

Modeling of human adenovirus B3 hexon protein

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ABSTRACT

Modeling of human adenovirus B3 hexon protein was done and models could be successfully made. Valuable structural details could be elucidated.

Key words: Modeling, human, adenovirus B3 , 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 is very important to know its structure and binding sites.

MATERIALS AND METHODS

Protein

Human adenovirus 3 gene for hexon, complete cds, strain: GB GenBank: AB330084.1 linear 2835 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

MATPSMMPQWAYMHIAQDASEYLSPLVQFARATDTYFSMGNKFRNPTVAPTHDVTDRSQRMLRFPVVDREDNTYSYKVRYTLAV	12
GDNRVLDMASTFFDIRGVLDGRPSFKPYSGTA	0
YNSLAPKGAPNTSQWIVTTNGDNAVTTTTNTFGIASMKGDNITKEGLQIGKDITTEGEEKPIYADKTYQPEPQVGEESWTDTDGTNE	24
KFGGRALKPATNMKPCYGSFARPTNIKGGQAK	0
NRKVKPTTEGGVETEEDIDMEFFDGRDAVAGALAPEIVLYTENVNLETPDSHVYKPKETSNNSHANLGQQAMPNRPNIYIFRDNFVG	36
LMYYNSTGNMGVLQAGASQLNAVVDLQDRNTE	0
LSYQLLLDSLGRTRYFSMWNAVDSDPDVRIENHIGIEDELPNYCFPLNGIGPGHTYQGIKVKTTDDTNGWEKDANVAPANEITIGN	48
NLAMEINIQANLWRSFLYSNVALYLPDVYKYT	0
PPNITLPTNTNTYEMNGRVVSPSLVDSYINIGARWSLDPMDNVNPFNNHNRNAGLRYSMLLGNGRYVPFHIQVPQKFFAVKNLLLLP	60
GSYTYEWNFRKDVNMVLQSSLGNDLRTDGATI	0
SFTSINLYATFFPMAHNTASTLEAMLRNDTNDQSFNDYLSAANMLYPIPANATNIPISIPSRNWAARFGRWSFTRLKTKETPSLGSGFD	72
PYFVYSGSIPYLDGTFFYLNHTFKKVSIMFDSS	0
VSWPGNDRLLSPNEFEIKRTVDGEGYNVAQCNMTKDWFVLQMLANYNIGYQGFYIPEGYKDRMYSFFRNFPMSRQVVDEVNYTDYKA	84

