



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2017 – 09:27 AM EDT

PDB ID : 5XQ1
Title : Structural basis of kindlin-mediated integrin recognition and activation
Authors : Li, H.; Yang, H.; Sun, K.; Zhang, Z.; Yu, C.; Wei, Z.
Deposited on : unknown
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

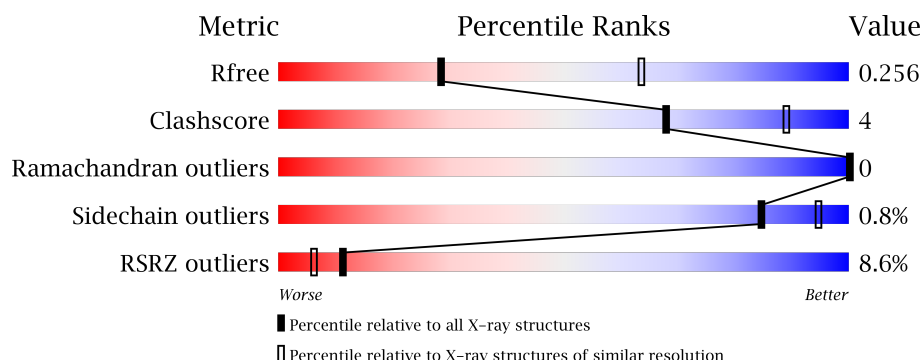
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$. 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	<div> <div>3%</div> <div>78%</div> <div>10%</div> <div>12%</div> </div>
1	B	485	<div> <div>12%</div> <div>74%</div> <div>11%</div> <div>15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6712 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 Fermitin family homolog 2, Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3447	2221	585	621	20			
1	B	411	Total	C	N	O	S	0	0	0
			3260	2101	548	591	20			

