

Full wwPDB X-ray Structure Validation Report (i)

Oct 1, 2023 – 11:11 PM EDT

PDB ID : 6MKD

Title : 4699 TCR bound to I-Ab Padi4

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Deposited on : 2018-09-25

Resolution : 3.20 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:

MolProbity : FAILED 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 3.20 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 5916 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 H-2 class II histocompatibility antigen, A-B alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	С	166	Total 1211	C 783	N 198	O 227	S 3	0	0	0

• Molecule 2 is a protein called Padi4 (92-105) peptide and MHC Class II I-Ab beta chain, H-2 class II histocompatibility antigen, A beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	201	Total 1584	C 1001	N 276	O 300	S 7	0	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	GLY	-	linker	UNP Q9Z183
D	-11	GLY	-	linker	UNP Q9Z183
D	-10	GLY	-	linker	UNP Q9Z183
D	-9	GLY	-	linker	UNP Q9Z183
D	-8	SER	-	linker	UNP Q9Z183
D	-7	LEU	-	linker	UNP Q9Z183
D	-6	VAL	-	linker	UNP Q9Z183
D	-5	PRO	-	linker	UNP Q9Z183
D	-4	ARG	-	linker	UNP Q9Z183
D	-3	GLY	-	linker	UNP Q9Z183
D	-2	SER	-	linker	UNP Q9Z183
D	-1	GLY	-	linker	UNP Q9Z183
D	0	GLY		linker	UNP Q9Z183
D	1	GLY	-	linker	UNP Q9Z183
D	2	GLY	_	linker	UNP Q9Z183

• Molecule 3 is a protein called 4699 TCR alpha chain.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	193	Total 1339	C 853	N 222	O 258	S 6	0	0	0

 \bullet Molecule 4 is a protein called 4699 TCR beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	В	239	Total 1782	C 1125	N 316	O 335	S 6	0	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	C 1 2 1	Depositor
Cell constants	255.45Å 73.64Å 64.57Å	Depositor
a, b, c, α , β , γ	90.00° 90.39° 90.00°	Depositor
Resolution (Å)	29.24 - 3.20	Depositor
% Data completeness	97.8 (29.24-3.20)	Depositor
(in resolution range)	,	
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.59 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.233 , 0.278	Depositor
Wilson B-factor (\mathring{A}^2)	70.3	Xtriage
Anisotropy	0.625	Xtriage
L-test for twinning ²	$< L > = 0.47, < L^2> = 0.29$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
Total number of atoms	5916	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.92% 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.



 $^{^1 {\}rm Intensities}$ 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)

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