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Modelling of hepatitis A virus capsid proteins

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Abstract

Modelling of capsid protein was done using SWISS-MODEL software. Valuable structural properties could be obtained.

Key words: Modeling, capsid protein, hepatitis A

Introduction

Viral proteins play an important role in their actions and study of their structural details would be of great importance.

Materials and Methods

Protein

Hepatitis A virus capsid proteins VP1, VP2, VP3, VP4, and P2A (P1 and P2 regions) genes, complete cds
GenBank: M59286.1 HPACAPPRO 2521 bp ss-RNA linear

```
source          1..2521
                     /organism="Hepatovirus A"
                     /mol_type="genomic RNA"
                     /isolate="CY145"
                     /db_xref="taxon:12092"
     CDS             1..>2521
                     /codon_start=1
                     /product="polyprotein"
                     /protein_id="AAA45473.1"
     mat_peptide     4..738
                     /product="capsid protein VP4"
     mat_peptide     739..1476
                     /product="capsid protein VP3"
     mat_peptide     1477..2376
                     /product="capsid protein VP1"
```

```
mat_peptide     2377..2520
                /product="capsid protein P2A"
```

The amino acid sequence was downloaded and used for modelling.

Modelling software

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

Results and Discussion

Project summary

```
MMNMARQGLFQTVGSGLDHILSLADVEEEQMIQSVDRTAVTGASYFTSVDQSSVHTAEVGSHQSEPLKTSVDKPGSKKTQGE  120
KFFLIHSADWLSTHALFHEVAKLDVVSLLYNEQFAVQG                                              0

LLRYHTYARFGIEIQVQINPTPFQQGGLICAMVPGDQGYGSIASLTVYPHGLLNCNINNVVRIKVPFIYTRGAYHFKDPQYP  240
VWELTIRVWSEFNIGTGTSAYTSLNVLARFTDLELHGL                                              0

TPLSTQMMRNEFRVSTTENVVNLSNYEDARAKMSFALDQENWRSDPSEGGGIKITHFSTWTSIPTLAAQFAFNASASVGQQI  360
KVIPVDPYFYQMTNSNPDQKYITALASICQMFCFWRGD                                              0

LVFDFQVFPTKYHSGRLQFCFVPGNELIEVTSITLKQATTAPCAVMDITGVQSTLRFRVPWISDTPYRVNCYIKSSHQKGEY  480
TAIEKLIVYCYNRLTSPSNVASHVRVNVYLSAINLECF                                              0

APLYHAMDVTSQTGDDSGGFSTTVSTEQNVPDPQVGITTPKDLKGKANKGKMDVSGVQAPVGAITTIEDPVLAKKVPETFPE  600
LKPGESRHTSDHMSVYKFMGRSHFLCTFTFNANNREYT                                              0

FPITLSSTSNPPHGSPSTLRWFFNLFQLYRGPLDLTIIIITGATDVDGMAWFTPVGLAVDTPWVEKQSALTIDYKTALGAIRF  720
NTRRTGNIQIRLPWYSYLYAVSGALDGLGDTTDSTFGL                                              0

VSIQIANYNHSDEYLSFSCYLSVTEQSEFFFPRAPLNSSAMMTSENMLDRIAGGDLESSVDDPRTDEDRRFESHIEKKPYKE  840
LRLEVGKQRFKYAREELSNEILPPPRKLKGLFSQSKIS                                              0
```

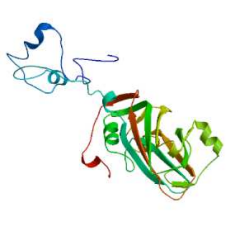
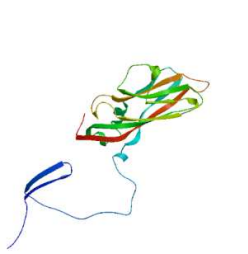
Template Results

A total of 2615 templates were found to match the target sequence. This list was filtered by a heuristic down to 50. The top templates are:

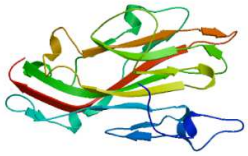
Template	Sequence Identity	Biounit Oligo State	Description
4qpi.1	93.14	hetero-trimer	Capsid protein VP1 Crystal structure of hepatitis A virus
4qpi.1	93.01	hetero-trimer	Capsid protein VP1 Crystal structure of hepatitis A virus
6jht.2	93.14	hetero-25-mer	VP1 The cryo-EM structure of HAV bound to a neutralizing antibody-F9

