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Research Article

## HUMAN ADENOVIRUS TYPE 2 HEXON CAPSID PROTEIN MODELLING

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### ABSTRACT

The modelling of human adenovirus 2 hexon capsid protein was done using Swiss-Model and valuable structural informations were obtained. The reacting sites of the protein could be visualised.

**Keywords:** Adenovirus, human, hexon capsid, modelling.

### INTRODUCTION

Adenoviruses are important infectious agents prevalent in almost all species. The hexon capsid protein is an important protein which helps in infectious process and also produces neutralising antibodies which participate in immunity against this disease. Hence it was considered essential to understand the

detailed structure of hexon protein and its reacting sites. Hence modelling of this protein using Swiss model was undertaken.

### MATERIALS AND METHODS

The human adenovirus 2 hexon capsid genome was downloaded from NCBI Pubmed and the aminoacid sequence was saved for use in modelling (Table 1).

**Table 1. Amino acid sequence used for modeling.**

```
MATPSMMPQWSYMHISGQDASEYLSPLGVQFARATETYFSLNNKFRNPTVAPTHDVTDRSQRLTLRFIPVDREDT  
AYSYKARFTLAVGDNRVLDMASTY  
FDIRGVLDGRPTFKPYSGTAYNALAPKGAPNSCEWEQTEDSGRAVAEDEEEEEDEDEEEEEEQNARDQATKKTH  
VYAQAPLSGETITKSGLQIGSDNAE  
TQAKPVYADPSYQPEPQIGESQWNEADANAAGGRVLKKTTPMKPCYGSYARPTNPFGGQSVLVPDEKGVPLPKVD  
LQFFSNTTSLNDRQGNATKPKVVLY  
SEVDNLETDPDTHLSYKPGKGDENSKAMLGQQSMPNRPNYIAFRDNFIGLMYYNSTGNMGVLAGQASQLNAVVDL  
QDRNTELSYQLLLDSIGDRTRYFSMW  
NQAVDSYDPDVRIENHGTEDELPNYCFPLGGIGVTDITYQAIKANGNGAGDNGNTTWTKDETFATRNEIGVGNNF  
AMEINLNANLWRNFLYSNIALYLPD
```

KLKYNPTNVEISDNPNNTYDYMNKRVVAPGLVDCYINLGARWVSLDYMDNVNPFNHHRNAGLRYRSMLLGNTRYV  
 PFHIQVPQKFFAIKNLLLLPGSYTYEW  
 NFRKDVNMVLQSSLGNDLRVDGASIKFDSICLYATFFPMAHNTASTLEAMLRNDTNDQSFNDYLSAANMLYPIPA  
 NATNVPISIPSRNWAFAFRGWAFTRL  
 KTKETPSLGSYDPYYTYSGSIPYLDGTFYLNHTFKKVAITFDSSVSWPGNDRLLTPNEFEIKRSVDGEGYNVAQCN  
 MTKDWFLVQMLANYNIGYQGFYI  
 PESYKDRMYSFFRNFPMSRQVVDDTKYKDYQQVGIHQHNNSGFVGYLAPTMREGQAYPANVPYPLIGKTAVDS  
 ITQKKFLCDRTLWRIPFSSNFMSMG  
 ALTDLQGNLLYANSAHALDMTFEVDPMDEPTLLYVLFVFDVVRVHQPHRGVIETVYLRTPFSAAGNATT

## Modeling

The target sequence was searched with BLAST against the primary amino acid sequence contained in the SMTL. An initial HHblits profile was built using the procedure of Remmert *et al.* (2009). The obtained profile was then searched against all profiles of the SMTL. A total of 37 templates were found. 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. Models are built based on the target-template alignment using ProMod3. 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. In case loop modelling with ProMod3 fails, an alternative model is built with PROMOD-II (Guex *et al.*, 2009).

The global and per-residue model quality has been assessed using the QMEAN scoring function (Benkert *et al.*, 2011). For improved performance, weights of the individual QMEAN terms have been trained specifically for SWISS-MODEL.

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 quaternary structure annotation of the template is used to model the target sequence in its oligomeric form. The method (Bertoni *et al.*, 2017) 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 (Waterhouse *et al.*, 2018).

