



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 12:40 AM BST

PDB ID : 6V9G  
Title : Kindlin-3 double deletion mutant long form  
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Deposited on : 2019-12-13  
Resolution : 2.35 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

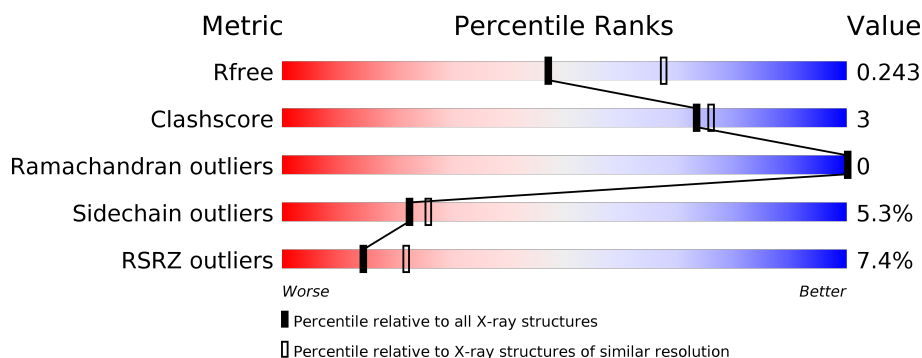
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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	492	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>16%</div> </div> </div>
1	B	492	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>10%</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6998 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
1	A	412	Total	C	N	O	S	0	2	0
			3402	2181	608	602	11			
1	B	411	Total	C	N	O	S	0	1	0
			3375	2162	606	596	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	664	LEU	-	expression tag	UNP Q86UX7
A	665	GLU	-	expression tag	UNP Q86UX7
A	666	HIS	-	expression tag	UNP Q86UX7
A	667	HIS	-	expression tag	UNP Q86UX7
A	668	HIS	-	expression tag	UNP Q86UX7
A	669	HIS	-	expression tag	UNP Q86UX7
A	670	HIS	-	expression tag	UNP Q86UX7
A	671	HIS	-	expression tag	UNP Q86UX7
B	664	LEU	-	expression tag	UNP Q86UX7
B	665	GLU	-	expression tag	UNP Q86UX7
B	666	HIS	-	expression tag	UNP Q86UX7
B	667	HIS	-	expression tag	UNP Q86UX7
B	668	HIS	-	expression tag	UNP Q86UX7
B	669	HIS	-	expression tag	UNP Q86UX7
B	670	HIS	-	expression tag	UNP Q86UX7
B	671	HIS	-	expression tag	UNP Q86UX7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	122	Total	O	0	0
			122	122		
2	B	99	Total	O	0	0
			99	99		

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.

Chain A:

74% 9% 16%

MET  
 ALA  
 GLY  
 MET  
 LYS  
 THR  
 ALA  
 SER  
 ASP  
 TYR  
 ILE  
 SER  
 S15  
 R19  
 V20  
 F21  
 V22  
 E25  
 D26  
 P27  
 E28  
 A29  
 L34  
 T37  
 G38  
 E39  
 V45  
 I49  
 N54  
 D51  
 P59  
 R107  
 R108  
 A109  
 L110  
 R111  
 L112  
 R113  
 L120  
 F121  
 L131  
 L141  
 L142  
 P145

E146  
 LNS  
 LYS  
 GLU  
 LNS  
 LYS  
 LNS  
 LNS  
 LNS  
 LNS  
 GLU  
 GLU  
 PRO  
 GLU  
 ASP  
 GLU  
 E160  
 L161  
 Y162  
 M197  
 L198  
 Q202  
 D221  
 E228  
 R228  
 S232  
 M237  
 I241  
 L247  
 R250  
 Y254  
 D258  
 P261  
 D264  
 R267  
 L268  
 G308  
 GLU  
 VAL  
 GLY  
 GLY  
 PRO  
 ALA  
 GLY  
 THR  
 ASP  
 PRO  
 TYR

