



Modeling of parvovirus VP2 protein

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ABSTRACT

Modeling of canine parvovirus vp2 protein was done using SWISS-MODEL software. Structural details could be elucidated.

Key words: Modeling, CPV, virus, VP2, protein.

INTRODUCTION

Canine parvovirus (CPV) is an important pathogen of dogs and causes serious disease conditions including fatality. The vp2 protein plays an important role in induction of immune response. Therefore it is useful to understand the structural details of the vp2 protein.

MATERIALS AND METHODS

Protein

Canine parvovirus VP2 gene for VP2, complete cds GenBank: AB128923.1 linear 1755 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

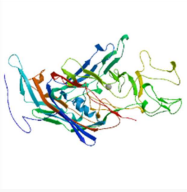
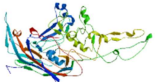
Project summary

MSDGA VQPDGGQPAVRNERATGSGNGSGGGGGGGSGGVGISTGT FNNQTEFKFLENGWVEITANSSRLVHLNMPESENYR	1
RVVVNNLDKTA VNGNMALDDTHAQIVTPWSLVDANAWGVW	2
	0
FNPGDWQLIVNTMSELHLVSFEQEIFNVVLKTVSESATQPPTKVYNNDLTASLMVALDSNNTMPPTPAAMRSETLGFYPWK	2
PTIPTPWRY YFQWDR TLIPSHTGTSGTPTNIYHGTD PDD	4
	0
VQFYTIENSVPVHLLRTGDEFATG TFFDCKPCRLTHTWQTNRALGLPPFLNSLPQAEGGTNFGYIGVQQDKRRGVTQMGN	3
TNYITEATIMRPAEVGY SAPYYSFEASTQGPFKTPIAAG	6
	0
RGGAQTDENQAADGDP RYAFGRQH GQKTTTTGETPERFTYIAHQDTGRYPEGDWIQNFNLPVTDDNVLLPTDPIGGKTG	4
INYTNIFNTYGLPTALNNVPPVYPNGQIWDKEFD TDLKP	8
	0
RLHVNAPFVCQNNCPGQLFVKVAPNL TNEYDPDASANMSRIVTYSDFWWKGKLVFKAKLRASHTWNPIQQMSINVDNQF	5
NYVPSNIGGMKIVYEKSQLAPRKLY	8
	4

Template Results

A total of 169 templates were found to match the target sequence. This list was filtered by a heuristic down to 16. The top templates are:

Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	4dpv.1.B	0.91	0.86 ± 0.05	monomer	1 x MG
	02	7na6.1.A	0.48	± 0.05	monomer	-

QMEAN Z-Scores

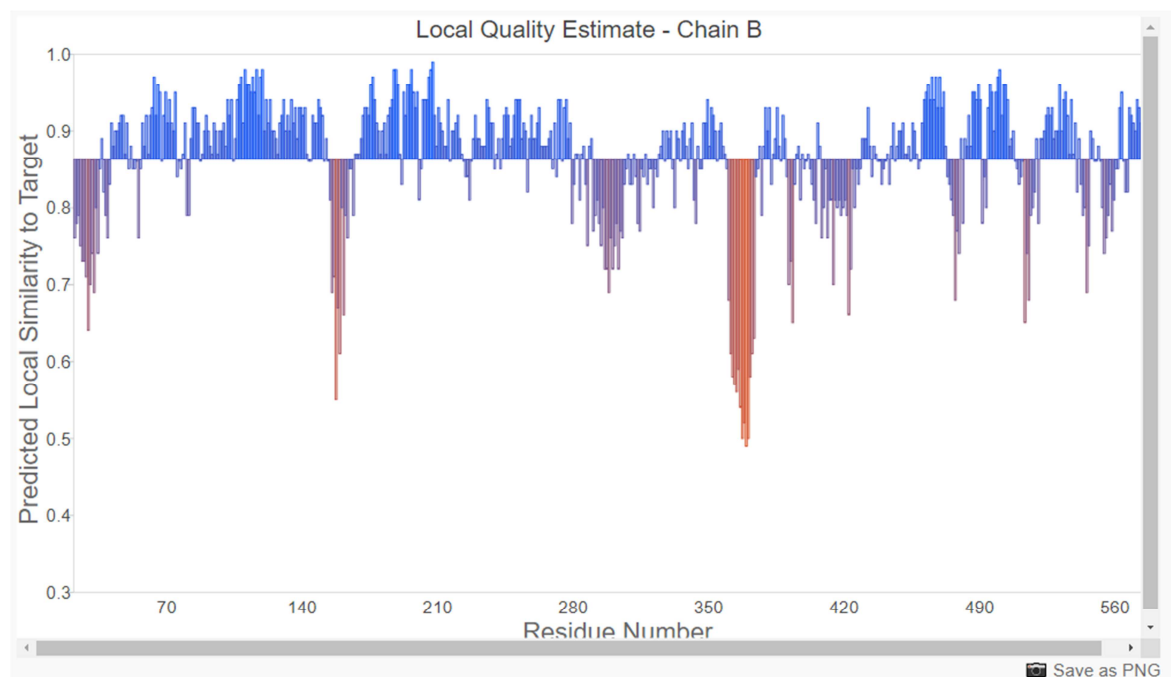
QMEAN -2.14

C β -2.33

All Atom -1.85

solvation -3.12

torsion -0.59



It is apparent that several 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 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.
- 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. IDDT: 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.