There are 484 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP Q8CIB5
A	-2	MET	-	expression tag	UNP Q8CIB5
A	-1	GLY	-	expression tag	UNP Q8CIB5
A	0	SER	-	expression tag	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	MET	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	MET	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	HIS	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	TRP	deletion	UNP Q8CIB5
A	?	-	PHE	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	VAL	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	VAL	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	VAL	deletion	UNP Q8CIB5
A	?	-	PHE	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	TRP	deletion	UNP Q8CIB5
A	?	-	CYS	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	PHE	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	CYS	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	ARG	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	HIS	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ARG	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	CYS	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	VAL	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	VAL	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	PHE	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	VAL	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	MET	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	TRP	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ARG	deletion	UNP Q8CIB5
A	?	-	CYS	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	HIS	deletion	UNP Q8CIB5
A	?	-	TRP	deletion	UNP Q8CIB5
A	?	-	MET	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	CYS	deletion	UNP Q8CIB5
A	?	-	ARG	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	GLY	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	THR	deletion	UNP Q8CIB5
A	?	-	MET	deletion	UNP Q8CIB5
A	?	-	ALA	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	TYR	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	GLU	deletion	UNP Q8CIB5
A	?	-	VAL	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	SER	deletion	UNP Q8CIB5
A	?	-	PHE	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	LYS	deletion	UNP Q8CIB5
A	?	-	MET	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	HIS	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ASN	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	LEU	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	?	-	PRO	deletion	UNP Q8CIB5
A	?	-	ASP	deletion	UNP Q8CIB5
A	?	-	GLN	deletion	UNP Q8CIB5
A	?	-	ILE	deletion	UNP Q8CIB5
A	761	LEU	-	linker	UNP Q8CIB5
A	762	VAL	-	linker	UNP Q8CIB5
A	763	PRO	-	linker	UNP Q8CIB5
A	764	ARG	-	linker	UNP Q8CIB5
A	765	GLY	-	linker	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	766	SER	-	linker	UNP Q8CIB5
A	767	GLY	-	linker	UNP Q8CIB5
A	768	SER	-	linker	UNP Q8CIB5
A	769	GLY	-	linker	UNP Q8CIB5
A	770	SER	-	linker	UNP Q8CIB5
A	771	GLY	-	linker	UNP Q8CIB5
A	772	SER	-	linker	UNP Q8CIB5
B	-3	HIS	-	expression tag	UNP Q8CIB5
B	-2	MET	-	expression tag	UNP Q8CIB5
B	-1	GLY	-	expression tag	UNP Q8CIB5
B	0	SER	-	expression tag	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	MET	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	MET	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	HIS	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	TRP	deletion	UNP Q8CIB5
B	?	-	PHE	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	VAL	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	VAL	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	VAL	deletion	UNP Q8CIB5
B	?	-	PHE	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	TRP	deletion	UNP Q8CIB5
B	?	-	CYS	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	PHE	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	CYS	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	ARG	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	HIS	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ARG	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	CYS	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	VAL	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	VAL	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	PHE	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	VAL	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	MET	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	TRP	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ARG	deletion	UNP Q8CIB5
B	?	-	CYS	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	HIS	deletion	UNP Q8CIB5
B	?	-	TRP	deletion	UNP Q8CIB5
B	?	-	MET	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	CYS	deletion	UNP Q8CIB5
B	?	-	ARG	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	GLY	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	THR	deletion	UNP Q8CIB5
B	?	-	MET	deletion	UNP Q8CIB5
B	?	-	ALA	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	TYR	deletion	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	GLU	deletion	UNP Q8CIB5
B	?	-	VAL	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	SER	deletion	UNP Q8CIB5
B	?	-	PHE	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	LYS	deletion	UNP Q8CIB5
B	?	-	MET	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	HIS	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ASN	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	LEU	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	?	-	PRO	deletion	UNP Q8CIB5
B	?	-	ASP	deletion	UNP Q8CIB5
B	?	-	GLN	deletion	UNP Q8CIB5
B	?	-	ILE	deletion	UNP Q8CIB5
B	761	LEU	-	linker	UNP Q8CIB5
B	762	VAL	-	linker	UNP Q8CIB5
B	763	PRO	-	linker	UNP Q8CIB5
B	764	ARG	-	linker	UNP Q8CIB5
B	765	GLY	-	linker	UNP Q8CIB5
B	766	SER	-	linker	UNP Q8CIB5
B	767	GLY	-	linker	UNP Q8CIB5
B	768	SER	-	linker	UNP Q8CIB5
B	769	GLY	-	linker	UNP Q8CIB5
B	770	SER	-	linker	UNP Q8CIB5
B	771	GLY	-	linker	UNP Q8CIB5
B	772	SER	-	linker	UNP Q8CIB5

- Molecule 2 is water.

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	75.97Å 75.97Å 387.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.99 – 2.95 37.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.5 (37.99-2.95) 95.4 (37.99-2.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.220 , 0.260 0.215 , 0.256	Depositor DCC
R_{free} test set	1355 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	82.2	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.042 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6712	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.25	1/3522 (0.0%)	0.39	0/4766
1	B	0.22	0/3331	0.39	0/4516
All	All	0.24	1/6853 (0.0%)	0.39	0/9282

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	640	GLU	CD-OE2	6.95	1.33	1.25

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	3447	0	3418	30	0
1	B	3260	0	3179	29	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
All	All	6712	0	6597	58	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 4.

