MODELING OF FOWL ADENOVIRUS 4 HEXON PROTEIN

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ABSTRACT
The fowl adenovirus 4 hexon protein was subjected to modelling using SWISS-MODEL software online. A total of 38 templates were found and the model built was viewed and analysed using software spdbv 4.10. The structural details provided valuable information on its compostion and surfaces.
Key Words: Protein modelling, FAV4, swiss-model.

INTRODUCTION

FAV4 is very important disease of chicken. Broilers are commonly infected and there is high mortality. Hexon protein is important in protection since antibody against this protein protects the birds (Barua and Rai, 2003). Hence modeling of hexon protein is can provide valuable information on its structure and reacting surfaces.

MATERIALS AND METHODS
Template

Template search was performed against the SWISS-MODEL template library (Bienert *et al*., 2017; Waterhouse *et al*., 2018). Initially a total of 49 templates were found and finally (Remmert *et al*., 2012) 38 templates were found to be of practical use. For each identified template, the template's quality was predicted from features of the target-template alignment.

The templates with the highest quality had then been selected for model building.

Model Building

Models were built online at SWISS-MODEL website based on the target-template alignment using ProMod3. In case loop modelling with ProMod3 failed, an alternative model was built with PROMOD-II (Guex *et al*., 2009). The global and per-residue model quality was assessed using the QMEAN scoring function (Benkert *et al*., 2011).The quaternary structure annotation of the template was used to model the target sequence (Bertoni *et al*., 2017).

Table 1: Primary amino acid sequence for which templates were searched and models were built.

MAALTPDLTTATPRLQYFHIAGPGTRE
YLSEDLQQFISATGSYFDLKNKFRQTV
VAPTRNVTTEKAQRLQIRFYPIQTDDT
STGYRVRYNINVGDGWVLDMGSTYF
DIKGILDRGPSFKPYCGTAYNPLAPKE

SMFNNWAETAPGQNVSASGQLSNVY
TNTSTTKDTTAAQVTKISGVFPNPNQG
PGINPLRQVNANTGVLGRFAKSQYNY
AYGAYVKPVAADGSQSLTQTPYWIM
NNAGTEYLGAVAVEDYTNSLSYPDT
MIVPPPEDYDDDNIGTTRALRPNYIGF
RDNFINLLYHDSGVCSGTLNSERSGM
NVVVELPDRNTELSYQYMLADMMSR
HHYFALWNQAVDQYDPEVRVFSNDG
YEEGAPSYAFNPEAVGAGEGYGPDLS
QIKLYTNNTAANDKNTAVTNATTNFY
FGTVPSYEIDISATQRRNFIMANIAEYL
PDRYKFSISGFDATSVAPTTYEYMNKR
VPLTNVVDMFTNVGARWSIDQMDNV
NPFNHHRNWGLKYRSQLLGNSRYVN
FHIQVPQKFFAIKNLLLLSGSYTYEWV
LRKDPNMILQSSLGNDLRADGASIVY
NEVNLMANFMPMDHNTSNQLELMLR
NATNDQTFVDYLGAKNALYSVPAGST
ALTINIPARTWEGMRGWSFTRIKAAET
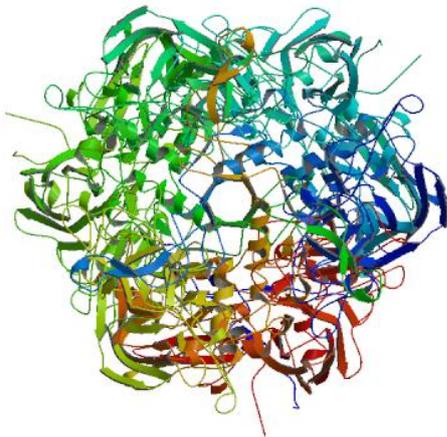PQLGAQYDVNFKYSGSIAYSDGGFYL
SHTFRNMSILFDTSINWPGNDR

LLTPNMFEIKRSVALDTEGFTMSQCDI
TKDWYLIQMATNYNFVYNGYRFWPD
RQYFHYDFLRNFDPMTRQGPNFALPG
LFDLVSYTPTTDNSGQQASQEA
VRNNSGFIAPRSWPVWSAHQGESWPA
NWPYPLCGQQAIQPGQVLSYKKFLCD
NYLWTIPFSSDFMYMGELTDLGQNPM
YTNNSHSMVINFELDPMDDPTYVYML
YGVFDTVRVNQPERNVLAMAYFRTPF
ATGNAV

