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Modeling of hepatitis D virus delta antigen protein and hepatitis E virus polyprotein

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Abstract

Modeling of human hepatitis D virus delta antigen protein and hepatitis E virus polyprotein was done and valuable structural details could be obtained.

Key words: Modeling, hepatitis D virus, delta antigen protein, hepatitis E virus polyprotein

Introduction

Human hepatitis D and E are of much interest because less information is available about them. A study of their structural details would help in understanding their functions and role in infections.

Materials and Methods

Protein

Hepatitis D virus delta antigen (HDAg) mRNA, complete cds GenBank: M55042.1 HPDAG 1679 bp ss-RNA linear was downloaded and amino acid sequence was used for modeling.

Hepatitis E virus, complete genome NCBI Reference Sequence: NC_001434.1 linear 7176 bp ss-RNA was downloaded and amino acid sequence was used for modelling.

Modeling software

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

Results and Discussion

Hepatitis D virus delta antigen (HDAg) protein

Project Summary

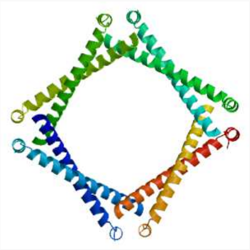
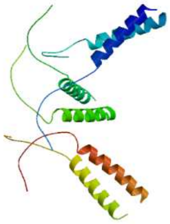
```
MSRSESRKNRGGREEILEQWVAGRKKLEELERDLRKTKKKLKKIEDENPWLGNIKGILGKKDKDGEGAPPAKRARTDQMEVDSGPRKR  12
PLRGGFTDKERQDHRRRKALENKKKQLSAGGK                                                           0

                                                                                          19
NLSKEEEEELRRLTEEDERRERRVAGPPVGGVNPLEGGSRGAPGGGFVPSLQGVPESPFSRTGEGLDIRGNRGFP                5
```

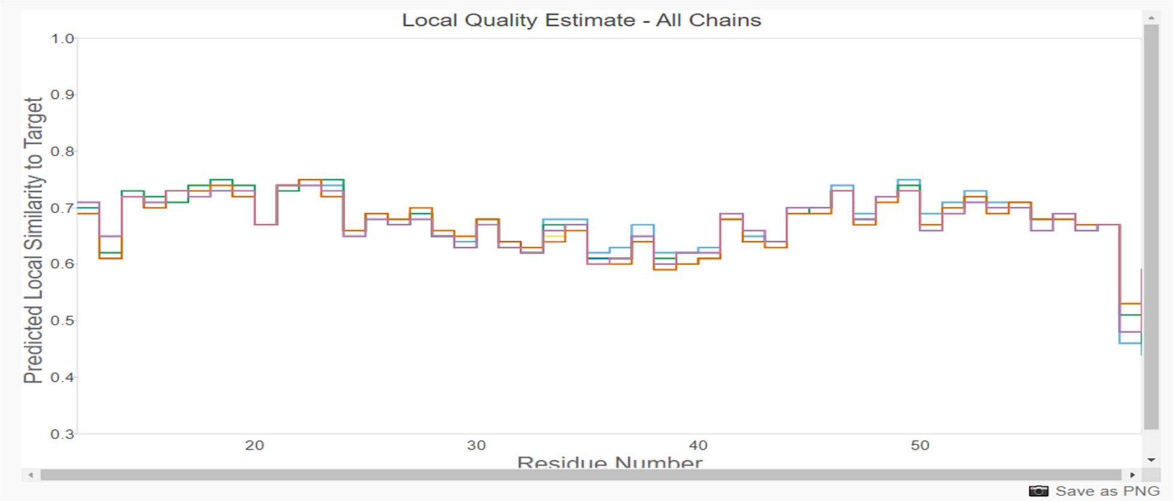
Template Results

A total of 43 templates were found to match the target sequence. This list was filtered by a heuristic down to 22. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
1a92.1	83.67	homo-octamer	DELTA ANTIGEN OLIGOMERIZATION DOMAIN OF HEPATITIS DELTA ANTIGEN
1a92.1	83.67	homo-octamer	DELTA ANTIGEN OLIGOMERIZATION DOMAIN OF HEPATITIS DELTA ANTIGEN
1a92.1	83.67	homo-octamer	DELTA ANTIGEN OLIGOMERIZATION DOMAIN OF HEPATITIS DELTA ANTIGEN
1cos.1	42.86	homo-trimer	COILED SERINE CRYSTAL STRUCTURE OF A SYNTHETIC TRIPLE-STRANDED ALPHA-HELICAL BUNDLE
1cos.1	42.86	homo-trimer	COILED SERINE CRYSTAL STRUCTURE OF A SYNTHETIC TRIPLE-STRANDED ALPHA-HELICAL BUNDLE

Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	1a92.1.C	0.13	0.67 ± 0.05	homo-octamer	-
	02	2wg6.1.A	0.04	± 0.06	homo-hexamer	-



