

Modeling of canine adenovirus 2 penton protein

Sadhna Yadav*, Nisha Dinkar*, Soni Devi

BTS Institute of Science & Technology, 197, Mundia Ahmednagar, Bareilly-243122, UP, India

*Khandelwal College of Management & Technology, Bareilly

**Corresponding author: sadhnayadav455@gmail.com

ABSTRACT

Modeling of cav2 penton protein was done successfully and valuable structural details could be visualized.

Key words: Modeling, canine, adenovirus, penton, protein

INTRODUCTION

Canine adenovirus (CAV), a non-enveloped dsDNA virus, is a member of the genus mastadenovirus under the family adenoviridae. Based on genetic and antigenic characteristics, canine adenoviruses are divided into two types: canine adenovirus type 1 (CAV-1) and canine adenovirus type 2 (CAV-2). Although CAV-1 affects the digestive tract and causes infectious canine hepatitis (ICH) accompanied by uveitis and interstitial nephritis in dogs, CAV-2 is mainly associated with respiratory type of disease. Modeling of cav2 penton protein may provide valuable data on its structure.

MATERIALS AND METHODS

Protein

Canine adenovirus 2 penton gene sequence was downloaded GenBank: MT737968.1 linear DNA 1434 bp and the amino acid sequence was used for modelling.

Modelling software

<https://swissmodel.expasy.org> was reached to model the protein.

RESULTS AND DISCUSSION

Project summary

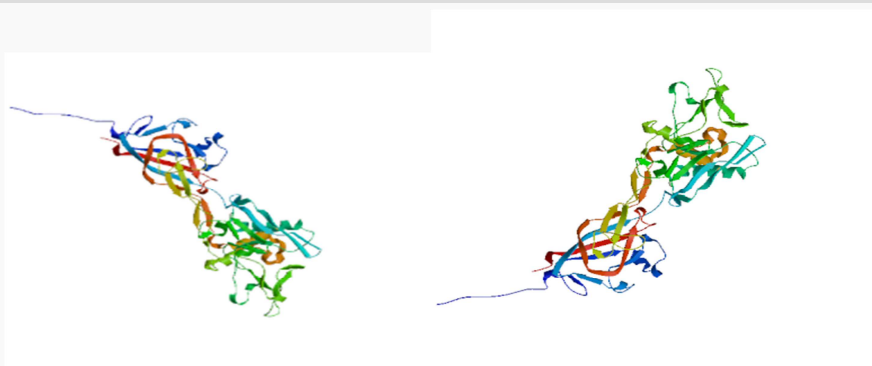
MEFSSPPPSYETVMAQVPSILAPLVPPRYKGATEGRNSIRYSQLPPLFDTTKLYLIDNKSSDIQALNYQNDHSNFLTTVVQNANYTP	12
MEASTQSIQLDERSRWGGFEKSI LHMNMPNVT	0
EYMFNSFKAYLPATADNFGKVLTYEWTTLTPEGNYSEVMLLDLLNNAVENYLAHGRQHNVR EEDMGLKFDTRNFHLGFD PETKLV	24
MPGFYTNEAFHPDIVLSPGCAVDFTHSRLN NF	0
LGIRKRLPYQEGFVITWEDLQGGNIPALLDLENYNPDIPGADITPLMYDSKGRPYHVGEDPSAGSTFTWYRSWFVAYNYGPADGIKSK	36
TVLVAPDITCGVEQIYWSLPDMAVDPVTF TSS	0
HNPSSYPVVGTELLP LPRS FYNGSSVYSQLLQESTSQ TQVFNRF PENAILKRPPAPTII SISENVPALSNHGTLP LKNNIPGVQ RVT	47
ITDARRRVCPYVYKSLGVVVPRVLSSKTF	7