RESULTS AND DISCUSSION

The SWISS-MODEL template library (SMTL version 2018-05-23, PDB release 2018-05-18) 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 86 templates were found. The model was built as shown in fig.1.
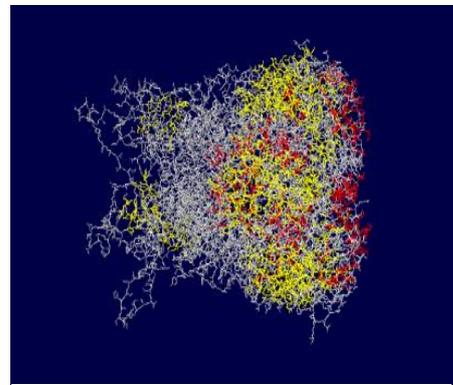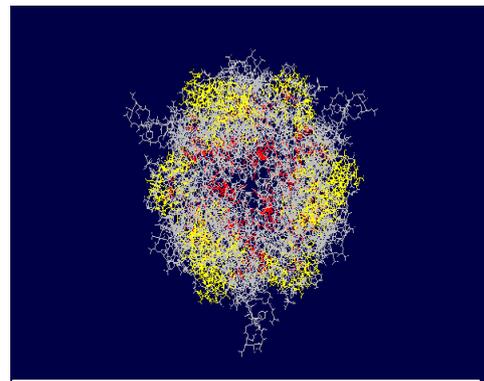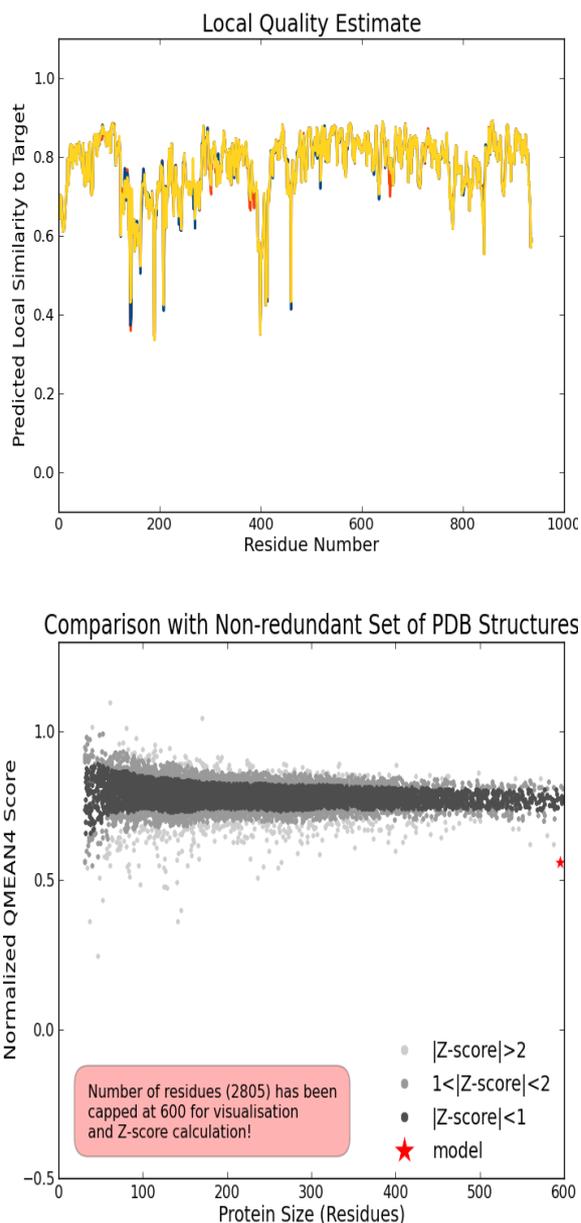

Figure 1. FAV4 protein model built using swiss-model and visualized using spdbv 4.1.0 software.

Figure 2. FAV4 protein showing color side chain.

Figure 3. FAV4 protein showing secondary structure.

Local Quality Estimate

Comparison with Non-redundant Set of PDB Structures

QMEAN	-5.68
Cβ	-2.50
All Atom	-3.52
Solvation	-2.44
Torsion	-4.47

Figure 4. Model building with oligo-state ligands GMQE QMEAN PDB ProMod3 V1.1.0.

It is evident that much clearer picture of structures of fav4 hexon protein was obtained.

REFERENCES

Barua S and Rai A (2003). Cloning of hexon gene of fowl adenovirus 4 in mammalian expression vector. Indian J Comp Microbiol Immunol Inf Dis. 24: 33-38.

Benkert P, Biasini M, Schwede T (2011). Toward the estimation of the absolute quality of individual protein structure models. Bioinformatics 27: 343-350.

Bertoni M, Kiefer F, Biasini M, Bordoli L, Schwede T (2017). Modeling protein quaternary structure of homo- and hetero-oligomers beyond binary interactions by homology. Scientific Reports 7.

Bienert S, Waterhouse A, de Beer TAP, Tauriello G, Studer G, Bordoli L, Schwede T. (2017). The SWISS-MODEL Repository - new features and functionality. Nucleic Acids Res. 45: D313-D319.

Camacho C, Coulouris G, Avagyan V, Ma N, Papadopoulos J, Bealer K, MaddenTL. (2009). BLAST+: architecture and applications. BMC Bioinformatics 10:421-430.

Guex N, Peitsch MC, Schwede T (2009). Automated comparative protein structure modeling with SWISS-MODEL and Swiss-PdbViewer: A historical perspective. Electrophoresis 30: S162-S173

Remmert M, Biegert A, Hauser A, Söding J (2012). HHblits: lightning-fast iterative protein sequence searching by HMM-HMM Prot alignment. Nat Methods 9: 173-175.

Waterhouse A, Bertoni M, Bienert S, Studer G, Tauriello G, Gumienny R, Heer FT, de Beer TAP, Rempfer C, Bordoli L, Lepore R, Schwede T (2018). SWISS-MODEL: homology modelling of protein structures and complexes. Nucleic Acids Res. gky427.