



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 04:00 PM BST

PDB ID : 6FQL  
Title : Crystal structure of Danio rerio Lin41 filamin-NHL domains in complex with mab-10 3'UTR 13mer RNA  
Authors : Kumari, P.; Aeschmann, F.; Gaidatzis, D.; Keusch, J.J.; Ghosh, P.; Neagu, A.; Pachulska-Wieczorek, K.; Bujnicki, J.M.; Gut, H.; Grosshans, H.; Ciosk, R.  
Deposited on : 2018-02-14  
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.

---

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  
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

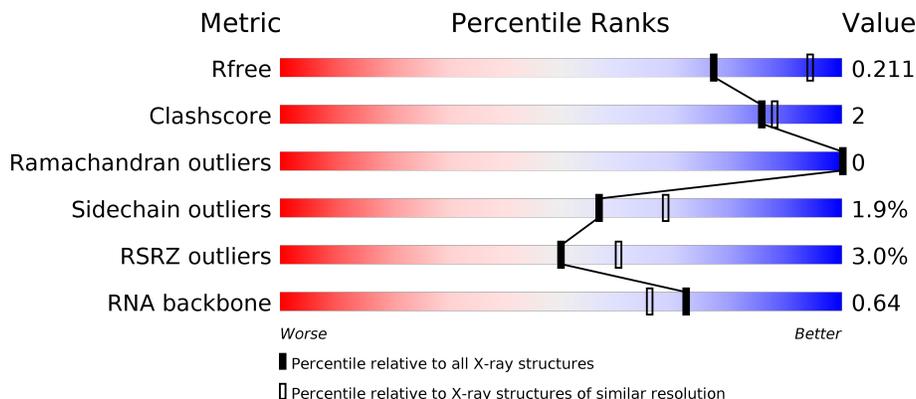
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

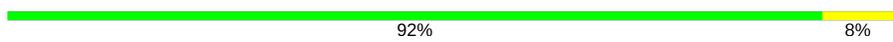
The reported resolution of this entry is 2.35 Å.

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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)
RNA backbone	3102	1027 (2.72-1.96)

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	409	 3% 89% 6% 5%
2	B	13	 92% 8%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3384 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 E3 ubiquitin-protein ligase TRIM71.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3013	1889	550	562	12	0	2	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	416	MET	-	initiating methionine	UNP E7FAM5
A	417	ALA	-	expression tag	UNP E7FAM5
A	418	HIS	-	expression tag	UNP E7FAM5
A	419	HIS	-	expression tag	UNP E7FAM5
A	420	HIS	-	expression tag	UNP E7FAM5
A	421	HIS	-	expression tag	UNP E7FAM5
A	422	HIS	-	expression tag	UNP E7FAM5
A	423	HIS	-	expression tag	UNP E7FAM5
A	424	SER	-	expression tag	UNP E7FAM5
A	425	SER	-	expression tag	UNP E7FAM5
A	426	GLY	-	expression tag	UNP E7FAM5
A	427	LEU	-	expression tag	UNP E7FAM5
A	428	GLU	-	expression tag	UNP E7FAM5
A	429	VAL	-	expression tag	UNP E7FAM5
A	430	LEU	-	expression tag	UNP E7FAM5
A	431	PHE	-	expression tag	UNP E7FAM5
A	432	GLN	-	expression tag	UNP E7FAM5
A	433	GLY	-	expression tag	UNP E7FAM5
A	434	PRO	-	expression tag	UNP E7FAM5

- Molecule 2 is a RNA chain called RNA (5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*UP\*AP\*AP\*UP\*GP\*CP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	13	271	123	46	90	12	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total Cl 8 8	0	0

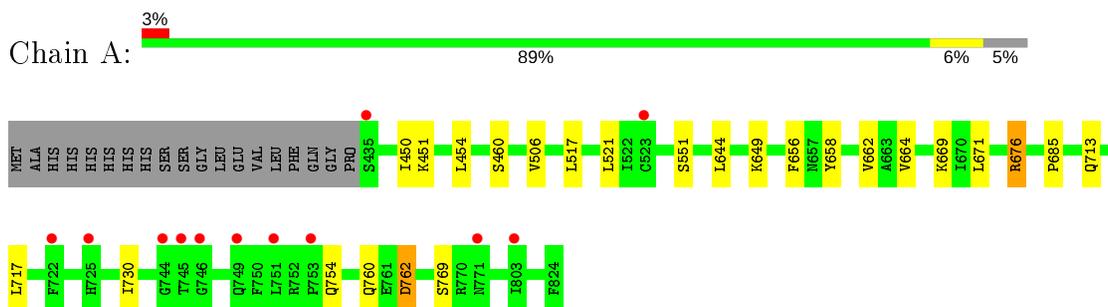
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	78	Total O 78 78	0	0
4	B	14	Total O 14 14	0	0