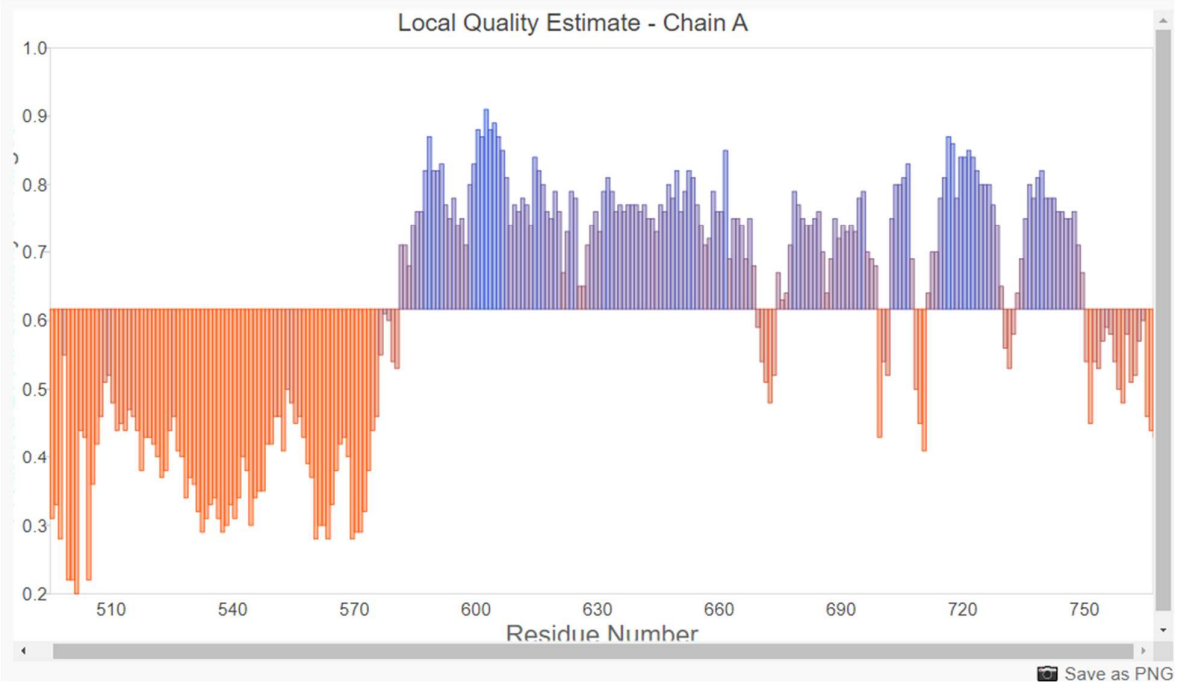
Template	Sequence Identity	Biounit Oligo State	Description
6jhr.3	93.14	hetero-30-mer	VP1 The cryo-EM structure of HAV bound to a neutralizing antibody-F6
5wth.2	93.14	hetero-25-mer	Polyprotein Cryo-EM structure for Hepatitis A virus complexed with FAB

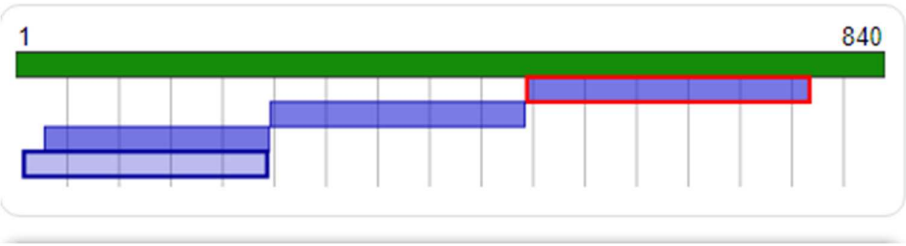
Model Results

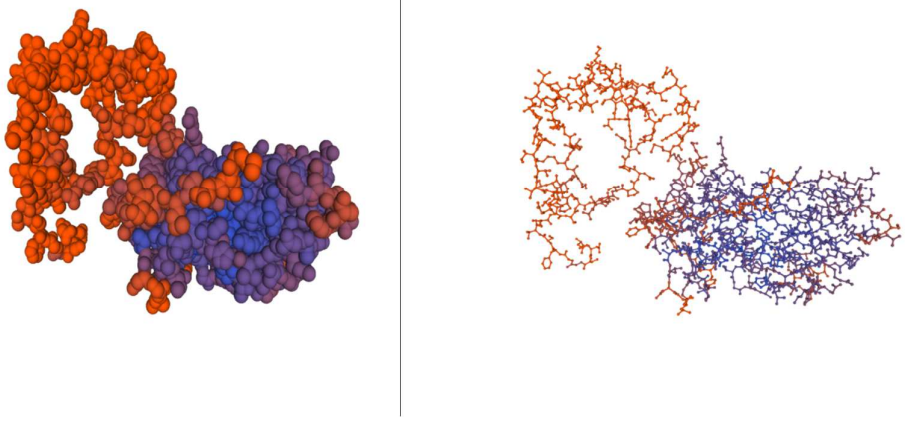
	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	4qpi.1.A	0.23	0.62 ± 0.05	monomer	-
	02	4qpg.1.C	0.22	± 0.05	monomer	-
	03	4qpi.1.B	0.21	0.65 ± 0.06	monomer	-

Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
04	5c9a.1.B	0.15	± 0.05	monomer	-









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