Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 04:37 PM JST

PDB ID	:	5WU5
Title	:	Crystal structure of apo human Tut1, form III
Authors	:	Yamashita, S.; Tomita, K.
Deposited on	:	2016-12-16
Resolution	:	3.40 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:

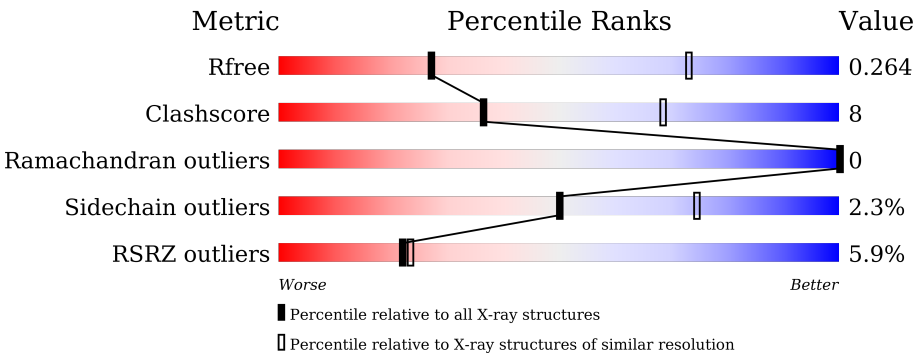
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	3%, 65%, 19%, •, 15%
1	B	573	5%, 68%, 16%, •, 16%
1	C	573	5%, 68%, 16%, 15%
1	D	573	6%, 67%, 17%, •, 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 15026 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	485	3760	2376	686	682	16	0	0	0
1	B	483	3752	2371	684	681	16	0	0	0
1	C	485	3763	2378	686	683	16	0	0	0
1	D	483	3751	2371	683	681	16	0	0	0

There are 724 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

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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	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

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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	501	ALA	CYS	engineered mutation	UNP Q9H6E5
B	504	SER	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
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
C	140	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	501	ALA	CYS	engineered mutation	UNP Q9H6E5
C	504	SER	CYS	engineered mutation	UNP Q9H6E5
C	?	-	GLU	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	?	-	GLN	deletion	UNP Q9H6E5
C	?	-	GLY	deletion	UNP Q9H6E5
C	?	-	GLY	deletion	UNP Q9H6E5

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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LYS	deletion	UNP Q9H6E5
C	?	-	GLY	deletion	UNP Q9H6E5
C	?	-	HIS	deletion	UNP Q9H6E5
C	?	-	GLU	deletion	UNP Q9H6E5
C	?	-	ALA	deletion	UNP Q9H6E5
C	?	-	ALA	deletion	UNP Q9H6E5
C	?	-	GLN	deletion	UNP Q9H6E5
C	?	-	GLU	deletion	UNP Q9H6E5
C	?	-	TRP	deletion	UNP Q9H6E5
C	?	-	SER	deletion	UNP Q9H6E5
C	875	LEU	-	expression tag	UNP Q9H6E5
C	876	GLU	-	expression tag	UNP Q9H6E5
C	877	HIS	-	expression tag	UNP Q9H6E5
C	878	HIS	-	expression tag	UNP Q9H6E5
C	879	HIS	-	expression tag	UNP Q9H6E5
C	880	HIS	-	expression tag	UNP Q9H6E5
C	881	HIS	-	expression tag	UNP Q9H6E5
C	882	HIS	-	expression tag	UNP Q9H6E5
D	140	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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

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

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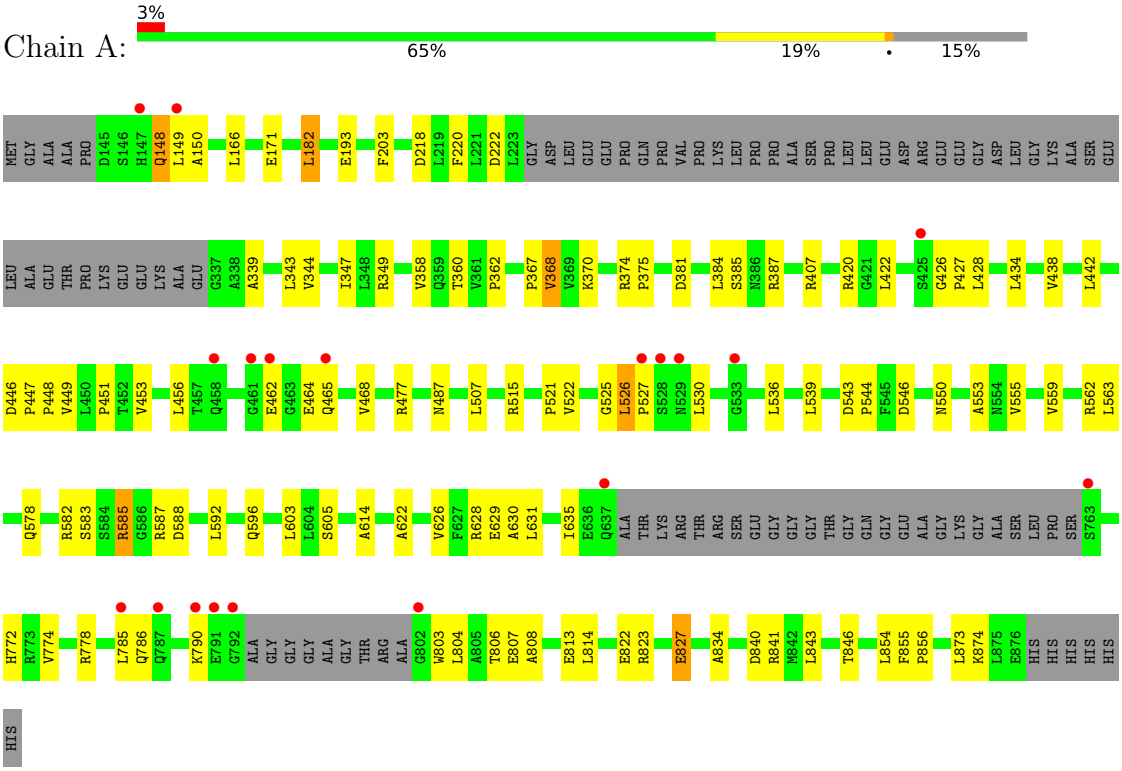
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP Q9H6E5
D	?	-	GLN	deletion	UNP Q9H6E5
D	?	-	PRO	deletion	UNP Q9H6E5
D	?	-	SER	deletion	UNP Q9H6E5
D	?	-	HIS	deletion	UNP Q9H6E5
D	?	-	ALA	deletion	UNP Q9H6E5
D	?	-	ALA	deletion	UNP Q9H6E5
D	?	-	LEU	deletion	UNP Q9H6E5
D	?	-	ALA	deletion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