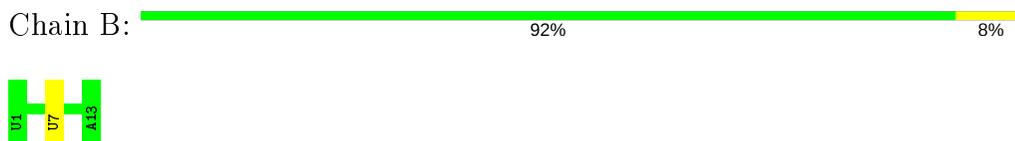
### 3 Residue-property plots [i](#)

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.

- Molecule 1: E3 ubiquitin-protein ligase TRIM71



- Molecule 2: RNA (5'-R(\*UP\*GP\*CP\*AP\*UP\*UP\*UP\*AP\*AP\*UP\*GP\*CP\*A)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.49Å 101.49Å 108.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.30 – 2.35 46.30 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.30-2.35) 99.4 (46.30-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.96 (at 2.34Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.172 , 0.211 0.172 , 0.211	Depositor DCC
$R_{free}$ test set	1369 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.3	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.030 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	3384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.41	0/3085	0.59	0/4163
2	B	0.53	0/302	0.90	0/468
All	All	0.42	0/3387	0.62	0/4631

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 [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	3013	0	2896	14	0
2	B	271	0	140	2	0
3	A	8	0	0	0	0
4	A	78	0	0	0	0
4	B	14	0	0	0	0
All	All	3384	0	3036	14	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 2.

All (14) 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:676[A]:ARG:HH22	2:B:7:U:H3	1.18	0.88
1:A:754:GLN:HG3	1:A:769:SER:HB3	1.88	0.55
1:A:450:ILE:HG13	1:A:451:LYS:HD3	1.91	0.53
1:A:676[A]:ARG:NH2	2:B:7:U:H3	1.99	0.49
1:A:649:LYS:HA	1:A:656:PHE:O	2.13	0.49
1:A:658:TYR:HD2	1:A:676[A]:ARG:HG3	1.77	0.49
1:A:713:GLN:HG2	1:A:762:ASP:OD1	2.13	0.48
1:A:717:LEU:HB2	1:A:730:ILE:HB	1.96	0.46
1:A:662:VAL:HA	1:A:671:LEU:O	2.16	0.45
1:A:664:VAL:HA	1:A:669:LYS:O	2.18	0.44
1:A:517:LEU:HD23	1:A:517:LEU:HA	1.83	0.43
1:A:760:GLN:N	1:A:760:GLN:OE1	2.52	0.42
1:A:460:SER:HA	1:A:506:VAL:O	2.20	0.41
1:A:454:LEU:HA	1:A:454:LEU:HD23	1.91	0.41

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	390/409 (95%)	377 (97%)	13 (3%)	0	<b>100</b> <b>100</b>

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	319/333 (96%)	312 (98%)	7 (2%)	52 63

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	LEU
1	A	551	SER
1	A	644	LEU
1	A	676[A]	ARG
1	A	676[B]	ARG
1	A	685	PRO
1	A	762	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	490	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	12/13 (92%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

## 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](#)

Of 8 ligands modelled in this entry, 8 are 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 [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, 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	390/409 (95%)	0.25	12 (3%) 49 59	41, 65, 94, 119	0
2	B	13/13 (100%)	-0.35	0 100 100	53, 68, 77, 79	0
All	All	403/422 (95%)	0.23	12 (2%) 50 60	41, 65, 93, 119	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	744	GLY	3.8
1	A	745	THR	3.7
1	A	771	ASN	2.8
1	A	523	CYS	2.8
1	A	435	SER	2.4
1	A	753	PRO	2.3
1	A	749	GLN	2.2
1	A	746	GLY	2.2
1	A	725	HIS	2.2
1	A	722	PHE	2.1
1	A	803[A]	ILE	2.1
1	A	751	LEU	2.1

### 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, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	CL	A	907	1/1	0.45	0.27	106,106,106,106	0
3	CL	A	905	1/1	0.63	0.39	91,91,91,91	0
3	CL	A	906	1/1	0.74	0.20	104,104,104,104	0
3	CL	A	901	1/1	0.77	0.14	91,91,91,91	0
3	CL	A	904	1/1	0.85	0.16	91,91,91,91	0
3	CL	A	903	1/1	0.87	0.10	95,95,95,95	0
3	CL	A	902	1/1	0.89	0.11	92,92,92,92	1
3	CL	A	908	1/1	0.97	0.44	88,88,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.