



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 4, 2022 – 08:26 PM EDT

PDB ID : 5K81
Title : Crystal Structure of a Primate APOBEC3G N-Terminal Domain
Authors : Xiao, X.; Li, S.-X.; Yang, H.; Chen, X.S.
Deposited on : 2016-05-27
Resolution : 2.01 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 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) : 2.27

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 2.01 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 10140 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 Apolipoprotein B mRNA editing enzyme, catalytic peptide-like 3G, Apolipoprotein B mRNA editing enzyme, catalytic peptide-like 3G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1603	1045	279	268	11			
1	B	191	Total	C	N	O	S	0	0	0
			1603	1045	279	268	11			
1	C	191	Total	C	N	O	S	0	0	0
			1603	1045	279	268	11			
1	D	186	Total	C	N	O	S	0	0	0
			1561	1018	272	261	10			
1	E	186	Total	C	N	O	S	0	0	0
			1561	1018	272	261	10			
1	F	186	Total	C	N	O	S	0	0	0
			1561	1018	272	261	10			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP M1GSK9
A	-3	PRO	-	expression tag	UNP M1GSK9
A	-2	ALA	-	expression tag	UNP M1GSK9
A	-1	GLY	-	expression tag	UNP M1GSK9
A	0	SER	-	expression tag	UNP M1GSK9
A	143	ALA	-	linker	UNP M1GSK9
A	144	GLU	-	linker	UNP M1GSK9
A	145	ALA	-	linker	UNP M1GSK9
A	146	GLY	-	linker	UNP M1GSK9
B	-4	GLY	-	expression tag	UNP M1GSK9
B	-3	PRO	-	expression tag	UNP M1GSK9
B	-2	ALA	-	expression tag	UNP M1GSK9
B	-1	GLY	-	expression tag	UNP M1GSK9
B	0	SER	-	expression tag	UNP M1GSK9
B	143	ALA	-	linker	UNP M1GSK9
B	144	GLU	-	linker	UNP M1GSK9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	145	ALA	-	linker	UNP M1GSK9
B	146	GLY	-	linker	UNP M1GSK9
C	-4	GLY	-	expression tag	UNP M1GSK9
C	-3	PRO	-	expression tag	UNP M1GSK9
C	-2	ALA	-	expression tag	UNP M1GSK9
C	-1	GLY	-	expression tag	UNP M1GSK9
C	0	SER	-	expression tag	UNP M1GSK9
C	143	ALA	-	linker	UNP M1GSK9
C	144	GLU	-	linker	UNP M1GSK9
C	145	ALA	-	linker	UNP M1GSK9
C	146	GLY	-	linker	UNP M1GSK9
D	-4	GLY	-	expression tag	UNP M1GSK9
D	-3	PRO	-	expression tag	UNP M1GSK9
D	-2	ALA	-	expression tag	UNP M1GSK9
D	-1	GLY	-	expression tag	UNP M1GSK9
D	0	SER	-	expression tag	UNP M1GSK9
D	143	ALA	-	linker	UNP M1GSK9
D	144	GLU	-	linker	UNP M1GSK9
D	145	ALA	-	linker	UNP M1GSK9
D	146	GLY	-	linker	UNP M1GSK9
E	-4	GLY	-	expression tag	UNP M1GSK9
E	-3	PRO	-	expression tag	UNP M1GSK9
E	-2	ALA	-	expression tag	UNP M1GSK9
E	-1	GLY	-	expression tag	UNP M1GSK9
E	0	SER	-	expression tag	UNP M1GSK9
E	143	ALA	-	linker	UNP M1GSK9
E	144	GLU	-	linker	UNP M1GSK9
E	145	ALA	-	linker	UNP M1GSK9
E	146	GLY	-	linker	UNP M1GSK9
F	-4	GLY	-	expression tag	UNP M1GSK9
F	-3	PRO	-	expression tag	UNP M1GSK9
F	-2	ALA	-	expression tag	UNP M1GSK9
F	-1	GLY	-	expression tag	UNP M1GSK9
F	0	SER	-	expression tag	UNP M1GSK9
F	143	ALA	-	linker	UNP M1GSK9
F	144	GLU	-	linker	UNP M1GSK9
F	145	ALA	-	linker	UNP M1GSK9
F	146	GLY	-	linker	UNP M1GSK9

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total 121	O 121	0	0
3	B	117	Total 117	O 117	0	0
3	C	125	Total 125	O 125	0	0
3	D	89	Total 89	O 89	0	0
3	E	99	Total 99	O 99	0	0
3	F	91	Total 91	O 91	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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	106.21Å 81.30Å 106.30Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	46.01 – 2.01	Depositor
% Data completeness (in resolution range)	94.8 (46.01-2.01)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.188 , 0.223	Depositor
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.294	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.469 for -h-l,k,h 0.469 for l,k,-h-l 0.036 for l,-k,h 0.035 for h,-k,-h-l 0.035 for -h-l,-k,l	Xtriage
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 6 ligands modelled in this entry, 6 are 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 ⓘ

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.