



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 2, 2023 – 02:30 AM EDT

PDB ID : 6MQE  
Title : Vaccine-elicited NHP FP-targeting HIV neutralizing antibody DFPH-a.15 in complex with HIV fusion peptide (residue 512-519)  
Authors : Xu, K.; Wang, Y.; Kwong, P.D.  
Deposited on : 2018-10-09  
Resolution : 2.46 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](mailto: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>.

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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 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.

## 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.

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	212	Total 1612	C 1007	N 269	O 331	S 5	0	0	0
1	L	212	Total 1612	C 1007	N 269	O 331	S 5	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	224	Total 1689	C 1064	N 283	O 337	S 5	0	0	0
2	H	224	Total 1689	C 1064	N 283	O 337	S 5	0	0	0

- Molecule 3 is a protein called HIV fusion peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	C	8	Total 51	C 35	N 8	O 8	0	0	0
3	D	8	Total 51	C 35	N 8	O 8	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	52	Total 52	O 52	0	0
4	A	52	Total 52	O 52	0	0
4	H	54	Total 54	O 54	0	0
4	L	44	Total 44	O 44	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	C	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		

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

### 3 Data and refinement statistics

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.23Å 147.73Å 172.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.28 – 2.46	Depositor
% Data completeness (in resolution range)	97.9 (37.28-2.46)	Depositor
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.45Å)	Xtrriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.192 , 0.245	Depositor
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtrriage
Anisotropy	0.463	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6909	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup> Intensities estimated from amplitudes.

<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.

## 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](#)

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### 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

### 5.1 Protein, DNA and RNA chains

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

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

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

### 5.3 Carbohydrates

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### 5.4 Ligands

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### 5.5 Other polymers

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