Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 04:14 PM JST

PDB ID	:	5WU6
Title	:	Crystal structure of apo human Tut1, form IV
Authors	:	Yamashita, S.; Tomita, K.
Deposited on	:	2016-12-16
Resolution	:	3.21 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:

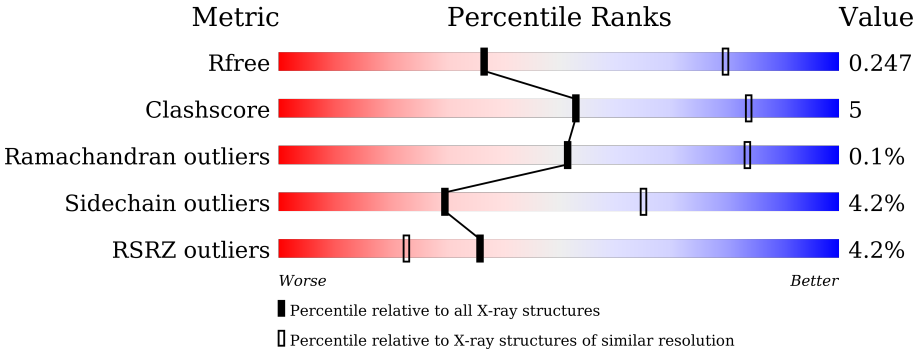
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.21 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	485	3%, 72%, 12%, •, 14%
1	B	485	3%, 71%, 14%, 15%
1	C	485	7%, 70%, 14%, •, 13%
1	D	485	59%, 11%, 30%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 12194 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	415	3183	2008	581	583	11	0	0	0
1	B	413	3163	1996	575	581	11	0	0	0
1	C	420	3224	2033	587	593	11	0	0	0
1	D	341	2617	1651	476	481	9	0	0	0

There are 340 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q9H6E5
A	?	-	CYS	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	PRO	deletion	UNP Q9H6E5
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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP Q9H6E5
A	?	-	THR	deletion	UNP Q9H6E5
A	?	-	LEU	deletion	UNP Q9H6E5
A	?	-	ALA	deletion	UNP Q9H6E5
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	600	LEU	-	expression tag	UNP Q9H6E5
A	601	GLU	-	expression tag	UNP Q9H6E5
A	602	HIS	-	expression tag	UNP Q9H6E5
A	603	HIS	-	expression tag	UNP Q9H6E5
A	604	HIS	-	expression tag	UNP Q9H6E5
A	605	HIS	-	expression tag	UNP Q9H6E5
A	606	HIS	-	expression tag	UNP Q9H6E5
A	607	HIS	-	expression tag	UNP Q9H6E5
B	53	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	399	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	574	ALA	CYS	conflict	UNP Q9H6E5
B	600	LEU	-	expression tag	UNP Q9H6E5
B	601	GLU	-	expression tag	UNP Q9H6E5
B	602	HIS	-	expression tag	UNP Q9H6E5
B	603	HIS	-	expression tag	UNP Q9H6E5
B	604	HIS	-	expression tag	UNP Q9H6E5
B	605	HIS	-	expression tag	UNP Q9H6E5
B	606	HIS	-	expression tag	UNP Q9H6E5
B	607	HIS	-	expression tag	UNP Q9H6E5
C	53	MET	-	initiating methionine	UNP Q9H6E5
C	?	-	ALA	deletion	UNP Q9H6E5
C	?	-	PRO	deletion	UNP Q9H6E5
C	?	-	GLU	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	PRO	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	LEU	deletion	UNP Q9H6E5
C	?	-	ASP	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	ALA	deletion	UNP Q9H6E5
C	?	-	LEU	deletion	UNP Q9H6E5
C	?	-	ALA	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	PRO	deletion	UNP Q9H6E5
C	?	-	LEU	deletion	UNP Q9H6E5
C	?	-	ASP	deletion	UNP Q9H6E5
C	?	-	PRO	deletion	UNP Q9H6E5
C	?	-	GLN	deletion	UNP Q9H6E5