All (58) 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:99:LEU:HD21	1:B:270:LEU:HD12	1.72	0.69
1:B:514:THR:HG23	1:B:516:VAL:H	1.56	0.68
1:A:20:LEU:HD12	1:A:35:VAL:HG11	1.77	0.65
1:B:137:GLU:OE2	1:B:659:ARG:NH2	2.31	0.65
1:A:32:THR:O	1:A:51:LYS:NZ	2.25	0.64
1:B:65:TRP:CZ3	1:B:68:LYS:HD3	2.33	0.63
1:A:101:LEU:HD11	1:A:126:ILE:HD13	1.82	0.62
1:A:550:SER:OG	1:B:557:ARG:NH2	2.33	0.61
1:A:514:THR:HG23	1:A:516:VAL:H	1.66	0.60
1:B:79:LEU:HD22	1:B:84:ILE:HD12	1.85	0.59
1:A:100:ARG:HE	1:A:110:LYS:HE2	1.68	0.58
1:B:20:LEU:HD12	1:B:35:VAL:HG21	1.85	0.57
1:A:137:GLU:OE2	1:A:659:ARG:NH2	2.37	0.57
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.87	0.56
1:B:104:PRO:HB3	1:B:297:GLN:HB2	1.87	0.56
1:A:610:SER:HB2	1:A:785:ARG:HD2	1.88	0.56
1:B:84:ILE:HD13	1:B:90:LEU:HD11	1.87	0.55
1:B:65:TRP:CH2	1:B:68:LYS:HD3	2.42	0.55
1:A:79:LEU:HD22	1:A:84:ILE:HD12	1.89	0.53
1:B:628:PHE:HB2	1:B:632:VAL:HB	1.89	0.53
1:B:585:LEU:HB2	1:B:596:MET:HB2	1.90	0.53
1:B:287:ASP:HB3	1:B:290:ARG:HB3	1.91	0.51
1:A:74:LYS:HG3	1:A:77:TRP:CD2	2.46	0.50
1:B:612:MET:HE1	1:B:654:ILE:HD11	1.93	0.50
1:B:656:LEU:O	1:B:659:ARG:HD3	2.12	0.49
1:A:104:PRO:HB3	1:A:297:GLN:HB2	1.94	0.48
1:B:97:LYS:HD3	1:B:266:GLU:HB2	1.94	0.48
1:A:97:LYS:HB3	1:A:266:GLU:HG3	1.94	0.48
1:A:119:VAL:HB	1:A:255:SER:HA	1.96	0.48
1:A:97:LYS:HB2	1:A:115:PHE:CE1	2.49	0.48
1:B:623:MET:HB2	1:B:637:ILE:HG12	1.95	0.48
1:B:119:VAL:HB	1:B:255:SER:HA	1.97	0.47
1:A:612:MET:HE1	1:A:654:ILE:HD11	1.96	0.47
1:A:240:GLN:OE1	1:A:240:GLN:N	2.46	0.47
1:A:622:LYS:HE2	1:A:640:GLU:HG3	1.97	0.46
1:A:144:PRO:HG3	1:A:248:THR:HG23	1.97	0.46
1:A:102:GLN:HB2	1:A:108:TYR:CE1	2.51	0.45
1:A:161:ASP:OD1	1:A:161:ASP:N	2.50	0.45
1:A:108:TYR:O	1:A:164:LEU:HB3	2.17	0.45
1:A:74:LYS:HG3	1:A:77:TRP:CE3	2.52	0.44
1:B:97:LYS:HB2	1:B:115:PHE:CE1	2.52	0.44
1:A:71:TRP:HB3	1:A:73:LEU:HG	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:MET:HB2	1:A:637:ILE:HG12	2.00	0.43
1:B:283:ASN:HA	1:B:284:PRO:HD2	1.89	0.43
1:B:613:LYS:HE3	1:B:629:ALA:HA	1.99	0.43
1:B:26:ASP:OD1	1:B:26:ASP:N	2.52	0.42
1:A:26:ASP:N	1:A:26:ASP:OD1	2.52	0.42
1:A:662:ASP:N	1:A:662:ASP:OD1	2.52	0.42
1:B:41:ILE:HG23	1:B:63:LEU:HD12	2.00	0.42
1:B:250:GLN:HG2	1:B:642:ASP:OD1	2.19	0.42
1:A:141:LEU:HB3	1:A:271:LEU:HB2	2.02	0.42
1:B:589:ALA:HB3	1:B:592:ARG:HG2	2.01	0.42
1:A:74:LYS:HD3	1:A:74:LYS:H	1.84	0.41
1:B:61:HIS:HA	1:B:94:PRO:HA	2.02	0.41
1:A:605:LYS:HD3	1:A:607:TRP:CZ2	2.56	0.41
1:B:613:LYS:HE2	1:B:784:TYR:OH	2.21	0.41
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.96	0.40
1:B:36:THR:HB	1:B:39:VAL:HG23	2.02	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	421/485 (87%)	408 (97%)	13 (3%)	0	100	100
1	B	403/485 (83%)	395 (98%)	8 (2%)	0	100	100
All	All	824/970 (85%)	803 (98%)	21 (2%)	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	369/433 (85%)	365 (99%)	4 (1%)	78	92
1	B	343/433 (79%)	341 (99%)	2 (1%)	89	96
All	All	712/866 (82%)	706 (99%)	6 (1%)	85	95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	LYS
1	A	260	MET
1	A	643	CYS
1	A	662	ASP
1	B	30	ASP
1	B	305	GLU

