

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

Oct 4, 2023 – 10:34 PM EDT

PDB ID : 6VB7

Title: HLA-B\*15:02 complexed with a synthetic peptide

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Deposited on : 2019-12-18

Resolution : 2.10 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 (i)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

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:  $X\text{-}RAY\ DIFFRACTION$ 

The reported resolution of this entry is 2.10 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 8 unique types of molecules in this entry. The entry contains 3485 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		Ato	oms			ZeroOcc	AltConf	Trace
1	A	276	Total 2256	C 1406	N 408	O 433	S 9	0	2	0

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

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
2	В	100	Total 837	C 533	N 141	O 159	S 4	0	0	0

There is a discrepancy between the modelled and reference sequences:

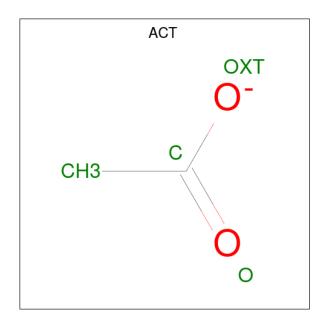
Chain	Residue	Modelled	Actual	Comment	Reference
В	0	MET	-	initiating methionine	UNP P61769

• Molecule 3 is a protein called Synthetic peptide THR-VAL-ARG-ALA-SER-GLY-HIS-SER -TYR.

Mol	Chain	Residues		Ator	$\mathbf{n}\mathbf{s}$	Atoms			Trace
3	С	9	Total 69	C 41	N 14	O 14	0	0	0

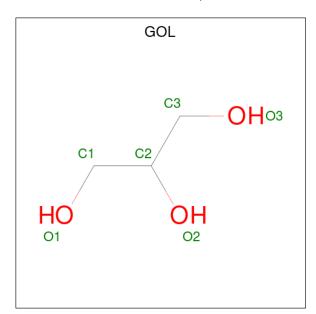
• Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

 $\bullet$  Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $\mathrm{C_3H_8O_3}).$ 



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0

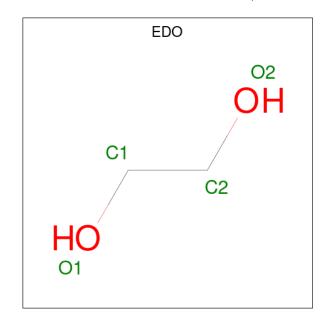
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0

• Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



$\mathbf{Mol}$	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	В	1	Total C O 4 2 2	0	0

• Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

$\mathbf{N}$	lol	Chain	Residues	Atoms	ZeroOcc	AltConf
	7	В	1	Total Na 1 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	219	Total O 219 219	0	0
8	В	61	Total O 61 61	0	0
8	С	8	Total O 8 8	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	50.91Å 81.52Å 110.15Å	Depositor	
a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	24.80 - 2.10	Depositor	
% Data completeness	96.1 (24.80-2.10)	Depositor	
(in resolution range)	,	_	
$R_{merge}$	(Not available)	Depositor	
$R_{sym}$	(Not available)	Depositor	
$< I/\sigma(I) > 1$	6.23  (at  2.10Å)	Xtriage	
Refinement program	PHENIX 1.13_2998	Depositor	
$R, R_{free}$	0.194 , $0.257$	Depositor	
Wilson B-factor $(A^2)$	32.3	Xtriage	
Anisotropy	0.258	Xtriage	
L-test for twinning <sup>2</sup>	$ < L > = 0.50, < L^2> = 0.34$	Xtriage	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	3485	wwPDB-VP	
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.41% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<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)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond



length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	В	ond leng	$_{ m gths}$	В	ond ang	gles
IVIOI	туре	Chain	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	EDO	В	102	-	3,3,3	0.45	0	2,2,2	0.31	0
6	EDO	A	306	-	3,3,3	0.44	0	2,2,2	0.24	0
4	ACT	A	301	-	3,3,3	0.97	0	3,3,3	1.01	0
4	ACT	A	302	-	3,3,3	1.00	0	3,3,3	0.85	0
5	GOL	A	303	-	5,5,5	0.50	0	5,5,5	1.11	0
5	GOL	A	304	-	5,5,5	0.53	0	5,5,5	0.27	0
5	GOL	A	305	-	5,5,5	0.50	0	5,5,5	0.44	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	В	102	-	-	0/1/1/1	-
6	EDO	A	306	-	-	0/1/1/1	-
5	GOL	A	303	-	-	2/4/4/4	_
5	GOL	A	304	-	-	2/4/4/4	-
5	GOL	A	305	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	303	GOL	C1-C2-C3-O3
5	A	304	GOL	C1-C2-C3-O3
5	A	305	GOL	C1-C2-C3-O3
5	A	304	GOL	O2-C2-C3-O3
5	A	305	GOL	O2-C2-C3-O3
5	A	303	GOL	O1-C1-C2-C3

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.