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ALA	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	GLU	deletion	UNP Q9H6E5
C	?	-	THR	deletion	UNP Q9H6E5
C	?	-	LEU	deletion	UNP Q9H6E5
C	?	-	ALA	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	PRO	deletion	UNP Q9H6E5
C	?	-	GLN	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	372	ALA	CYS	conflict	UNP Q9H6E5
C	399	ALA	CYS	conflict	UNP Q9H6E5
C	415	ALA	CYS	conflict	UNP Q9H6E5
C	501	ALA	CYS	conflict	UNP Q9H6E5
C	504	SER	CYS	conflict	UNP Q9H6E5
C	574	ALA	CYS	conflict	UNP Q9H6E5
C	600	LEU	-	expression tag	UNP Q9H6E5
C	601	GLU	-	expression tag	UNP Q9H6E5
C	602	HIS	-	expression tag	UNP Q9H6E5
C	603	HIS	-	expression tag	UNP Q9H6E5
C	604	HIS	-	expression tag	UNP Q9H6E5
C	605	HIS	-	expression tag	UNP Q9H6E5
C	606	HIS	-	expression tag	UNP Q9H6E5
C	607	HIS	-	expression tag	UNP Q9H6E5
D	53	MET	-	initiating methionine	UNP Q9H6E5
D	?	-	ALA	deletion	UNP Q9H6E5
D	?	-	PRO	deletion	UNP Q9H6E5
D	?	-	GLU	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	?	-	PRO	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	?	-	LEU	deletion	UNP Q9H6E5
D	?	-	ASP	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	?	-	ALA	deletion	UNP Q9H6E5
D	?	-	LEU	deletion	UNP Q9H6E5
D	?	-	ALA	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	?	-	PRO	deletion	UNP Q9H6E5
D	?	-	LEU	deletion	UNP Q9H6E5
D	?	-	ASP	deletion	UNP Q9H6E5
D	?	-	PRO	deletion	UNP Q9H6E5

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

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	LEU	deletion	UNP Q9H6E5
D	?	-	ALA	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	?	-	GLU	deletion	UNP Q9H6E5
D	?	-	THR	deletion	UNP Q9H6E5
D	?	-	LEU	deletion	UNP Q9H6E5
D	?	-	ALA	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	?	-	PRO	deletion	UNP Q9H6E5
D	?	-	GLN	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	372	ALA	CYS	conflict	UNP Q9H6E5
D	399	ALA	CYS	conflict	UNP Q9H6E5
D	415	ALA	CYS	conflict	UNP Q9H6E5
D	501	ALA	CYS	conflict	UNP Q9H6E5
D	504	SER	CYS	conflict	UNP Q9H6E5
D	574	ALA	CYS	conflict	UNP Q9H6E5
D	600	LEU	-	expression tag	UNP Q9H6E5
D	601	GLU	-	expression tag	UNP Q9H6E5
D	602	HIS	-	expression tag	UNP Q9H6E5
D	603	HIS	-	expression tag	UNP Q9H6E5
D	604	HIS	-	expression tag	UNP Q9H6E5
D	605	HIS	-	expression tag	UNP Q9H6E5
D	606	HIS	-	expression tag	UNP Q9H6E5
D	607	HIS	-	expression tag	UNP Q9H6E5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

