



## *In-silico* analysis of 2A protease as a prophylactic and therapeutic target against Hand, Foot, and Mouth disease

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### Supplementary Tables

Table 1 — Physicochemical parameters of EV - 71 2A<sup>pro</sup> analyzed by Protparam server

Molecular Weight	242657.25 Da
Pi	6.37
Half Life	
1. in mammalian reticulocytes	30 hours
2. Yeast	>20 hours
2. <i>E.coli</i>	>10 hours
Instability index	37.42
Aliphatic index	83.16 %
Hydrophobicity grand average	-0.199

Table 2 — Physicochemical parameters vaccine construct analysed by Protparam server

Molecular Weight	5937 Da
pI	8.52
Half Life	
1. in mammalian reticulocytes	1 hour
2. Yeast	30 min
2. <i>E.coli</i>	>10 hours
Instability index	18.86
Aliphatic index	68.39%
Hydrophobicity grand average	-0.37

## Supplementary Figures

```
GOR4 :  
Alpha helix (Hh) : 628 is 28.64%  
310 helix (Gg) : 0 is 0.00%  
Pi helix (Ii) : 0 is 0.00%  
Beta bridge (Bb) : 0 is 0.00%  
Extended strand (Ee) : 455 is 20.75%  
Beta turn (Tt) : 0 is 0.00%  
Bend region (Ss) : 0 is 0.00%  
Random coil (Cc) : 1110 is 50.62%  
Ambiguous states (?) : 0 is 0.00%  
Other states : 0 is 0.00%
```

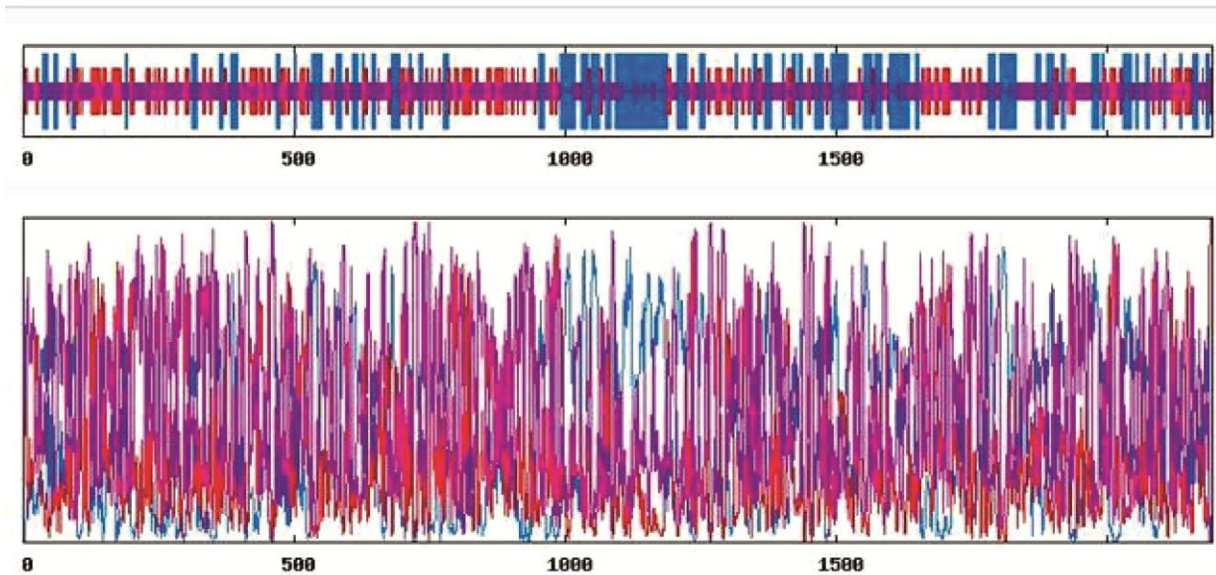


Fig. 1 — Secondary Structure of 2A polyprotein EV-71 using GOR IV server.

