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Modeling of human adenovirus penton protein

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Abstract

Modeling of human adenovirus penton protein was done and valuable information about its structural details was revealed.

Key words: Modeling, human adenovirus, penton, protein

Introduction

Viral proteins play an important role in their actions and study of their structural details would be of great importance.

Materials and Methods

Protein

The amino acid sequence of human adenovirus penton gene GenBank: MT150576.1 protein sequence was downloaded from GenBank and used for modeling.

Modelling software

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

Template Search

Template search with BLAST and HHblits has been performed against the SWISS-MODEL template library (SMTL, last update: 2026-03-11, last included PDB release: 2026-03-06).

The target sequence was searched with BLAST against the primary amino acid sequence contained in the SMTL. A total of 26 templates were found.

An initial HHblits profile has been built using the procedure outlined in (Steinegger et al.), followed by 1 iteration of HHblits against Uniclust30 (Mirdita, von den Driesch et al.). The obtained profile has then be searched against all profiles of the SMTL. A total of 36 templates were found.

Template Selection

For each identified template, the template's quality has been predicted from features of the target-template alignment. The templates with the highest quality have then been selected for model building.

Model Building

Models are built based on the target-template alignment using ProMod3 (Studer et al.). Coordinates which are conserved between the target and the template are copied from the template to the model. Insertions and deletions are remodelled using a fragment library. Side chains are then rebuilt. Finally, the geometry of the resulting model is regularized by using a force field.

Model Quality Estimation

The global and per-residue model quality has been assessed using the QMEAN scoring function (Studer et al.).

Ligand Modelling

Ligands present in the template structure are transferred by homology to the model when the following criteria are met: (a) The ligands are annotated as biologically relevant in the template library, (b) the ligand is in contact with the model, (c) the ligand is not clashing with the protein, (d) the residues in contact with the ligand are conserved between the target and the template. If any of these four criteria is not satisfied, a certain ligand will not be included in the model. The model summary includes information on why and which ligand has not been included.

Oligomeric State Conservation

The quaternary structure annotation of the template is used to model the target sequence in its oligomeric form. The method (Bertoni et al.) is based on a supervised machine learning algorithm, Support Vector Machines (SVM), which combines interface conservation, structural clustering, and other template features to provide a quaternary structure quality estimate (QSQE). The QSQE score is a number between 0 and 1, reflecting the expected accuracy of the interchain contacts for a model built based a given alignment and template. Higher numbers indicate higher reliability. This complements the GMQE score which estimates the accuracy of the tertiary structure of the resulting model.

Results and Discussion

Project Summary

Target 1	MRRAVGVPPVMAYAEGPPPSYESVMGSADSPATLEALYVPPRYLGPTEGRNSIRYSELAPLYDTTRVYLVDNKSADIASLNYQNDHSNFQTTVVQNNDFTPAEAGTQTINFDERSRWGADLKTILRTNMP	130
Target 1	NINEFMSTNKFKARLMVEKKNKETGLPRYEWFEFTLPEGNYSETMTIDLMNNAIVDNYLEVGRQNGVLESDIGVKFDTRNFRLGWDPVTKLVMPGVYTNEAFHPDIVLLPGCGVDFTQSRLSNLLGIRKR	260
Target 1	LPFQEGFQIMYEDLEGGNIPALLDVAKYEASIQKAKEEGKEIGDDTFATRPQDLVIEPVAKDSKNRSYNLLPNDQNNTAYRSWFLAYNYGDPKKGVQSWTLLTTADVTCGSQQVYWSLPDMMQDPVTFRP	390

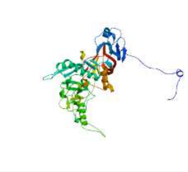
Target 1	STQVSNYPVVGVELLPVHAKSFYNEQAVYSQLIRQSTALTHVFNRFPENQILVRPPAPTITT VSENVPALTDHGTLPLRSSISGVQRVTITDARRRTCPYVHKALGIVAPKVLSSRTF	508

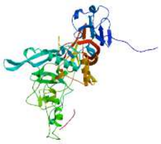
Template Results

A total of 60 templates were found to match the target sequence. This list was filtered by a heuristic down to 43. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
A0A5B1BAK1.1	79.80	monomer	Uncharacterized protein AlphaFold DB model of A0A5B1BAK1_MYCSI (ge
6z7n.1	100.00	hetero-34-mer	Penton protein The atomic structure of HAdV-F41 at pH 7.4
9r78.1	77.69	hetero-28-mer	Penton protein Human Adenovirus D 10 Capsid Structure
7tau.1	77.69	hetero-31-mer	Penton protein Refined capsid structure of human adenovirus D26 at
7s78.2	79.96	hetero-31-mer	Penton protein Structure of a cell-entry defective human adenovirus p

Model Results

	Id	Template	GMQE	QMEANDisCo Global
	01	A0A5B1BAK1.1.A	0.87	

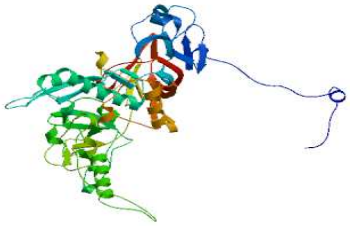
	Id	Template	GMQE	QMEANDisCo Global
	02	6z7n.1.W	0.78	± 0.05

Show full model results

Model Results Schwede GroupContact UsTerms of use

Order by: GMQEQMEANDisCoOligo StateLigandsSeq IdentitySimilarityCoverage
1508

Model 01



Compare

Oligo-State

Monomer

GMQE

0.87

Template

A0A5B1BAK1.1.A Uncharacterized protein

AlphaFold DB model of A0A5B1BAK1_MYCSI (gene: A0A5B1BAK1_MYCSI, organism: Mycobacterium simiae (Mycobacterium habana))

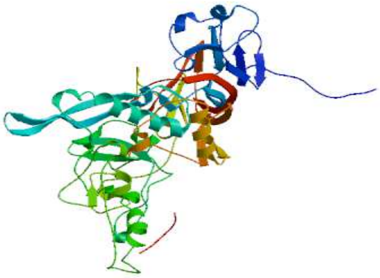
Seq Identity

79.80%

Coverage

Model-Template Alignment

Model 02



Compare

Oligo-State

Monomer

GMQE

0.78

QMEANDisCo Global:

± 0.05

Ligands

1 x PHE-ASN-PRO-VAL-TYR-PRO-TYR

QMEANDisCo Local

QMEAN Z-Scores

Template

6z7n.1.W Penton protein

The atomic structure of HAdV-F41 at pH 7.4

Seq Identity

100.00%

Coverage

Model-Template Alignment

Model #01	File	Built with	Oligo-State	Ligands	GMQE
	PDB	ProMod3 3.6.0	monomer	None	0.87

Template	Seq Identity	Oligo-state	QS QE	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
A0A5B1BAK1.1.A	79.80	monomer	-	AFDB search	AlphaFold v2	-	0.55	13 - 508	0.97	Uncharacterized protein

Model #02	File	Built with	Oligo-State	Ligands	GMQE	QMEANDisCo Global

Template	Seq Identity	Oligo-state	QSQE	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
	PDB	ProMod3 3.6.0	monomer	1 x PHE-ASN-PRO-VAL-TYR-PRO-TYR: Fiber protein;	0.78	0.73 ± 0.05				

Template	Seq Identity	Oligo-state	QSQE	Found by	Method	Resolution	Seq Similarity	Range	Coverage	Description
6z7n.1.W	100.00	monomer	0.00	HHblits	EM	3.77Å	0.62	33 - 508	1.00	Penton protein

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