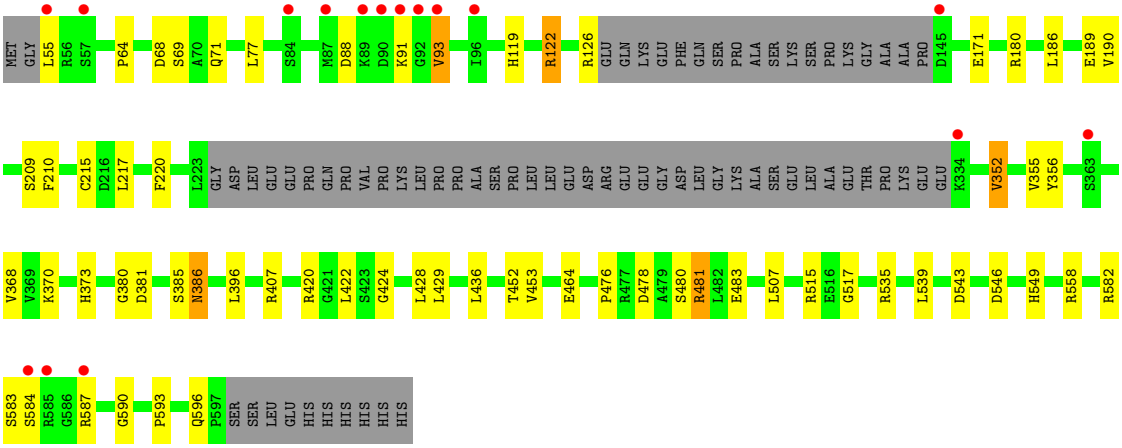
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	2	Total Mg 2 2	0	0
2	D	1	Total Mg 1 1	0	0

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.

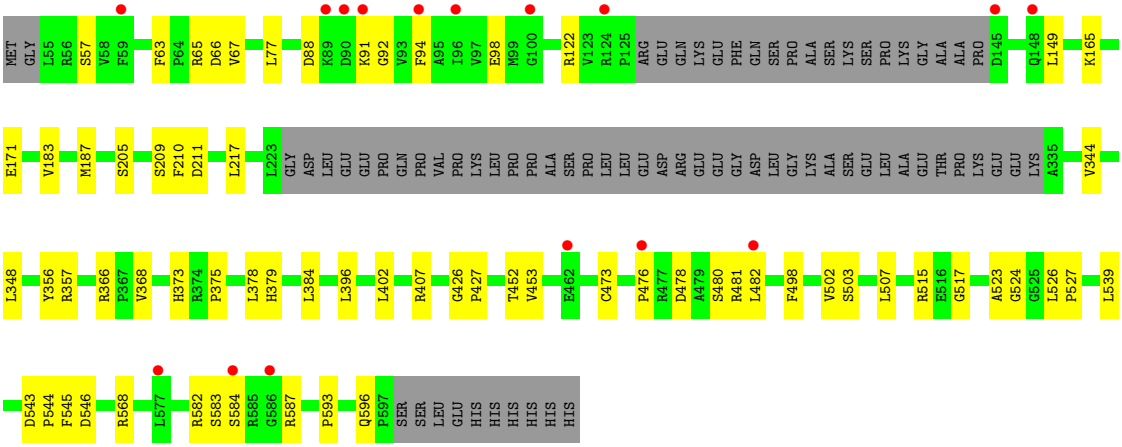
• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase

Chain A:



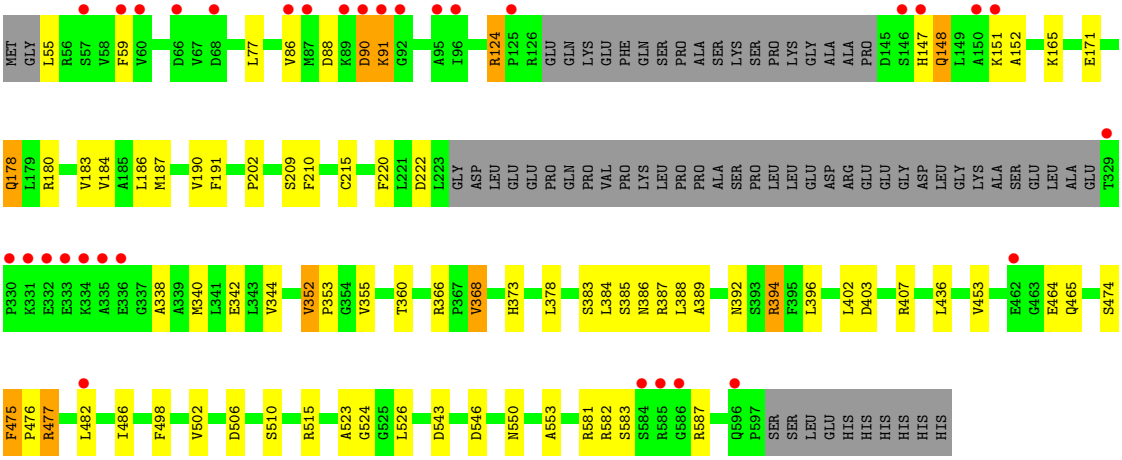
• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase