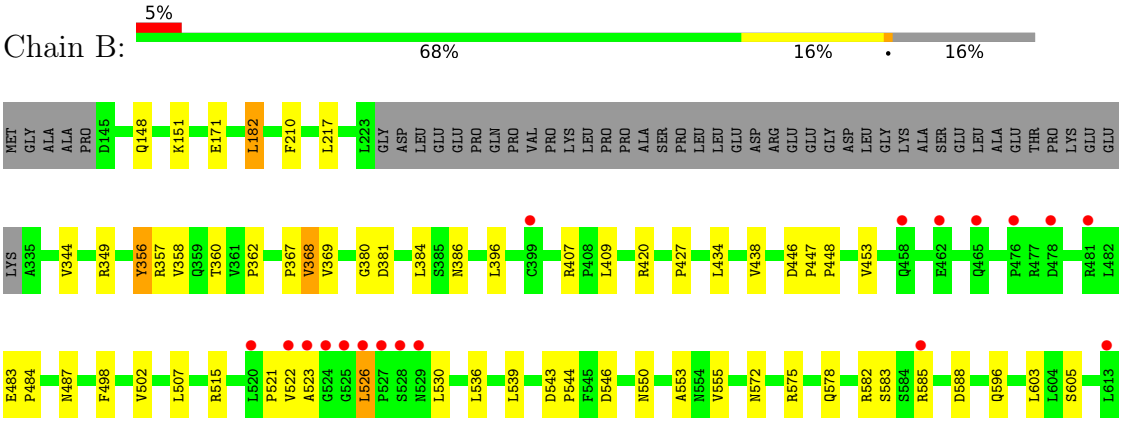
3 Residue-property plots (i)

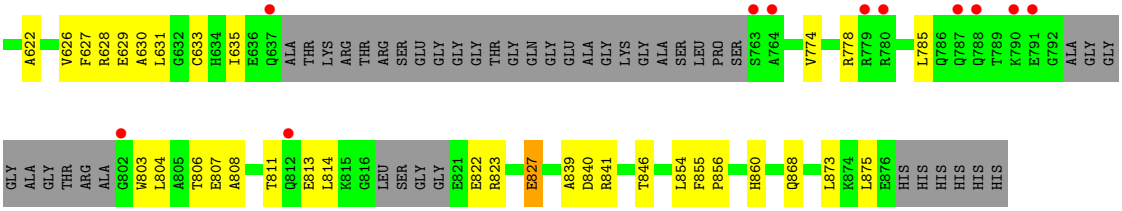
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



