

Full wwPDB X-ray Structure Validation Report (i)

Dec 14, 2023 – 03:29 am GMT

PDB ID	:	4BLG
Title	:	Crystal structure of MHV-68 Latency-associated nuclear antigen (LANA) C-
		terminal DNA binding domain
Authors	:	Correia, B.; Cerqueira, S.A.; Beauchemin, C.; Pires De Miranda, M.; Li, S.;
		Ponnusamy, R.; Rodrigues, L.; Schneider, T.R.; Carrondo, M.A.; Kaye, K.M.;
		Simas, J.P.; McVey, C.E.
Deposited on		
Resolution	:	2.20 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 (i)) 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)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\hbox{-}RAY\,DIFFRACTION$

The reported resolution of this entry is 2.20 Å.

There are no overall percentile quality scores available for this entry.

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO



2 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	88.58Å 61.68 Å 63.68 Å	Depositor
a, b, c, α , β , γ	90.00° 99.36° 90.00°	
Resolution (Å)	30.84 - 2.20	Depositor
% Data completeness	100.0 (30.84-2.20)	Depositor
(in resolution range)		
R _{merge}	0.06	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.42 (at 2.20 \text{\AA})$	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.171 , 0.203	Depositor
Wilson B-factor $(Å^2)$	39.8	Xtriage
Anisotropy	0.231	Xtriage
L-test for twinning ²	$< L > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2027	wwPDB-VP
Average B, all atoms $(Å^2)$	45.0	wwPDB-VP

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

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

3 Model quality (i)

3.1 Standard geometry (i)

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

3.2 Too-close contacts (i)

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

3.3 Torsion angles (i)

3.3.1 Protein backbone (i)

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

3.3.2 Protein sidechains (i)

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

3.3.3 RNA (i)

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

3.4 Non-standard residues in protein, DNA, RNA chains (i)

validation-pack failed to run properly - this section is therefore empty.

3.5 Carbohydrates (i)

validation-pack failed to run properly - this section is therefore empty.

3.6 Ligand geometry (i)

validation-pack failed to run properly - this section is therefore empty.

3.7 Other polymers (i)

validation-pack failed to run properly - this section is therefore empty.



3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



4 Fit of model and data (i)

4.1 Protein, DNA and RNA chains (i)

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

4.2 Non-standard residues in protein, DNA, RNA chains (i)

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

4.3 Carbohydrates (i)

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

4.4 Ligands (i)

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

4.5 Other polymers (i)

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

