



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2023 – 06:12 PM JST

PDB ID : 5XQ0
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 : 2017-06-05
Resolution : 2.75 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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

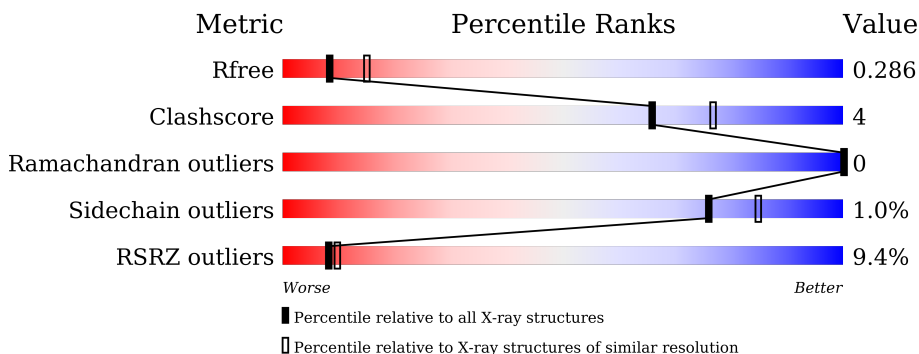
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 $\leq 5\%$. 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	
1	B	485	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6670 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-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	424	3410	2203	578	609	20	0	0	0
1	B	410	3225	2078	541	586	20	0	0	0

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	681	LEU	-	linker	UNP Q8CIB5
A	682	VAL	-	linker	UNP Q8CIB5
A	774	PRO	-	linker	UNP Q8CIB5
A	775	ARG	-	linker	UNP Q8CIB5
A	776	GLY	-	linker	UNP Q8CIB5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	777	SER	-	linker	UNP Q8CIB5
A	778	GLY	-	linker	UNP Q8CIB5
A	779	SER	-	linker	UNP Q8CIB5
A	780	GLY	-	linker	UNP Q8CIB5
A	781	SER	-	linker	UNP Q8CIB5
A	782	GLY	-	linker	UNP Q8CIB5
A	783	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	772	LEU	-	linker	UNP Q8CIB5
B	773	VAL	-	linker	UNP Q8CIB5
B	774	PRO	-	linker	UNP Q8CIB5
B	775	ARG	-	linker	UNP Q8CIB5
B	776	GLY	-	linker	UNP Q8CIB5
B	777	SER	-	linker	UNP Q8CIB5
B	778	GLY	-	linker	UNP Q8CIB5
B	779	SER	-	linker	UNP Q8CIB5
B	780	GLY	-	linker	UNP Q8CIB5
B	781	SER	-	linker	UNP Q8CIB5
B	782	GLY	-	linker	UNP Q8CIB5
B	783	SER	-	linker	UNP Q8CIB5

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C O	0	0
			6	3 3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	9	Total	O	0	0
			9	9		

4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	75.87Å 75.87Å 384.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.86 – 2.75 45.86 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.86-2.75) 95.1 (45.86-2.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.73Å)	Xtrriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.232 , 0.284 0.237 , 0.286	Depositor DCC
R_{free} test set	1734 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6670	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL

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	1/3487 (0.0%)	0.36	0/4722
1	B	0.20	0/3295	0.35	0/4474
All	All	0.23	1/6782 (0.0%)	0.36	0/9196

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	640	GLU	CD-OE2	6.87	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	3410	0	3390	21	0
1	B	3225	0	3118	35	0
2	A	6	0	8	1	0
3	A	20	0	0	0	0
3	B	9	0	0	0	0
All	All	6670	0	6516	53	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.

The worst 5 of 53 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:114:ASN:ND2	1:B:117:ASP:OD2	2.25	0.70
1:B:104:PRO:HB3	1:B:297:GLN:HB2	1.79	0.64
1:A:287:ASP:HB3	1:A:290:ARG:HB3	1.80	0.63
1:B:628:PHE:HB2	1:B:632:VAL:HG23	1.81	0.62
1:B:40:HIS:HA	1:B:78:THR:HA	1.82	0.62

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	416/485 (86%)	406 (98%)	10 (2%)	0	100	100
1	B	402/485 (83%)	390 (97%)	12 (3%)	0	100	100
All	All	818/970 (84%)	796 (97%)	22 (3%)	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	366/433 (84%)	364 (100%)	2 (0%)	88	92
1	B	336/433 (78%)	331 (98%)	5 (2%)	65	78
All	All	702/866 (81%)	695 (99%)	7 (1%)	76	85

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	92	PHE
1	B	124	SER
1	B	653	TYR
1	B	513	THR
1	B	22	VAL

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	801	-	5,5,5	0.37	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	801	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O1-C1-C2-C3
2	A	801	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	1	0

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	424/485 (87%)	0.23	13 (3%) 49 58	33, 61, 96, 125	0
1	B	410/485 (84%)	0.89	65 (15%) 1 2	41, 76, 163, 204	0
All	All	834/970 (85%)	0.55	78 (9%) 8 10	33, 67, 152, 204	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	45	MET	10.5
1	B	49	VAL	9.7
1	B	48	LEU	8.9
1	B	39	VAL	7.9
1	B	52	LEU	7.3

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(\AA^2)	Q<0.9
2	GOL	A	801	6/6	0.76	0.27	58,81,83,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.