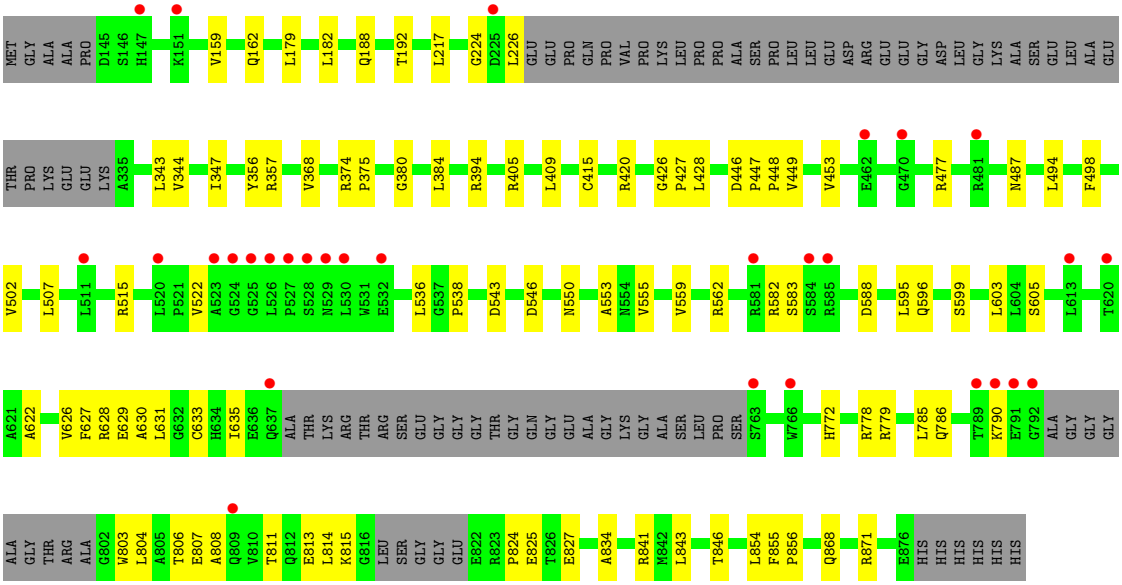
• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase





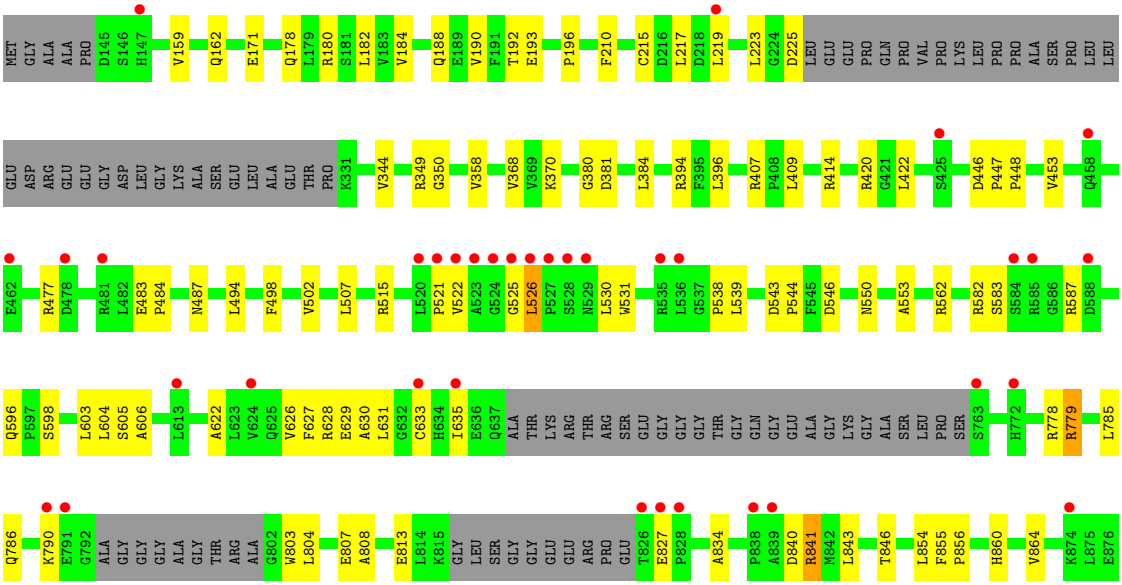
• Molecule 1: Speckle targeted PIP5K1A-regulated poly(A) polymerase

Chain C:



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

Chain D:



HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	173.14Å 173.14Å 208.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.40 48.02 – 3.40	Depositor EDS
% Data completeness (in resolution range)	89.7 (19.99-3.40) 89.8 (48.02-3.40)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.214 , 0.258 0.218 , 0.264	Depositor DCC
R_{free} test set	1984 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	15026	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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)

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	0/3843	0.44	0/5222
1	B	0.23	0/3834	0.45	0/5209
1	C	0.23	0/3845	0.44	0/5224
1	D	0.23	0/3832	0.42	0/5204
All	All	0.23	0/15354	0.44	0/20859

