



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 05:31 AM EDT

PDB ID : 6N5D
Title : Broadly protective antibodies directed to a subdominant influenza hemagglutinin epitope
Authors : Bajic, G.; Schmidt, A.G.
Deposited on : 2018-11-21
Resolution : 3.00 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 ⓘ 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 : **FAILED**
Xtrriage (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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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

There are 3 unique types of molecules in this entry. The entry contains 16356 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	282	2188	1374	382	421	11	0	0	0
1	B	282	2188	1374	382	421	11	0	0	0
1	K	282	2188	1374	382	421	11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	ASP	ASN	conflict	UNP P03437
B	188	ASP	ASN	conflict	UNP P03437
K	188	ASP	ASN	conflict	UNP P03437

- Molecule 2 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	222	1684	1066	276	334	8	0	0	0
2	E	222	1684	1066	276	334	8	0	0	0
2	L	222	1684	1066	276	334	8	0	0	0

- Molecule 3 is a protein called antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	N	212	1580	995	265	316	4	0	0	0
3	F	212	1580	995	265	316	4	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	212	1580	995	265	316	4	0	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 31	Depositor
Cell constants a, b, c, α , β , γ	153.19Å 153.19Å 94.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.37 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (44.37-3.00)	Depositor
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.217 , 0.244	Depositor
Wilson B-factor (Å ²)	57.5	Xtrriage
Anisotropy	0.244	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.19$	Xtrriage
Estimated twinning fraction	0.127 for -h,-k,l 0.129 for h,-h-k,-l 0.397 for -k,-h,-l	Xtrriage
Reported twinning fraction	0.460 for -k,-h,-l	Depositor
Outliers	0 of 49440 reflections	Xtrriage
Total number of atoms	16356	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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.

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](#)

There are no ligands in this entry.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues

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.