



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2023 – 01:35 AM EDT

PDB ID : 7MNN  
Title : Crystal structure of the N-terminal domain of NUP358/RanBP2 (residues 1-752) T653I mutant in complex with Fab fragment  
Authors : Bley, C.J.; Nie, S.; Mobbs, G.W.; Petrovic, S.; Gres, A.T.; Liu, X.; Mukherjee, S.; Harvey, S.; Huber, F.M.; Lin, D.H.; Brown, B.; Tang, A.W.; Rundlet, E.J.; Correia, A.R.; Chen, S.; Regmi, S.G.; Stevens, T.A.; Jette, C.A.; Dasso, M.; Patke, A.; Palazzo, A.F.; Kossiakoff, A.A.; Hoelz, A.  
Deposited on : 2021-05-01  
Resolution : 6.70 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](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 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  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

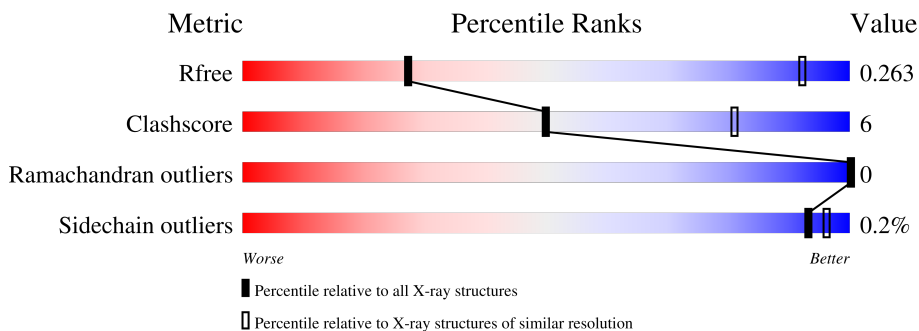
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 6.70 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	1002 (9.50-3.90)
Clashscore	141614	1066 (9.50-3.90)
Ramachandran outliers	138981	1000 (9.50-3.90)
Sidechain outliers	138945	1000 (9.50-3.86)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	753	86% (green), 14% (yellow)
1	B	753	69% (green), 12% (yellow), 20% (grey)
2	H	240	81% (green), 13% (yellow), 5% (grey)
2	K	240	78% (green), 16% (yellow), 5% (grey)
3	L	215	89% (green), 10% (yellow), . (grey)
3	M	215	90% (green), 9% (yellow), . (grey)

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 34833 atoms, of which 17334 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 SUMO-protein ligase RanBP2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	750	12093	3839	6052	1042	1132	28	0	0	0
1	B	604	9691	3074	4850	838	906	23	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P49792
A	599	MET	ILE	engineered mutation	UNP P49792
A	653	ILE	THR	engineered mutation	UNP P49792
B	0	SER	-	expression tag	UNP P49792
B	599	MET	ILE	engineered mutation	UNP P49792
B	653	ILE	THR	engineered mutation	UNP P49792

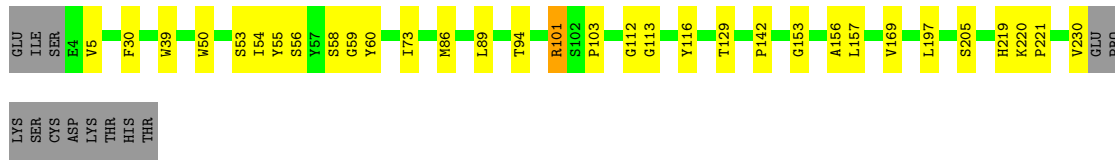
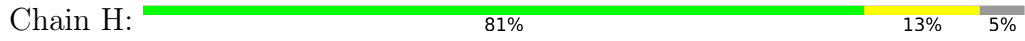
- Molecule 2 is a protein called Antibody Fab14 Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	227	3329	1072	1636	282	334	5	0	0	0
2	K	227	3329	1072	1636	282	334	5	0	0	0

