Modeling of human parvovirus VP1 and VP2 proteins

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Abstract

Modeling of human parvovirus VP1 and VP2 proteins was done using SWISS-MODEL software. Valuable structural properties could be obtained.

Key words: Modeling, human parvovirus, VP1, VP2 protein.

Introduction

Human parvovirus infection is of great importance. It is useful to study the structural details of their proteins.

Materials and Methods

Protein sequence

Human parvovirus B19 isolate Vn147 NS1 (NS1), 7.5 kDa protein (NS1), VP1, 9.5 kDa protein (VP1), and VP2 genes, complete cds GenBank: DQ357064.1 linear 4500 bp DNA was downloaded and used the amino acid sequence for modeling.

Modelling software

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

Results and Discussion

VP1 Protein

Project Summary

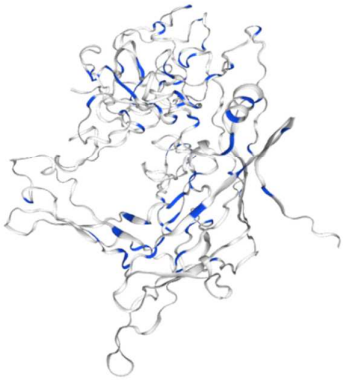
```
MSKESSKWWESDDKFAKAVYQQFVQFYEKVTGTDLELIQILKDHYNISLHNPLENPSSLFDLVARIKNNLKNSPDLYSHHFQSHGQLS  12
DHPHALSSSSSHAEPRGENAVLSSEDLHKPGQ                                                           0

VSVQLPGTNYVGPGNELQAGPPQSAVDSAARIHDFRYSQLAKLGINPYTHWTVADEELLKNIKNETGFQAQVVKDYFTLKGAAAPVAY  24
FQGSLPEVPAYNASEKYPSMTSVNSAEAITGA                                                            0

GGGGSNSVKSMWSEGATFTANSVTCTFSRQFLIPYDPEHHYKVFSPAASSCHNASGKEAKVCTISPIMGYSTPWRYLDFNALNLFFSP  36
LEFQHLIEKYGSIAPDALTVTISEIAVKDVTD                                                            0

KTGGGVQVTDSTTGRLCMLVDHEYKYPYVLGQGQDTLAPELPIWVYFPPQYAYLSVGDVNTQGISGDSKKLASEESAFYVLEHSSFQL  48
LGTGGSASMSYKFPAVPPENLEGCSQHFYEMY                                                            0

NPLYGSCLGVPHTLGGDPKFRSLTHEDHAIQPQNFMPWPLVNSVSTNEGDSSNTGAGKALTGLRKGTSQNTRISLRPGPVSQPYHHWD  60
                                                                                            0
```

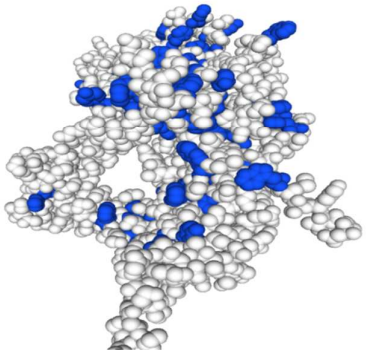
```
TDKYVTGINAISHGQTTYGNAEDKEYHQGVGR

FPNEKEQLKQLQGLNMHTYFPNKGTQQYTDQIERPLMVGSVWNRRALHYESQLWSKIPNLDDSFKTQFAALGGWGLHQPPPQIFLKIL  720
PQSGPIGGIKSMGITTLVQYAVGIRTVTMTFK                                                          0

LGPRKATGRWNPQPGVYPPHAAGHLPYGLYDPTATDAKQHHRHGYEKPEELWTAKSRVHPL                             781
                                                                                           1
```

Template Results

A total of 209 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
1s58.1	96.39	homo-60-mer	B19 parvovirus capsid The structure of B19 parvovirus capsid
1s58.1	96.50	homo-60-mer	B19 parvovirus capsid The structure of B19 parvovirus capsid
6nn3.1	96.75	hetero-trimer	VP2 of B19 parvovirus Structure of parvovirus B19 decorated with Fab molecules from a human antibody
6nn3.1	96.87	hetero-trimer	VP2 of B19 parvovirus Structure of parvovirus B19 decorated with Fab molecules from a
7ud4.1	25.39	homo-60-mer	Capsid protein VP1 Cryo-EM structure of AAV-PHP.eB





VP2 Protein

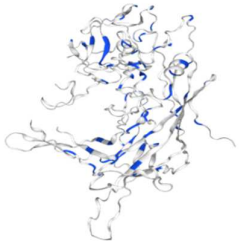
Project Summary

```
MTSVNSAEAITGAGGGGSNSVKSMWSEGATFTANSVTCTFSRQFLIPYDPEHHYKVFSPAASSCHNASGKEAKVCTISPIMGYSTPWR  120
YLDFNALNLFFSPLEFQHLIEKYGSIAPDALT                                                           
                                                                                            
VTISEIAVKDVTDKTGGGVQVTDSTTGRLCMLVDHEYKYPYVLGQGQDTLAPELPIWVYFPPQYAYLSVGDVNTQGISGDSKKLASEE  240
SAFYVLEHSSFQLLGTGGSASMSYKFPAVPPE                                                           
                                                                                            
NLEGCSQHFYEMYNPLYGSCLGVPHTLGGDPKFRSLTHEDHAIQPQNFMPWPLVNSVSTNEGDSSNTGAGKALTGLRKGTSQNTRISL  360
RPGPVSQPYHHWDTDKYVTGINAISHGQTTYG                                                           
                                                                                            
NAEDKEYHQGVGRFPNEKEQLKQLQGLNMHTYFPNKGTQQYTDQIERPLMVGSVWNRRALHYESQLWSKIPNLDDSFKTQFAALGGWG  480
LHQPPPQIFLKILPQSGPIGGIKSMGITTLVQ                                                           
                                                                                            
YAVGIRTVTMTFKLGPRKATGRWNPQPGVYPPHAAGHLPYGLYDPTATDAKQHHRHGYEKPEELWTAKSRVHPL                554
```

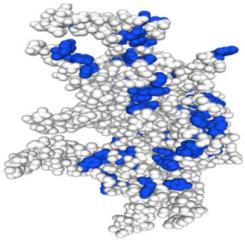
Template Results

A total of 161 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
6nn3.1	96.75	hetero-trimer	VP2 of B19 parvovirus Structure of parvovirus B19 decorated with Fab molecules from a human antibody
1s58.1	96.39	homo-60-mer	B19 parvovirus capsid The structure of B19 parvovirus capsid
6cbe.1	24.70	homo-60-mer	Capsid protein VP1 Atomic structure of a rationally engineered gene delivery vector, AAV2.5
7rwt.1	24.36	homo-60-mer	Capsid protein VP1 Adeno-associated virus type 2
6u0v.1	24.16	homo-60-mer	Capsid protein VP1 Atomic-Resolution Cryo-EM Structure of AAV2 VLP



cartoon



spacefill

It is evident that detailed valuable structural parameters could be found.

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