



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 7, 2022 – 06:07 PM 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

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	:	2.28.1
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)	:	2.28.1

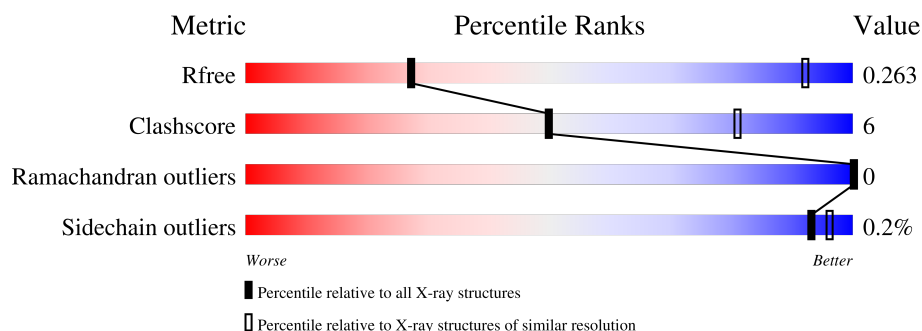
1 Overall quality at a glance

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 ≥ 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% 14%
1	B	753	69% 12% 20%
2	H	240	81% 13% 5%
2	K	240	78% 16% 5%
3	L	215	89% 10% .
3	M	215	90% 9% .

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
1	A	750	Total	C	H	N	O	S	0	0	0
			12093	3839	6052	1042	1132	28			
1	B	604	Total	C	H	N	O	S	0	0	0
			9691	3074	4850	838	906	23			

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
2	H	227	Total	C	H	N	O	S	0	0	0
			3329	1072	1636	282	334	5			
2	K	227	Total	C	H	N	O	S	0	0	0
			3329	1072	1636	282	334	5			

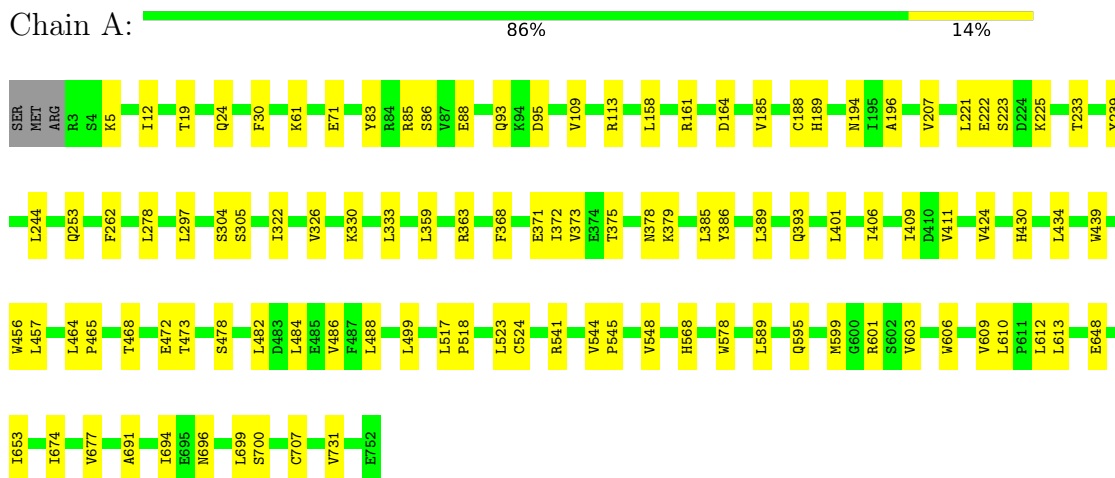
- Molecule 3 is a protein called Antibody Fab14 Light Chain.

