



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 8, 2025 – 05:40 pm BST

PDB ID : 9SKP / pdb\_00009skp  
Title : Crystal structure of HLA-A0201 in complex with peptide SLLWNGPMAV  
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Deposited on : 2025-09-02  
Resolution : 1.89 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**  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

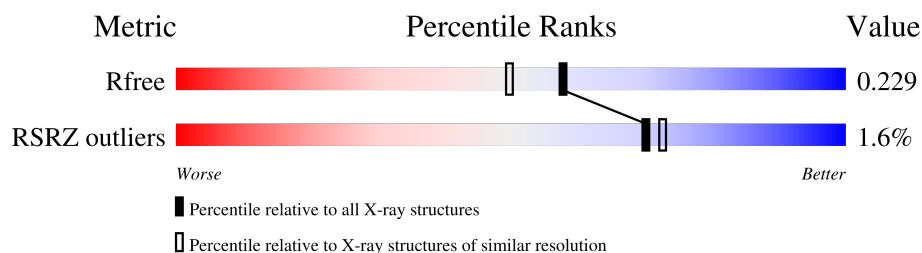
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.89 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	7293 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3575 atoms, of which 78 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	A	275	Total	C	N	O	S	0	4	0
			2278	1423	414	432	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A5I8L1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	1	0
			832	528	143	158	3			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called SLLWNGPMAV peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	S	0	0	0
			76	50	12	13	1			

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Cl	0	0
			3	3		
4	B	2	Total	Cl	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	Na 3	0	0
6	B	1	Total 1	Na 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	190	Total 190	O 190	0	0
7	B	54	Total 54	O 54	0	0
7	C	6	Total 6	O 6	0	0

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

### 3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.63Å 79.96Å 109.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.68 – 1.89 19.68 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.68-1.89) 99.7 (19.68-1.89)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.10 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.21.2-5419	Depositor
R, $R_{free}$	0.186 , 0.229 0.186 , 0.229	Depositor DCC
$R_{free}$ test set	2144 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.8	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 39.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3575	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 oligosaccharides in this entry.

### 4.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	EDO	A	305	-	3,3,3	0.32	0	2,2,2	0.42	0
5	EDO	A	307	-	3,3,3	0.35	0	2,2,2	0.10	0
5	EDO	B	102	-	3,3,3	0.27	0	2,2,2	0.23	0
5	EDO	B	106	-	3,3,3	0.30	0	2,2,2	0.48	0
5	EDO	A	309	-	3,3,3	0.32	0	2,2,2	0.33	0
5	EDO	A	302	-	3,3,3	0.32	0	2,2,2	0.22	0
5	EDO	A	313	-	3,3,3	0.31	0	2,2,2	0.06	0
5	EDO	B	101	-	3,3,3	0.28	0	2,2,2	0.60	0
5	EDO	A	310	-	3,3,3	0.30	0	2,2,2	0.41	0
5	EDO	A	312	-	3,3,3	0.32	0	2,2,2	0.28	0
5	EDO	C	101	-	3,3,3	0.29	0	2,2,2	0.51	0
5	EDO	A	306	-	3,3,3	0.32	0	2,2,2	0.28	0
5	EDO	B	104	-	3,3,3	0.35	0	2,2,2	0.43	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	305	-	-	1/1/1/1	-
5	EDO	A	307	-	-	1/1/1/1	-
5	EDO	B	102	-	-	1/1/1/1	-
5	EDO	B	106	-	-	1/1/1/1	-
5	EDO	A	309	-	-	1/1/1/1	-
5	EDO	A	302	-	-	1/1/1/1	-
5	EDO	A	313	-	-	1/1/1/1	-
5	EDO	B	101	-	-	1/1/1/1	-
5	EDO	A	310	-	-	1/1/1/1	-
5	EDO	A	312	-	-	1/1/1/1	-
5	EDO	C	101	-	-	0/1/1/1	-
5	EDO	A	306	-	-	0/1/1/1	-
5	EDO	B	104	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
5	A	307	EDO	O1-C1-C2-O2
5	B	104	EDO	O1-C1-C2-O2
5	A	302	EDO	O1-C1-C2-O2
5	A	312	EDO	O1-C1-C2-O2
5	A	313	EDO	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](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	275/276 (99%)	-0.38	3 (1%) 77 79	9, 22, 37, 58	4 (1%)
2	B	98/100 (98%)	-0.18	0 100 100	15, 27, 49, 52	1 (1%)
3	C	10/10 (100%)	1.02	3 (30%) 1 1	19, 26, 51, 59	0
All	All	383/386 (99%)	-0.29	6 (1%) 70 72	9, 24, 40, 59	5 (1%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	5.4
3	C	6	GLY	4.1
3	C	5	ASN	3.5
3	C	4	TRP	2.8
1	A	16	GLY	2.1

### 5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EDO	A	309	4/4	0.76	0.34	36,49,55,61	0
4	CL	A	303	1/1	0.77	0.20	55,55,55,55	0
5	EDO	B	104	4/4	0.79	0.14	35,42,45,45	0
5	EDO	B	106	4/4	0.82	0.17	37,45,49,58	0
5	EDO	B	102	4/4	0.83	0.32	26,33,42,51	0
5	EDO	B	101	4/4	0.84	0.12	37,46,55,55	0
5	EDO	A	307	4/4	0.85	0.25	27,36,54,65	0
5	EDO	A	305	4/4	0.85	0.20	32,39,47,47	0
5	EDO	A	310	4/4	0.85	0.12	34,41,49,50	0
5	EDO	A	313	4/4	0.85	0.25	26,35,42,51	0
6	NA	A	314	1/1	0.86	0.09	40,40,40,40	0
5	EDO	A	302	4/4	0.87	0.15	32,46,59,59	0
6	NA	B	105	1/1	0.89	0.11	45,45,45,45	0
4	CL	B	107	1/1	0.91	0.25	43,43,43,43	0
5	EDO	A	312	4/4	0.91	0.26	25,35,43,51	0
5	EDO	A	306	4/4	0.91	0.11	26,35,43,52	0
6	NA	A	311	1/1	0.92	0.10	46,46,46,46	0
4	CL	B	103	1/1	0.92	0.31	54,54,54,54	0
5	EDO	C	101	4/4	0.92	0.11	28,38,46,46	0
4	CL	A	301	1/1	0.95	0.09	40,40,40,40	0
6	NA	A	304	1/1	0.96	0.05	34,34,34,34	0
4	CL	A	308	1/1	0.97	0.39	58,58,58,58	0

## 5.5 Other polymers ⓘ

There are no such residues in this entry.