



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2017 – 12:37 PM EST

PDB ID : 5L81
Title : Crystal structure of the PH domain of murine kindlin-3
Authors : Ni, T.; Harlos, K.; Gilbert, R.J.C.
Deposited on : 2016-06-06
Resolution : 2.23 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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20028442

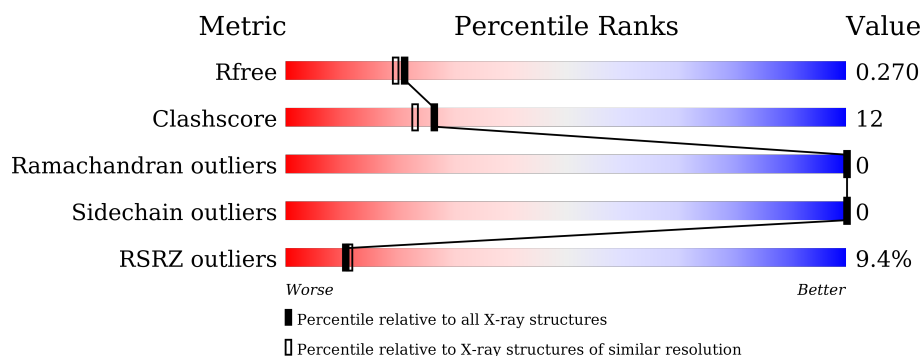
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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}	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	150	<div> <div>3%</div> <div>68%</div> <div>21%</div> <div>11%</div> </div>
1	B	150	<div> <div>14%</div> <div>63%</div> <div>24%</div> <div>12%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2137 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	133	Total	C	N	O	S	0	0	0
			1066	677	183	199	7			
1	B	132	Total	C	N	O	S	0	0	0
			1057	671	182	197	7			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	SER	-	expression tag	UNP Q8K1B8
A	331	ASP	-	expression tag	UNP Q8K1B8
A	332	LEU	-	expression tag	UNP Q8K1B8
A	333	SER	-	expression tag	UNP Q8K1B8
A	334	SER	-	expression tag	UNP Q8K1B8
A	335	GLY	-	expression tag	UNP Q8K1B8
A	336	LEU	-	expression tag	UNP Q8K1B8
A	337	GLU	-	expression tag	UNP Q8K1B8
A	338	VAL	-	expression tag	UNP Q8K1B8
A	339	LEU	-	expression tag	UNP Q8K1B8
A	340	PHE	-	expression tag	UNP Q8K1B8
A	341	GLN	-	expression tag	UNP Q8K1B8
A	342	GLY	-	expression tag	UNP Q8K1B8
A	343	THR	-	expression tag	UNP Q8K1B8
A	479	GLY	-	expression tag	UNP Q8K1B8
B	330	SER	-	expression tag	UNP Q8K1B8
B	331	ASP	-	expression tag	UNP Q8K1B8
B	332	LEU	-	expression tag	UNP Q8K1B8
B	333	SER	-	expression tag	UNP Q8K1B8
B	334	SER	-	expression tag	UNP Q8K1B8
B	335	GLY	-	expression tag	UNP Q8K1B8
B	336	LEU	-	expression tag	UNP Q8K1B8
B	337	GLU	-	expression tag	UNP Q8K1B8
B	338	VAL	-	expression tag	UNP Q8K1B8
B	339	LEU	-	expression tag	UNP Q8K1B8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	340	PHE	-	expression tag	UNP Q8K1B8
B	341	GLN	-	expression tag	UNP Q8K1B8
B	342	GLY	-	expression tag	UNP Q8K1B8
B	343	THR	-	expression tag	UNP Q8K1B8
B	479	GLY	-	expression tag	UNP Q8K1B8

