Modeling of canine parvovirus NS1 protein

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

ABSTRACT

Modeling of canine parvovirus NS1 protein was done using SWISS-MODEL software. Structural details could be elucidated.
Key words: Modeling, CPV, virus, NS1, protein.

INTRODUCTION

Canine parvovirus (CPV) is an important pathogen of dogs and causes serious disease conditions including fatality. The NS1 is a capsid protein. Therefore it is useful to understand the structural details of the vp1 protein.

MATERIALS AND METHODS

Protein

Canine parvovirus isolate Canine/SH/1/2019, complete genome MN840830.1 linear 4269 bp DNA 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

|	
MSGNQYTEEVMEGVNWLKKHAENEAFSFVFKCDNVQLNGKDVRWNNYTKPIQNEELTSLIRGAQTAMDQTEEEEMDWESEVDSLAKKQVQTFDALIKKCLFEVFVSKNIEPNECVWFIQH	120
EWGKDQGWHCHVLLHSKNLQQATGKWLRRQMNMYWSRWLVTLCSVNLTPTEKIKLREIAEDSEWVTILTYRHKQTKKDYVKMVHFGNMIAYYFLTKKKIVHMTKESGYFLSTDSGWKFNF	240
MKYQDRQIVSTLYTEQMKPETVETTVTTAQETKRGRIQTKKEVSIKCTLRDLVSKRVTSPEDWMMLQPDSYIEMMAQPGGENLLKNTLEICTLTLARTKTAFELILEKADNTKLTKFDLA	360
NSRTCQIFRMHGWNWIKVCHAIACVLNRQGGKRNTVLFHGPASTGKSIIAQAIAQAVGNVGCYNAANVNFPFNDCTNKNLIWIEEAGNFGQQVNQFKAICSGQTIRIDQKGKGSKQIEPT	480
PVIMTTNENITIVRIGCEERPEHTQPIRDRMLNIKLVCKLPGDFGLVDKEEWPLICAWLVKHGYESTMANYTHHWGKVPEWDENWAEPKIQKGINSPGCKDLETQAASNPQSQDQVLTPL	600
TPDVVDLALEPWSTPDTPIAETANQQSNQLGVTHKDVQASPTWSEIEADLRAIFTSEQLEEDFRDDLD	668

Template Results

A total of 12193 templates were found to match the target sequence. This list was filtered by a heuristic down to 50. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
7jsi.1	28.61	homo-hexamer	Protein Rep68 Adeno-Associated Virus 2 Rep68 HD Hexamer-ssDNA with ATPgS
7jsi.1	28.61	homo-hexamer	Protein Rep68 Adeno-Associated Virus 2 Rep68 HD Hexamer-ssDNA with ATPgS
7jsi.1	28.61	homo-hexamer	Protein Rep68 Adeno-Associated Virus 2 Rep68 HD Hexamer-ssDNA with ATPgS
7jsi.1	28.61	homo-hexamer	Protein Rep68 Adeno-Associated Virus 2 Rep68 HD Hexamer-ssDNA with ATPgS
7jsi.1	28.61	homo-hexamer	Protein Rep68 Adeno-Associated Virus 2 Rep68 HD Hexamer-ssDNA with ATPgS

Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	02	3wrn.1.A	0.34	0.72 ± 0.05	monomer	1 x ZN
	01	7jsi.1.A	0.30	± 0.05	homo-hexamer	

Local Quality Estimate - Chain A
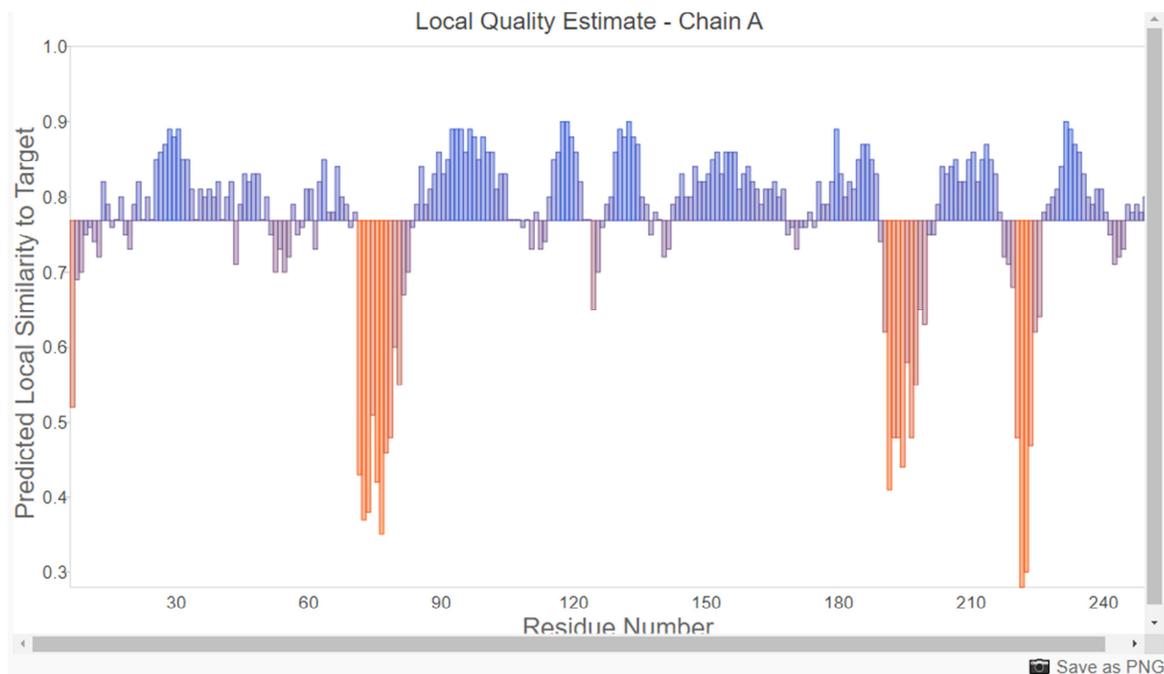
It is apparent that two models could be constructed and structural details could be elucidated.

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.

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, 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.