Modeling of human adenovirus 2 hexon protein

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ABSTRACT

Modeling of human adenovirus 2 hexon protein was done and models could be successfully made. Valuable structural details could be elucidated.

Key words: Modeling, human, adenovirus 2 , 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 detail. In this context study of structural details of hexon protein of adenovirus 2 is very important to know its structure and binding sites.

MATERIALS AND METHODS

Protein

Human adenovirus type 2 hexon gene for hexon, isolate 105 GenBank: AJ293903.1 linear 2910 bp 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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MATPSMMPQWSYMHISGQDASEYLSPGLVQFARATETYFSLNNKFRNPTVAPTHDVTTDRSQRLTLRFIPVDREDTAYSYK  12
ARFTLAVGDNRVLDMASTYFDIRGVLDRGPTFKPYSGTA                                               0

YNALAPKGAPNSCEWEQTEDSGRAVAEDEEEEEDEDEEEEEEEQNARDQATKKTHVYAQAPLSGETITKSGLQIGSDNAET  24
QAKPVYADPSYQPEPQIGESQWNEADANAAGGRVLKKTT                                              0

PMKPCYGSYARPTNPFGGQSVLVPDEKGVPLPKVDLQFFSNTTSLNDRQGNATKPKVVLYSEDVNLETPDTHLSYKPGKG   36
DENSKAMLGQQSMPNRPNYIAFRDNFIGLMYYNSTGNMGV                                              0

LAGQASQLNAVVDLQDRNTELSYQLLLDSIGDRTRYFSMWNQAVDSYDPDVRIIENHGTEDELPNYCFPLGGIGVTDTYQA  48
IKANGNGAGDNGNTTWTKDETFATRNEIGVGNNFAMEIN                                               0

LNANLWRNFLYSNIALYLPDKLKYNPTNVEISDNPNTYDYMNKRVVAPGLVDCYINLGARWSLDYMDNVNPFNHHRNAG  60
LRYRSMLLGNGRYVPFHIQVPQKFFAIKNLLLLPGSYTYEW                                             0

NFRKDVNMVLQSSLGNDLRVDGASIKFDSICLYATFFPMAHNTASTLEAMLRNDTNDQSFNDYLSAANMLYPIPANATNV  72
PISIPSRNWAAFRGWAFTRLKTKETPSLGSGYDPYYTYSG                                              0

SIPYLDGTFYLNHTFKKVAITFDSSVSWPGNDRLLTPNEFEIKRSVDGEGYNVAQCNMTKDWFLVQMLANYNIGYQGFYIP  84
ESYKDRMYSFFRNFQPMSRQVVDDTKYKDYQQVGIIHQH                                               0
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NNSGFVGYLAPTMREGQAYPANVPYPLIGKTAVDSITQKKFLCDRTLWRIPFSSNFMSMGALTDLGQNLLYANSAHALDM 960
TFEVDPMDEPTLLYVLFEVFDVVRVHQPHRGVIETVYLRT

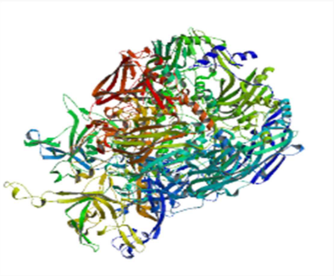
PFSAGNATT 969

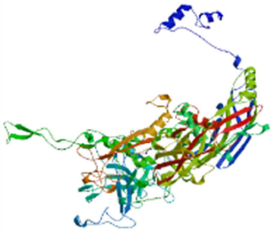
Template Results

A total of 361 templates were found to match the target sequence. This list was filtered by a heuristic down to 36. The top templates are:

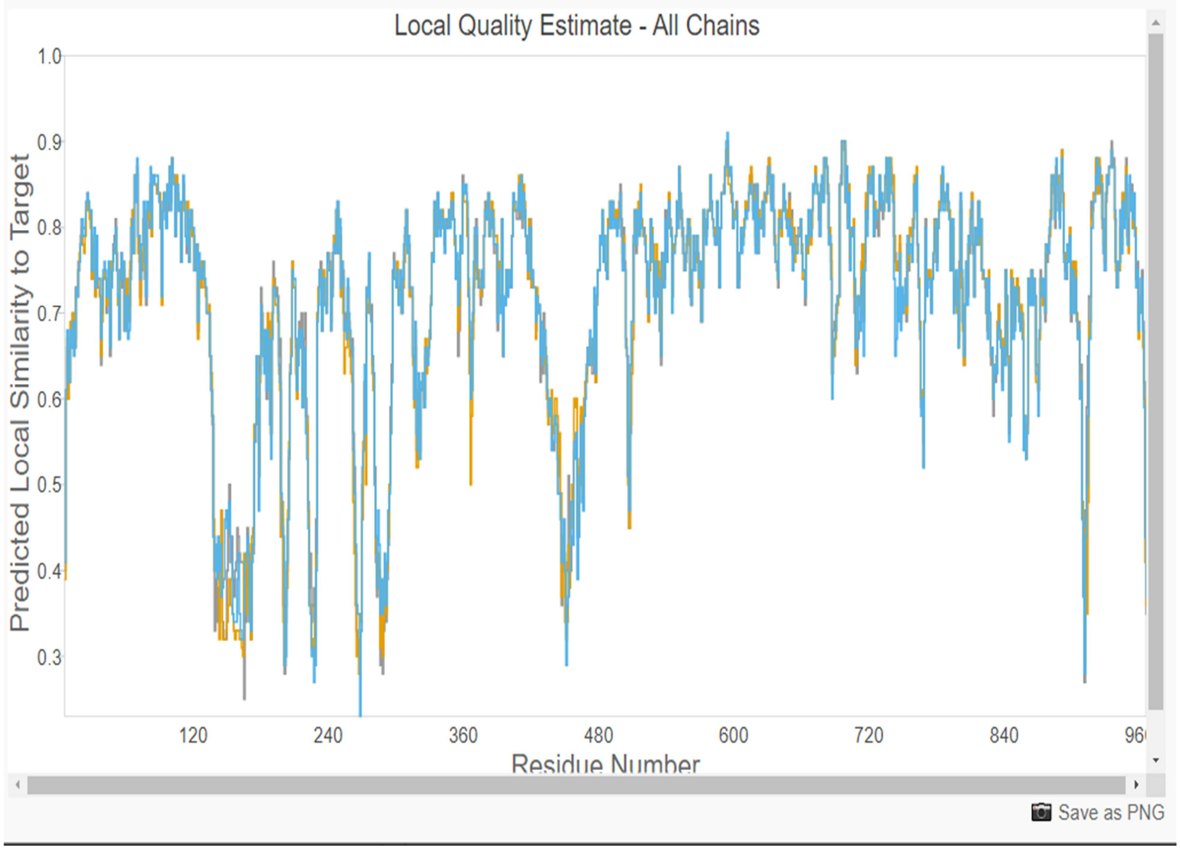
Template	Sequence Identity	Biounit Oligo State	Description
2obe.1	80.97	homo-trimer	Hexon protein Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
2obe.1	81.08	homo-trimer	Hexon protein Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
1p2z.1	99.48	homo-trimer	Hexon protein Refinement of Adenovirus Type 2 Hexon with CNS
1p2z.1	99.07	homo-trimer	Hexon protein Refinement of Adenovirus Type 2 Hexon with CNS
6b1t.1	88.64	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
	01	2obe.1.A	0.74	0.72 ± 0.05	homo-trimer	14 x 2HP



Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
02	7rd1.1.S	0.74	± 0.05	monomer	-



It is evident that valuable structural models could be constructed.

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