

Modeling of infectious bursal disease virus VP2 protein

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ABSTRACT

Modeling of infectious bursal disease virus VP2 protein was done using SWISS-MODEL software. Structural details could be elucidated.

Key words: Modeling, IBD virus, vp2, protein

INTRODUCTION

Infectious bursal disease virus (IBDV) is an important pathogen of chicken and causes fatality as well as drop in egg production. VP 2 protein plays an important role in induction of immune response. Therefore it is useful to understand the structural details of the VP 2 protein.

MATERIALS AND METHODS

Protein

IBD virus vp2 gene sequence was downloaded GenBank: GenBank: OM307063.1 linear 3121 bp RNA and the amino acid sequence was used for modelling.

Modelling software

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

RESULTS AND DISCUSSION

Project summary

RSLLMPTTGPASIPDDTLEKHTLRSETSTYNLTVGDTGSLIVFFPGFPGSIVGAHYTLQSDGNYKFDQMLL	1
TAQNLPASYNCRSLVSRSLTVRSSTLPGGVYALNGTINAVTFQGSLS	2
	0
LTDVSYNGLMSATANINDKIGNVLVGEGVTVLSTLPTSYDLGYVRLGDPPIAIGLDPKMOVATCDSSDRPRV	2
YTITAADNYQFSSQYKTGGVTITLFSANIDAITSLSVGGELVFKTSIQNL	4
	0
VLGATIYLLIGFDGTAVITRAVAANNGLTAGIDNLMFNLVIPTSEITQPITSIKLEIVTSKSDGQVGEQMSWS	3
ASGSLAVTIHGGNYPGALRPVTLVAYERVAKGSVTVAGVSNFELIP	6
	0
NPELAKNLVTEYGRFDPGAMNYTKLILSERDRLGIKTVWPTREYTDREYFMEVADLNSPLKIAGAFGFK	4
DIIRAIRRIAVPVVSTLFPPAAPLAHAIGEGVDYLLGDEAQAASGTARAA	8
	0
SGK	4
	8
	3

Template results

A total of 34 templates were found to match the target sequence. This list was filtered by a heuristic down to 8. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
2df7.1	95.13	homo-60-mer	structural polyprotein VP2 Crystal structure of infectious bursal disease virus VP2 subviral particle
2df7.1	95.19	homo-60-mer	structural polyprotein VP2 Crystal structure of infectious bursal disease virus VP2 subviral particle
2df7.1	95.13	homo-60-mer	structural polyprotein VP2 Crystal structure of infectious bursal disease virus VP2 subviral particle
3fbm.1	95.59	homo-60-mer	Polyprotein D431N Mutant VP2 Protein of Infectious Bursal Disease Virus; Derived T=1 Particles
2df7.1	95.19	homo-60-mer	structural polyprotein VP2 Crystal structure of infectious bursal disease virus VP2 subviral particle

Model results

Id	Template	GMQE QMEANDisCo		Oligo State	Ligands	
		Global	Oligo State			
01	2df7.1.A	0.78	0.84 ± 0.050	homo-60-mer	20 x <u>CA</u>	20 x <u>CA</u>

QMEAN Z-Scores

QMEAN -0.28

Cβ -0.83

All Atom -0.93

solvation -1.40

torsion 0.33

Template

[2df7.1.A](#) structural polypeptide VP2 Crystal structure of infectious bursal disease virus VP2 subviral particle

Seq Identity 95.13%

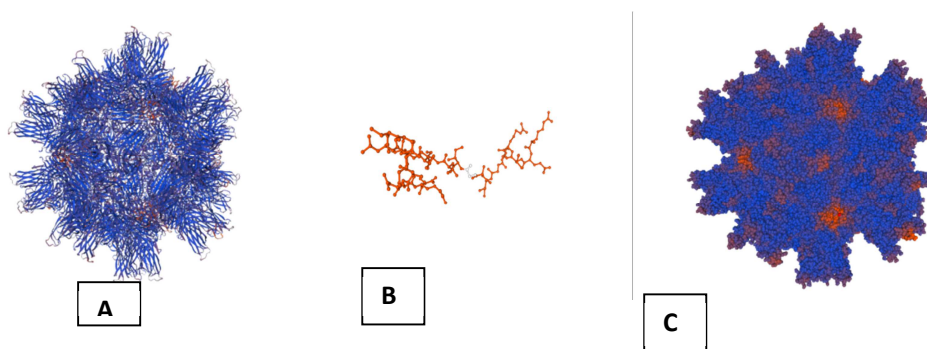
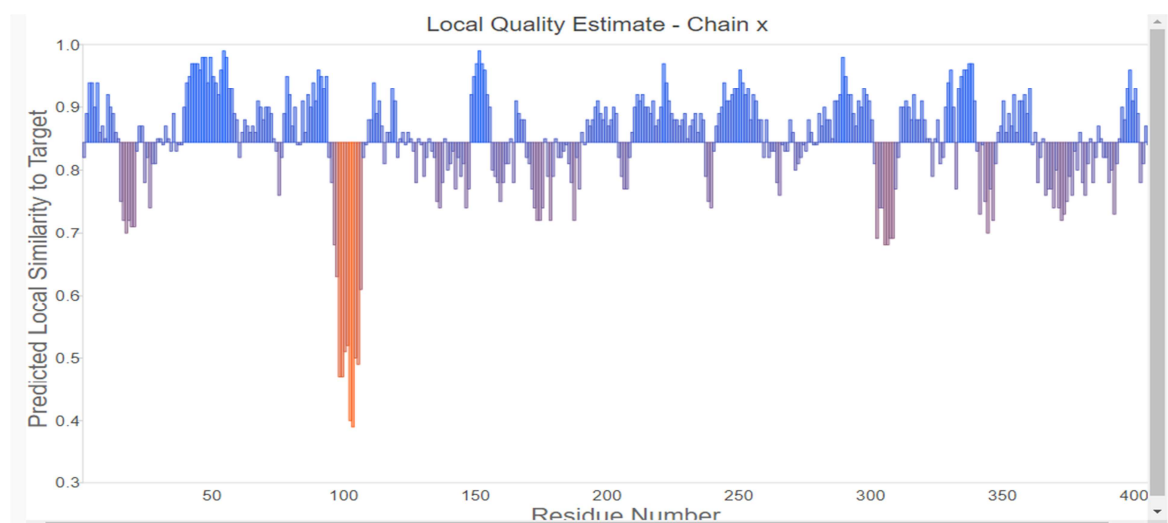


Fig. IBD VP2 A-cartoon. B- ball &



It is evident that details of the protein structure could be deduced.

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.

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.



Devi, 2022. Biotechnology International 15:13- 16.

www.biotechnologyinternational.org

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.

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

Mariani, V., Biasini, M., Barbato, A., Schwede, T. 2013. lDDT: a local superposition-free score for comparing protein structures and models using distance difference tests. *Bioinformatics* 29: 2722-2728.

Schwede, T., Kopp, J., Guex, N., Peitsch, M.C. 2003. SWISS-MODEL: an automated protein homology-modeling server. *Nucleic Acids Res.* 31, 3381-3385.

Studer, G., Rempfer, C., Waterhouse, A.M., Gumienny, R., Haas, J., Schwede, T. 2020. QMEANDisCo - distance constraints applied on model quality estimation. *Bioinformatics* 36: 1765-1771.

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(W1), W296-W303.