Some 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	429/485 (88%)	0.27	16 (3%) 42 27	41, 81, 139, 193	0
1	B	411/485 (84%)	0.68	56 (13%) 3 2	57, 98, 163, 217	0
All	All	840/970 (86%)	0.47	72 (8%) 11 6	41, 89, 154, 217	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	87	ASP	7.5
1	B	39	VAL	6.6
1	B	41	ILE	5.9
1	B	84	ILE	5.5
1	B	79	LEU	5.2
1	B	20	LEU	4.9
1	B	27	LEU	4.5
1	B	48	LEU	4.4
1	B	35	VAL	4.2
1	B	44	VAL	4.2
1	B	228	THR	4.1
1	B	98	LEU	4.0
1	B	92	PHE	4.0
1	B	673	TYR	4.0
1	B	782	ILE	3.9
1	A	84	ILE	3.8
1	B	63	LEU	3.8
1	B	45	MET	3.8
1	B	675	LEU	3.7
1	B	779	PHE	3.6
1	B	49	VAL	3.6
1	B	33	LEU	3.6
1	B	88	ALA	3.5
1	B	266	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	20	LEU	3.4
1	A	640	GLU	3.4
1	B	58	TRP	3.3
1	A	540	LEU	3.2
1	B	43	GLY	3.1
1	A	218	PRO	3.0
1	A	88	ALA	3.0
1	B	640	GLU	3.0
1	B	24	VAL	3.0
1	B	26	ASP	3.0
1	B	54	VAL	3.0
1	B	75	THR	2.9
1	B	56	LYS	2.9
1	B	100	ARG	2.9
1	B	82	CYS	2.9
1	B	77	TRP	2.9
1	B	660	ALA	2.8
1	B	25	THR	2.7
1	B	112	LYS	2.7
1	B	674	LYS	2.7
1	B	40	HIS	2.7
1	A	35	VAL	2.7
1	B	53	ASP	2.6
1	B	220	ILE	2.5
1	B	85	GLN	2.5
1	A	533	LYS	2.5
1	B	777	SER	2.4
1	B	57	ASP	2.4
1	A	41	ILE	2.4
1	B	668	ASP	2.4
1	A	519	GLU	2.4
1	B	21	SER	2.3
1	B	99	LEU	2.3
1	A	628	PHE	2.3
1	A	18	TRP	2.2
1	B	110	LYS	2.2
1	B	108	TYR	2.2
1	B	107	LYS	2.2
1	B	267	ASN	2.2
1	B	42	GLY	2.1
1	B	280	PHE	2.1
1	A	516	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	36	THR	2.1
1	B	34	ARG	2.1
1	B	36	THR	2.1
1	A	534	GLN	2.1
1	A	517	ASN	2.1
1	B	532	SER	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 carbohydrates 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.