18.4 Tyagi, 2025. Biotechnology International 18: 17- 23.
https://www.biotechnologyinternational.org

Modeling of hepatitis C virus E1 structural and nucleocapsid proteins

Manjusha Tyagi

Department of Microbiology, SGRR University, Dehradun-248001
corresponding author: manjushatyagi2008@gmail.com

Abstract

Modeling of hepatitis C virus E1 structural and nucleocapsid proteins was done using SWISS-MODEL software. Valuable structural details could be revealed.

Key words: Modeling, hepatitis C virus, E1 structural protein, nucleocapsid protein

Introduction

Hepatitis C virus is an important pathogen of human and study of its proteins structural details will yield valuable information.

Materials and Methods

Protein

Hepatitis C virus E1 structural protein mRNA GenBank: X84985 linear 378 bp mRNA and synthetic gene for hepatitis C virus nucleocapsid protein GenBank: X71611. linear 645 bp RNA were downloaded. and amino acid sequence were used in modelling.

Modeling software

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

Results and Discussion

E1 structural Protein

Project Summary

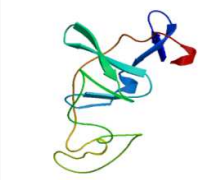
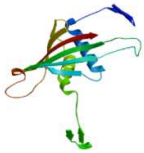
```
QVRNSTGLYHVTNDCPNSSIVYEAADAILHTPGCVPCVREGNVSKCWVAVTPTVATRDGKLPTTQLRRHIDLLVGSATLCSALYVGDL  120
CGSVFLVGQLFTFSPRRHWTTQDCNCSIYPGH                                                          0

ITGHR                                                                                      125
```

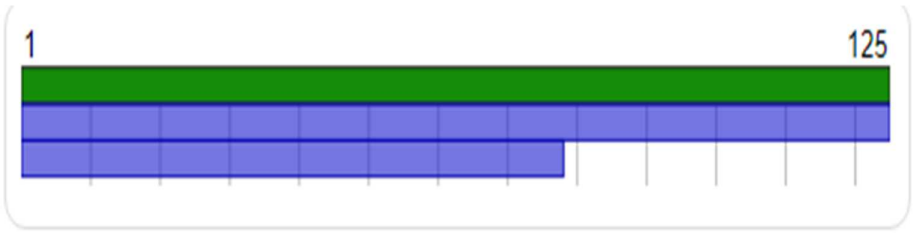
Template Results

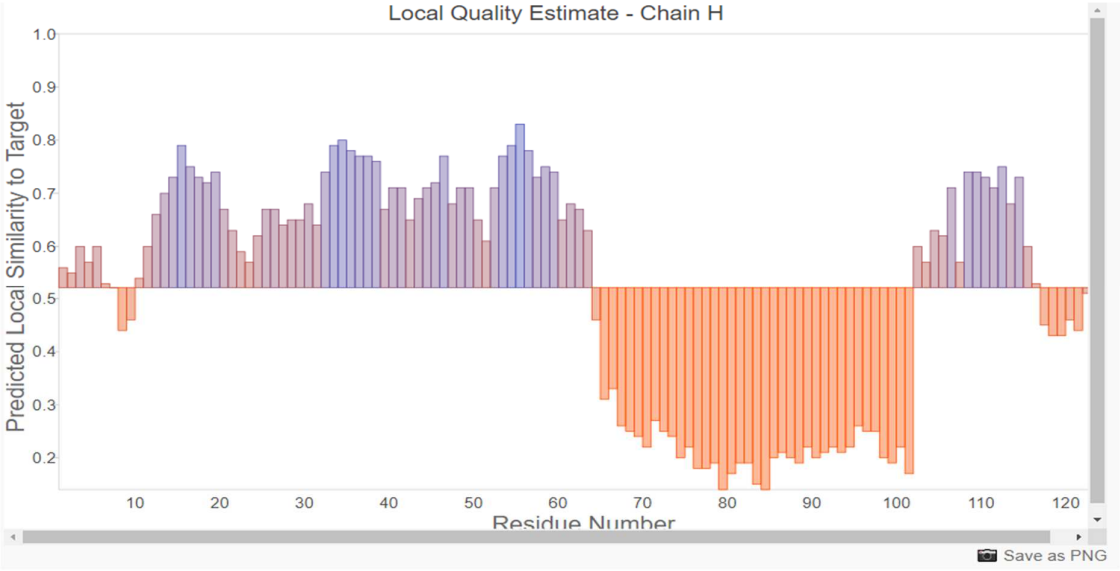
A total of 15 templates were found to match the target sequence. This list was filtered by a heuristic down to 7. The top templates are:

