

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 02:28 AM EDT

PDB ID : 6UZP

Title: HLA-B*15:01 complexed with a synthetic peptide

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Deposited on : 2019-11-15

Resolution : 2.08 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
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-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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 3476 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 2262	C 1407	N 414	O 433	S 8	0	1	0

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

\mathbf{Mol}	Chain	Residues	Atoms					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:

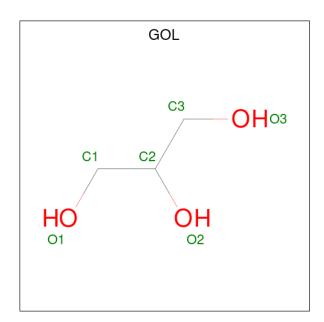
Chain	n Residue Modelled Act		Actual	Comment	Reference	
В	0	MET	-	initiating methionine	UNP P61769	

• Molecule 3 is a protein called Synthetic peptide HIS-LEU-ALA-SER-SER-GLY-HIS-SER-L EU.

Mol	Chain	Residues	1	Ator	$\mathbf{n}\mathbf{s}$	ZeroOcc	AltConf	Trace
3	С	9	Total 71		N 15	0	1	0

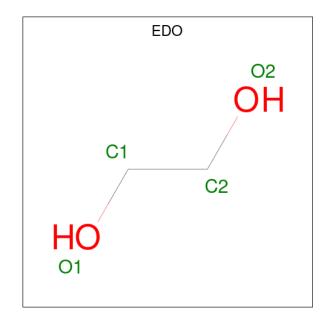
• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total C C 6 3 3)	0	0

 \bullet Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\mathrm{C_2H_6O_2}).$



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

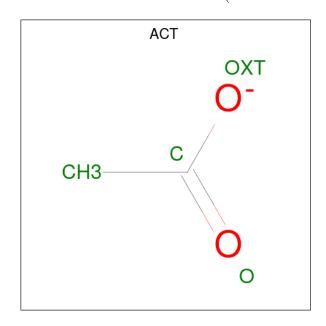
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total C O 4 2 2	0	0

• Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

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

Mol	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	216	Total O 216 216	0	0
8	В	49	Total O 49 49	0	0
8	С	10	Total O 10 10	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	50.96Å 81.67Å 109.61Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.69 - 2.08	Depositor
% Data completeness	99.7 (29.69-2.08)	Depositor
(in resolution range)	,	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.13 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.182 , 0.248	Depositor
Wilson B-factor (A^2)	31.5	Xtriage
Anisotropy	0.373	Xtriage
L-test for twinning ²	$ < L > = 0.50, < L^2> = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3476	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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)

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	Tuno	Chain	Res	Link	В	ond leng	Bond angles			
MIOI	Type	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	303	-	3,3,3	0.45	0	2,2,2	0.11	0
6	ACT	A	305	-	3,3,3	0.93	0	3,3,3	0.92	0
5	EDO	В	101	-	3,3,3	0.45	0	2,2,2	0.09	0
5	EDO	A	302	-	3,3,3	0.41	0	2,2,2	0.30	0
6	ACT	С	101	-	3,3,3	1.02	0	3,3,3	1.04	0
5	EDO	A	304	-	3,3,3	0.43	0	2,2,2	0.51	0
4	GOL	A	301	-	5,5,5	0.41	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
5	EDO	A	303	-	-	0/1/1/1	-
5	EDO	В	101	-	-	0/1/1/1	-
5	EDO	A	302	-	-	0/1/1/1	-
5	EDO	A	304	-	-	0/1/1/1	-
4	GOL	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GOL	O1-C1-C2-C3
4	A	301	GOL	O1-C1-C2-O2

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.

