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Modeling of human adenovirus penton protein

Soni Devi and Anant Rai*
BTS Institute of Science & Technology, Mundia Ahmednagar, Bareilly-243122, UP
*Corresponding author: raia48@gmail.com

Abstract

Modeling of human adenovirus penton protein was done using SWISS-MODEL software. Valuable structural properties could be obtained.

Key words: Modeling, human, adenovirus, penton, protein.

Introduction

Human adenoviruses are one of the most important pathogens detected in acute respiratory diseases in pediatrics and immunocompromised patients. To date, more than 110 types of human adenoviruses have been described, with different cellular tropisms. They can cause respiratory and gastrointestinal symptoms, even urinary tract inflammation, although most infections are asymptomatic. However, there is a population at risk that can develop serious and even lethal conditions. These viruses have a double-stranded DNA genome, 25–48 kb, 90 nm in diameter, without an envelope, are stable in the environment, and resistant to fat-soluble detergents (Contreras et.al., 2023). They can cause infections at any age but most commonly in pediatric population, especially in young children and infants. By the time 10 years old, most children have at least one episode of adenovirus infection. Adenoviruses can cause many symptoms similar to common cold, including rhinorrhea, fever, cough, and sore throat. Lower respiratory infections such as bronchitis, bronchiolitis, and pneumonia can be severe and even fatal. Other diseases such as conjunctivitis, gastroenteritis, cystitis, myocarditis, cardiomyopathy, and meningoencephalitis can also be associated with adenovirus infections (Shieh,2022). Adenoviruses are medium-sized,70–100 nm in diameter, non-enveloped icosahedral viruses composed of double-stranded linear DNA genome with an average length of 26–45 kb. In humans more than 100 adenovirus types have been identified and classified into seven species (A to G) based on hemagglutination properties, oncogenicity in rodents, DNA homology, and genomic organization. Human adenoviruses cause significant numbers of respiratory, ocular, and gastrointestinal diseases and incidences of severe diseases caused by adenoviruses most occur in immunocompromised individuals or toddlers. Recent outbreaks of adenovirus infections are at least partly due to newly evolving adenovirus types from constant molecular evolution (Zhang et al., 2021).

Materials and Methods

Protein sequence

Human adenovirus sp. Isolate 1955/Beijing/08/2019 penton gene, complete cds GenBank: MT150576.1 linear 1527 bp DNA was downloaded and used the amino acid sequence for modeling.

Modelling software

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

Results and Discussion

Project Summary

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MRRAVGVPPVMAYAEGPPPSYESVMGSADSPATLEALYVPPRYLGPTEGRNSIRYSELAPLYDTTRVYLVDNKSAD  120
IASLNYQNDHSNFQTTVVQNNDFTPAEAGTQTINFDERSRWGAD

LKTILRTNMPNINEFMSTNKFKARLMVEKKNKETGLPRYEWFEFTLPEGNYSETMTIDLMNNAIVDNYLEVGRQNG  240
VLESDIGVKFDTRNFRLGWDPVTKLVMPGVYTNEAFHPDIVLLP

GCGVDFTQSRLSNLLGIRKRLPFQEGFQIMYEDLEGGNIPALLDVAKYEASIQKAKEEGKEIGDDTFATRPQDLVI  360
EPVAKDSKNRSYNLLPNDQNNTAYRSWFLAYNYGDPKKGVQSWT

LLTTADVTCGSQQVYWSLPDMMQDPVTFRPSTQVSNYPVVGVELLPVHAKSFYNEQAVYSQLIRQSTALTHVFNRF  480
PENQILVRPPAPTITTVSENVPALTDHGTLPLRSSISGVQRVTI