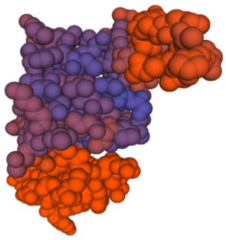
Template	Sequence Identity	Biounit Oligo State	Description
7t6x.1	94.40	hetero-octamer	Envelope glycoprotein E1 Cryo-EM structure of full-length hepatitis C virus E1E2 glycoprotein in complex with AR4A, AT12009, and IGH505 Fabs
4uoi.2	93.59	homo-dimer	GENOME POLYPROTEIN Unexpected structure for the N-terminal domain of Hepatitis C virus envelope glycoprotein E1
4uoi.3	93.59	homo-dimer	GENOME POLYPROTEIN Unexpected structure for the N-terminal domain of Hepatitis C virus envelope glycoprotein E1
4uoi.3	93.59	homo-dimer	GENOME POLYPROTEIN Unexpected structure for the N-terminal domain of Hepatitis C virus envelope glycoprotein E1
4uoi.2	93.59	homo-dimer	GENOME POLYPROTEIN Unexpected structure for the N-terminal domain of Hepatitis C virus envelope glycoprotein E1

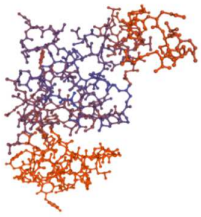
Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	7t6x.1.H	0.52	0.52 ± 0.07	monomer	-
	02	4uoi.2.A	0.34	± 0.07	homo-dimer	-

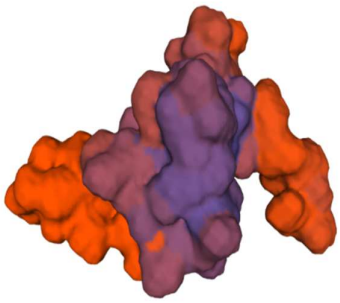


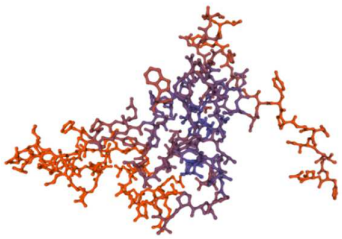






Spacefill **Ball + Stick**





Surface **Hyperball**

Nucleocapsid Protein

Project Summary

```
MSTIPKPQRKTKRNTNRRPQDVKFPGGGQIVGGVYLLPRRGPRLGVRATRKTSERSQPRGRRQPIPKVRRPEGRTWAQPGYPWPLYGN  120
EGCGWAGWLLSPRGSRPSWGPTDPRRRSRNLG

KVIDTLTCGFADLMGYIPLVGAPLGGAARALAHGVRVLEDGVNYATGNLPGCSFSIFLLALLSCLTVPASAYQVRK  196
```

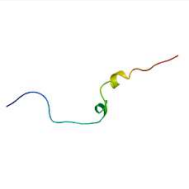
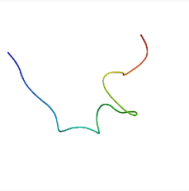
Template Results

