12	0	0	0

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 (three-letter code: CL) (formula: Cl).

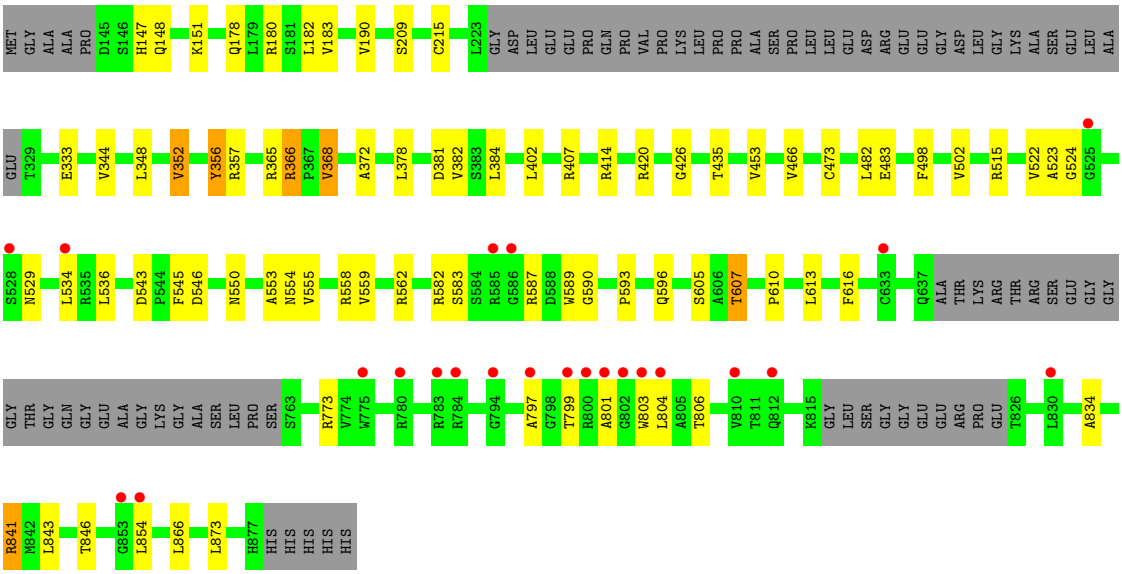
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	1	1	1	0	0
			Total	Cl		
2	B	1	1	1	0	0

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.

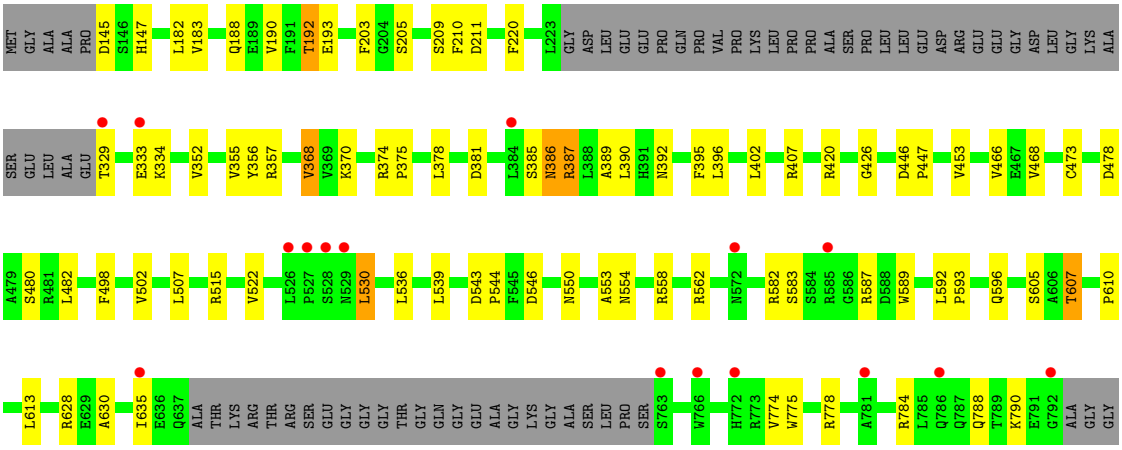
• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase