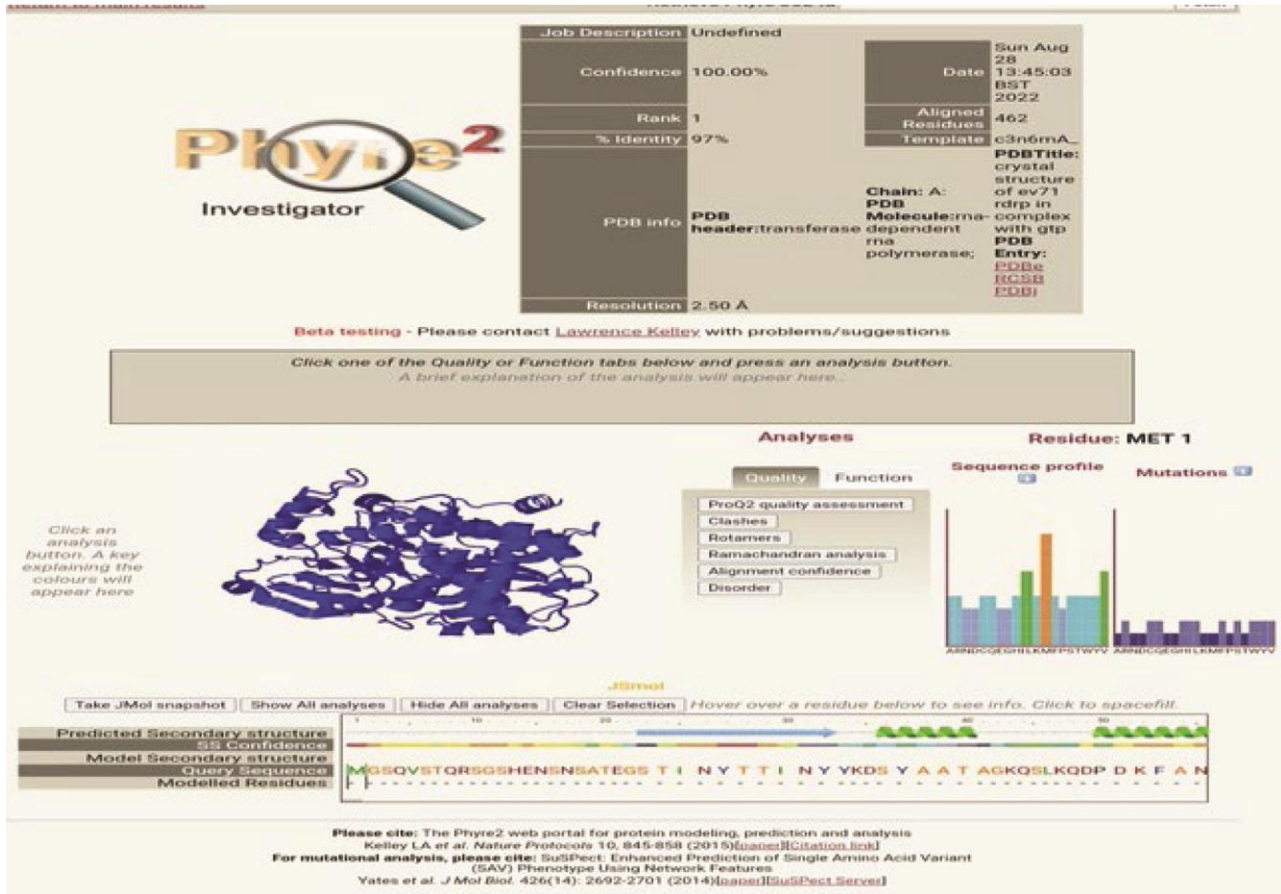


Fig. 2 — Tertiary structure prediction of 2A polyprotein EV-71 using Phyre tool.