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	3760	0	3773	71	1
1	B	3752	0	3761	59	1
1	C	3763	0	3773	53	1
1	D	3751	0	3765	66	0
All	All	15026	0	15072	237	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (237) 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:D:210:PHE:HB3	1:D:414:ARG:HH22	1.40	0.86
1:A:521:PRO:HG2	1:A:525:GLY:HA3	1.59	0.83
1:A:344:VAL:HG21	1:A:384:LEU:HD21	1.68	0.74
1:D:420:ARG:NH2	1:D:596:GLN:O	2.21	0.73
1:A:526:LEU:HD23	1:A:530:LEU:HD21	1.72	0.72
1:C:420:ARG:NH2	1:C:596:GLN:O	2.23	0.70
1:D:522:VAL:HA	1:D:526:LEU:HD22	1.72	0.70
1:C:868:GLN:OE1	1:C:871:ARG:NH1	2.25	0.70
1:A:874:LYS:HB3	1:C:224:GLY:HA2	1.72	0.70
1:D:785:LEU:HD11	1:D:813:GLU:HG3	1.75	0.68
1:A:605:SER:HB2	1:A:846:THR:HG22	1.76	0.68
1:B:778:ARG:HG2	1:B:814:LEU:HD11	1.76	0.67
1:A:420:ARG:O	1:A:562:ARG:NH1	2.27	0.67
1:C:785:LEU:HD11	1:C:813:GLU:HG3	1.76	0.67
1:B:344:VAL:HG21	1:B:384:LEU:HD21	1.76	0.67
1:A:827:GLU:OE2	1:A:827:GLU:HA	1.95	0.66
1:D:370:LYS:HG2	1:D:381:ASP:OD2	1.96	0.66
1:D:779:ARG:HA	1:D:779:ARG:HH11	1.61	0.65
1:D:420:ARG:O	1:D:562:ARG:NH2	2.30	0.65
1:A:874:LYS:HG2	1:C:226:LEU:HG	1.77	0.65
1:C:605:SER:HB2	1:C:846:THR:HG22	1.79	0.64
1:A:453:VAL:HB	1:A:515:ARG:HA	1.79	0.64
1:B:420:ARG:NH2	1:B:596:GLN:O	2.30	0.64
1:A:420:ARG:NH2	1:A:596:GLN:O	2.31	0.63
1:B:578:GLN:NE2	1:B:588:ASP:O	2.31	0.63
1:A:778:ARG:HH21	1:A:807:GLU:HG3	1.63	0.62
1:D:605:SER:HB2	1:D:846:THR:HG22	1.81	0.61
1:C:344:VAL:HG21	1:C:384:LEU:HD21	1.83	0.61
1:D:223:LEU:HD11	1:D:384:LEU:HD22	1.83	0.60
1:B:522:VAL:HG13	1:B:536:LEU:HD13	1.83	0.60
1:B:360:THR:HG22	1:B:369:VAL:HG22	1.83	0.60
1:A:149:LEU:HD11	1:A:166:LEU:HD13	1.84	0.59
1:B:446:ASP:HB3	1:B:447:PRO:HD3	1.84	0.59
1:A:370:LYS:HD3	1:B:357:ARG:HH21	1.66	0.59
1:B:778:ARG:HH21	1:B:807:GLU:HG3	1.67	0.58
1:D:422:LEU:HD21	1:D:562:ARG:HE	1.68	0.58
1:A:446:ASP:HB3	1:A:447:PRO:HD3	1.84	0.58
1:D:344:VAL:HG21	1:D:384:LEU:HD21	1.85	0.58
1:C:446:ASP:HB3	1:C:447:PRO:HD3	1.85	0.58
1:D:171:GLU:OE1	1:D:407:ARG:NH2	2.34	0.57
1:A:840:ASP:OD1	1:A:841:ARG:N	2.37	0.57
1:C:453:VAL:HB	1:C:515:ARG:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HG2	1:A:381:ASP:OD2	2.04	0.57
1:D:446:ASP:HB3	1:D:447:PRO:HD3	1.85	0.57
1:D:521:PRO:HG2	1:D:525:GLY:HA3	1.86	0.57
1:B:572:ASN:OD1	1:B:575:ARG:NH2	2.35	0.57
1:A:362:PRO:HA	1:A:367:PRO:HB3	1.86	0.56
1:A:785:LEU:HD11	1:A:813:GLU:HG3	1.87	0.56
1:A:804:LEU:HG	1:A:873:LEU:HD21	1.88	0.55
1:A:171:GLU:OE1	1:A:407:ARG:NH2	2.32	0.55
1:A:614:ALA:O	1:A:841:ARG:NH2	2.39	0.55
1:D:394:ARG:HD3	1:D:477:ARG:HH22	1.71	0.54
1:D:778:ARG:HH21	1:D:807:GLU:HG3	1.71	0.54
1:D:827:GLU:OE2	1:D:827:GLU:N	2.40	0.54
1:D:453:VAL:HB	1:D:515:ARG:HA	1.89	0.54