TDARRRTCPYVHKALGIVAPKVLSSRTF                                                  508
```

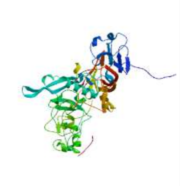
Template Results

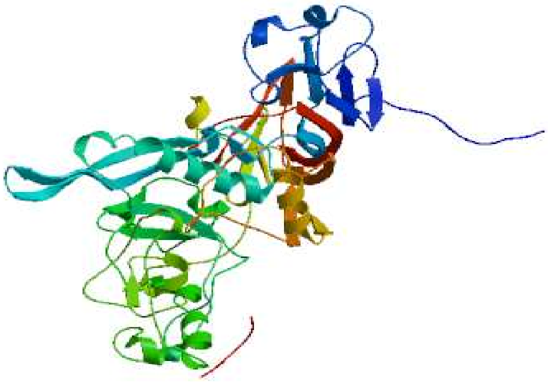
A total of 34 templates were found to match the target sequence. This list was filtered by a heuristic down to 27. The top templates are:

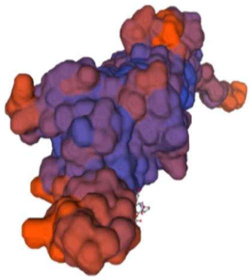
Template	Sequence Identity	Biounit Oligo State	Description
6z7n.1	100.00	hetero-34-mer	Penton protein The atomic structure of HAdV-F41 at pH 7.4
7tau.1	77.69	hetero-31-mer	Penton protein Refined capsid structure of human adenovirus D26 at 3.4 A resolution

Template	Sequence Identity	Biounit Oligo State	Description
7s78.2	79.96	hetero-31-mer	Penton protein Structure of a cell-entry defective human adenovirus provides insights into precursor proteins and capsid maturation
7s78.2	76.45	hetero-31-mer	Penton protein Structure of a cell-entry defective human adenovirus provides insights into precursor proteins and capsid maturation
7tau.1	80.67	hetero-31-mer	Penton protein Refined capsid structure of human adenovirus D26 at 3.4 A resolution

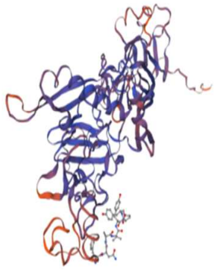
Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	6z7n.1.W	0.78	0.73 ± 0.05	monomer	1 x PHE-ASN-PRO-VAL-TYR-PRO-T

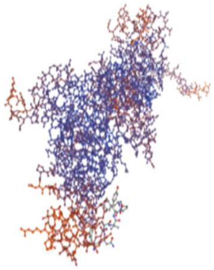




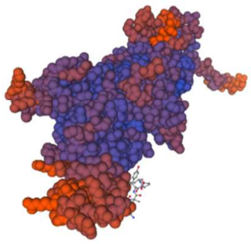
surface



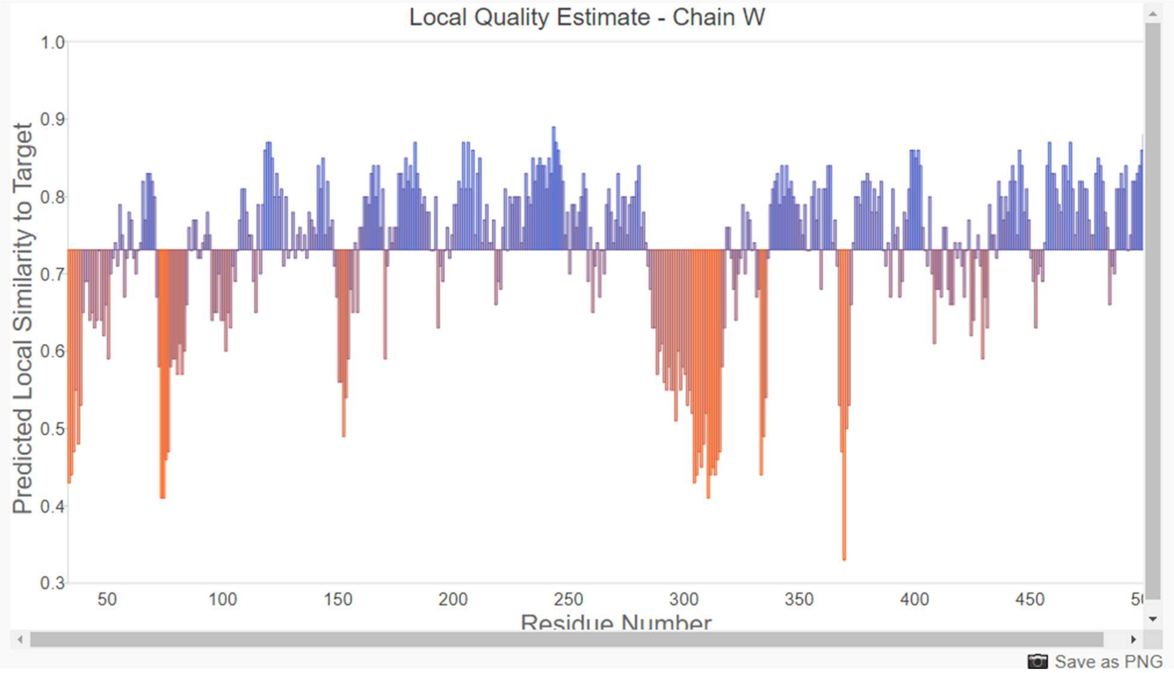
cartoon



ball+stick



spacefill



It is evident that detailed valuable structural parameters could be found.

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