

Modeling of canine adenovirus 2 hexon 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

Modelling of cav2 hexon protein was done using SWISS-MODEL software and structural details could be visualized and a 3-D image was obtained.

Key words: Modelling, adenovirus, hexon, 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 hexon protein may provide valuable data on its structure.

MATERIALS AND METHODS

Protein sequence

Canine adenovirus 2 hexon gene sequence was downloaded GenBank: EU794687, 12718 bp DNA linear and the amino acid sequence was used for modelling.

Modelling software

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

RESULTS AND DISCUSSION

The results obtained are given below.

Target

MATPSMLPQWSYMHIAGQDAEYLSPALVQFAQATSSYFKLDNKFRNPTVAPTHDVTTERSQRQLQLRFV	1
PVMQEDGQTYKTRFQLAVGDNRVLDMASTYFDIRGTLDRGSPFKPYSGTA	2
	0

YNALAPKAGANNCLFNGQGANINTLAQVPSAGAITVNGQAAVTNNTYQPEPQLGPESWVDGSLAELGDA	2
SGRALKASTPRMPCYGSYAPPTNENGGQATGPVESRFYKVTTNNNNEADAM	4
	0

LYTEDVNLQAPDTHLVHQVPEGQVTGVQGLGQQAPNRPNYIGFRDNFIGLMMYYNSNGNLGVLAGQSSQ	3
LNAVVDLQDRNTELSYQLLLDALTDRSRYFSMWNQAVDSYDQDVRIIDNHG	6
	0

VEDDMPNYCYPLSGMGPLTNMTMKVNNQNFQAENANVGPIQKIGFGNVEAMEINLNANLFKSFLYSNV	4
ALYLPDAFKYTPEIVAPANVNTYAYMNVRPAANLIDTFVNIGARWSPDV	8
	0

MDTVNPFHHRNAGLRYRSQLLGNGRYCSFHIQVPQKFFAIKNLLLLPGTYTYEWSFRKDVNMLQSSLG	6
NDLRVDGATINIQSINLYASFFPMAHNTASTLEAMLRNDVNDQSFADYLS	0
	0

SANMLYPIPANTTLPISIPARNWAGFRGWSFTRIKQRETPALGSPYDPYFTYSGSIPYLDATFYLSHTFRR	7
VSIMFDSSVSWPGNDRLTPNEFEIKRYVDGEGYNVAQSNMTKDWFMV	2
QMLAHYNIGYQGYHLPESYKDRMYSFLRNFEPMCRQLVDVANYAAQPVTVGHQHNNSGYASALSAFN	8
PREGHPYPANWPYPLIGANAVPTVTQKKFLCDRSLWRIPFSSNFMSMGTLD	4
LGQNLLYSNSAHAldMTFEVDAMNEPTLLYVLFEVFDVARVHQPHRGVIEVVYLRTPFSAgnATT	9
	0
	5

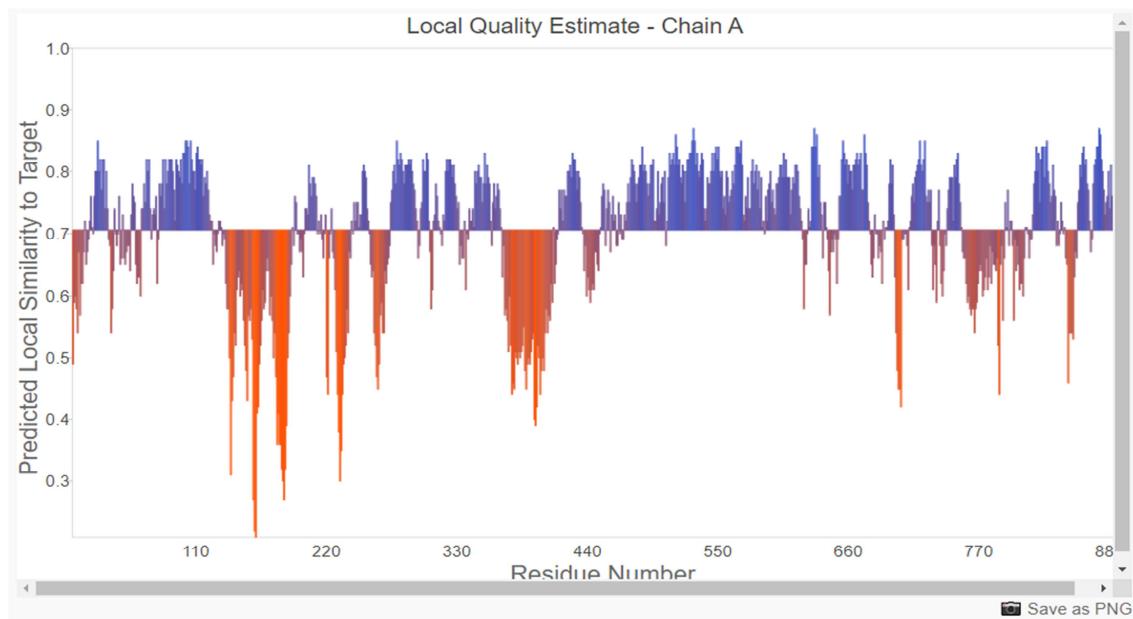
Template Results

A total of 361 templates were found to match the target sequence. This list was filtered by a heuristic down to 50. The top templates are:

Template	Sequence	Biounit		Description
		Identity	Oligo State	
1p2z.1	71.75	homo-trimer		Hexon protein Refinement of Adenovirus Type 2 Hexon with CNS
2obe.1	71.59	homo-trimer		Hexon protein Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
6b1t.1	71.37	hetero-25-mer		Hexon protein Improved cryoEM structure of human adenovirus type 5 with atomic details of minor proteins VI and VII
6b1t.1	71.37	hetero-25-mer		Hexon protein Improved cryoEM structure of human adenovirus type 5 with atomic details of minor proteins VI and VII
6b1t.1	71.37	hetero-25-mer		Hexon protein Improved cryoEM structure of human adenovirus type 5 with atomic details of minor proteins VI and VII

Model Results

Id Template GMQE QMEANDisCo Global Oligo State Ligands



QMEANDisCo Global: ± 0.05

QMEAN Z-Scores

QMEAN	-2.03
C β	-2.19
All Atom	-1.97
solvation	-2.46
torsion	-0.79

★Comparison with Non-redundantSet of PDB StructuresNormalized QMEAN4Protein Size (Residues)

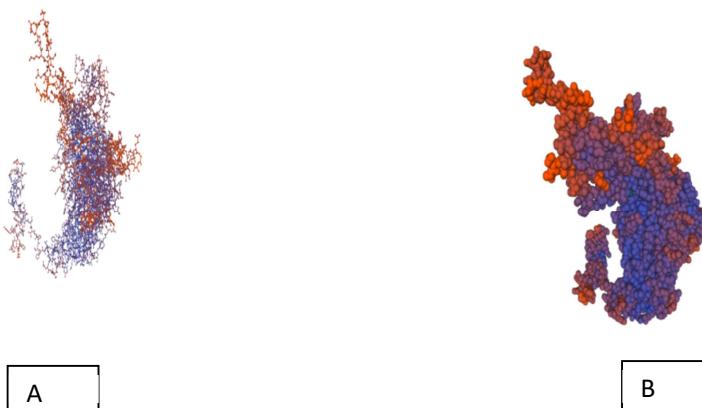


Fig. CAV2 hexon protein as ball and stick(A) and as spacefill (B) model.

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.