1:B:582:ARG:HG2	1:B:583:SER:H	1.72	0.54
1:C:582:ARG:HG2	1:C:583:SER:H	1.72	0.53
1:D:840:ASP:OD1	1:D:841:ARG:N	2.42	0.53
1:C:217:LEU:O	1:C:380:GLY:HA3	2.08	0.53
1:C:394:ARG:HD3	1:C:477:ARG:HH22	1.74	0.52
1:C:420:ARG:O	1:C:562:ARG:NH1	2.41	0.52
1:D:582:ARG:HG2	1:D:583:SER:H	1.74	0.52
1:C:630:ALA:H	1:C:808:ALA:HB2	1.75	0.52
1:D:834:ALA:HB1	1:D:843:LEU:HD11	1.90	0.52
1:B:778:ARG:NH2	1:B:807:GLU:HG3	2.24	0.52
1:D:210:PHE:O	1:D:414:ARG:NH2	2.42	0.52
1:A:778:ARG:NH2	1:A:807:GLU:HG3	2.24	0.52
1:B:453:VAL:HB	1:B:515:ARG:HA	1.92	0.52
1:C:507:LEU:HB3	1:C:538:PRO:O	2.09	0.51
1:C:427:PRO:O	1:C:555:VAL:HA	2.11	0.51
1:B:349:ARG:HD3	1:B:358:VAL:HB	1.93	0.51
1:B:840:ASP:OD1	1:B:841:ARG:N	2.43	0.51
1:C:772:HIS:CD2	1:C:815:LYS:HD2	2.45	0.51
1:A:522:VAL:HA	1:A:526:LEU:HD22	1.91	0.51
1:A:550:ASN:HB3	1:A:553:ALA:HB2	1.93	0.51
1:D:779:ARG:HH11	1:D:779:ARG:CA	2.23	0.51
1:C:543:ASP:HB3	1:C:546:ASP:O	2.11	0.51
1:C:428:LEU:HA	1:C:559:VAL:HG11	1.91	0.51
1:C:628:ARG:HH21	1:C:635:ILE:HD11	1.75	0.50
1:A:447:PRO:O	1:A:487:ASN:HB2	2.12	0.50
1:D:446:ASP:O	1:D:448:PRO:HD3	2.12	0.50
1:C:405:ARG:NH1	1:C:487:ASN:OD1	2.44	0.50
1:D:521:PRO:O	1:D:526:LEU:HD13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:583:SER:OG	1:D:587:ARG:HB2	2.12	0.49
1:C:446:ASP:O	1:C:448:PRO:HD3	2.12	0.49
1:B:785:LEU:HD11	1:B:813:GLU:HG3	1.94	0.49
1:A:442:LEU:HB3	1:A:449:VAL:HB	1.94	0.49
1:B:630:ALA:H	1:B:808:ALA:HB2	1.78	0.49
1:B:774:VAL:HG12	1:B:778:ARG:NH1	2.28	0.48
1:D:210:PHE:HB3	1:D:414:ARG:NH2	2.19	0.48
1:D:409:LEU:HD11	1:D:494:LEU:HB3	1.93	0.48
1:A:585:ARG:HH21	1:A:587:ARG:HH21	1.60	0.48
1:B:446:ASP:O	1:B:448:PRO:HD3	2.12	0.48
1:C:629:GLU:C	1:C:631:LEU:H	2.17	0.48
1:C:550:ASN:HB3	1:C:553:ALA:HB2	1.94	0.48
1:B:171:GLU:OE1	1:B:407:ARG:NH2	2.45	0.48
1:C:622:ALA:O	1:C:626:VAL:HG23	2.14	0.48
1:D:526:LEU:HG	1:D:530:LEU:HD21	1.95	0.48
1:B:362:PRO:HA	1:B:367:PRO:HB3	1.95	0.48
1:B:521:PRO:O	1:B:526:LEU:HD13	2.14	0.48
1:B:356:TYR:H	1:B:356:TYR:HD2	1.61	0.47
1:A:446:ASP:O	1:A:448:PRO:HD3	2.14	0.47
1:B:605:SER:HB2	1:B:846:THR:HG22	1.95	0.47
1:D:543:ASP:HB3	1:D:546:ASP:O	2.14	0.47
1:A:543:ASP:HB3	1:A:546:ASP:O	2.15	0.47
1:A:339:ALA:HB1	1:D:350:GLY:HA2	1.97	0.47
1:D:184:VAL:HG22	1:D:219:LEU:HD21	1.97	0.47
1:D:562:ARG:NH1	1:D:606:ALA:HB2	2.29	0.47
1:D:420:ARG:NE	1:D:598:SER:OG	2.43	0.47
1:D:629:GLU:C	1:D:631:LEU:H	2.19	0.46
1:D:498:PHE:O	1:D:502:VAL:HG22	2.14	0.46
1:B:629:GLU:C	1:B:631:LEU:H	2.19	0.46
1:D:447:PRO:O	1:D:487:ASN:HB2	2.16	0.46
1:C:188:GLN:NE2	1:C:192:THR:OG1	2.42	0.46
1:C:834:ALA:HB1	1:C:843:LEU:HD11	1.97	0.46
1:A:427:PRO:O	1:A:555:VAL:HA	2.16	0.46
1:C:384:LEU:HD23	1:C:384:LEU:HA	1.78	0.46
1:D:210:PHE:CE2	1:D:396:LEU:HB3	2.51	0.46