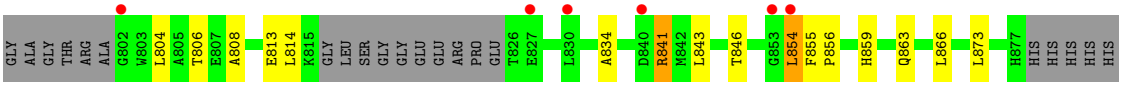
Chain A:



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

Chain B:




GLY
ALA
GLY
THR
ARG
ALA
G802
W803
L804
A805
T806
E807
A808
E813
L814
K815
GLY
LEU
SER
GLY
GLY
GLU
GLU
ARG
PRO
GLU
T826
E827
L830
A834
D840
R841
M842
L843
T846
G853
L854
F855
P856
H859
Q863
L866
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	77.63Å 87.78Å 185.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 48.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.98-2.80) 99.8 (48.30-2.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.253 , 0.297 0.257 , 0.301	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)	0.32 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	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.*

[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: 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	0.22	0/3892	0.41	0/5289
1	B	0.21	0/3842	0.40	0/5221
All	All	0.22	0/7734	0.41	0/10510

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	3808	0	3827	41	0
1	B	3759	0	3779	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	7569	0	7606	93	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.

All (93) 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
1:B:834:ALA:HB1	1:B:843:LEU:HD11	1.79	0.65
1:B:605:SER:HB2	1:B:846:THR:HG22	1.82	0.61
1:A:834:ALA:HB1	1:A:843:LEU:HD11	1.83	0.61
1:A:562:ARG:HE	1:A:607:THR:HB	1.66	0.60
1:B:507:LEU:HD13	1:B:539:LEU:HD13	1.83	0.59
1:A:344:VAL:HG21	1:A:384:LEU:HD21	1.85	0.58
1:B:530:LEU:HD23	1:B:530:LEU:H	1.68	0.58
1:B:558:ARG:HH11	1:B:610:PRO:HG2	1.69	0.57
1:A:178:GLN:NE2	1:B:375:PRO:O	2.33	0.57
1:A:180:ARG:NH2	1:A:215:CYS:O	2.38	0.57
1:B:188:GLN:HE21	1:B:192:THR:HG23	1.70	0.57
1:A:190:VAL:HG21	1:A:352:VAL:HB	1.87	0.56
1:A:843:LEU:HD23	1:A:866:LEU:HD13	1.87	0.56
1:B:420:ARG:NH2	1:B:596:GLN:O	2.40	0.55
1:B:453:VAL:HB	1:B:515:ARG:HA	1.87	0.55
1:A:414:ARG:NH2	1:A:435:THR:OG1	2.39	0.55
1:A:797:ALA:O	1:A:799:THR:HG23	2.07	0.55
1:A:582:ARG:HG2	1:A:583:SER:H	1.72	0.53
1:B:843:LEU:HD23	1:B:866:LEU:HD13	1.90	0.53
1:B:498:PHE:O	1:B:502:VAL:HG22	2.08	0.53
1:A:357:ARG:HB2	1:A:372:ALA:HB3	1.90	0.53
1:B:203:PHE:HB3	1:B:390:LEU:HD12	1.92	0.52
1:A:498:PHE:O	1:A:502:VAL:HG22	2.10	0.52
1:B:387:ARG:HB3	1:B:468:VAL:HG11	1.91	0.51
1:A:558:ARG:HH11	1:A:610:PRO:HG2	1.75	0.51
1:B:190:VAL:HG21	1:B:352:VAL:HB	1.92	0.51
1:B:582:ARG:HG2	1:B:583:SER:H	1.75	0.51
1:B:630:ALA:HA	1:B:808:ALA:HA	1.93	0.51
1:A:555:VAL:HG13	1:A:559:VAL:HB	1.93	0.50
1:B:613:LEU:HG	1:B:841:ARG:NH1	2.26	0.49
1:A:426:GLY:O	1:A:554:ASN:ND2	2.45	0.49
1:B:589:TRP:H	1:B:592:LEU:HD12	1.78	0.49
1:B:774:VAL:HG12	1:B:778:ARG:NH1	2.28	0.48
