

Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 03:19 AM EDT

PDB ID : 6UTA

Title : Crystal structure of Z004 iGL Fab in complex with ZIKV EDIII

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Deposited on : 2019-10-29

Resolution : 3.10 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 (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 3.10 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 8038 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 Z004 iGL Fab heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Н	221	Total 1636	C 1029	11	O 323	S 6	0	0	0
1	A	218	Total 1622	C 1022			S 6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Н	221	HIS	-	expression tag	UNP S6C4S0
Н	222	HIS	-	expression tag	UNP S6C4S0
Н	223	HIS	-	expression tag	UNP S6C4S0
Н	224	HIS	-	expression tag	UNP S6C4S0
Н	225	HIS	-	expression tag	UNP S6C4S0
A	221	HIS	-	expression tag	UNP S6C4S0
A	222	HIS	-	expression tag	UNP S6C4S0
A	223	HIS	-	expression tag	UNP S6C4S0
A	224	HIS	-	expression tag	UNP S6C4S0
A	225	HIS	-	expression tag	UNP S6C4S0

• Molecule 2 is a protein called Z004 iGL Fab light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	L	212	Total 1638	C 1029	N 273	O 331	S 5	0	0	0
						331	0			
2	В	212	1638	C 1029	N 273	331	5 5	0	0	0

• Molecule 3 is a protein called Env.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Е	99	Total 751	C 477	N 124	O 144	S 6	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	99	Total 753	C 479	N 124	O 144	S 6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ε	298	MET	-	initiating methionine	UNP A0A1X9PPI0
С	298	MET	-	initiating methionine	UNP A0A1X9PPI0

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 43 21 2	Depositor
Cell constants	85.91Å 85.91Å 327.46Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.42 - 3.10	Depositor
% Data completeness	93.7 (38.42-3.10)	Depositor
(in resolution range)	,	•
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.56 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.274 , 0.291	Depositor
Wilson B-factor (A^2)	67.7	Xtriage
Anisotropy	0.167	Xtriage
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8038	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 8.90% 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)

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)

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