Hepatitis E virus polyprotein

Project Summary

```
MEAHQFIKAPGITTAIEQAALAAANSALANAVVVRPFLSHQQIEILINLMQPRQLVFRPEVFWNHPIQRVIHNELELYCRARSGRCLE  12
IGAHPRSINDNPNVVHRCFLRPAGRDVQRWYT                                                            0

APTRGPAANCRRSALRGLPAADRTYCFDGFSGCNFPAETGVALYSLHDMSPSDVAEAMFRHGMTRLYAALHLPPEVLLPPGTYRTASY  24
LLIHDGRRVVVTYEGDTSAGYNHDVSNLRSWI                                                            0

RTTKVTGDHPLVIERVRAIGCHFVLLLTAAPEPSPTPYVPYPRSTEVYVRSIFGPGGTPSLFPTSCSTKSTFHAVPAHIWDRLMLFGA  36
TLDDQAFCCSRLMTYLRGISYKVTVGTLVANE                                                            0

GWNASEVALTAVITAAYLTICHQRYLRTQAISKGMRRLEREHAQKFITRLYSWLFEKSGRDYIPGRQLEFYAQCRRWLSAGFHLDPRV  48
LVFDESAPCHCRTAIRKAVSKFCCFMKWLGQE                                                            0

CTCFLQPAEGAVGDQGHDNEAYEGSDVDPAESAISDISGSYVVPGTALQPLYQALDLPAEIVARAGRLTATVKVSQVDGRIDCETLLG  60
NKTFRTSFVDGAVLETNGPERHNLSFDASQST                                                            0

MAAGPFSLTYAASAAGLEVRYVAAGLDHRAVFAPGVSPRSAPGEVTAFCSALYRFNREAQRLSLTGNFWFHPEGLLGPFAPFSPGHVW  72
ESANPFCGESTLYTRTWSEVDAVSSPAQPDLG                                                            0

FISEPSIPSRAATLTPAAPLPPPAPDPSPTPSAPARGEPAPGATARAPAITHQAARHRRLLFTYPDGSKVFAGSLFESTCTWLVNASN  84
VDHRPGGGLCHAFYQRYPASFDAASFVMRDGA                                                            0

AAYTLTPRPIIHAVAPDYRLEHNPKMLEAAYRETCSRLGTAAYPLLGTGIYQVPIGPSFDAWERNHRPGDELYLPELAARWFEANRPT  96
CPTLTITEDVARTANLAIELDSATDVGRACAG                                                            0

CRVTPGVVQYQFTAGVPGSGKSRSITQADVDVVVVPTRELRNAWRRRGFAAFTPHTAARVTQGRRVVIDEAPSLPPHLLLLHMQRAAT  10
VHLLGDPNQIPAIDFEHAGLVPAIRPDLAPTS                                                           80

WWHVTHRCPADVCELIRGAYPMIQTTSRVLRSLFWGEPAVGQKLVFTQAAKAANPGSVTVHEAQGATYTETTIIATADARGLIQSSRA  12
HAIVALTRHTEKCVIIDAPGLLREVGISDAIV                                                           00

NNFFLAGGEIGHQRPSVIPRGNPDANVDTLAAFPPSCQISAFHQLAEELGHRPAPVAAVLPPCPELEQGLLYLPQELTTCDSVVTFEL  13
TDIVHCRMAAPSQRKAVLSTLVGHYGRRTKLY                                                           20

NASHSDVRDSLARFIPAIGHVQVTTCELYELVEAMVEKGQDGSAVLELDLCNRDVSRITFFQKDCNKFTTGETIAHGKVGQGISAWSK  14
```

```
TFCALFGPWFRAIEKAILALLPQGVFYGDAFD                                                                      40

DTVFSAAVAAARASMVFENDFSEFDSTQNNFSLGLECAIMVECGMPQWLIRLYHLIRSAWILQAPKESLRGFWKKHSGEPGTLLWNTV            15
WNMAVITHCYDFRDLQVAAFKGDDSIVLCSEY                                                                      60

RQSPGAAVLIAGCGLKLKVDFRPIGLYAGVVVAPGLGALPDVVRFAGRLTEKNWGPGPERAKQLRLAVSDFLRKLTNVAQMCVDVVSR            16
VYGVSPGLVHNLIGMLQAVADGKAHFTESVKP                                                                      80

                                                                                                      16
VLDLTNSILCRVE                                                                                         93
```

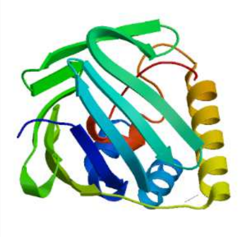
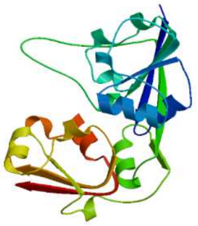
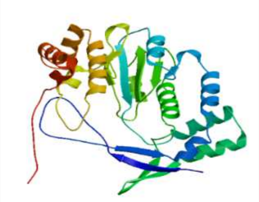
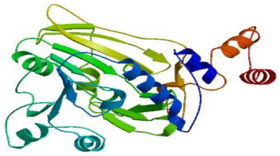
Template Results