1:B:558:ARG:NH1	1:B:610:PRO:HG2	2.28	0.48
1:A:183:VAL:HG21	1:A:378:LEU:HD12	1.96	0.48
1:A:522:VAL:HG13	1:A:536:LEU:HD13	1.96	0.48
1:A:368:VAL:HG21	1:A:381:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLN:HA	1:A:151:LYS:HE2	1.96	0.48
1:A:550:ASN:HB3	1:A:553:ALA:HB2	1.96	0.47
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.75	0.47
1:B:220:PHE:HE1	1:B:385:SER:HA	1.78	0.47
1:B:368:VAL:HG21	1:B:381:ASP:HB3	1.96	0.47
1:B:453:VAL:HG21	1:B:544:PRO:HB3	1.97	0.47
1:A:613:LEU:HG	1:A:841:ARG:NH1	2.30	0.46
1:A:466:VAL:HG13	1:A:473:CYS:HB2	1.97	0.46
1:B:183:VAL:HG21	1:B:378:LEU:HD12	1.97	0.46
1:A:182:LEU:HD23	1:B:182:LEU:HD23	1.98	0.46
1:B:402:LEU:HD21	1:B:482:LEU:HD12	1.98	0.46
1:A:804:LEU:HG	1:A:873:LEU:HD21	1.98	0.46
1:A:523:ALA:HA	1:A:524:GLY:HA2	1.45	0.45
1:B:356:TYR:CD2	1:B:357:ARG:HG3	2.52	0.45
1:B:583:SER:OG	1:B:587:ARG:HB2	2.17	0.45
1:A:402:LEU:HD21	1:A:482:LEU:HD12	1.98	0.44
1:B:628:ARG:HE	1:B:635:ILE:HG12	1.81	0.44
1:B:775:TRP:CH2	1:B:854:LEU:HD13	2.53	0.44
1:B:859:HIS:O	1:B:863:GLN:HG3	2.18	0.44
1:B:592:LEU:HB2	1:B:593:PRO:HD3	1.99	0.44
1:B:522:VAL:HG13	1:B:536:LEU:HD13	2.00	0.43
1:B:392:ASN:HA	1:B:395:PHE:HB3	2.00	0.43
1:A:365:ARG:HG2	1:A:366:ARG:HD2	2.01	0.43
1:B:446:ASP:HB3	1:B:447:PRO:HD3	1.99	0.43
1:A:483:GLU:OE1	1:A:483:GLU:N	2.49	0.43
1:A:773:ARG:HD3	1:A:773:ARG:HA	1.89	0.43
1:B:370:LYS:HG2	1:B:381:ASP:OD2	2.19	0.43
1:B:784:ARG:NH2	1:B:813:GLU:HB3	2.34	0.42
1:B:466:VAL:HG13	1:B:473:CYS:HB2	2.01	0.42
1:B:790:LYS:NZ	1:B:790:LYS:HB2	2.34	0.42
1:B:784:ARG:NH1	1:B:788:GLN:OE1	2.52	0.42
1:B:804:LEU:HG	1:B:873:LEU:HD21	2.02	0.42
1:B:329:THR:HB	1:B:333:GLU:HG3	2.01	0.42
1:A:420:ARG:NH2	1:A:596:GLN:O	2.52	0.42
1:A:543:ASP:HB3	1:A:546:ASP:O	2.20	0.42
1:A:583:SER:OG	1:A:587:ARG:HB2	2.19	0.42
1:B:543:ASP:HB3	1:B:546:ASP:O	2.19	0.42
1:B:386:ASN:ND2	1:B:389:ALA:H	2.18	0.42
1:A:348:LEU:HD11	1:A:382:VAL:HG21	2.01	0.41
1:B:478:ASP:OD2	1:B:480:SER:HB2	2.21	0.41
1:B:855:PHE:N	1:B:856:PRO:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ARG:HB3	1:B:375:PRO:HD3	2.03	0.41
1:B:426:GLY:O	1:B:554:ASN:ND2	2.48	0.41
1:A:356:TYR:H	1:A:356:TYR:HD1	1.69	0.41
1:B:190:VAL:O	1:B:193:GLU:HB3	2.21	0.41
1:B:210:PHE:CE2	1:B:396:LEU:HB3	2.56	0.41
1:A:590:GLY:O	1:A:593:PRO:HD2	2.21	0.40
1:A:473:CYS:HA	1:A:545:PHE:CD1	2.56	0.40
1:A:582:ARG:HG3	1:A:589:TRP:CZ2	2.57	0.40
1:B:550:ASN:HB3	1:B:553:ALA:HB2	2.03	0.40
1:B:205:SER:O	1:B:211:ASP:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/573 (85%)	461 (95%)	23 (5%)	1 (0%)	47	78
1	B	474/573 (83%)	455 (96%)	19 (4%)	0	100	100
All	All	959/1146 (84%)	916 (96%)	42 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	801	ALA