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

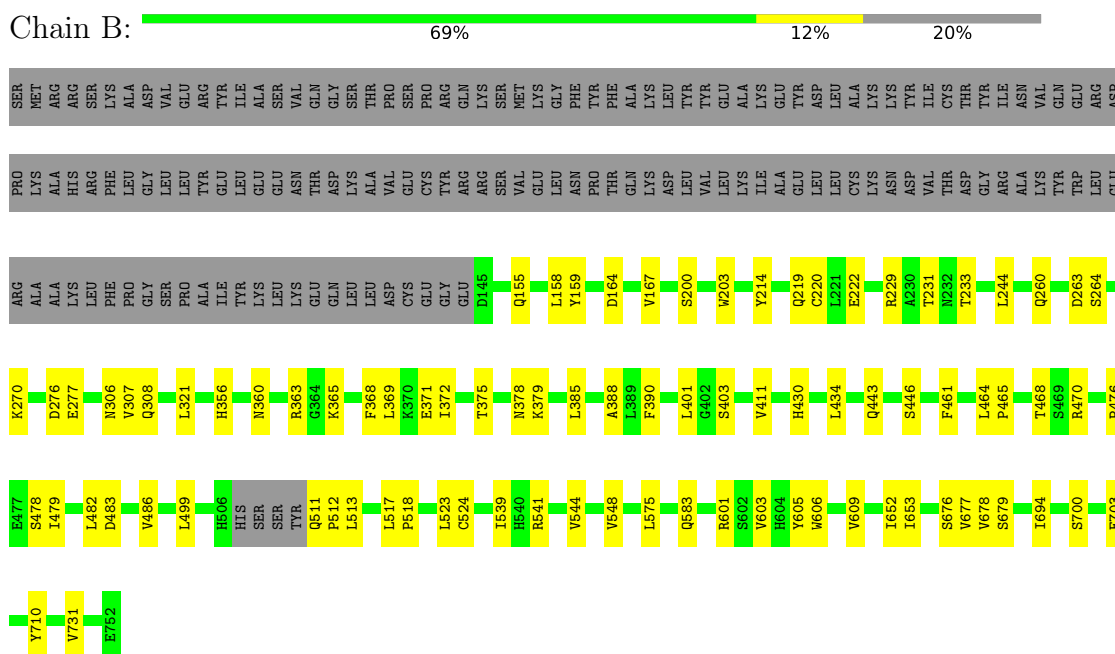
3 Residue-property plots

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. 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. 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 SUMO-protein ligase RanBP2



- Molecule 1: E3 SUMO-protein ligase RanBP2



- Molecule 2: Antibody Fab14 Heavy Chain

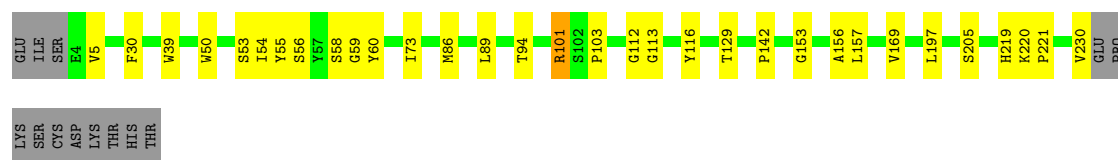


Figure 1: A bar chart showing the number of amino acid mutations in the SARS-CoV-2 spike protein across different regions. The regions are: N1, N2, N3, N4, N5, N6, N7, N8, N9, N10, N11, N12, N13, N14, N15, N16, N17, N18, N19, N20, N21, N22, N23, N24, N25, N26, N27, N28, N29, N30, N31, N32, N33, N34, N35, N36, N37, N38, N39, N40, N41, N42, N43, N44, N45, N46, N47, N48, N49, N50, N51, N52, N53, N54, N55, N56, N57, N58, N59, N60, N61, N62, N63, N64, N65, N66, N67, N68, N69, N70, N71, N72, N73, N74, N75, N76, N77, N78, N79, N80, N81, N82, N83, N84, N85, N86, N87, N88, N89, N90, N91, N92, N93, N94, N95, N96, N97, N98, N99, N100. The bars are color-coded by region: N1-N10 (blue), N11-N20 (orange), N21-N30 (green), N31-N40 (red), N41-N50 (purple), N51-N60 (brown), N61-N70 (pink), N71-N80 (grey), N81-N90 (light blue), N91-N100 (light orange). The y-axis represents the number of mutations, ranging from 0 to 100. The x-axis represents the amino acid positions, from 1 to 1000.

SFR	D2	I3	L12	V20	R25	V30	Q38	L48	S61	A52	L55	D71	Q91	S94	I97	I107	F119	S122	L136	L137	V151	Q167	E214	CYS
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SER
D2
L12
S13
V20
V34
Q38
L48
S51
A52
Q90
S94
I97
R109
T110
Y141
V151
S160
L180
L202
V206
G213
GLU
CYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 6.58Å)	Xtriage
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 ²)	384.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 223.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	34833	wwPDB-VP
Average B, all atoms (Å ²)	363.0	wwPDB-VP

Xtriage'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.*

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

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	0.27	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

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.