



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 27, 2026 – 04:05 PM EDT

PDB ID : 9Z00 / pdb_00009z00
Title : Kindlin-3/Integrin Beta3 Cytoplasmic Tail Complex
Authors : Xu, Z.; Ma, Y.Q.
Deposited on : 2025-10-30
Resolution : 2.20 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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

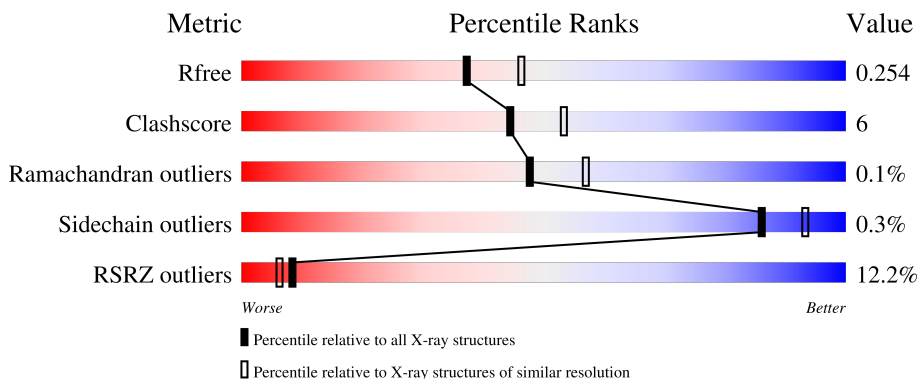
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	489	
1	B	489	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6776 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 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3500	2241	626	622	11	0	0	0
1	B	371	3062	1963	543	545	11	0	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q86UX7
A	?	-	VAL	deletion	UNP Q86UX7
A	?	-	VAL	deletion	UNP Q86UX7
A	?	-	LEU	deletion	UNP Q86UX7
A	?	-	ALA	deletion	UNP Q86UX7
A	?	-	GLY	deletion	UNP Q86UX7
A	?	-	GLY	deletion	UNP Q86UX7
A	?	-	VAL	deletion	UNP Q86UX7
A	?	-	ALA	deletion	UNP Q86UX7
A	?	-	PRO	deletion	UNP Q86UX7
A	?	-	ALA	deletion	UNP Q86UX7
A	?	-	LEU	deletion	UNP Q86UX7
A	?	-	PHE	deletion	UNP Q86UX7
A	?	-	ARG	deletion	UNP Q86UX7
A	?	-	GLY	deletion	UNP Q86UX7
A	?	-	MET	deletion	UNP Q86UX7
A	?	-	PRO	deletion	UNP Q86UX7
A	?	-	ALA	deletion	UNP Q86UX7
A	?	-	HIS	deletion	UNP Q86UX7
A	?	-	PHE	deletion	UNP Q86UX7
A	?	-	SER	deletion	UNP Q86UX7
A	?	-	ASP	deletion	UNP Q86UX7
A	?	-	SER	deletion	UNP Q86UX7
A	?	-	ALA	deletion	UNP Q86UX7
A	?	-	GLN	deletion	UNP Q86UX7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	deletion	UNP Q86UX7
A	?	-	GLU	deletion	UNP Q86UX7
A	?	-	ALA	deletion	UNP Q86UX7
A	?	-	CYS	deletion	UNP Q86UX7
A	664	LEU	-	expression tag	UNP Q86UX7
A	665	LEU	-	expression tag	UNP Q86UX7
A	666	VAL	-	expression tag	UNP Q86UX7
A	667	PRO	-	expression tag	UNP Q86UX7
A	668	ARG	-	expression tag	UNP Q86UX7
A	669	GLY	-	expression tag	UNP Q86UX7
A	670	SER	-	expression tag	UNP Q86UX7
A	671	GLY	-	expression tag	UNP Q86UX7
A	672	SER	-	expression tag	UNP Q86UX7
A	673	GLY	-	expression tag	UNP Q86UX7
A	674	SER	-	expression tag	UNP Q86UX7
A	675	GLY	-	expression tag	UNP Q86UX7
A	676	SER	-	expression tag	UNP Q86UX7
A	677	LYS	-	expression tag	UNP Q86UX7
A	678	GLU	-	expression tag	UNP Q86UX7
A	679	ALA	-	expression tag	UNP Q86UX7
A	680	THR	-	expression tag	UNP Q86UX7
A	681	SER	-	expression tag	UNP Q86UX7
A	682	THR	-	expression tag	UNP Q86UX7
A	683	PHE	-	expression tag	UNP Q86UX7
A	684	THR	-	expression tag	UNP Q86UX7
A	685	ASN	-	expression tag	UNP Q86UX7
A	686	ILE	-	expression tag	UNP Q86UX7
A	687	THR	-	expression tag	UNP Q86UX7
A	688	TYR	-	expression tag	UNP Q86UX7
A	689	ARG	-	expression tag	UNP Q86UX7
A	690	GLY	-	expression tag	UNP Q86UX7
A	691	THR	-	expression tag	UNP Q86UX7
A	692	LEU	-	expression tag	UNP Q86UX7
A	693	GLU	-	expression tag	UNP Q86UX7
A	694	HIS	-	expression tag	UNP Q86UX7
A	695	HIS	-	expression tag	UNP Q86UX7
A	696	HIS	-	expression tag	UNP Q86UX7
A	697	HIS	-	expression tag	UNP Q86UX7
A	698	HIS	-	expression tag	UNP Q86UX7
B	?	-	LYS	deletion	UNP Q86UX7
B	?	-	VAL	deletion	UNP Q86UX7
B	?	-	VAL	deletion	UNP Q86UX7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LEU	deletion	UNP Q86UX7
B	?	-	ALA	deletion	UNP Q86UX7
B	?	-	GLY	deletion	UNP Q86UX7
B	?	-	GLY	deletion	UNP Q86UX7
B	?	-	VAL	deletion	UNP Q86UX7
B	?	-	ALA	deletion	UNP Q86UX7
B	?	-	PRO	deletion	UNP Q86UX7
B	?	-	ALA	deletion	UNP Q86UX7
B	?	-	LEU	deletion	UNP Q86UX7
B	?	-	PHE	deletion	UNP Q86UX7
B	?	-	ARG	deletion	UNP Q86UX7
B	?	-	GLY	deletion	UNP Q86UX7
B	?	-	MET	deletion	UNP Q86UX7
B	?	-	PRO	deletion	UNP Q86UX7
B	?	-	ALA	deletion	UNP Q86UX7
B	?	-	HIS	deletion	UNP Q86UX7
B	?	-	PHE	deletion	UNP Q86UX7
B	?	-	SER	deletion	UNP Q86UX7
B	?	-	ASP	deletion	UNP Q86UX7
B	?	-	SER	deletion	UNP Q86UX7
B	?	-	ALA	deletion	UNP Q86UX7
B	?	-	GLN	deletion	UNP Q86UX7
B	?	-	THR	deletion	UNP Q86UX7
B	?	-	GLU	deletion	UNP Q86UX7
B	?	-	ALA	deletion	UNP Q86UX7
B	?	-	CYS	deletion	UNP Q86UX7
B	664	LEU	-	expression tag	UNP Q86UX7
B	665	LEU	-	expression tag	UNP Q86UX7
B	666	VAL	-	expression tag	UNP Q86UX7
B	667	PRO	-	expression tag	UNP Q86UX7
B	668	ARG	-	expression tag	UNP Q86UX7
B	669	GLY	-	expression tag	UNP Q86UX7
B	670	SER	-	expression tag	UNP Q86UX7
B	671	GLY	-	expression tag	UNP Q86UX7
B	672	SER	-	expression tag	UNP Q86UX7
B	673	GLY	-	expression tag	UNP Q86UX7
B	674	SER	-	expression tag	UNP Q86UX7
B	675	GLY	-	expression tag	UNP Q86UX7
B	676	SER	-	expression tag	UNP Q86UX7
B	677	LYS	-	expression tag	UNP Q86UX7
B	678	GLU	-	expression tag	UNP Q86UX7
B	679	ALA	-	expression tag	UNP Q86UX7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	680	THR	-	expression tag	UNP Q86UX7
B	681	SER	-	expression tag	UNP Q86UX7
B	682	THR	-	expression tag	UNP Q86UX7
B	683	PHE	-	expression tag	UNP Q86UX7
B	684	THR	-	expression tag	UNP Q86UX7
B	685	ASN	-	expression tag	UNP Q86UX7
B	686	ILE	-	expression tag	UNP Q86UX7
B	687	THR	-	expression tag	UNP Q86UX7
B	688	TYR	-	expression tag	UNP Q86UX7
B	689	ARG	-	expression tag	UNP Q86UX7
B	690	GLY	-	expression tag	UNP Q86UX7
B	691	THR	-	expression tag	UNP Q86UX7
B	692	LEU	-	expression tag	UNP Q86UX7
B	693	GLU	-	expression tag	UNP Q86UX7
B	694	HIS	-	expression tag	UNP Q86UX7
B	695	HIS	-	expression tag	UNP Q86UX7
B	696	HIS	-	expression tag	UNP Q86UX7
B	697	HIS	-	expression tag	UNP Q86UX7
B	698	HIS	-	expression tag	UNP Q86UX7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	101	Total O 101 101	0	0
2	B	113	Total O 113 113	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.25Å 103.00Å 111.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.20 49.15 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.15-2.20) 96.5 (49.15-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.218 , 0.254 0.220 , 0.254	Depositor DCC
R_{free} test set	2607 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6776	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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	0.11	0/3584	0.33	0/4854
1	B	0.13	0/3136	0.34	0/4248
All	All	0.12	0/6720	0.34	0/9102

