



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:27 AM EDT

PDB ID : 6N7Q
Title : Plasmodium falciparum FVO apical membrane antigen 1 (AMA1) bound to cyclised RON2 peptide
Authors : McGowan, S.; Drinkwater, N.
Deposited on : 2018-11-28
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 ⓘ 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**
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

The following experimental techniques were used to determine the structure:

X-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 3 unique types of molecules in this entry. The entry contains 2346 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 Apical membrane antigen-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	266	2077	1318	347	399	13	1	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	expression tag	UNP Q1PBJ5
A	267	GLU	GLN	conflict	UNP Q1PBJ5
A	433	HIS	-	expression tag	UNP Q1PBJ5
A	434	PRO	-	expression tag	UNP Q1PBJ5
A	435	ILE	-	expression tag	UNP Q1PBJ5
A	436	GLU	-	expression tag	UNP Q1PBJ5
A	437	VAL	-	expression tag	UNP Q1PBJ5
A	438	GLU	-	expression tag	UNP Q1PBJ5

- Molecule 2 is a protein called RON2 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	13	105	67	18	17	3	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	C	1	Total 1	O 1	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 a, b, c, α , β , γ	122.56Å 37.98Å 72.02Å 90.00° 91.06° 90.00°	Depositor
Resolution (Å)	36.27 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (36.27-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.207 , 0.243	Depositor
Wilson B-factor (Å ²)	19.3	Xtrriage
Anisotropy	0.753	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtrriage
Total number of atoms	2346	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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](#)

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4.3.2 Protein sidechains [i](#)

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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

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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