## RESULTS AND DISCUSSION

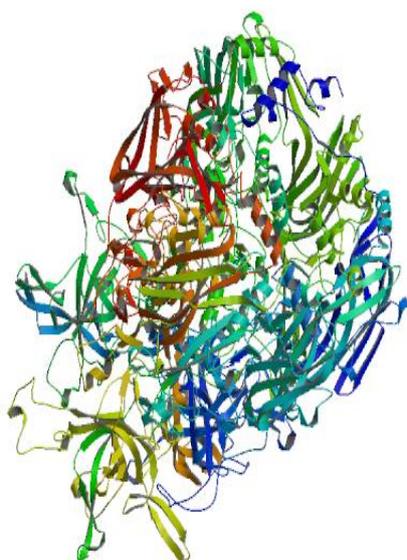
The SWISS-MODEL template library (SMTL version 2018-06-01, PDB release 2018-05-25) was searched with BLAST (Camacho *et al.*, 2009) and HHblits (Remmert *et al.*, 2012) for evolutionary related structures matching the target sequence in Table 1. Overall 74

templates were found but those giving satisfactory results are shown in Table 2

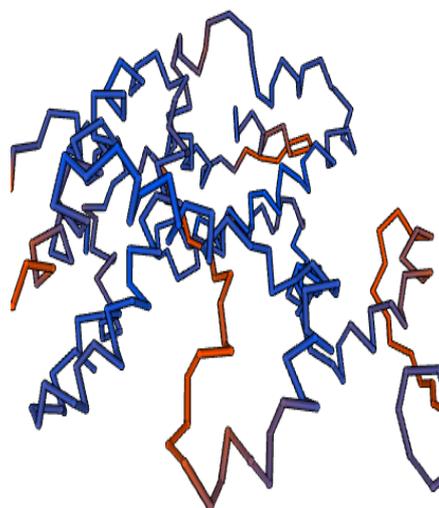
and models constructed were homo-trimer (Fig. 1) and monomer (Fig. 2).

**Table 2. Templates found matching target sequence.**

Template Description	Seq Identity	Oligo-state	QSQE	Method	Resolution	Similarity	Coverage
1p2z.1.A	99.07	homo-trimer	0.84	HHblits X-ray	2.20Å	0.62	1.00 Hexon
1p2z.1.A	99.07	homo-trimer	0.83	BLAST X-ray	2.20Å	0.62	1.00 Hexon
2obe.1.A	81.08	homo-trimer	0.87	BLAST X-ray	2.10Å	0.56	0.96 Hexon
2obe.1.A	80.86	homo-trimer	0.87	HHblits X-ray	2.10Å	0.56	0.96 Hexon
5ogi.1.A	88.75	monomer		BLAST X-ray	2.80Å	0.58	0.98 Hexon
6eqc.1.A	88.75	homo-trimer	0.79	BLASTEM	NA	0.58	0.98 Hexon
6eqc.1.B	88.75	homo-trimer	0.79	BLASTEM	NA	0.58	0.98 Hexon
6eqc.1.C	88.75	homo-trimer	0.79	BLASTEM	NA	0.58	0.98 Hexon
5ogi.1.A	88.75	monomer		HHblits X-ray	2.80Å	0.58	0.98 Hexon
6eqc.1.A	88.75	homo-trimer	0.79	HHblitsEM	NA	0.58	0.98 Hexon
6eqc.1.B	88.75	homo-trimer	0.79	HHblitsEM	NA	0.58	0.98 Hexon
6eqc.1.C	88.75	homo-trimer	0.79	HHblitsEM	NA	0.58	0.98 Hexon
5tx1.1.A	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon
5tx1.1.F	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon
5tx1.1.B	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon
5tx1.1.D	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon
5tx1.1.E	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon
5tx1.1.G	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon
5tx1.1.H	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon
5tx1.1.C	78.46	homo-12-mer	0.78	BLASTEM	NA	0.55	0.98 Hexon



**Fig 1. Model 1 Homo-trimer.**



**Fig.2. Model 2 Monomer**

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