



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 3, 2023 – 08:14 AM EDT

PDB ID : 6PUH  
Title : Structure of human MAIT A-F7 TCR in complex with human MR1-Ribityl-less  
Authors : Awad, W.; Keller, A.N.; Rossjohn, J.  
Deposited on : 2019-07-18  
Resolution : 1.88 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>.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (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

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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 7 unique types of molecules in this entry. The entry contains 15614 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	265	Total	C	N	O	S	0	13	0
			2246	1441	388	404	13			
1	C	268	Total	C	N	O	S	0	18	0
			2299	1475	387	422	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called Human TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	199	Total	C	N	O	S	0	24	0
			1674	1070	260	333	11			
2	D	194	Total	C	N	O	S	0	8	0
			1529	976	240	303	10			

- Molecule 3 is a protein called Human TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	242	Total	C	N	O	S	0	13	0
			1949	1234	331	372	12			
3	G	244	Total	C	N	O	S	0	22	0
			2033	1284	345	391	13			

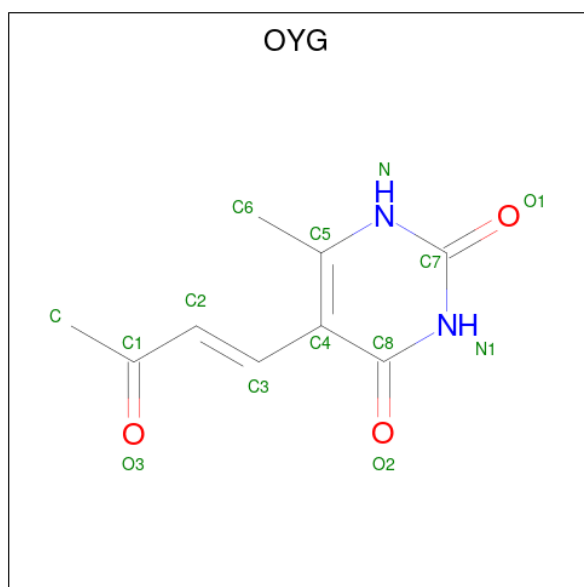
- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	100	Total	C	N	O	S	0	3	0
			840	540	141	154	5			
4	H	98	Total	C	N	O	S	0	1	0
			793	510	135	145	3			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is 6-methyl-5-[(1E)-3-oxobut-1-en-1-yl]pyrimidine-2,4(1H,3H)-dione (three-letter code: OYG) (formula: C<sub>9</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			13	9	2	2		
5	C	1	Total	C	N	O	0	0
			13	9	2	2		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Na	0	0
			1	1		
6	G	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	378	Total 378	O 378	0	0
7	B	344	Total 344	O 344	0	0
7	C	393	Total 393	O 393	0	0
7	D	176	Total 176	O 176	0	0
7	E	244	Total 244	O 244	0	0
7	F	150	Total 150	O 150	0	0
7	G	417	Total 417	O 417	0	0
7	H	121	Total 121	O 121	0	0

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

### 3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	218.48Å 70.56Å 143.98Å 90.00° 104.74° 90.00°	Depositor
Resolution (Å)	48.43 – 1.88	Depositor
% Data completeness (in resolution range)	99.8 (48.43-1.88)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.26 (at 1.88Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.160 , 0.195	Depositor
Wilson B-factor (Å <sup>2</sup> )	27.3	Xtrriage
Anisotropy	0.476	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15614	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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](#)

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	OYG	A	301	1	12,13,14	1.09	1 (8%)	15,17,19	2.53	2 (13%)
5	OYG	C	801	1	12,13,14	0.67	0	15,17,19	1.64	1 (6%)

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	OYG	A	301	1	-	1/4/4/5	0/1/1/1
5	OYG	C	801	1	-	1/4/4/5	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	301	OYG	C3-C2	3.09	1.40	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	301	OYG	C1-C2-C3	-9.09	115.53	125.84
5	C	801	OYG	C1-C2-C3	-5.86	119.19	125.84
5	A	301	OYG	C2-C3-C4	-2.63	122.23	127.02

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	301	OYG	C2-C3-C4-C5
5	C	801	OYG	C2-C3-C4-C5

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

### 5.1 Protein, DNA and RNA chains

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

### 5.2 Non-standard residues in protein, DNA, RNA chains

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

### 5.3 Carbohydrates

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

### 5.4 Ligands

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

### 5.5 Other polymers

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