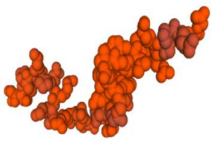
A total of 19 templates were found to match the target sequence. This list was filtered by a heuristic down to 15. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
1cwx.1	97.73	monomer	HEPATITIS C VIRUS CAPSID PROTEIN SOLUTION STRUCTURE OF THE HEPATITIS C VIRUS N-TERMINAL CAPSID PROTEIN 2-45 [C-HCV(2-45)]
1xcq.2	97.73	hetero-tetramer	Capsid protein C Complex HCV core-Fab 19D9D6-Protein L mutant (D55A,L57H,Y64W) in space group P21
1xcq.4	97.73	hetero-tetramer	Capsid protein C Complex HCV core-Fab 19D9D6-Protein L mutant (D55A,L57H,Y64W) in space group P21
1xcq.1	97.73	hetero-tetramer	Capsid protein C Complex HCV core-Fab 19D9D6-Protein L mutant (D55A,L57H,Y64W) in

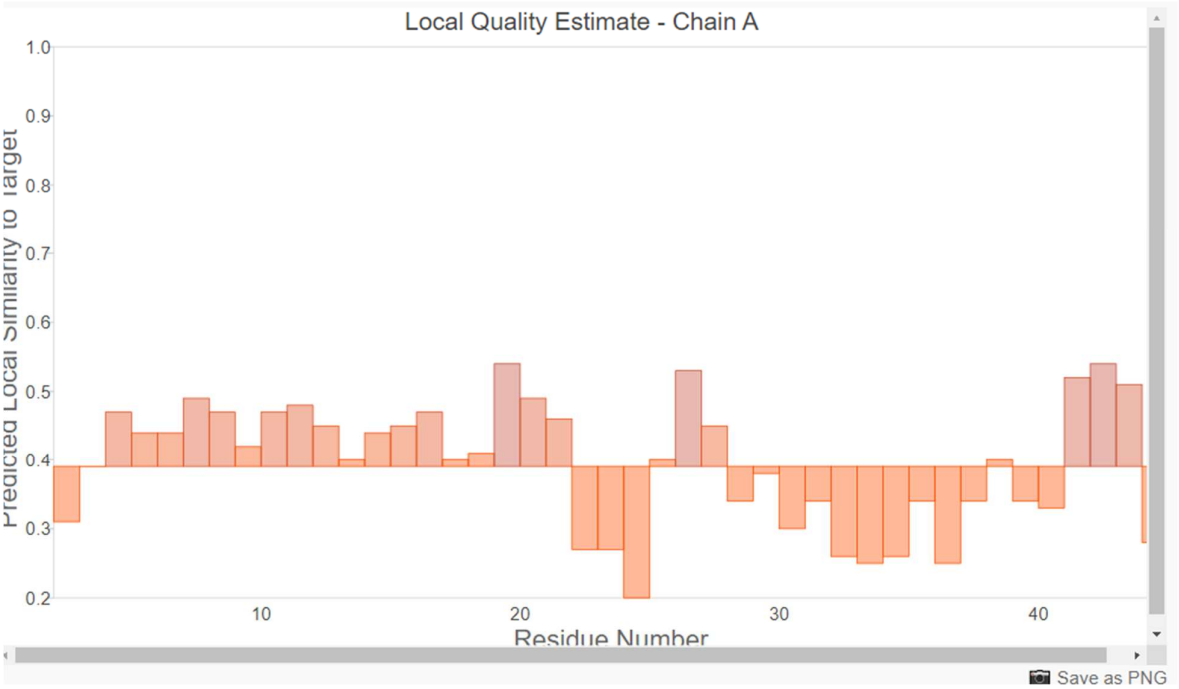
Template	Sequence Identity	Biounit Oligo State	Description
			space group P21
1xct.1	97.73	hetero-tetramer	Capsid protein C Complex HCV core-Fab 19D9D6-Protein L mutant (D55A, L57H, Y64W) in space group P21212

Model Results

Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	1cwx.1.A	0.07	± 0.12	monomer	-
	04	7kdp.1.A	0.07	± 0.12	monomer	-
	02	1xcq.4.A	0.05	± 0.12	monomer	-
	03	2lif.1.A	0.00	± 0.12	monomer	-



Ball +stick **spacefill**



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

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. 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.