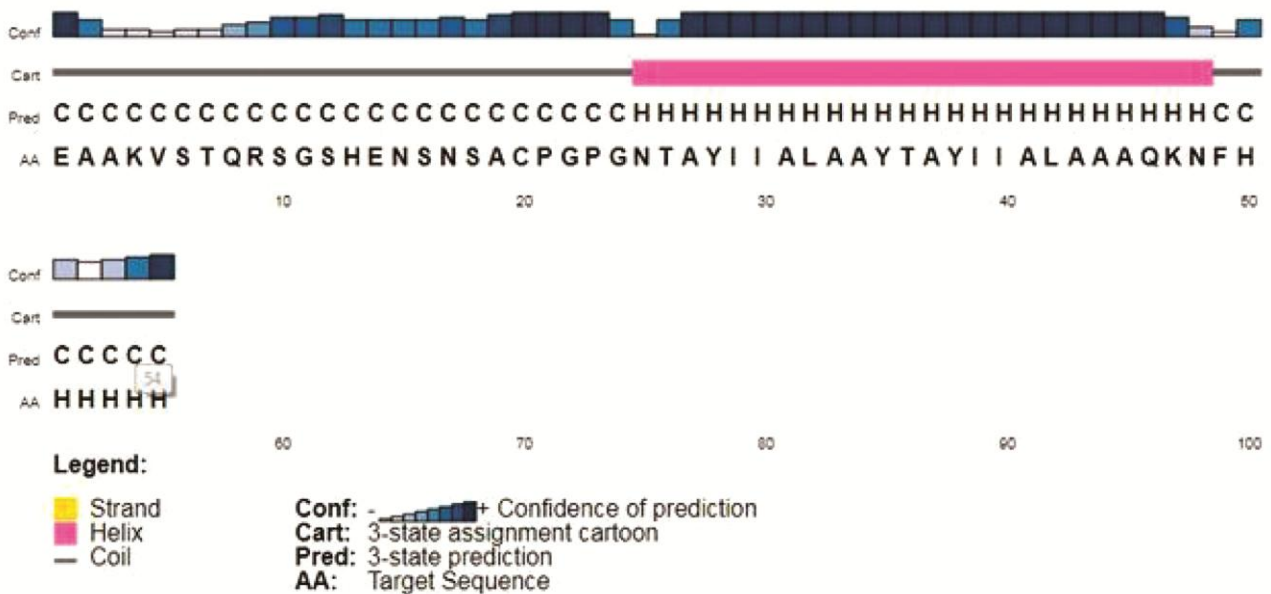


Fig. 3 — Secondary structure prediction of vaccine construct by using PSIPRED tool.

Job Description	VACCINE_...
Confidence	90.39%
Rank	1
% Identity	56%
PDB info	PDB header:virus/viral protein, receptor
Resolution	UNK
Date	Wed Sep 21 16:09:49 BST 2022
Aligned Residues	16
Template	c1dgl4_
Chain	4: PDB Molecule:vp4
PDB	Fragment:poliovirus fragments vp1,vp2,vp3,vp4; PDBTitle: PDB Entry: PDBe RCSB PDBj

Beta testing - Please contact [Lawrence Kelley](#) with problems/suggestions

Click one of the Quality or Function tabs below and press an analysis button.  
A brief explanation of the analysis will appear here..

Analyses

Residue: GLU 1

Quality Function

- ProQ2 quality assessment
- Clashes
- Rotamers
- Ramachandran analysis
- Alignment confidence
- Disorder

Sequence profile Mutations

Click an analysis button. A key explaining the colours will appear here

Take JMol snapshot Show All analyses Hide All analyses Clear Selection Hover over a residue below to see info. Click to spacefill.

Predicted Secondary structure SS Confidence

Model Secondary structure Query Sequence Modelled Residues

EAAKV S T Q RSGSHENSNSACPGPNT A Y I I A L A A Y T A Y I I A L A A A Q K N F T

AKV S T Q RSGSHENSNS-

Please cite: The Phyre2 web portal for protein modeling, prediction and analysis  
Kelley LA et al. Nature Protocols 10, 845-858 (2015)[paper][Citation link]

For mutational analysis, please cite: SuSPect: Enhanced Prediction of Single Amino Acid Variant (SAV) Phenotype Using Network Features  
Yates et al. J Mol Biol. 426(14): 2692-2701 (2014)[paper][SuSPect Server]

Fig. 4 — Tertiary structure prediction of vaccine construct by Phyreserver.