

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 02:30 AM EDT

:	6 MQE
:	Vaccine-elicited NHP FP-targeting HIV neutralizing antibody DFPH-a.15 in
	complex with HIV fusion peptide (residue 512-519)
:	Xu, K.; Wang, Y.; Kwong, P.D.
:	2018-10-09
:	2.46 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:

:	FAILED
:	1.13
:	FAILED
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	2.35.1
	: : : :

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 2.46 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.



6MQE

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6909 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	В	212	Total	С	Ν	Ο	\mathbf{S}	0	0	0
			1612	1007	269	331	5			
1	т	212	Total	С	Ν	0	S	0	0	0
		212	1612	1007	269	331	5	0	0	0

• Molecule 1 is a protein called DFPHa.15 antibody Fab light chain.

• Molecule 2 is a protein called DFPHa.15 antibody Fab heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
0	٨	224	Total	С	Ν	0	S	0	0	0
	\mathcal{L} A		1689	1064	283	337	5			
0	Ц	Н 224	Total	С	Ν	0	S	0	0	0
	2 H		1689	1064	283	337	5	0	0	0

• Molecule 3 is a protein called HIV fusion peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	С	8	Total	С	Ν	0	0	0	0
0	3 0	0	51	35	8	8			
2	Л	0	Total	С	Ν	0	0	0	0
0	5 D	0	51	35	8	8	0		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	52	Total O 52 52	0	0
4	А	52	Total O 52 52	0	0
4	Н	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
4	L	44	Total O 44 44	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total O 1 1	0	0
4	D	2	Total O 2 2	0	0

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



3 Data and refinement statistics (i)

Property	Value	Source	
Space group	C 2 2 21	Depositor	
Cell constants	71.23Å 147.73Å 172.71Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	37.28 - 2.46	Depositor	
% Data completeness	97.9 (37.28-2.46)	Depositor	
(in resolution range)		Depositor	
R _{merge}	0.19	Depositor	
R _{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$1.09 (at 2.45 \text{\AA})$	Xtriage	
Refinement program	PHENIX (1.12_2829: ???)	Depositor	
R, R_{free}	0.192 , 0.245	Depositor	
Wilson B-factor $(Å^2)$	41.1	Xtriage	
Anisotropy	0.463	Xtriage	
L-test for twinning ²	$ < L >=0.49, < L^2>=0.33$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	6909	wwPDB-VP	
Average B, all atoms $(Å^2)$	43.0	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 4.38% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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)

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 (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.

