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Modeling of canine parvovirus VP1 protein

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ABSTRACT

Modeling of canine parvovirus vp1 protein was done using SWISS-MODEL software. Structural details could be elucidated.

Key words: Modeling, CPV, virus, VP1, protein.

INTRODUCTION

Canine parvovirus (CPV) is an important pathogen of dogs and causes serious disease conditions including fatality. The vp1 protein is a structural 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.

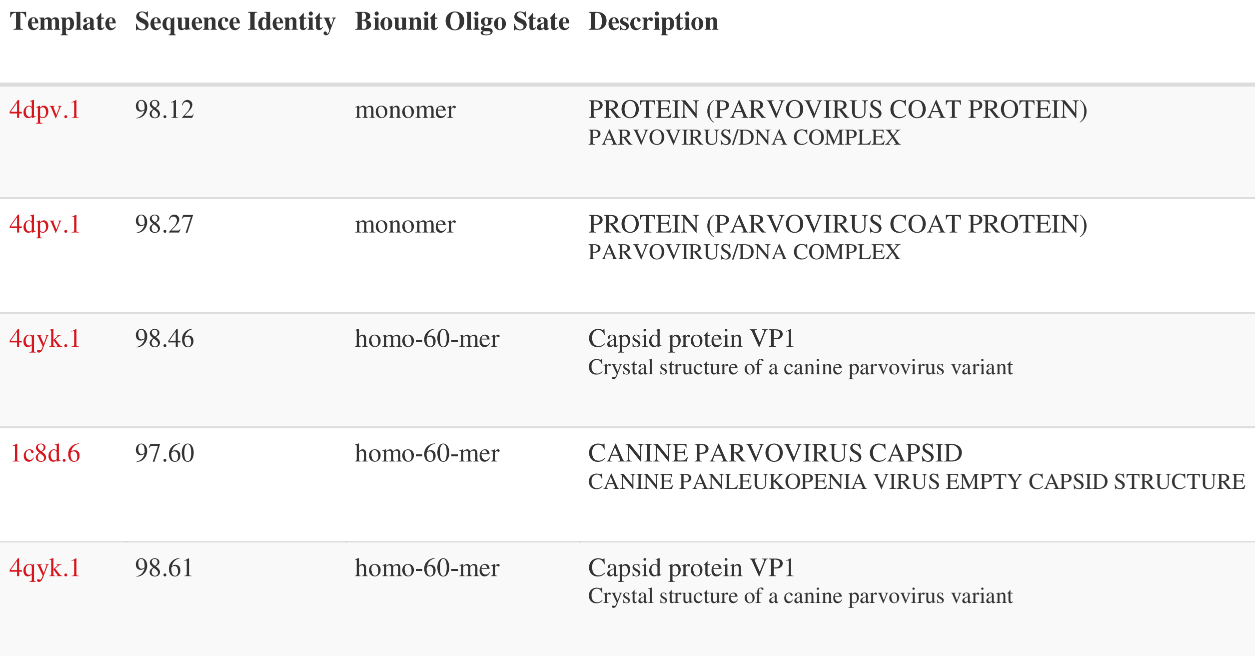
RESULTS AND DISCUSSION

Project summary

```
MAPPAKRARRGLVPPGYKYLGPGNSLDQGEPTNPSDAAAKEPDEAYAAYLRSGKNPYLYFSPADQRFIDQTKDAKDWGGKIGHYFFRA  12
KKAIAPVLTDTPDHPSTSRPTKPTKRSKPPPH                                                            0

IFINLAKKKKAGAGQVKRDNLAPMSDGGVQPDGGQPAVRNERATGSGNGSGGGGGGGSGGVGISTGTFNNQTEFKFLENGWVEITANS  24
SRLVHLNMPESENYRRVVVNNLDKTAVNGNMA                                                            0

LDDTHAQIVTPWSLVDANAWGVWFNPGDWQLIVNTMSELHLVSFEQEIFNVVLKTVSESATQPPTKVYNNDLTASLMVALDSNNTMPF  36
TPAAMRSETLGFYPWKPTIPTPWRYYFQWDRT                                                            0

LIPSHTGTSGTPTNIYHGTDPDDVQFYTIENSVPVHLLRTGDEFATGTFYFDCKPCRLTHTWQTNRALGLPPFLNSLPQAEGGTNFGY  48
IGVQQDKRRGVTQMGNTNIITEATIMRPAEVG                                                            0

YSAPYYSFEASTQGPFKTPIAAGRGGAQTDENRAADGDPRYAFGRQHGQKTTTTGETPERFTYIAHQDTGRYPEGDWIQNINFNLPVT  60
EDNVLLPTDPIGGKTGINYTNIFNTYGPLTAL                                                            0

NNVPPVYPNGQIWDKEFDTDLKPRLHVNAPFVCQNNCPGQLFVKVAPNLTNEYDPDASANMSRIVTYSDFWWKGKLVFKAKLRASHTW  72
NPIQQMSINVDNQFNYVPSNIGGMKIVYEKSQ                                                            0

                                                                                           72
LAPRKLY
                                                                                            7
```