LEU  
 LEU  
 ASP  
 ASP  
 LEU  
 LEU  
 ASP  
 VAL  
 HIS  
 HIS  
 HIS  
 HIS  
 HIS  
 ASN  
 LEU  
 LEU  
 VAL  
 LEU  
 LEU  
 GLY  
 GLY  
 SER  
 ALA  
 PRO  
 THR  
 ASP  
 VAL  
 LEU  
 ALA  
 GLU  
 G496  
 R509  
 Q529  
 G550  
 I566  
 I577  
 R594  
 N597  
 Y630  
 T639  
 R640  
 E641  
 R642  
 ALA  
 ARG  
 GLY  
 GLU  
 E647  
 Q655  
 G659  
 HIS  
 ALA

[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.73Å 129.17Å 134.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.73 – 2.35 47.73 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.73-2.35) 99.6 (47.73-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.214 , 0.245 0.214 , 0.243	Depositor DCC
$R_{free}$ test set	2101 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.48	0/3492	0.66	0/4730
1	B	0.45	0/3460	0.66	0/4688
All	All	0.46	0/6952	0.66	0/9418

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

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	3402	0	3382	20	0
1	B	3375	0	3351	25	0
2	A	122	0	0	1	0
2	B	99	0	0	0	0
All	All	6998	0	6733	44	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 3.

All (44) 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:120:LEU:HB3	1:A:232:SER:HA	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:GLU:O	1:A:642:ARG:HB2	1.93	0.67
1:A:110:LEU:HD13	1:A:197:MET:CE	2.24	0.67
1:A:110:LEU:HD13	1:A:197:MET:HE1	1.76	0.66
1:A:264:ASP:HB3	1:A:267:ARG:HB3	1.79	0.64
1:B:508:GLN:HA	1:B:512:LYS:HG3	1.82	0.61
1:B:206:ASP:HB3	1:B:209:LEU:HB2	1.82	0.61
1:B:264:ASP:HB3	1:B:267:ARG:HB3	1.86	0.58
1:A:121:PHE:HB3	1:A:232:SER:HB2	1.87	0.57
1:A:221:ASP:OD1	1:B:589:ARG:NH2	2.36	0.53
1:A:509:ARG:NH2	2:A:701:HOH:O	2.42	0.53
1:A:142:LEU:HD11	1:A:250:ARG:HD3	1.90	0.52
1:A:145:PRO:HA	1:A:228:ARG:HD3	1.91	0.52
1:B:16:TRP:CE3	1:B:36:VAL:HG23	2.44	0.51
1:B:58:ASP:OD1	1:B:60:SER:HB2	2.10	0.51
1:B:291:MET:CE	1:B:504:ALA:H	2.24	0.51
1:A:241:ILE:HG12	1:A:247:LEU:HD21	1.93	0.50
1:A:34:LEU:HD11	1:A:49:ILE:HG13	1.95	0.48
1:B:79:THR:HG23	1:B:82:LYS:H	1.78	0.47
1:B:609:PHE:HE2	1:B:615:VAL:CG1	2.26	0.47
1:B:291:MET:HE3	1:B:504:ALA:H	1.80	0.46
1:B:208:LEU:HD12	1:B:212:ARG:HH11	1.81	0.45
1:B:120:LEU:HB3	1:B:232:SER:HA	1.98	0.45
1:A:261:PRO:HA	1:A:268:LEU:HD22	1.98	0.45
1:A:99:PRO:HD3	1:A:113:ARG:HH21	1.82	0.44
1:B:609:PHE:HE2	1:B:615:VAL:HG11	1.82	0.44
1:A:37:THR:C	1:A:39:GLU:H	2.21	0.44
1:A:108:ARG:HE	1:A:202:GLN:HG2	1.82	0.43
1:B:68:GLN:NE2	1:B:90:ARG:HG3	2.34	0.43
1:B:24:GLU:HG3	1:B:25:GLU:H	1.82	0.43
1:B:512:LYS:HB3	1:B:516:LEU:HD23	2.00	0.43
1:B:86:LEU:HB2	1:B:88:ASP:OD1	2.19	0.43
1:B:34:LEU:HD22	1:B:48:LYS:HB3	2.02	0.42
1:B:134:ARG:HD3	1:B:264:ASP:OD1	2.20	0.42
1:A:110:LEU:HD23	1:A:112:LEU:HD21	2.01	0.41
1:B:571:ASN:HA	1:B:634:TYR:CD1	2.55	0.41
1:B:607:ILE:HB	1:B:615:VAL:HG13	2.01	0.41
1:B:107:ARG:HD2	1:B:277:TRP:CD2	2.56	0.41
1:A:566:ILE:HB	1:A:577:ILE:HB	2.03	0.41
1:B:558:PHE:CE2	1:B:576:ARG:HG3	2.56	0.40
1:A:141:LEU:HD13	1:A:247:LEU:HD13	2.03	0.40
1:B:142:LEU:HB2	1:B:248:TRP:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:CD2	1:A:550:GLY:HA2	2.57	0.40
1:B:254:TYR:CG	1:B:550:GLY:HA2	2.57	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	406/492 (82%)	398 (98%)	8 (2%)	0	100	100
1	B	404/492 (82%)	391 (97%)	13 (3%)	0	100	100
All	All	810/984 (82%)	789 (97%)	21 (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	366/431 (85%)	351 (96%)	15 (4%)	30	37
1	B	360/431 (84%)	337 (94%)	23 (6%)	17	18
All	All	726/862 (84%)	688 (95%)	38 (5%)	22	27