Template results

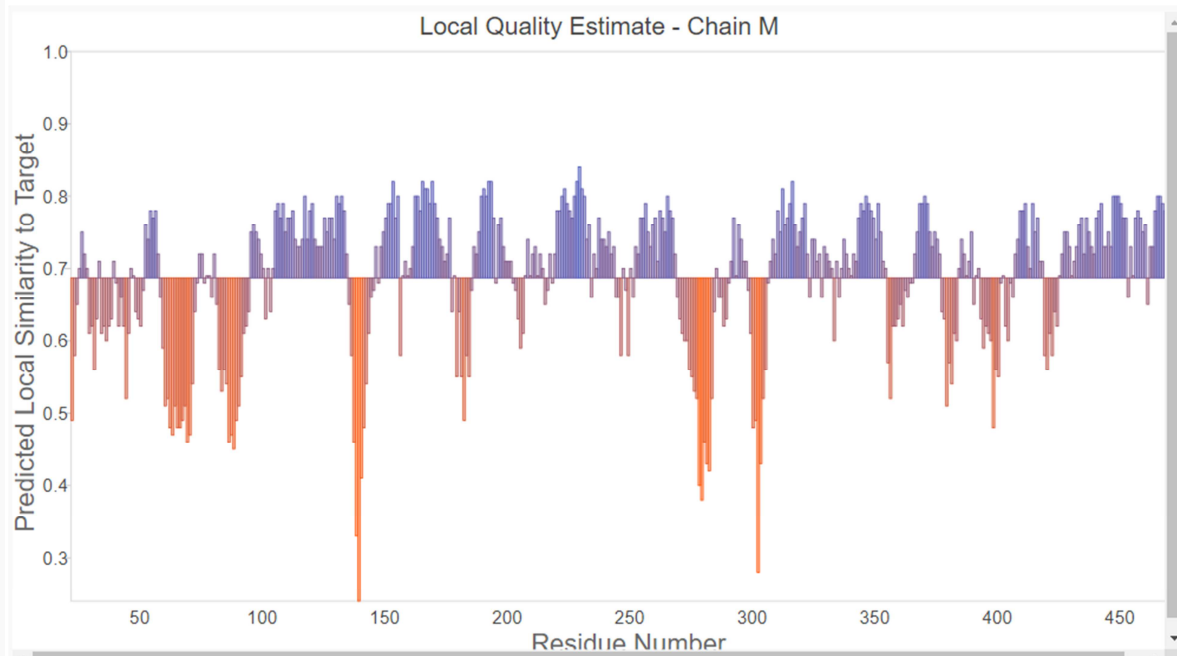
A total of 53 templates were found to match the target sequence. This list was filtered by a heuristic down to 30. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
6b1t.2	64.98	hetero-25-mer	Penton protein Improved cryoEM structure of human adenovirus type 5 with atomic details of minor proteins VI and VII
7s78.2	64.98	hetero-31-mer	Penton protein Structure of a cell-entry defective human adenovirus provides insights into precursor proteins and capsid maturation
7tau.1	62.92	hetero-31-mer	Penton protein Refined capsid structure of human adenovirus D26 at 3.4 Å resolution
3zif.1	67.48	hetero-18-mer	Penton protein Cryo-EM structures of two intermediates provide insight into adenovirus assembly and disassembly
6z7n.1	63.71	hetero-34-mer	Penton protein The atomic structure of HAdV-F41 at pH 7.4

Model results



Oligo-State	GMQE	QMEANDisCo Global: QMEANDisCo Local
Monomer	0.76	0.69 ± 0.05



Local Quality Estimate - Chain M Predicted Local Similarity to Target Residue Number 1.00.80.60.45010015020025030035

QMEAN Z-Scores

Template

6b1t.2.M Penton protein

Improved cryoEM structure of human adenovirus type 5 with atomic details of minor proteins VI and VII Seq Identity 64.98%

Model-Template Alignment

REFERENCES

- Berman, H., Westbrook J., Feng Z., Gilliland G., Bhat T. N., Weissig I., Shindyalov I., Bourne P. E. 2000. The Protein Data Bank. *Nucleic Acids Res.* 28: 235-242.
- Berman, H., Henrick, K., Nakamura, H. and Markley, J.L. 2007. The worldwide Protein Data Bank (wwPDB): ensuring a single, uniform archive of PDB data. *Nucleic Acids Res.* 35: D301-303.
- Bertoni, M., Kiefer, F., Biasini, M., Bordoli, L., Schwede, T. 2017. Modeling protein quaternary structure of homo- and hetero-oligomers beyond binary interactions by homology. *Scientific Reports* 7.
- Bienert, S., Waterhouse, A., de Beer, T.A.P., Tauriello, G., Studer, G., Bordoli, L., Schwede, T. 2017. The SWISS-MODEL Repository - new features and functionality. *Nucleic Acids Res.* 45: D313-D319.
- Bordoli, L., Schwede T. 2012. Automated protein structure modeling with SWISS-MODEL Workspace and the Protein Model Portal. *Methods Mol. Biol.* 857:107-136.
- Guex, N., Peitsch, M.C., Schwede, T. 2009. Automated comparative protein structure modeling with SWISS-MODEL and Swiss-PdbViewer: A historical perspective. *Electrophoresis* 30: S162-S173.
- Mariani, V., Biasini, M., Barbato, A., Schwede, T. 2013. IDDT: a local superposition-free score for comparing protein structures and models using distance difference tests. *Bioinformatics* 29: 2722-2728.
- Schwede, T., Kopp, J., Guex, N., Peitsch, M.C. 2003. SWISS-MODEL: an automated protein homology-modeling server. *Nucleic Acids Res.* 31, 3381-3385.
- Studer, G., Rempfer, C., Waterhouse, A.M., Gumienny, R., Haas, J., Schwede, T. 2020. QMEANDisCo - distance constraints applied on model quality estimation. *Bioinformatics* 36: 1765-1771.
- Waterhouse, A., Bertoni, M., Bienert, S., Studer, G., Tauriello, G., Gumienny, R., Heer, F.T., de Beer, T.A.P., Rempfer, C., Bordoli, L., Lepore, R., Schwede, T. 2018. SWISS-MODEL: homology modelling of protein structures and complexes. *Nucleic Acids Res.* 46(W1), W296-W303.