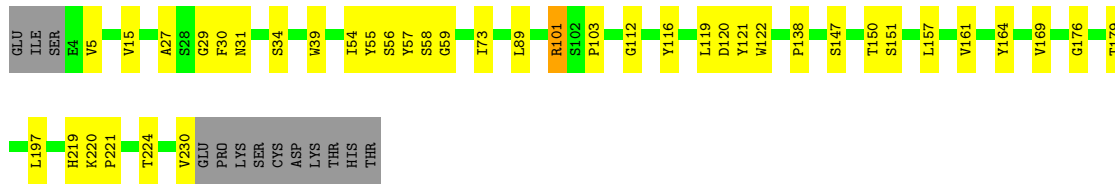
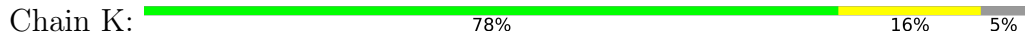
- Molecule 3 is a protein called Antibody Fab14 Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	213	3203	1009	1583	273	333	5	0	0	0
3	M	212	3188	1004	1577	272	330	5	0	0	0

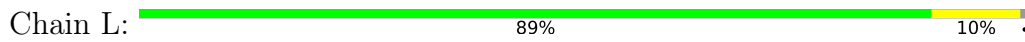




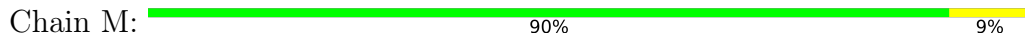
● Molecule 2: Antibody Fab14 Heavy Chain



● Molecule 3: Antibody Fab14 Light Chain



● Molecule 3: Antibody Fab14 Light Chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.54Å 161.54Å 647.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 6.70 30.00 – 6.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-6.70) 100.0 (30.00-6.70)	Depositor EDS
$R_{merge}$	0.78	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 6.58Å)	Xtrriage
Refinement program	PHENIX 1.17.1	Depositor
R, $R_{free}$	0.217 , 0.263 0.217 , 0.263	Depositor DCC
$R_{free}$ test set	457 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	384.2	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 223.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	34833	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	363.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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](#)

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	0.27	0/6167	0.42	0/8342
1	B	0.27	0/4940	0.42	0/6688
2	H	0.28	0/1738	0.48	0/2370
2	K	0.28	0/1738	0.48	0/2370
3	L	0.27	0/1652	0.47	0/2241
3	M	0.27	0/1643	0.49	0/2229
All	All	0.27	0/17878	0.45	0/24240

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	6041	6052	6051	72	0
1	B	4841	4850	4848	64	0
2	H	1693	1636	1636	25	0
2	K	1693	1636	1636	31	0
3	L	1620	1583	1583	16	0
3	M	1611	1577	1577	14	0
All	All	17499	17334	17331	201	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 201 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:677:VAL:HG21	1:B:731:VAL:HG13	1.47	0.97
2:H:54:ILE:HD11	2:H:73:ILE:HG23	1.66	0.76
2:K:116:TYR:HD2	3:M:97:ILE:HD11	1.48	0.76
2:H:50:TRP:HE1	2:H:53:SER:HG	1.31	0.75
1:A:677:VAL:HG21	1:A:731:VAL:HG13	1.68	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	748/753 (99%)	736 (98%)	12 (2%)	0	100	100
1	B	600/753 (80%)	592 (99%)	8 (1%)	0	100	100
2	H	225/240 (94%)	219 (97%)	6 (3%)	0	100	100
2	K	225/240 (94%)	220 (98%)	5 (2%)	0	100	100
3	L	211/215 (98%)	208 (99%)	3 (1%)	0	100	100
3	M	210/215 (98%)	208 (99%)	2 (1%)	0	100	100
All	All	2219/2416 (92%)	2183 (98%)	36 (2%)	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	670/673 (100%)	669 (100%)	1 (0%)	93	96
1	B	541/673 (80%)	541 (100%)	0	100	100
2	H	187/200 (94%)	186 (100%)	1 (0%)	88	93
2	K	187/200 (94%)	186 (100%)	1 (0%)	88	93
3	L	188/190 (99%)	188 (100%)	0	100	100
3	M	187/190 (98%)	187 (100%)	0	100	100
All	All	1960/2126 (92%)	1957 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	696	ASN
2	H	101	ARG
2	K	101	ARG

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](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.