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	1	0

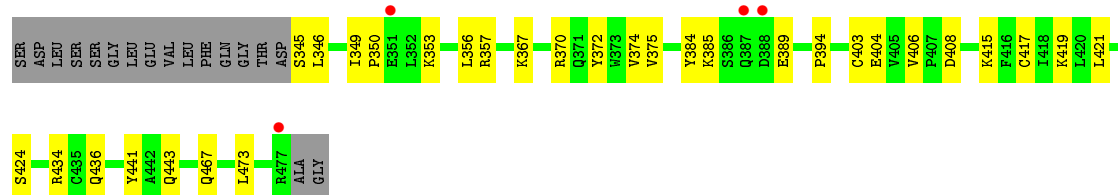
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	4	Total O 4 4	0	0

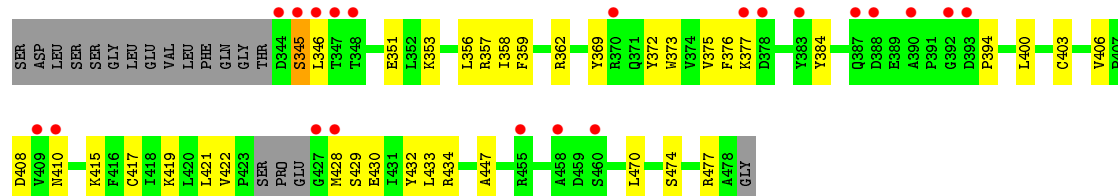
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Fermitin family homolog 3



• Molecule 1: Fermitin family homolog 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	132.04Å 36.19Å 52.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.73 – 2.23 31.73 – 2.23	Depositor EDS
% Data completeness (in resolution range)	96.2 (31.73-2.23) 96.2 (31.73-2.23)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.219 , 0.271 0.219 , 0.270	Depositor DCC
R_{free} test set	617 reflections (4.96%)	DCC
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2137	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.33% 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: NA

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	0.35	0/1088	0.63	0/1471
1	B	0.42	0/1077	0.69	0/1454
All	All	0.39	0/2165	0.66	0/2925

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	B	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	B	345	SER	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	1066	0	1071	21	0
1	B	1057	0	1061	31	0
2	B	1	0	0	0	0
3	A	9	0	0	4	0
3	B	4	0	0	0	0
All	All	2137	0	2132	52	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 12.