All (38) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	22	VAL
1	A	45	VAL
1	A	54	ASN
1	A	107	ARG
1	A	108	ARG
1	A	131	LEU
1	A	160	GLU
1	A	198	LEU
1	A	237	MET
1	A	258	ASP
1	A	529	GLN
1	A	597	ASN
1	A	630	TYR
1	A	639	THR
1	A	642	ARG
1	B	16	TRP
1	B	22	VAL
1	B	41	HIS
1	B	45	VAL
1	B	60	SER
1	B	79	THR
1	B	103	ARG
1	B	163	ASP
1	B	198	LEU
1	B	208	LEU
1	B	209	LEU
1	B	215	ARG
1	B	297	LEU
1	B	304	LEU
1	B	306	GLN
1	B	516	LEU
1	B	557	ARG
1	B	562	ARG
1	B	589	ARG
1	B	603	ARG
1	B	630	TYR
1	B	639	THR
1	B	642	ARG

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 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	412/492 (83%)	0.34	16 (3%) 39 52	29, 47, 87, 105	0
1	B	411/492 (83%)	0.62	45 (10%) 5 9	32, 55, 104, 128	0
All	All	823/984 (83%)	0.48	61 (7%) 14 22	29, 51, 98, 128	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	516	LEU	8.5
1	B	513	ALA	7.7
1	B	500	TYR	7.0
1	B	515	GLN	6.9
1	B	208	LEU	6.9
1	B	514	LYS	5.3
1	B	54	ASN	5.3
1	B	209	LEU	5.0
1	B	147	LYS	5.0
1	B	508	GLN	4.4
1	B	518	PRO	4.0
1	B	37	THR	3.8
1	B	146	GLU	3.6
1	A	29	ALA	3.6
1	A	308	GLY	3.4
1	B	81	ASP	3.3
1	B	16	TRP	3.3
1	A	25	GLU	3.1
1	B	521	LEU	3.1
1	B	56	LYS	3.1
1	B	306	GLN	3.0
1	B	308	GLY	3.0
1	A	162	TYR	2.9
1	B	642	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	196	HIS	2.9
1	B	499	PRO	2.9
1	B	299	TYR	2.9
1	B	212	ARG	2.9
1	A	81	ASP	2.8
1	B	519	ARG	2.8
1	B	160	GLU	2.8
1	A	26	ASP	2.7
1	A	27	PRO	2.7
1	B	525	GLN	2.6
1	B	33	THR	2.6
1	B	498	ASN	2.6
1	B	520	ILE	2.6
1	B	88	ASP	2.6
1	B	211	GLN	2.6
1	A	54	ASN	2.6
1	B	307	SER	2.5
1	A	655	GLN	2.5
1	A	597	ASN	2.5
1	A	659	GLY	2.5
1	B	523	ALA	2.4
1	A	37	THR	2.4
1	A	19	ARG	2.3
1	B	213	LEU	2.3
1	B	87	ALA	2.3
1	B	161	LEU	2.2
1	A	594	ARG	2.2
1	B	19	ARG	2.2
1	B	18	LEU	2.2
1	B	86	LEU	2.1
1	B	527	VAL	2.1
1	A	21	PHE	2.1
1	B	21	PHE	2.1
1	B	507	PHE	2.1
1	B	529	GLN	2.0
1	B	595	GLN	2.0
1	A	146	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.