Modeling of hepatitis B virus core protein and polymerase protein

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Abstract

Modeling of HBV core protein and polymerase protein was done using SWISS-MODEL software. Valuable structural properties could be obtained.

Key words: Modeling, HBV, core protein, polymerase protein

Introduction

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

Materials and Methods

Protein sequence

Hepatitis B virus isolate G376-A6, complete genome GenBank: AF384372 circular 3125 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

Core Protein

Project Summary

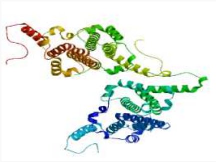
```
MDIDPYKEFGASVELLSFLPSDFFPSVRDLLDTASALYREALESPEHCSPHHTALRQAILCWVELMNLATWVGSNLEDPASRELVVSY  12
VNVNMGLKIRQLLWFHISCLTFGRETVLEYLV                                                            0

                                                                                            18
SFGVWIRTPPAYRPQNAPILSTLPETTVVRRRCRSPRRRTPSPRRRRSQSPRRRRSQSRESQC                              3
```

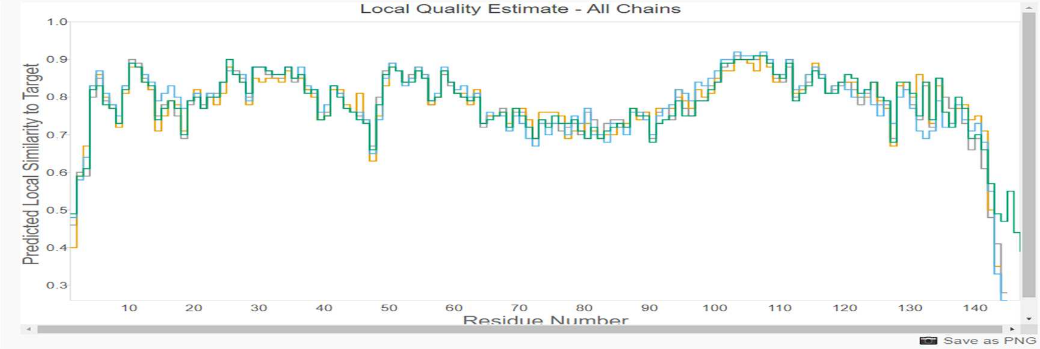
Template Results

A total of 289 templates were found to match the target sequence. This list was filtered by a heuristic down to 38. The top templates are:

Template	Sequence Identity	Biounit Oligo State	Description
7abl.1	97.81	homo-tetramer	Capsid protein HBV pgRNA T=4 NCP icosahedral symmetry
7abl.1	97.81	homo-tetramer	Capsid protein HBV pgRNA T=4 NCP icosahedral symmetry
7abl.1	97.81	homo-tetramer	Capsid protein HBV pgRNA T=4 NCP icosahedral symmetry
5t2p.1	91.28	homo-hexamer	Core protein Hepatitis B virus core protein Y132A mutant in complex with sulfamoylbenzamide (SBA_R01)
5gmz.1	91.28	homo-hexamer	Core protein Hepatitis B virus core protein Y132A mutant in complex with 4-methyl heteroaryldihydropyrimidine

Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	01	7abl.1.A	0.72	0.78 ± 0.05	homo-tetramer	-



Polymerase Protein

Project Summary

```
MPLSYQHFRKLLLLDDDAGPLEEELPRLADEGLNRRVAEDLNLGNLNVSIPWTHKVGNFTGLYSSTVPVFNPEWQTPSFPHIHLQEDI  12
INRCQQYVGPLTVNEKRRLKLIMPARFYPNIT                                                           0
```