Chain B:



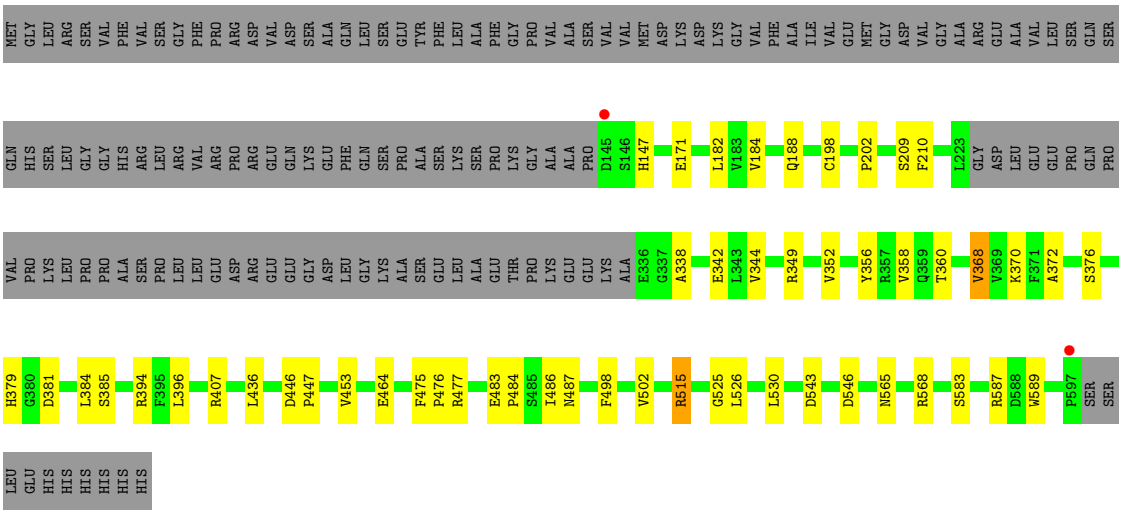
• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase

Chain C:



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

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	142.53Å 142.53Å 282.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.21 49.61 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-3.21) 99.9 (49.61-3.21)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.202 , 0.242 0.211 , 0.247	Depositor DCC
R_{free} test set	2420 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	70.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12194	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: MG

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	0.21	0/3247	0.40	0/4403
1	B	0.22	0/3227	0.40	0/4378
1	C	0.22	0/3289	0.41	0/4460
1	D	0.21	0/2671	0.40	0/3629
All	All	0.22	0/12434	0.40	0/16870

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	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	386	ASN	Peptide
1	D	385	SER	Peptide

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	3183	0	3194	32	0
1	B	3163	0	3168	36	0
1	C	3224	0	3233	37	0
1	D	2617	0	2624	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	1	0	0	0	0
All	All	12194	0	12219	132	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 5.