1:A:822:GLU:O	1:A:823:ARG:HB2	2.16	0.46
1:C:447:PRO:O	1:C:487:ASN:HB2	2.16	0.46
1:A:453:VAL:HG21	1:A:544:PRO:HB3	1.98	0.46
1:C:778:ARG:HH21	1:C:807:GLU:HG3	1.81	0.46
1:A:193:GLU:OE2	1:B:868:GLN:HG2	2.16	0.45
1:A:451:PRO:HG2	1:A:456:LEU:HD21	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:PHE:O	1:C:502:VAL:HG22	2.16	0.45
1:B:627:PHE:O	1:B:633:CYS:HB2	2.16	0.45
1:B:522:VAL:HA	1:B:526:LEU:HD22	1.97	0.45
1:D:530:LEU:HB3	1:D:531:TRP:CE3	2.51	0.45
1:A:150:ALA:HA	1:A:592:LEU:HD21	1.98	0.45
1:A:834:ALA:HB1	1:A:843:LEU:HD11	1.98	0.45
1:B:217:LEU:O	1:B:380:GLY:HA3	2.16	0.45
1:B:521:PRO:C	1:B:523:ALA:H	2.20	0.45
1:A:374:ARG:HB3	1:A:375:PRO:HD3	1.99	0.45
1:A:629:GLU:C	1:A:631:LEU:H	2.21	0.45
1:A:630:ALA:H	1:A:808:ALA:HB2	1.82	0.45
1:C:405:ARG:NH2	1:C:449:VAL:HG13	2.31	0.45
1:D:384:LEU:HD23	1:D:384:LEU:HA	1.83	0.45
1:D:786:GLN:O	1:D:790:LYS:HG2	2.17	0.45
1:A:806:THR:HG23	1:A:807:GLU:N	2.32	0.44
1:A:628:ARG:HH21	1:A:635:ILE:HD11	1.82	0.44
1:B:806:THR:HG23	1:B:807:GLU:N	2.33	0.44
1:D:210:PHE:HE2	1:D:396:LEU:HB3	1.81	0.44
1:B:875:LEU:HD23	1:D:223:LEU:O	2.17	0.44
1:C:179:LEU:HG	1:D:864:VAL:HG21	1.97	0.44
1:C:343:LEU:O	1:C:347:ILE:HG13	2.17	0.44
1:D:855:PHE:N	1:D:856:PRO:HD2	2.33	0.44
1:B:550:ASN:HB3	1:B:553:ALA:HB2	2.00	0.44
1:B:855:PHE:N	1:B:856:PRO:HD2	2.33	0.44
1:D:453:VAL:HG21	1:D:544:PRO:HB3	2.00	0.44
1:D:217:LEU:O	1:D:380:GLY:HA3	2.18	0.44
1:D:507:LEU:HG	1:D:539:LEU:HD13	2.00	0.44
1:A:428:LEU:HA	1:A:559:VAL:HG11	2.00	0.44
1:B:434:LEU:O	1:B:438:VAL:HG23	2.17	0.44
1:B:804:LEU:HA	1:B:804:LEU:HD23	1.85	0.44
1:A:368:VAL:HG21	1:A:381:ASP:HB3	2.00	0.44
1:A:587:ARG:HA	1:A:587:ARG:HD3	1.71	0.44
1:A:622:ALA:O	1:A:626:VAL:HG23	2.18	0.43
1:A:772:HIS:NE2	1:A:814:LEU:HB3	2.33	0.43
1:C:588:ASP:OD1	1:C:588:ASP:N	2.51	0.43
1:C:415:CYS:HB3	1:C:595:LEU:HD22	2.00	0.43
1:D:507:LEU:HB3	1:D:538:PRO:O	2.19	0.43
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.90	0.43
1:C:786:GLN:O	1:C:790:LYS:HG2	2.18	0.43
1:D:804:LEU:HD23	1:D:804:LEU:HA	1.84	0.43
1:A:220:PHE:HE1	1:A:385:SER:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:PHE:O	1:C:633:CYS:HB2	2.19	0.43
1:C:772:HIS:CG	1:C:815:LYS:HD2	2.54	0.43
1:C:394:ARG:HD3	1:C:477:ARG:NH2	2.34	0.43
1:A:370:LYS:HD3	1:B:357:ARG:NH2	2.33	0.43
1:A:526:LEU:HD12	1:A:526:LEU:HA	1.85	0.43
1:A:855:PHE:N	1:A:856:PRO:HD2	2.33	0.43
1:A:774:VAL:HG12	1:A:778:ARG:NH1	2.34	0.43
1:C:374:ARG:HB3	1:C:375:PRO:HD3	2.00	0.42
1:B:498:PHE:O	1:B:502:VAL:HG22	2.20	0.42
1:B:811:THR:O	1:B:814:LEU:HB2	2.19	0.42
1:A:203:PHE:CZ	1:A:218:ASP:HB3	2.54	0.42
1:A:582:ARG:HG2	1:A:583:SER:H	1.83	0.42
1:B:839:ALA:HA	1:B:840:ASP:HA	1.91	0.42
1:C:522:VAL:HG13	1:C:536:LEU:HD13	2.01	0.42