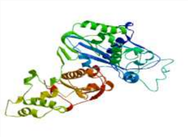
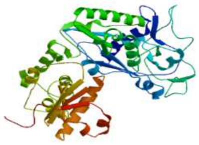
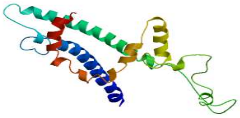
```
KYLPLDKGIKPYYPEHAVNHYFQTRHYLHTLWKAGILYKRETTRSASFCGSPYSWEQELQHGRLVFQTSTRHGDKSFCSQSSGKSGRS  24
GSIRARVHPTTRRSFGVEPSGSGHIDNGASST                                                            0

SSCLHQSAVRKTAYSHLSTSKRQSSSGHAVELHHIPPSSARPQSEGPILSCWWLQFRNSKPCSDYCLTHIVNLLEDWGPCTEHGEHNI  36
RIPRTPARVTGGVFLVDKNPHNTTESRLVVDF                                                            0

SQFSRGSTHVSWPKFAVPNLQSLTNLLSSNLSWLSLDVSAAFYHIPLHPAAMPHLLVGSSGLPRYVARLSSTSRNINYNYNHGTMQDL  48
HDSCSRNLYVSLLLLYKTFGRKLHLYSHPIIL                                                            0

GFRKIPMGVGLSPFLLAQFTSAICSVVRRAFPHCLAFSYMDDVVLGAKSVQHLESLFTSITNFLLSLGIHLNPNKTKRWGYSLNFMGY  60
VIGSWGTLPQDHIVLKIKQCFRKLPVNRPIDW                                                            0

KVCQRIVGLLGFAAPFTQCGYPALMPLYACIQSKQAFTFSPTYKAFLCKQYLNLYPVARQRSGVCQVFADATPTGWGLAIGHRRMRGT  72
FVAPLPIHTAELLAACFARSRSGAKLIGTDNS                                                            0

VVLSRKYTSFPWLLGCAANWILRGTSFVYVPSALNPADDPSRGRLGLYRPLLLLPFRPTTGRTSLYAVSPSVPSHLPARVHFASPLHV  81
AWRPP                                                                                       3
```

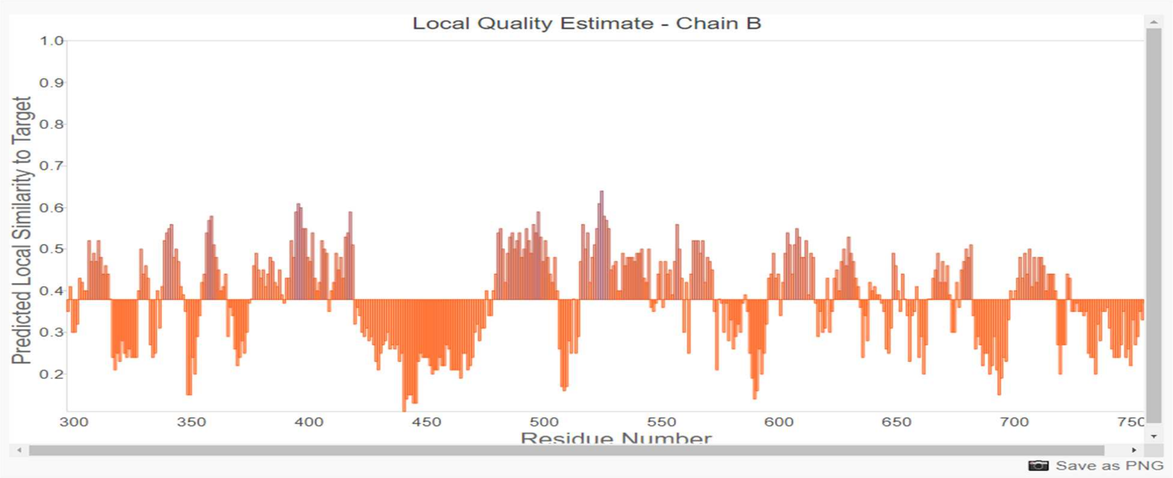
Template Results

A total of 566 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
7o0g.1	17.11	Monomer	Pr125Pol Structure of the foamy viral protease-reverse transcriptase in complex with RNA/DNA hybrid.
4ol8.1	19.79	homo-dimer	Reverse transcriptase/ribonuclease H Ty3 reverse transcriptase bound to DNA/RNA
7o0h.1	17.32	homo-dimer	Pr125Pol Structure of the foamy viral protease-reverse transcriptase dRH in complex with ds DNA.
5dmq.1	18.18	hetero-dimer	Reverse transcriptase/ribonuclease H p80 Crystal structure of mouse eRF1 in complex with Reverse Transcriptase (RT) of Moloney Murine Leukemia Virus
4hkq.1	17.86	Monomer	Reverse transcriptase/ribonuclease H p80 XMRV reverse transcriptase in complex with RNA/DNA hybrid

Model Results

	Id	Template	GMQE	QMEANDisCo Global	Oligo State	Ligands
	02	4ol8.1.B	0.25	0.38 ± 0.05	monomer	-
	01	7o0g.1.A	0.24	± 0.05	monomer	-
	03	7sep.1.A	0.20	0.33 ± 0.05	monomer	-
	05	7tuk.1.A	0.04	± 0.06	monomer	-
	04	7kft.1.D	0.04	0.29 ± 0.07	monomer	-



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

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