

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 4, 2023 – 07:22 PM EDT

PDB ID	:	6U1T
Title	:	Crystal structure of anti-Nipah virus (NiV) F 5B3 antibody Fab fragment
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Deposited on	:	2019-08-16
Resolution	:	1.48 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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

Clashscore

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 1.48 Å.

141614

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.

4955 (1.50-1.46)





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# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4135 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 antigen-binding (Fab) fragment, heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Н	221	Total 1791	C 1148	N 281	O 346	S 16	0	31	0

• Molecule 2 is a protein called antigen-binding (Fab) fragment, light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	L	214	Total 1786	C 1139	N 275	O 359	S 13	0	33	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Н	1	Total Cl 1 1	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	282	Total O   282 282	0	0
4	L	275	Total O 275 275	0	0

SEQUENCE-PLOTS INFOmissingINFO



# 3 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	78.12Å 95.01Å 137.20Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	68.60 - 1.48	Depositor
% Data completeness	99.6 (68.60-1.48)	Depositor
(in resolution range)	55.0 (00.00-1.40)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$< I/\sigma(I) > 1$	$1.36 (at 1.48 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
$R, R_{free}$	0.137 , $0.173$	Depositor
Wilson B-factor $(Å^2)$	17.6	Xtriage
Anisotropy	0.217	Xtriage
L-test for twinning <sup>2</sup>	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4135	wwPDB-VP
Average B, all atoms $(Å^2)$	23.0	wwPDB-VP

EDS failed to run properly - this section is therefore incomplete.

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 4 Model quality (i)

# 4.1 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).

Mal	Chain	Bond	lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	Н	0.45	0/1927	0.66	0/2627	
2	L	0.44	0/1920	0.62	0/2607	
All	All	0.44	0/3847	0.64	0/5234	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 4.2 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	Н	1791	0	1809	11	0
2	L	1786	0	1789	12	0
3	Н	1	0	0	0	0
4	Н	282	0	0	1	0
4	L	275	0	0	1	0
All	All	4135	0	3598	21	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 (21) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



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Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
2:L:175[B]:MET:HE1	2:L:177:SER:HB2	1.64	0.80
1:H:189:VAL:CG2	1:H:192[A]:THR:HG23	2.19	0.73
1:H:169[B]:HIS:HE1	2:L:137:ASN:OD1	1.82	0.63
1:H:110:GLN:CD	1:H:110:GLN:H	2.05	0.60
1:H:216:GLN:HE21	1:H:217:PRO:HD2	1.69	0.57
1:H:169[B]:HIS:CE1	2:L:137:ASN:OD1	2.59	0.56
1:H:12[A]:VAL:HG11	1:H:86:LEU:HD13	1.89	0.55
2:L:28[B]:THR:HG23	4:L:496:HOH:O	2.08	0.54
1:H:189:VAL:HG23	1:H:192[A]:THR:HG23	1.89	0.52
1:H:4:LEU:O	1:H:110:GLN:NE2	2.43	0.51
2:L:146[B]:VAL:HG21	2:L:175[B]:MET:CE	2.42	0.49
2:L:15:LEU:HG	2:L:106[A]:ILE:HD11	1.98	0.46
2:L:35:TRP:CE2	2:L:73:PHE:HB2	2.51	0.45
2:L:21[B]:ILE:HD12	2:L:102:THR:HG21	1.99	0.44
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.00	0.43
2:L:146[B]:VAL:HG21	2:L:175[B]:MET:HE1	2.01	0.42
2:L:83:PHE:CG	2:L:106[B]:ILE:HG12	2.54	0.42
1:H:134:GLY:O	4:H:401:HOH:O	2.22	0.41
1:H:189:VAL:HG22	1:H:192[B]:THR:OG1	2.21	0.40
1:H:110:GLN:CD	1:H:110:GLN:N	2.72	0.40

There are no symmetry-related clashes.

## 4.3 Torsion angles (i)

#### 4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

#### 4.3.2 Protein sidechains (i)

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

#### 4.3.3 RNA (i)

There are no RNA molecules in this entry.

### 4.4 Non-standard residues in protein, DNA, RNA chains (i)

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



### 4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

# 4.6 Ligand geometry (i)

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.

## 4.7 Other polymers (i)

There are no such residues in this entry.

## 4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



# 5 Fit of model and data (i)

# 5.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 5.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

## 5.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

## 5.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

### 5.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