All (132) 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:C:209:SER:O	1:C:407:ARG:NH1	2.03	0.92
1:B:209:SER:O	1:B:407:ARG:NH1	2.10	0.83
1:A:209:SER:O	1:A:407:ARG:NH1	2.13	0.81
1:D:209:SER:O	1:D:407:ARG:NH1	2.17	0.78
1:A:535:ARG:HH12	1:A:549:HIS:HA	1.49	0.75
1:D:525:GLY:HA3	1:D:526:LEU:HD13	1.70	0.73
1:C:394:ARG:HH21	1:C:477:ARG:HG3	1.54	0.71
1:C:178:GLN:HG2	1:D:376:SER:HA	1.76	0.68
1:C:344:VAL:HG21	1:C:384:LEU:HD21	1.80	0.64
1:B:402:LEU:HD21	1:B:482:LEU:HD12	1.80	0.63
1:D:188:GLN:NE2	1:D:198:CYS:O	2.31	0.62
1:D:349:ARG:HD3	1:D:358:VAL:HB	1.80	0.62
1:A:420:ARG:NH2	1:A:596:GLN:O	2.33	0.62
1:B:344:VAL:HG21	1:B:384:LEU:HD21	1.81	0.62
1:C:152:ALA:HB1	1:C:165:LYS:HE3	1.83	0.61
1:C:222:ASP:OD1	1:C:387:ARG:NH2	2.33	0.61
1:A:370:LYS:HG2	1:A:381:ASP:OD2	2.01	0.61
1:D:210:PHE:HE2	1:D:396:LEU:HB3	1.66	0.60
1:B:481:ARG:HH11	1:B:481:ARG:HA	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLU:OE1	1:D:407:ARG:NH2	2.36	0.59
1:A:68:ASP:HB3	1:A:71:GLN:HG3	1.85	0.59
1:D:453:VAL:HB	1:D:515:ARG:HA	1.84	0.58
1:C:464:GLU:OE2	1:C:476:PRO:HA	2.03	0.58
1:B:210:PHE:HE2	1:B:396:LEU:HB3	1.68	0.58
1:A:558:ARG:HH11	1:A:558:ARG:HA	1.69	0.57
1:C:402:LEU:HD21	1:C:482:LEU:HD12	1.86	0.57
1:C:148:GLN:HA	1:C:151:LYS:HE2	1.86	0.57
1:B:88:ASP:HB3	1:B:92:GLY:HA3	1.88	0.56
1:B:63:PHE:HB2	1:B:67:VAL:HG11	1.88	0.56
1:D:184:VAL:HG21	1:D:202:PRO:HG3	1.86	0.56
1:D:344:VAL:HG21	1:D:384:LEU:HD21	1.87	0.56
1:C:186:LEU:HD21	1:C:353:PRO:HG2	1.88	0.55
1:A:478:ASP:OD2	1:A:480:SER:OG	2.24	0.55
1:D:446:ASP:HB3	1:D:447:PRO:HD3	1.88	0.55
1:A:476:PRO:HB3	1:A:481:ARG:HE	1.73	0.54
1:D:565:ASN:OD1	1:D:568:ARG:NH2	2.40	0.54
1:D:464:GLU:OE2	1:D:477:ARG:HG2	2.08	0.53
1:B:217:LEU:HD22	1:B:378:LEU:HD13	1.91	0.53
1:D:583:SER:OG	1:D:587:ARG:N	2.42	0.53
1:A:210:PHE:HE2	1:A:396:LEU:HB3	1.73	0.53
1:A:453:VAL:HB	1:A:515:ARG:HA	1.91	0.53
1:C:210:PHE:HE2	1:C:396:LEU:HB3	1.72	0.53
1:A:88:ASP:OD2	1:A:91:LYS:HB2	2.09	0.52
1:C:506:ASP:O	1:C:510:SER:OG	2.25	0.52
1:C:59:PHE:HB3	1:C:124:ARG:HG3	1.90	0.52
1:A:171:GLU:OE1	1:A:407:ARG:NH2	2.43	0.52
1:B:481:ARG:HA	1:B:481:ARG:NH1	2.24	0.51
1:A:220:PHE:HE1	1:A:385:SER:HA	1.75	0.51
1:A:190:VAL:HG21	1:A:352:VAL:HB	1.93	0.51
1:C:582:ARG:HG2	1:C:583:SER:H	1.77	0.50
1:C:180:ARG:NH2	1:C:215:CYS:O	2.44	0.50
1:C:389:ALA:HA	1:C:392:ASN:ND2	2.26	0.50
1:C:453:VAL:HB	1:C:515:ARG:HA	1.93	0.50
1:B:183:VAL:HG21	1:B:378:LEU:HD12	1.93	0.49
1:D:368:VAL:HG21	1:D:381:ASP:HB3	1.93	0.49
1:B:171:GLU:OE1	1:B:407:ARG:NH2	2.45	0.49
1:A:582:ARG:HG2	1:A:583:SER:H	1.76	0.49
1:D:447:PRO:HD2	1:D:487:ASN:HD22	1.79	0.48
1:A:122:ARG:HH22	1:A:587:ARG:HD2	1.78	0.48
1:A:507:LEU:HG	1:A:539:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:OE2	1:A:476:PRO:HA	2.14	0.48
1:B:503:SER:HB2	1:B:568:ARG:HD3	1.96	0.48
1:A:64:PRO:HD3	1:A:119:HIS:HB2	1.96	0.48
1:B:210:PHE:CE2	1:B:396:LEU:HB3	2.48	0.48
1:D:543:ASP:HB3	1:D:546:ASP:O	2.13	0.47
1:D:498:PHE:O	1:D:502:VAL:HG22	2.14	0.47
1:D:210:PHE:CE2	1:D:396:LEU:HB3	2.49	0.47
1:B:582:ARG:HG2	1:B:583:SER:H	1.80	0.47
1:A:424:GLY:N	1:A:429:LEU:O	2.38	0.47