1:A:786:GLN:O	1:A:790:LYS:HG2	2.19	0.42
1:B:628:ARG:HE	1:B:635:ILE:HD11	1.84	0.42
1:C:804:LEU:HD23	1:C:804:LEU:HA	1.80	0.42
1:D:190:VAL:O	1:D:193:GLU:HB3	2.19	0.42
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.86	0.42
1:C:824:PRO:HD2	1:C:827:GLU:HG3	2.02	0.42
1:D:630:ALA:H	1:D:808:ALA:HB2	1.83	0.42
1:B:875:LEU:HD13	1:D:196:PRO:O	2.20	0.42
1:D:188:GLN:NE2	1:D:192:THR:OG1	2.47	0.42
1:D:349:ARG:HG3	1:D:358:VAL:HG21	2.02	0.42
1:A:434:LEU:O	1:A:438:VAL:HG23	2.19	0.42
1:B:526:LEU:HD23	1:B:530:LEU:HD21	2.01	0.42
1:B:483:GLU:HA	1:B:484:PRO:HD3	1.95	0.42
1:B:543:ASP:HB3	1:B:546:ASP:O	2.20	0.42
1:B:210:PHE:HE2	1:B:396:LEU:HB3	1.85	0.42
1:B:622:ALA:O	1:B:626:VAL:HG23	2.20	0.42
1:A:525:GLY:O	1:A:527:PRO:HD3	2.20	0.41
1:D:778:ARG:NH2	1:D:807:GLU:HG3	2.33	0.41
1:A:182:LEU:HD23	1:B:860:HIS:CE1	2.56	0.41
1:C:778:ARG:H	1:D:178:GLN:NE2	2.17	0.41
1:C:806:THR:HG23	1:C:807:GLU:N	2.35	0.41
1:A:530:LEU:HD21	1:A:536:LEU:HD11	2.02	0.41
1:B:804:LEU:HG	1:B:873:LEU:HD21	2.02	0.41
1:D:180:ARG:NH2	1:D:215:CYS:O	2.53	0.41
1:A:507:LEU:HG	1:A:539:LEU:HD13	2.02	0.41
1:B:822:GLU:O	1:B:823:ARG:HB2	2.21	0.41
1:A:222:ASP:CG	1:A:387:ARG:HH22	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:OE2	1:A:477:ARG:HG2	2.20	0.41
1:B:447:PRO:HB2	1:B:487:ASN:HD22	1.86	0.41
1:C:356:TYR:CE2	1:C:357:ARG:HG3	2.56	0.41
1:A:804:LEU:HD23	1:A:804:LEU:HA	1.87	0.41
1:B:507:LEU:HG	1:B:539:LEU:HD13	2.03	0.41
1:C:409:LEU:HD11	1:C:494:LEU:HB3	2.03	0.41
1:D:627:PHE:O	1:D:633:CYS:HB2	2.21	0.41
1:D:628:ARG:HH21	1:D:635:ILE:HD11	1.86	0.41
1:A:587:ARG:O	1:A:592:LEU:HD22	2.21	0.41
1:B:182:LEU:HD12	1:B:182:LEU:HA	1.88	0.41
1:C:426:GLY:HA3	1:C:427:PRO:HD2	1.91	0.41
1:C:855:PHE:N	1:C:856:PRO:HD2	2.36	0.41
1:D:159:VAL:O	1:D:162:GLN:HB2	2.21	0.41
1:D:483:GLU:HA	1:D:484:PRO:HD3	1.93	0.41
1:D:622:ALA:O	1:D:626:VAL:HG23	2.21	0.41
1:A:349:ARG:HD3	1:A:358:VAL:HB	2.03	0.41
1:A:426:GLY:HA3	1:A:427:PRO:HD2	1.93	0.41
1:A:578:GLN:NE2	1:A:588:ASP:O	2.43	0.41
1:C:825:GLU:H	1:C:825:GLU:CD	2.24	0.41
1:D:779:ARG:HA	1:D:779:ARG:HD3	1.60	0.41
1:C:811:THR:O	1:C:814:LEU:HB2	2.21	0.40
1:A:148:GLN:CD	1:B:148:GLN:HB2	2.40	0.40
1:B:368:VAL:HG21	1:B:381:ASP:HB3	2.03	0.40
1:B:427:PRO:O	1:B:555:VAL:HA	2.21	0.40
1:B:453:VAL:HG21	1:B:544:PRO:HB3	2.03	0.40
1:A:343:LEU:O	1:A:347:ILE:HG13	2.22	0.40
1:A:422:LEU:HD13	1:A:563:LEU:HD12	2.02	0.40
1:C:159:VAL:O	1:C:162:GLN:HB2	2.22	0.40
1:D:550:ASN:HB3	1:D:553:ALA:HB2	2.02	0.40
1:A:387:ARG:HB3	1:A:468:VAL:HG11	2.03	0.40
1:D:604:LEU:HD11	1:D:860:HIS:CE1	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:GLU:OE2	1:C:599:SER:OG[5_554]	1.97	0.23
1:A:462:GLU:OE2	1:A:465:GLN:NE2[8_554]	2.09	0.11

