

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

#### Oct 4, 2023 – 07:55 PM EDT

PDB ID	:	$6 \mathrm{UJQ}$
Title	:	HHAT Wild Type Peptide KQWLVWLLL Presented by HLA-A206
Authors	:	Devlin, J.R.; Baker, B.M.; Singh, N.K.
Deposited on		
Resolution	:	2.55  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:  $X\hbox{-}RAY\,DIFFRACTION$ 

The reported resolution of this entry is 2.55 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.



#### 6UJQ

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3247 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 MHC class I antigen.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	275	Total 2248	C 1403	N 409	0 427	${ m S} 9$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	0	MET	-	initiating methionine	UNP U5YJP1

• Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	100	Total 837	C 533	N 141	0 159	${S \over 4}$	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called Protein-cysteine N-palmitoyltransferase HHAT.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	Trace		
3	С	9	Total 86	C 62	N 13	O 11	0	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	54	$\begin{array}{cc} \text{Total} & \text{O} \\ 54 & 54 \end{array}$	0	0
4	В	21	Total O 21 21	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	С	1	Total O 1 1	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 1 2 1	Depositor
Cell constants	97.03Å $38.28$ Å $116.35$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $92.27^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	44.12 - 2.55	Depositor
% Data completeness	94.5 (44.12-2.55)	Depositor
(in resolution range)		-
$R_{merge}$	0.13	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.94 (at 2.54 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
$R, R_{free}$	0.194 , $0.228$	Depositor
Wilson B-factor $(Å^2)$	33.1	Xtriage
Anisotropy	0.233	Xtriage
L-test for twinning <sup>2</sup>	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
Total number of atoms	3247	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	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 8.09% 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)

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.