1:B:356:TYR:CD2	1:B:357:ARG:HG3	2.50	0.47
1:C:498:PHE:O	1:C:502:VAL:HG22	2.15	0.47
1:C:583:SER:OG	1:C:587:ARG:HB2	2.15	0.47
1:B:476:PRO:HG2	1:B:482:LEU:HD11	1.97	0.47
1:B:593:PRO:HA	1:B:596:GLN:HB2	1.96	0.47
1:C:373:HIS:HE1	1:D:182:LEU:HD21	1.80	0.47
1:C:90:ASP:N	1:C:91:LYS:HA	2.30	0.46
1:A:483:GLU:OE1	1:A:483:GLU:N	2.42	0.46
1:C:183:VAL:HG21	1:C:378:LEU:HD12	1.96	0.46
1:B:498:PHE:O	1:B:502:VAL:HG22	2.15	0.46
1:C:465:GLN:HA	1:C:474:SER:HB3	1.97	0.46
1:B:453:VAL:HB	1:B:515:ARG:HA	1.98	0.46
1:D:370:LYS:HG2	1:D:381:ASP:OD2	2.16	0.46
1:A:220:PHE:CE1	1:A:385:SER:HA	2.51	0.46
1:B:373:HIS:CE1	1:B:375:PRO:HD2	2.51	0.46
1:C:220:PHE:HE1	1:C:385:SER:HA	1.80	0.46
1:D:372:ALA:HA	1:D:379:HIS:HA	1.98	0.46
1:A:422:LEU:O	1:A:428:LEU:HB3	2.16	0.45
1:C:338:ALA:O	1:C:342:GLU:HG2	2.16	0.45
1:D:583:SER:HB2	1:D:589:TRP:HB3	1.99	0.45
1:A:68:ASP:OD1	1:A:69:SER:N	2.50	0.45
1:A:543:ASP:HB3	1:A:546:ASP:O	2.17	0.45
1:B:426:GLY:HA3	1:B:427:PRO:HD2	1.85	0.45
1:C:187:MET:HE3	1:C:191:PHE:HE2	1.82	0.45
1:A:355:VAL:HA	1:A:373:HIS:HA	1.99	0.44
1:D:447:PRO:HB3	1:D:486:ILE:HG13	2.00	0.44
1:B:478:ASP:OD2	1:B:480:SER:HB2	2.18	0.44
1:D:338:ALA:O	1:D:342:GLU:HG2	2.18	0.44
1:B:543:ASP:HB3	1:B:546:ASP:O	2.18	0.43
1:A:180:ARG:NH2	1:A:215:CYS:O	2.50	0.43
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.80	0.43
1:B:584:SER:H	1:B:587:ARG:NH2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:VAL:HG21	1:B:544:PRO:HB3	2.00	0.43
1:D:483:GLU:HA	1:D:484:PRO:HD3	1.88	0.43
1:B:88:ASP:HB2	1:B:94:PHE:CZ	2.52	0.43
1:C:523:ALA:HA	1:C:524:GLY:HA2	1.70	0.43
1:C:184:VAL:HG21	1:C:202:PRO:HG3	2.01	0.43
1:C:581:ARG:HG2	1:C:582:ARG:N	2.31	0.43
1:B:66:ASP:OD1	1:B:66:ASP:N	2.52	0.43
1:B:57:SER:HA	1:B:98:GLU:HA	2.01	0.42
1:D:464:GLU:OE2	1:D:476:PRO:HA	2.19	0.42
1:B:523:ALA:HA	1:B:524:GLY:HA2	1.60	0.42
1:C:91:LYS:H	1:C:91:LYS:HD2	1.85	0.42
1:B:452:THR:HG22	1:B:517:GLY:HA3	2.02	0.42
1:B:187:MET:HE3	1:B:348:LEU:HD21	2.02	0.42
1:A:590:GLY:O	1:A:593:PRO:HD2	2.20	0.41
1:B:526:LEU:N	1:B:527:PRO:HD3	2.35	0.41
1:A:546:ASP:OD2	1:A:549:HIS:HB2	2.20	0.41
1:C:210:PHE:CE2	1:C:396:LEU:HB3	2.54	0.41
1:C:394:ARG:HD2	1:C:475:PHE:CZ	2.55	0.41
1:C:550:ASN:HB3	1:C:553:ALA:HB2	2.01	0.41
1:B:205:SER:O	1:B:211:ASP:HB3	2.21	0.41
1:C:543:ASP:HB3	1:C:546:ASP:O	2.21	0.41
1:D:394:ARG:HD2	1:D:475:PHE:HE1	1.84	0.41
1:A:452:THR:HG22	1:A:517:GLY:HA3	2.01	0.41
1:C:368:VAL:HG23	1:C:383:SER:HB2	2.02	0.41
1:B:473:CYS:HA	1:B:545:PHE:CD1	2.56	0.41
1:A:584:SER:H	1:A:587:ARG:HH21	1.67	0.41
1:C:171:GLU:OE1	1:C:407:ARG:NH2	2.53	0.41
1:D:446:ASP:HB3	1:D:447:PRO:CD	2.50	0.41
1:B:507:LEU:HG	1:B:539:LEU:HD13	2.03	0.40
1:C:190:VAL:HG21	1:C:352:VAL:HA	2.03	0.40
1:A:217:LEU:O	1:A:380:GLY:HA3	2.21	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	409/485 (84%)	398 (97%)	10 (2%)	1 (0%)	47	79
1	B	407/485 (84%)	385 (95%)	22 (5%)	0	100	100
1	C	414/485 (85%)	397 (96%)	17 (4%)	0	100	100
1	D	337/485 (70%)	325 (96%)	12 (4%)	0	100	100
All	All	1567/1940 (81%)	1505 (96%)	61 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	VAL