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	ASN	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3500	0	3480	38	0
1	B	3062	0	3033	42	0
2	A	101	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	113	0	0	1	0
All	All	6776	0	6513	79	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 79 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:A:55:ARG:HH12	1:A:57:GLN:NE2	1.70	0.88
1:B:529:GLN:OE1	1:B:529:GLN:N	2.08	0.86
1:A:559:LYS:HZ2	1:A:560:GLY:H	1.26	0.79
1:A:120:LEU:HB3	1:A:232:SER:HA	1.67	0.76
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.49	0.75

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	416/489 (85%)	410 (99%)	5 (1%)	1 (0%)	43	51
1	B	361/489 (74%)	354 (98%)	7 (2%)	0	100	100
All	All	777/978 (79%)	764 (98%)	12 (2%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLY

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	376/428 (88%)	375 (100%)	1 (0%)	86	93
1	B	331/428 (77%)	330 (100%)	1 (0%)	86	93
All	All	707/856 (83%)	705 (100%)	2 (0%)	86	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	LEU
1	B	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	211	GLN
1	A	270	GLN
1	A	614	ASN
1	B	544	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	426/489 (87%)	0.79	48 (11%) 10 8	33, 48, 74, 98	0
1	B	371/489 (75%)	0.76	49 (13%) 7 5	31, 46, 80, 100	0
All	All	797/978 (81%)	0.77	97 (12%) 8 6	31, 48, 78, 100	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	659	GLY	9.2
1	A	494	ALA	5.2
1	A	690	GLY	5.2
1	A	308	GLY	5.1
1	B	527	VAL	4.8

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 oligosaccharides 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.