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	409/467 (88%)	395 (97%)	14 (3%)	37	71
1	B	407/467 (87%)	393 (97%)	14 (3%)	37	71
All	All	816/934 (87%)	788 (97%)	28 (3%)	37	71

All (28) 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	803	TRP
1	A	806	THR
1	A	841	ARG
1	A	854	LEU
1	B	145	ASP
1	B	147	HIS
1	B	192	THR
1	B	334	LYS
1	B	355	VAL
1	B	368	VAL
1	B	386	ASN
1	B	387	ARG
1	B	530	LEU
1	B	607	THR
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	GLN
1	A	529	ASN
1	A	618	GLN
1	A	772	HIS
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 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%)	0.40	23 (4%)	31	22	34, 69, 130, 198	0
1	B	484/573 (84%)	0.44	22 (4%)	33	23	30, 71, 127, 176	0
All	All	977/1146 (85%)	0.42	45 (4%)	32	22	30, 70, 129, 198	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	799	THR	12.3
1	A	802	GLY	6.0
1	A	586	GLY	6.0
1	A	800	ARG	5.6
1	A	801	ALA	5.6
1	B	528	SER	4.6
1	B	585	ARG	4.2
1	B	802	GLY	4.2
1	A	854	LEU	4.0
1	B	527	PRO	3.9
1	B	763	SER	3.9
1	A	803	TRP	3.9
1	A	585	ARG	3.8
1	B	781	ALA	3.7
1	B	854	LEU	3.6
1	B	329	THR	3.5
1	A	525	GLY	3.5
1	B	830	LEU	3.1
1	B	333	GLU	2.9
1	B	766	TRP	2.9
1	A	780	ARG	2.9
1	A	810	VAL	2.9
1	A	830	LEU	2.8
1	A	633	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	529	ASN	2.8
1	B	526	LEU	2.7
1	A	853	GLY	2.7
1	A	794	GLY	2.7
1	B	792	GLY	2.7
1	A	528	SER	2.6
1	A	797	ALA	2.5
1	B	853	GLY	2.5
1	A	812	GLN	2.5
1	A	804	LEU	2.5
1	B	827	GLU	2.4
1	B	772	HIS	2.4
1	B	384	LEU	2.3
1	A	783	ARG	2.3
1	B	572	ASN	2.3
1	B	786	GLN	2.2
1	A	775	TRP	2.2
1	A	784	ARG	2.1
1	B	840	ASP	2.1
1	A	534	LEU	2.1
1	B	635	ILE	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
2	CL	A	1001	1/1	0.88	0.15	76,76,76,76	0
2	CL	B	1001	1/1	0.94	0.08	70,70,70,70	0

6.5 Other polymers (i)

There are no such residues in this entry.