Devi and Rai (2021). Biotechnology International 14:1-4.
www. biotechnologyinternational.org

Modeling of human adenovirus 35 hexon protein

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ABSTRACT

Modeling of human adenovirus 35 hexon protein was done and models could be successfully made. Valuable structural details could be elucidated.

Key words: Modeling, human, adenovirus 35, virus, hexon, protein

INTRODUCTION

Adenoviruses cause several infections in human and thus are very important pathogen. The hexon protein of adenoviruses plays important role in development of immune responses and thus it has been studied in detil. In this context study of structural details of hexon protein is very important to know its structure and binding sites.

MATERIALS AND METHODS

Protein

Human adenovirus 35 gene for hexon, complete cds, strain: Holden GenBank: AB330116.1 linear 2859 bp DNA and amino acid sequence was used for modelling.

Modelling software

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

RESULTS AND DISCUSSION

Project summary

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MATPSMLPQWAYMHIAGQDASEYLSPGLVQFARATDTYFNLGNKFRNPTVAPTHDVTTDRSQRLMLRFVPVDREDNTYSYKVRYTLAV   12
GDNRVLDMASTFFDIRGVLDRGPSFKPYSGTA                                                             0

YNSLAPKGAPNASQWIAKGVPTAAAAGNGEEEHETEEKTATYTFANAPVKAEAQITKEGLPIGLEISAENESKPIYADKLYQPEPQVG   24
DETWTDLDGKTEEYGGRALKPTTNMKPCYGSY                                                             0

AKPTNLKGGQAKPKNSEPSSEKIEYDIDMEFFDNSSQRTNFSPKIVMYAENVGLETPDTHVVYKPGTEDTSSEANLGQQSMPNRPNYI   36
GFRDNFIGLMYYNSTGNMGVLAGQASQLNAVV                                                             0

DLQDRNTELSYQLLLDSLGDRTRYFSMWNQAVDSYDPDVRVIENHGVEDELPNYCFPLDGIGVPTTSYKSIVPNGEDNNNWKEPEVNG   48
TSEIGQGNLFAMEINLQANLWRSFLYSNVALY                                                             0

LPDSYKYTPSNVTLPENKNTYDYMNGRVVPPSLVDTYVNIGARWSLDAMDNVNPFNHHRNAGLRYRSMLLGNGRYVPFHIQVPQKFFA   60
VKNLLLLPGSYTYEWNFRKDVNMVLQSSLGND                                                             0

LRVDGASISFTSINLYATFFPMAHNTASTLEAMLRNDTNDQSFNDYLSAANMLYPIPANATNIPISIPSRNWAAFRGWSFTRLKTKET   72
PSLGSGFDPYFVYSGSIPYLDGTFYLNHTFKK                                                             0

VSIMFDSSVSWPGNDRLLSPNEFEIKRTVDGEGYNVAQCNMTKDWFLVQMLANYNIGYQGFYIPEGYKDRMYSFFRNFQPMSRQVVDE   84
VNYKDFKAVAIPYQHNNSGFVGYMAPTMRQGQ                                                             0

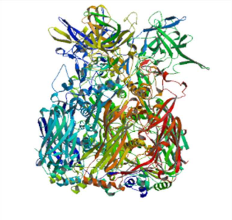
PYPANYPYPLIGTTAVNSVTQKKFLCDRTMWRIPFSSNFMSMGALTDLGQNMLYANSAHALDMTFEVDPMDEPTLLYLLFEVFDVVRV   95
HQPHRGIIEAVYLRTPFSAGNATT                                                                     2
```

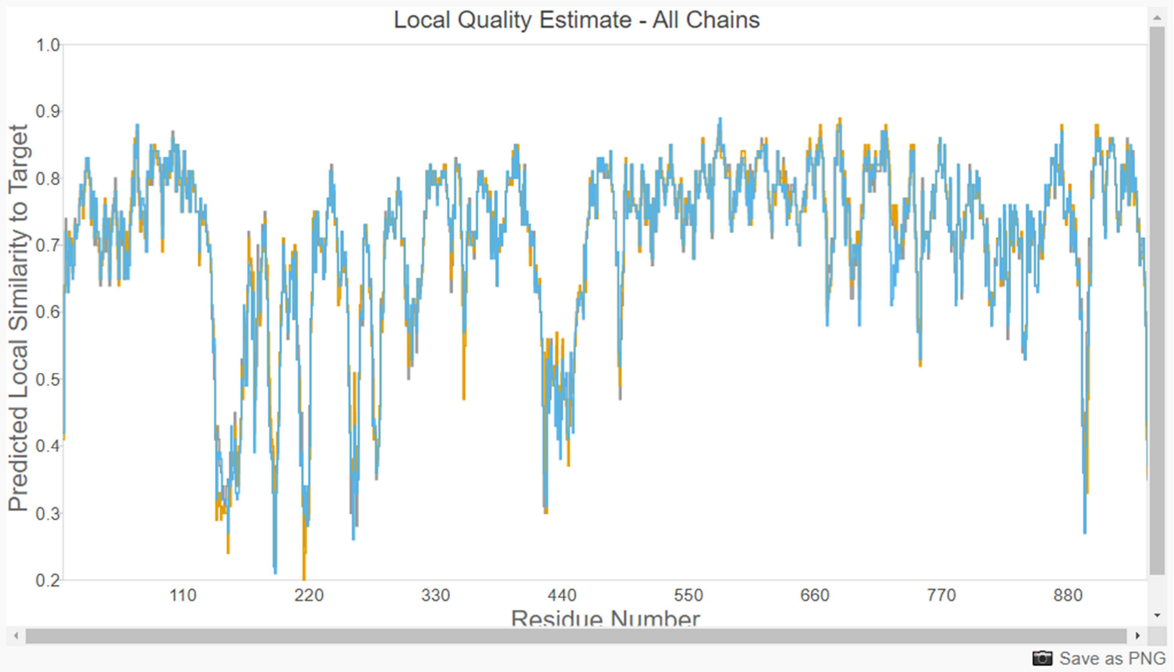
Template Results

A total of 361 templates were found to match the target sequence. This list was filtered by a heuristic down to 38. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
2obe.1	85.81	homo-trimer	Hexon protein Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
2obe.1	86.02	homo-trimer	Hexon protein Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
1p2z.1	78.92	homo-trimer	Hexon protein Refinement of Adenovirus Type 2 Hexon with CNS
1p2z.1	79.53	homo-trimer	Hexon protein Refinement of Adenovirus Type 2 Hexon with CNS
5ogi.1	78.43	hetero-dimer	Hexon protein Complex of a binding protein and human adenovirus C 5 hexon

Model Results

Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands	
	01	2obe.1.A	0.74	0.71 ± 0.05	homo-trimer	16 x 2HP
	02	5tx1.1.A	0.72	± 0.05	monomer	-



It is evident that valuable structural models could be constructed.

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