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	343/402 (85%)	330 (96%)	13 (4%)	33	67
1	B	341/402 (85%)	332 (97%)	9 (3%)	46	76
1	C	348/402 (87%)	323 (93%)	25 (7%)	14	47
1	D	283/402 (70%)	275 (97%)	8 (3%)	43	74
All	All	1315/1608 (82%)	1260 (96%)	55 (4%)	30	65

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	77	LEU
1	A	93	VAL
1	A	122	ARG
1	A	126	ARG
1	A	186	LEU
1	A	189	GLU

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Mol	Chain	Res	Type
1	A	352	VAL
1	A	356	TYR
1	A	368	VAL
1	A	386	ASN
1	A	436	LEU
1	A	481	ARG
1	B	65	ARG
1	B	77	LEU
1	B	91	LYS
1	B	122	ARG
1	B	149	LEU
1	B	165	LYS
1	B	366	ARG
1	B	368	VAL
1	B	379	HIS
1	C	55	LEU
1	C	77	LEU
1	C	86	VAL
1	C	88	ASP
1	C	90	ASP
1	C	91	LYS
1	C	124	ARG
1	C	147	HIS
1	C	148	GLN
1	C	178	GLN
1	C	340	MET
1	C	352	VAL
1	C	355	VAL
1	C	360	THR
1	C	366	ARG
1	C	368	VAL
1	C	386	ASN
1	C	388	LEU
1	C	394	ARG
1	C	403	ASP
1	C	436	LEU
1	C	475	PHE
1	C	477	ARG
1	C	486	ILE
1	C	526	LEU
1	D	147	HIS
1	D	352	VAL