VTLPYQHNNSGFVGYLAPTRQGEPYPANYPY

0

PLIGTTAVKSVTQKKFLCDRTMWRIPFSSNFMSMGALDGLQNMLYANSAHALDMTFEVDPMDEPTLLYLLFEVFDVVRVHQPHRGVI
EAVYLRTPFSAGNATT

94
4

Template Results

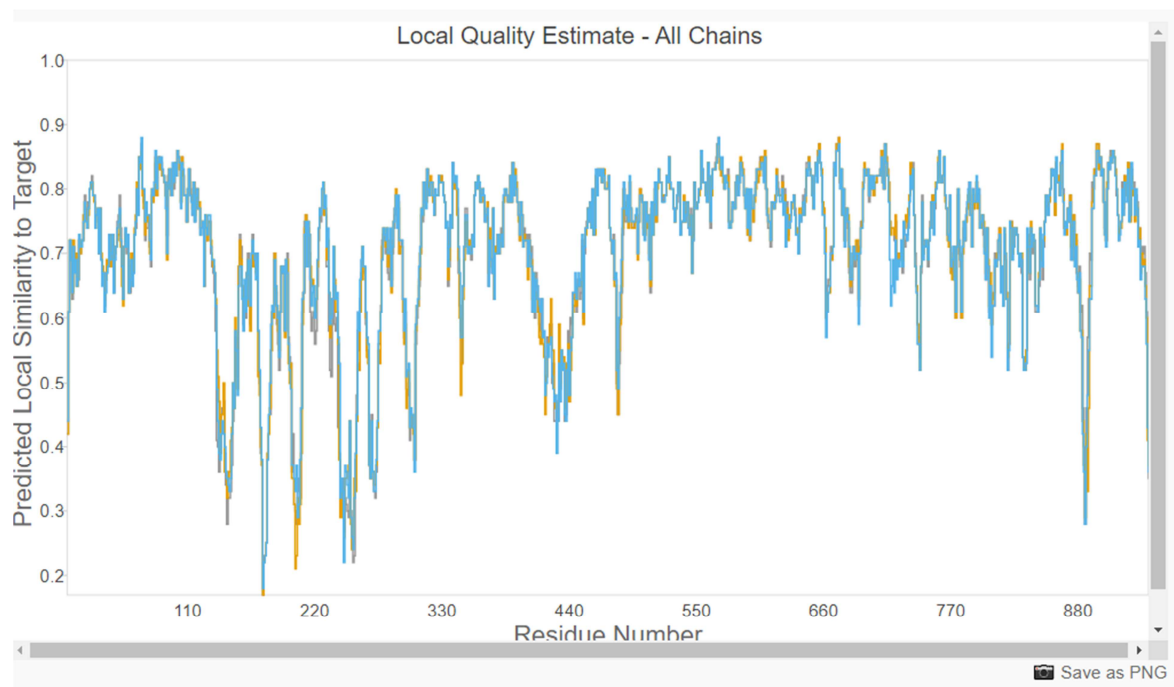
A total of 273 templates were found to match the target sequence. This list was filtered by a heuristic down to 38. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
2obe.1	87.11	homo-trimer	Hexon protein Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
2obe.1	87.00	homo-trimer	Hexon protein Crystal Structure of Chimpanzee Adenovirus (Type 68/Simian 25) Major Coat Protein Hexon
1p2z.1	79.42	homo-trimer	Hexon protein Refinement of Adenovirus Type 2 Hexon with CNS
1p2z.1	80.32	homo-trimer	Hexon protein Refinement of Adenovirus Type 2 Hexon with CNS
6b1t.1	79.89	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	0.75	0.75 ± 0.05	homo-trimer	18 x 2HP



It is evident that valuable structural models could be constructed.

REFERENCES

- Berman, H., Westbrook J., Feng Z., Gilliland G., Bhat T. N., Weissig I., Shindyalov I., Bourne P. E. 2000. The Protein Data Bank. *Nucleic Acids Res*, 28: 235-242.
- Berman, H., Henrick, K., Nakamura, H. and Markley, J.L. 2007. The worldwide Protein Data Bank (wwPDB): ensuring a single, uniform archive of PDB data. *Nucleic Acids Res*, 35: D301-303.
- Bienert, S., Waterhouse, A., de Beer, T.A.P., Tauriello, G., Studer, G., Bordoli, L., Schwede, T. 2017. The SWISS-MODEL Repository - new features and functionality. *Nucleic Acids Res*. 45: D313-D319
- Bordoli, L., Schwede T. 2012. Automated protein structure modeling with SWISS-MODEL Workspace and the Protein Model Portal. *Methods Mol. Biol*. 857: 107-136.
- Grosdidier A, Zoete V, Michielin O. 2011. SwissDock, a protein-small molecule docking web service based on EADock DSS. *Nucleic Acids Res*, 39: W270-7.
- Grosdidier A, Zoete V, Michielin O. 2011. Fast docking using the CHARMM force field with EADock DSS. *J Comput Chem*. 32: 2149-2159.



Studer, G., Tauriello, G., Bienert, S., Biasini, M., Johner, N., Schwede, T. 2021. ProMod3 - A versatile homology modelling toolbox. PLOS Comp. Biol. 17: e1008667.

Steinegger, M., Meier, M., Mirdita, M., Vöhringer, H., Haunsberger, S. J., Söding, J. 2019. HH-suite3 for fast remote homology detection and deep protein annotation. BMC Bioinformatics 20: 473.

Studer, G., Tauriello, G., Bienert, S., Waterhouse, A.M., Bertoni, M., Bordoli, L., Schwede, T., Lepore, R. 2019. Modeling of Protein Tertiary and Quaternary Structures Based on Evolutionary Information. Methods Mol. Biol. 1851: 301-316.

The UniProt Consortium. 2017. UniProt: the universal protein knowledgebase. Nucleic Acids Res. 45: D158-D169.

Waterhouse, A., Bertoni, M., Bienert, S., Studer, G., Tauriello, G., Gumienny, R., Heer, F.T., de Beer, T.A.P., Rempfer, C., Bordoli, L., Lepore, R., Schwede, T. 2018. SWISS-MODEL: homology modelling of protein structures and complexes. Nucleic Acids Res. 46: W296-W303.