



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 04:01 AM EDT

PDB ID : 6NFM  
Title : Crystal Structure of the Cancer Genomic DNA Mutator APOBEC3B with loop 7 from APOBEC3G  
Authors : Shi, K.; Aihara, H.  
Deposited on : 2018-12-20  
Resolution : 2.53 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](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**  
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 2.53 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

There are 3 unique types of molecules in this entry. The entry contains 1533 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 DNA dC->dU-editing enzyme APOBEC-3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	183	1510	954	268	276	12	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	MET	-	initiating methionine	UNP Q9UH17
A	200	SER	PHE	engineered mutation	UNP Q9UH17
A	228	SER	TRP	engineered mutation	UNP Q9UH17
A	230	LYS	LEU	engineered mutation	UNP Q9UH17
A	250	SER	ALA	engineered mutation	UNP Q9UH17
A	?	-	LYS	deletion	UNP Q9UH17
A	?	-	ASN	deletion	UNP Q9UH17
A	?	-	LEU	deletion	UNP Q9UH17
A	?	-	LEU	deletion	UNP Q9UH17
A	?	-	CYS	deletion	UNP Q9UH17
A	?	-	GLY	deletion	UNP Q9UH17
A	?	-	PHE	deletion	UNP Q9UH17
A	?	-	TYR	deletion	UNP Q9UH17
A	308	LYS	PHE	engineered mutation	UNP Q9UH17
A	315	ASP	TYR	engineered mutation	UNP Q9UH17
A	316	GLN	ASP	engineered mutation	UNP Q9UH17
A	317	GLY	PRO	engineered mutation	UNP Q9UH17
A	318	ARG	LEU	engineered mutation	UNP Q9UH17
A	319	CYS	TYR	engineered mutation	UNP Q9UH17
A	320	GLN	LYS	engineered mutation	UNP Q9UH17
A	379	LEU	-	expression tag	UNP Q9UH17
A	380	GLU	-	expression tag	UNP Q9UH17
A	381	HIS	-	expression tag	UNP Q9UH17
A	382	HIS	-	expression tag	UNP Q9UH17
A	383	HIS	-	expression tag	UNP Q9UH17
A	384	HIS	-	expression tag	UNP Q9UH17
A	385	HIS	-	expression tag	UNP Q9UH17

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Chain	Residue	Modelled	Actual	Comment	Reference
A	386	HIS	-	expression tag	UNP Q9UH17

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	22	Total O 22 22	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	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.31Å 50.31Å 149.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.77 – 2.53	Depositor
% Data completeness (in resolution range)	99.9 (41.77-2.53)	Depositor
$R_{merge}$	0.18	Depositor
$R_{sym}$	0.18	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (dev_3357: ???)	Depositor
R, $R_{free}$	0.218 , 0.276	Depositor
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtrriage
Anisotropy	0.310	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.05% 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 monosaccharides in this entry.

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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](#)

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.