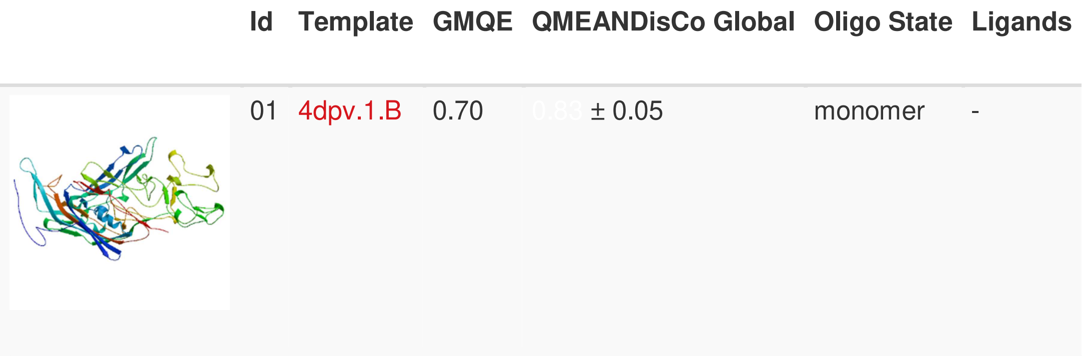
Template Results

A total of 206 templates were found to match the target sequence. This list was filtered by a heuristic down to 50. The top templates are:

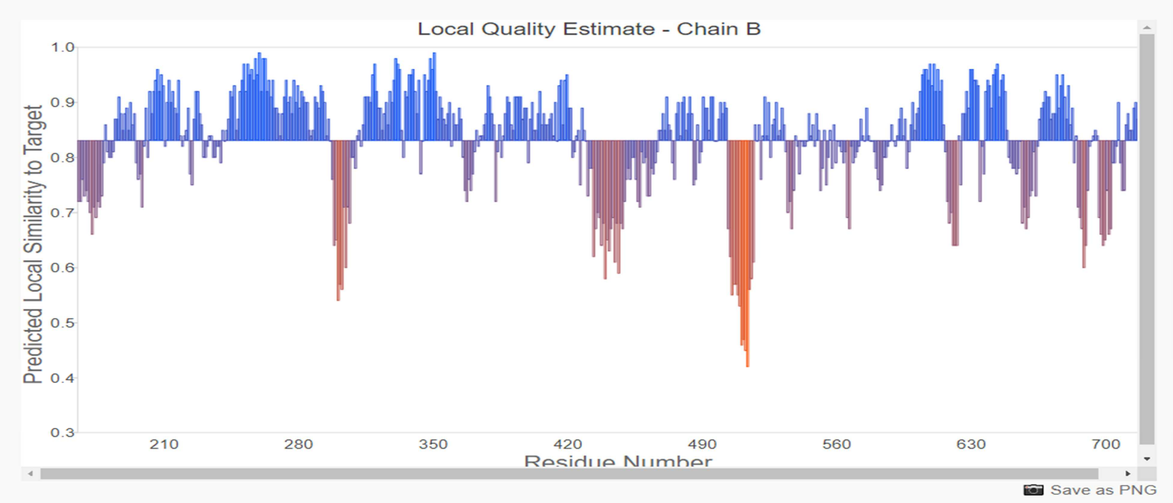


Template	Sequence Identity	Biounit Oligo State	Description
4dpv.1	98.12	monomer	PROTEIN (PARVOVIRUS COAT PROTEIN) PARVOVIRUS/DNA COMPLEX
4dpv.1	98.27	monomer	PROTEIN (PARVOVIRUS COAT PROTEIN) PARVOVIRUS/DNA COMPLEX
4qyk.1	98.46	homo-60-mer	Capsid protein VP1 Crystal structure of a canine parvovirus variant
1c8d.6	97.60	homo-60-mer	CANINE PARVOVIRUS CAPSID CANINE PANLEUKOPENIA VIRUS EMPTY CAPSID STRUCTURE
4qyk.1	98.61	homo-60-mer	Capsid protein VP1 Crystal structure of a canine parvovirus variant

Model Results



	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	4dpv.1.B	0.70	0.83 ± 0.05	monomer	-



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 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.