Devi. 2022. Biotechnology International 15:17-21.
www. biotechnologyinternational.org

Modeling of classical swine fever virus E2 protein

Soni Devi*
BTS Institute of Science & Technology,
Mundia Ahmednagar, Pilibhit Road, Bareilly-243122, UP, India
*sonigangwar12q@gmail.com

ABSTRACT

Modeling of classical swine fever virus E2 protein could be successfully done using SWISS-MODEL software. Valuable structural details of E2 protein were revealed.

Key words: Modeling, classical swine fever,virus, E2, protein

INTRODUCTION

Classical swine fever (hog cholera) virus is an important pathogen of swine in India and causes much fatality. E2 protein plays an important role in inducing protective immunological responses in pigs and thus is of paramount importance. Modeling of this protein could reveal valuable information about its structure and reactive sites.

MATERIALS AND METHODS

Protein

Classical swine fever E 2 gene sequence was downloaded GenBank: AY430287.1
1125 bp mRNA linear 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

MQLACKEDYRYAISSTNEIGLLGAGGLTTTWKEYNHDLQLNDGTVKAICVAGSFKVTALNVVSRRYLASLHKEASLTSVTF 120
ELLFDGTNPSTEEMGDDFGFGLCPFDTSPVVKGKYNTTL

LNGSAYYLVCPIGWTGVIECTAVSPTTLRTEVVKTFRRDKPFPHRMDCVTTTVENEDLFYCKLGGNWTCVKGEPVVYTGG 240
LVKQCRWCGFDFNEPDGLPHYPIGKCILANETGYRIVDST

DCNRDGVVISTEGSHECLIGNTTVKVHASDERLGPMPCRPKEIVSSAGPVRKTSCTFNYAKTLKNKYYEPRDSYFQQYMLK 360
GEYQYWFDLDVTDRHSDYFAEFVVLVVVALLGGRYVLWL

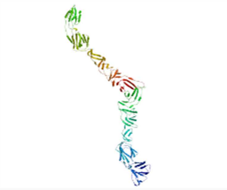
IVTYIVLTEQLAAG 374

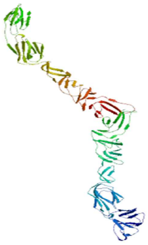
Template results

A total of 23 templates were found to match the target sequence. This list was filtered by a heuristic down to 19. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
4jnt.1	60.53	homo-dimer	Envelope glycoprotein E2 Crystal structure of the ectodomain of Bovine viral diarrhea virus 1 E2 envelope protein
4jnt.1	60.53	homo-dimer	Envelope glycoprotein E2 Crystal structure of the ectodomain of Bovine viral diarrhea virus 1 E2 envelope protein
4jnt.1	60.53	homo-dimer	Envelope glycoprotein E2 Crystal structure of the ectodomain of Bovine viral diarrhea virus 1 E2 envelope protein
4jnt.1	60.53	homo-dimer	Envelope glycoprotein E2 Crystal structure of the ectodomain of Bovine viral diarrhea virus 1 E2 envelope protein
2yq2.1	59.40	homo-dimer	BVDV1 E2 Structure of BVDV1 envelope glycoprotein E2, pH8

Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	4jnt.1.A	0.74	0.76 ± 0.05	homo-dimer	-
	02	2yq3.1.A	0.66	± 0.05	homo-dimer	-
	03	7vzr.1.C	0.00	0.56 ± 0.12	monomer	-



Model 01

Oligo-State Homo-dimer (matching prediction)

GMQE 0.74 **QMEANDisCo Global:** ± 0.05 **QMEANDisCo Local**

Local Quality Estimate - All ChainsPredicted LocalSimilarity to TargetResidue Number1.00.80.60.440801201602002402803 20

QMEAN Z-Scores

Template 4jnt.1.A nvelope glycoprotein E2 Crystal structure of the ectodomain of Bovine viral diarrhea virus 1 E2 envelope protein **Seq Identity** 60.53% **Coverage**

Model-Template Alignment

☑

Model 02

Oligo-State Homo-dimer (matching prediction) **GMQE** 0.66 **QMEANDisCo Global:** ± 0.05

QMEANDisCo Local **QMEAN Z-Scores Template**

2yq3.1.A BVDV1 E2 Structure of BVDV1 envelope glycoprotein E2, pH5 **Seq Identity** 59.40% **Coverage**

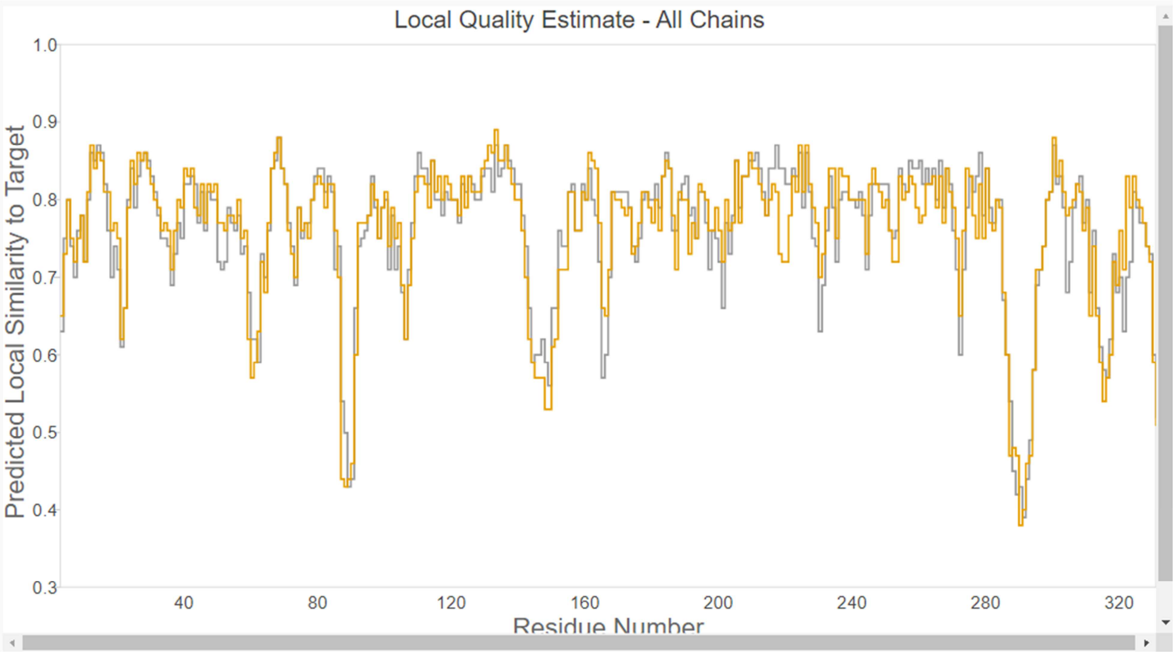
Model-Template Alignment

Model 03

Oligo-State Monomer **GMQE** 0.00 **QMEANDisCo Global:** ± 0.12 **QMEANDisCo Local** **QMEAN Z-Scores**

Template 7vzr.1.C PscE Structure of the Acidobacteria homodimeric reaction center bound with cytochrome c (the smaller form)

Seq Identity 30.77% **Coverage**



It may be seen that models could be constructed and structural details were elucidated.

REFERENCES

Berman, H., Westbrook J., Feng Z., Gilliland G., Bhat T. N., Weissig I., Shindyalov I., Bourne P. E. 2000. The Proten 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.