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Mol	Chain	Res	Type
1	D	356	TYR
1	D	360	THR
1	D	368	VAL
1	D	436	LEU
1	D	515	ARG
1	D	530	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	373	HIS
1	C	148	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 7 ligands modelled in this entry, 7 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	415/485 (85%)	0.24	16 (3%)	39	25	39, 66, 126, 192	0
1	B	413/485 (85%)	0.29	16 (3%)	39	25	44, 72, 136, 190	0
1	C	420/485 (86%)	0.31	32 (7%)	13	7	40, 68, 136, 211	0
1	D	341/485 (70%)	-0.01	2 (0%)	89	83	37, 56, 99, 165	0
All	All	1589/1940 (81%)	0.22	66 (4%)	36	23	37, 66, 126, 211	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	ASP	6.4
1	A	90	ASP	6.1
1	C	91	LYS	5.7
1	B	91	LYS	5.5
1	B	89	LYS	5.2
1	C	330	PRO	5.0
1	B	462	GLU	4.4
1	C	329	THR	4.4
1	C	333	GLU	4.1
1	D	145	ASP	4.1
1	B	90	ASP	4.1
1	C	147	HIS	3.9
1	C	331	LYS	3.8
1	A	91	LYS	3.7
1	B	586	GLY	3.7
1	C	92	GLY	3.6
1	C	146	SER	3.5
1	C	586	GLY	3.4
1	C	332	GLU	3.4
1	A	585	ARG	3.4
1	C	57	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	145	ASP	3.1
1	B	584	SER	3.1
1	A	93	VAL	3.1
1	C	89	LYS	3.0
1	B	577	LEU	2.9
1	A	89	LYS	2.9
1	A	87	MET	2.8
1	C	86	VAL	2.7
1	A	92	GLY	2.7
1	A	334	LYS	2.7
1	C	87	MET	2.6
1	A	84	SER	2.6
1	A	584	SER	2.6
1	B	100	GLY	2.6
1	B	96	ILE	2.6
1	B	145	ASP	2.6
1	C	596	GLN	2.5
1	A	587	ARG	2.5
1	B	476	PRO	2.5
1	C	585	ARG	2.5
1	C	68	ASP	2.4
1	C	336	GLU	2.4
1	C	151	LYS	2.3
1	B	148	GLN	2.3
1	B	482	LEU	2.3
1	A	96	ILE	2.3
1	C	334	LYS	2.3
1	C	66	ASP	2.2
1	C	462	GLU	2.2
1	C	584	SER	2.2
1	C	95	ALA	2.2
1	A	57	SER	2.1
1	C	96	ILE	2.1
1	C	150	ALA	2.1
1	B	124	ARG	2.1
1	B	94	PHE	2.1
1	B	59	PHE	2.1
1	C	125	PRO	2.1
1	A	55	LEU	2.1
1	C	59	PHE	2.0
1	C	60	VAL	2.0
1	C	335	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	363	SER	2.0
1	C	482	LEU	2.0
1	D	597	PRO	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	MG	A	1002	1/1	0.64	0.23	94,94,94,94	0
2	MG	C	1001	1/1	0.75	0.33	57,57,57,57	0
2	MG	A	1001	1/1	0.89	0.26	57,57,57,57	0
2	MG	B	1002	1/1	0.93	0.46	48,48,48,48	0
2	MG	B	1001	1/1	0.93	0.44	46,46,46,46	0
2	MG	C	1002	1/1	0.93	0.33	40,40,40,40	0
2	MG	D	701	1/1	0.95	0.33	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.