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	477/573 (83%)	456 (96%)	21 (4%)	0	100	100
1	B	473/573 (82%)	449 (95%)	24 (5%)	0	100	100
1	C	475/573 (83%)	457 (96%)	18 (4%)	0	100	100
1	D	473/573 (82%)	455 (96%)	18 (4%)	0	100	100
All	All	1898/2292 (83%)	1817 (96%)	81 (4%)	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	410/471 (87%)	400 (98%)	10 (2%)	49	74
1	B	409/471 (87%)	398 (97%)	11 (3%)	44	70
1	C	410/471 (87%)	403 (98%)	7 (2%)	60	80
1	D	409/471 (87%)	400 (98%)	9 (2%)	52	75
All	All	1638/1884 (87%)	1601 (98%)	37 (2%)	50	74

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	182	LEU

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Mol	Chain	Res	Type
1	A	360	THR
1	A	368	VAL
1	A	526	LEU
1	A	585	ARG
1	A	603	LEU
1	A	803	TRP
1	A	827	GLU
1	A	854	LEU
1	B	151	LYS
1	B	182	LEU
1	B	356	TYR
1	B	368	VAL
1	B	386	ASN
1	B	526	LEU
1	B	585	ARG
1	B	603	LEU
1	B	803	TRP
1	B	827	GLU
1	B	854	LEU
1	C	182	LEU
1	C	368	VAL
1	C	603	LEU
1	C	779	ARG
1	C	803	TRP
1	C	841	ARG
1	C	854	LEU
1	D	182	LEU
1	D	225	ASP
1	D	368	VAL
1	D	526	LEU
1	D	603	LEU
1	D	779	ARG
1	D	803	TRP
1	D	841	ARG
1	D	854	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no ligands in this entry.

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	485/573 (84%)	0.30	19 (3%)	39	38	21, 48, 106, 148	0
1	B	483/573 (84%)	0.32	29 (6%)	21	23	20, 50, 107, 156	0
1	C	485/573 (84%)	0.42	30 (6%)	20	21	23, 50, 100, 155	0
1	D	483/573 (84%)	0.60	36 (7%)	14	16	22, 63, 116, 197	0
All	All	1936/2292 (84%)	0.41	114 (5%)	22	23	20, 52, 110, 197	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	528	SER	12.6
1	B	763	SER	9.6
1	D	527	PRO	8.1
1	D	525	GLY	6.9
1	C	790	LYS	6.8
1	C	525	GLY	6.7
1	C	524	GLY	5.8
1	C	528	SER	5.5
1	D	526	LEU	5.2
1	A	790	LYS	5.1
1	C	763	SER	5.0
1	D	791	GLU	4.9
1	D	523	ALA	4.8
1	C	527	PRO	4.8
1	B	791	GLU	4.8
1	B	528	SER	4.7
1	D	462	GLU	4.6
1	C	613	LEU	4.3
1	B	527	PRO	4.2
1	B	529	ASN	4.2
1	A	791	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	827	GLU	4.0
1	D	585	ARG	3.9
1	C	791	GLU	3.9
1	D	529	ASN	3.8
1	B	525	GLY	3.8
1	A	528	SER	3.7
1	C	585	ARG	3.6
1	D	874	LYS	3.6
1	A	787	GLN	3.6
1	C	529	ASN	3.6
1	D	524	GLY	3.5
1	B	523	ALA	3.4
1	C	581	ARG	3.4
1	A	763	SER	3.4
1	B	637	GLN	3.3
1	B	520	LEU	3.3
1	C	462	GLU	3.3
1	B	526	LEU	3.2
1	B	476	PRO	3.2
1	C	532	GLU	3.2
1	A	792	GLY	3.2
1	B	764	ALA	3.2
1	D	763	SER	3.2
1	C	637	GLN	3.1
1	C	792	GLY	3.1
1	D	522	VAL	3.0
1	A	527	PRO	3.0
1	C	470	GLY	3.0
1	D	790	LYS	2.9
1	D	425	SER	2.8
1	B	780	ARG	2.8
1	A	637	GLN	2.8
1	C	789	THR	2.8
1	B	802	GLY	2.8
1	A	462	GLU	2.8
1	D	520	LEU	2.7
1	C	523	ALA	2.7
1	B	481	ARG	2.7
1	C	526	LEU	2.7
1	D	458	GLN	2.7
1	D	838	PRO	2.7
1	B	478	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	812	GLN	2.6
1	B	790	LYS	2.6
1	C	530	LEU	2.6
1	D	828	PRO	2.6
1	D	633	CYS	2.6
1	D	521	PRO	2.5
1	B	787	GLN	2.5
1	D	584	SER	2.5
1	B	524	GLY	2.4
1	B	613	LEU	2.4
1	B	462	GLU	2.4
1	A	458	GLN	2.4
1	B	522	VAL	2.4
1	D	613	LEU	2.4
1	B	788	GLN	2.4
1	A	533	GLY	2.4
1	A	529	ASN	2.4
1	B	465	GLN	2.3
1	D	839	ALA	2.3
1	C	520	LEU	2.3
1	D	624	VAL	2.3
1	D	147	HIS	2.3
1	D	588	ASP	2.3
1	A	461	GLY	2.3
1	C	511	LEU	2.3
1	D	536	LEU	2.3
1	D	826	THR	2.2
1	C	809	GLN	2.2
1	B	779	ARG	2.2
1	A	147	HIS	2.2
1	B	399	CYS	2.2
1	D	478	ASP	2.1
1	C	151	LYS	2.1
1	A	149	LEU	2.1
1	C	147	HIS	2.1
1	A	425	SER	2.1
1	D	535	ARG	2.1
1	D	772	HIS	2.1
1	A	465	GLN	2.1
1	B	458	GLN	2.1
1	C	620	THR	2.1
1	C	481	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	481	ARG	2.1
1	A	802	GLY	2.1
1	D	635	ILE	2.0
1	C	766	TRP	2.0
1	C	584	SER	2.0
1	C	225	ASP	2.0
1	A	785	LEU	2.0
1	D	219	LEU	2.0
1	B	585	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.