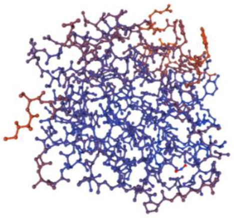
A total of 7202 templates were found to match the target sequence. This list was filtered by a heuristic down to 50. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
7y38.1	19.87	hetero-14-mer	RNA-directed RNA polymerase nsP4 Molecular architecture of the chikungunya virus replication complex
7vw5.2	18.85	monomer	RNA-directed RNA polymerase nsP4 Crystal structures of alphavirus nonstructural protein 4 (nsP4) reveal an intrinsically dynamic RNA-dependent RNA polymerase fold
7vw5.1	18.85	monomer	RNA-directed RNA polymerase nsP4 Crystal structures of alphavirus nonstructural protein 4 (nsP4) reveal an intrinsically dynamic RNA-dependent RNA polymerase fold
7vb4.1	18.85	homo-dimer	RNA-directed RNA polymerase nsP4 A crystal structure of alphavirus nonstructural protein 4 (nsP4) reveals an intrinsically dynamic RNA-dependent RNA polymerase
6nu9.1	100.00	monomer	Zinc-Binding Non-Structural Protein Crystal Structure of a Zinc-Binding Non-Structural Protein from the Hepatitis E Virus

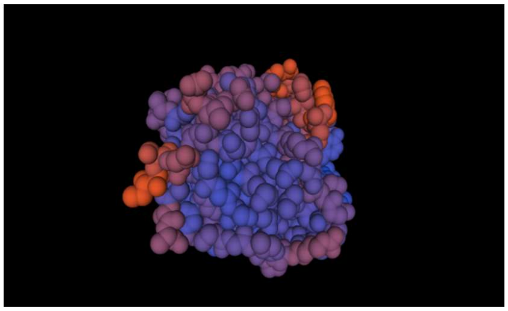
Model Results

Id	Template	GMQE	QMEANDisCo lobal	Oligo State	Ligands

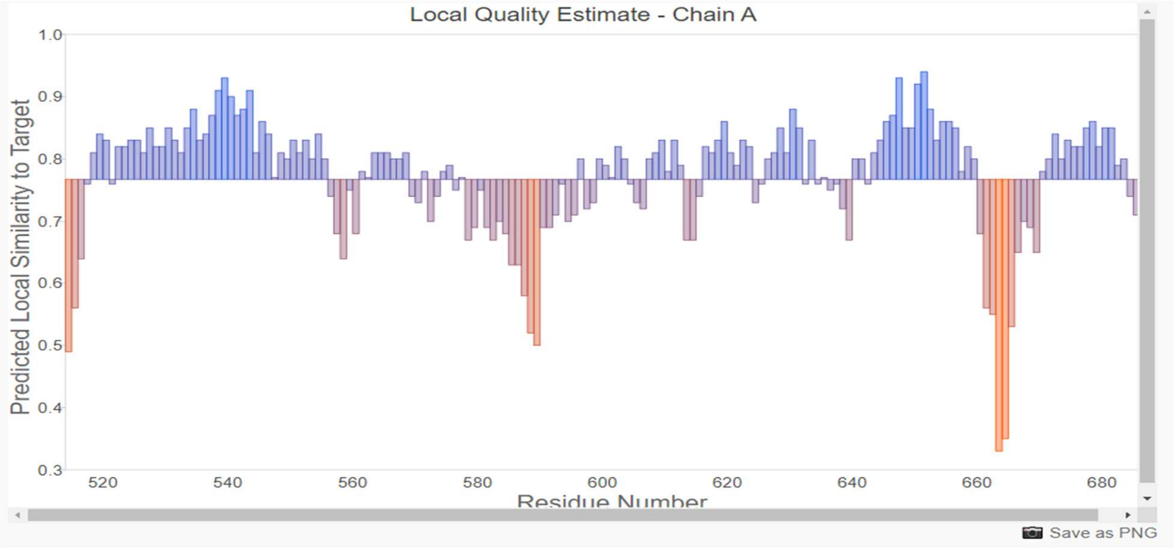
	Id	Template	GMQE	QMEANDisCo lobal	Oligo State	Ligands
	02	6nu9.1.A	0.11	0.77 ± 0.07	monomer	1 x NO2
	04	3vkw.1.A	0.08	± 0.06	monomer	-
	01	7y38.1.M	0.07	0.43 ± 0.05	monomer	-
	03	7fgi.1.A	0.06	± 0.05	monomer	-
	05	6jdr.1.A	0.05	0.44 ± 0.06	monomer	-



Hyperball



Spacefill



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

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