All (52) 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:467:GLN:OE1	3:A:501:HOH:O	1.86	0.92
1:A:415:LYS:HG3	1:A:434:ARG:HH12	1.37	0.89
1:B:369:TYR:HE2	1:B:434:ARG:HG3	1.38	0.88
1:B:369:TYR:CE2	1:B:434:ARG:HG3	2.19	0.75
1:A:367:LYS:HG3	1:A:370:ARG:HE	1.56	0.71
1:B:415:LYS:HG3	1:B:434:ARG:NH1	2.09	0.67
1:B:351:GLU:OE1	1:B:353:LYS:NZ	2.29	0.64
1:A:443:GLN:NE2	3:A:504:HOH:O	2.33	0.62
1:B:415:LYS:HG3	1:B:434:ARG:HH12	1.66	0.60
1:B:417:CYS:HB2	1:B:434:ARG:NH1	2.16	0.60
1:A:356:LEU:HD12	1:A:374:VAL:HG11	1.82	0.60
1:B:406:VAL:HB	1:B:419:LYS:HB3	1.83	0.59
1:A:415:LYS:HG3	1:A:434:ARG:NH1	2.14	0.59
1:B:359:PHE:HB2	1:B:369:TYR:CD1	2.38	0.59
1:B:362:ARG:NH1	1:B:429:SER:OG	2.37	0.57
1:A:406:VAL:HB	1:A:419:LYS:HB2	1.85	0.56
1:A:357:ARG:HH22	1:A:436:GLN:HG2	1.70	0.56
1:A:384:TYR:CD1	1:A:394:PRO:HA	2.42	0.55
1:A:408:ASP:HB3	1:A:417:CYS:HB3	1.89	0.55
1:A:345:SER:OG	1:A:346:LEU:N	2.41	0.53
1:A:370:ARG:HB2	1:A:372:TYR:CZ	2.44	0.52
1:B:373:TRP:HD1	1:B:384:TYR:HD2	1.58	0.52
1:B:408:ASP:O	1:B:417:CYS:HB3	2.10	0.51
1:B:376:PHE:CE2	1:B:447:ALA:HB1	2.45	0.51
1:B:353:LYS:HG2	1:B:375:VAL:HG22	1.91	0.51
1:A:353:LYS:HG2	1:A:375:VAL:HG22	1.93	0.50
1:B:357:ARG:HH22	1:B:434:ARG:HD2	1.76	0.50
1:A:384:TYR:CE1	1:A:394:PRO:HA	2.47	0.49
1:B:421:LEU:HD23	1:B:430:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:LYS:CG	1:B:434:ARG:HH12	2.24	0.49
1:B:376:PHE:HE1	1:B:400:LEU:HD12	1.79	0.48
1:A:424:SER:N	3:A:503:HOH:O	2.20	0.47
1:A:424:SER:O	3:A:503:HOH:O	2.20	0.47
1:B:345:SER:HB2	1:B:346:LEU:HA	1.95	0.47
1:B:421:LEU:CD2	1:B:430:GLU:HG2	2.45	0.47
1:A:403:CYS:HB2	1:A:421:LEU:O	2.14	0.47
1:A:441:TYR:HD2	1:A:473:LEU:HD11	1.80	0.47
1:B:403:CYS:HB3	1:B:422:VAL:HG22	1.96	0.46
1:B:419:LYS:HG3	1:B:432:TYR:HE1	1.81	0.46
1:B:351:GLU:OE2	1:B:377:LYS:HD3	2.16	0.46
1:B:384:TYR:CD1	1:B:394:PRO:HA	2.51	0.45
1:A:404:GLU:HB2	1:A:421:LEU:HB2	1.99	0.45
1:B:422:VAL:O	1:B:428:MET:HG3	2.16	0.45
1:B:474:SER:HA	1:B:477:ARG:NH1	2.33	0.43
1:B:357:ARG:NH2	1:B:434:ARG:HD2	2.35	0.41
1:A:385:LYS:HB2	1:A:389:GLU:OE1	2.21	0.41
1:B:358:ILE:HB	1:B:372:TYR:HD2	1.86	0.41
1:B:419:LYS:HG3	1:B:432:TYR:CE1	2.56	0.41
1:B:356:LEU:HD13	1:B:433:LEU:HD23	2.01	0.41
1:B:410:ASN:CB	1:B:415:LYS:HE2	2.51	0.40
1:A:349:ILE:HD12	1:A:350:PRO:HD2	2.03	0.40
1:B:470:LEU:HA	1:B:470:LEU:HD23	1.89	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	131/150 (87%)	128 (98%)	3 (2%)	0	100	100
1	B	128/150 (85%)	125 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	259/300 (86%)	253 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	118/131 (90%)	118 (100%)	0	100	100
1	B	116/131 (88%)	116 (100%)	0	100	100
All	All	234/262 (89%)	234 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	133/150 (88%)	0.50	4 (3%) 54 57	53, 75, 111, 165	0
1	B	132/150 (88%)	1.07	21 (15%) 3 3	56, 83, 137, 243	0
All	All	265/300 (88%)	0.78	25 (9%) 11 11	53, 80, 131, 243	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	SER	8.0
1	B	346	LEU	6.7
1	B	393	ASP	6.6
1	A	477	ARG	5.6
1	B	388	ASP	5.5
1	B	344	ASP	4.8
1	B	392	GLY	4.3
1	B	455	ARG	3.7
1	B	428	MET	3.7
1	B	427	GLY	3.6
1	B	387	GLN	3.2
1	B	458	ALA	3.1
1	A	351	GLU	2.8
1	B	347	THR	2.7
1	B	370	ARG	2.6
1	B	409	VAL	2.5
1	A	388	ASP	2.5
1	A	387	GLN	2.4
1	B	377	LYS	2.3
1	B	383	TYR	2.2
1	B	410	ASN	2.2
1	B	460	SER	2.2
1	B	348	THR	2.2
1	B	378	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	390	ALA	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NA	B	501	1/1	-	-	-	13,13,13,13	1

6.5 Other polymers [i](#)

There are no such residues in this entry.