

Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 09:26 PM EDT

PDB ID : 6VJN

Title : Structure of NHP D11A.B5Fab in complex with 16055 V2b peptide

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Deposited on : 2020-01-16

Resolution : 2.00 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 (1)) were used in the production of this report:

MolProbity : FAILED 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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3708 atoms, of which 28 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 D11A.B5 Fab Heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Н	214	Total 1589	C 1010	N 262	O 310	S 7	0	2	0

• Molecule 2 is a protein called D11A.B5 Fab Light chain.

\mathbf{Mol}	Chain	Residues		-	Ator	$\mathbf{n}\mathbf{s}$			ZeroOcc	AltConf	Trace	
2	L	212	Total 1586	C 973	H 28	N 262	O 319	S 4	6	3	0	

• Molecule 3 is a protein called V2b peptide.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	G	19	Total 157			0	0	0
3	F	10	Total 76		N 15	0	0	0

• Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Н	1	Total Na 1 1	0	0
4	L	3	Total Na 3 3	0	0
4	G	1	Total Na 1 1	0	0
4	F	1	Total Na 1 1	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Н	153	Total O 153 153	0	0
5	L	125	Total O 125 125	0	0
5	G	16	Total O 16 16	0	0

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



3 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	64.78Å 74.78Å 101.45Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	41.98 - 2.00	Depositor	
% Data completeness	99.3 (41.98-2.00)	Depositor	
(in resolution range)	,	Depositor	
R_{merge}	(Not available)	Depositor	
R_{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	2.06 (at 2.00Å)	Xtriage	
Refinement program	PHENIX 1.14_3260, PHENIX 1.14_3260	Depositor	
R, R_{free}	0.180 , 0.236	Depositor	
Wilson B-factor (\mathring{A}^2)	26.9	Xtriage	
Anisotropy	0.792	Xtriage	
L-test for twinning ²	$< L > = 0.47, < L^2> = 0.30$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3708	wwPDB-VP	
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.27% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $< L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

4.3.2 Protein sidechains (i)

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

4.3.3 RNA (i)

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

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 6 ligands modelled in this entry, 6 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.

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.

