

Supplementary Materials

Elucidating the Substrate Envelope of Enterovirus 68-3C Protease: Structural Basis of Specificity and Potential Resistance

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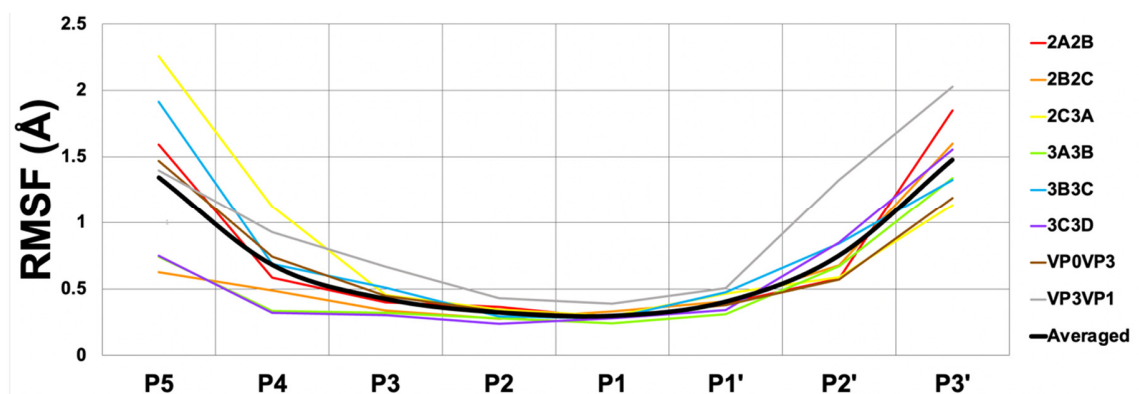


Figure S1. Substrate peptide fluctuations during 150 ns molecular dynamics (MD) simulations of molecular models bound to EV68-3C protease. The root-mean-squared fluctuations (RMSF) of viral substrate backbone were calculated (colored lines), and then averaged at each position (bolded black line).

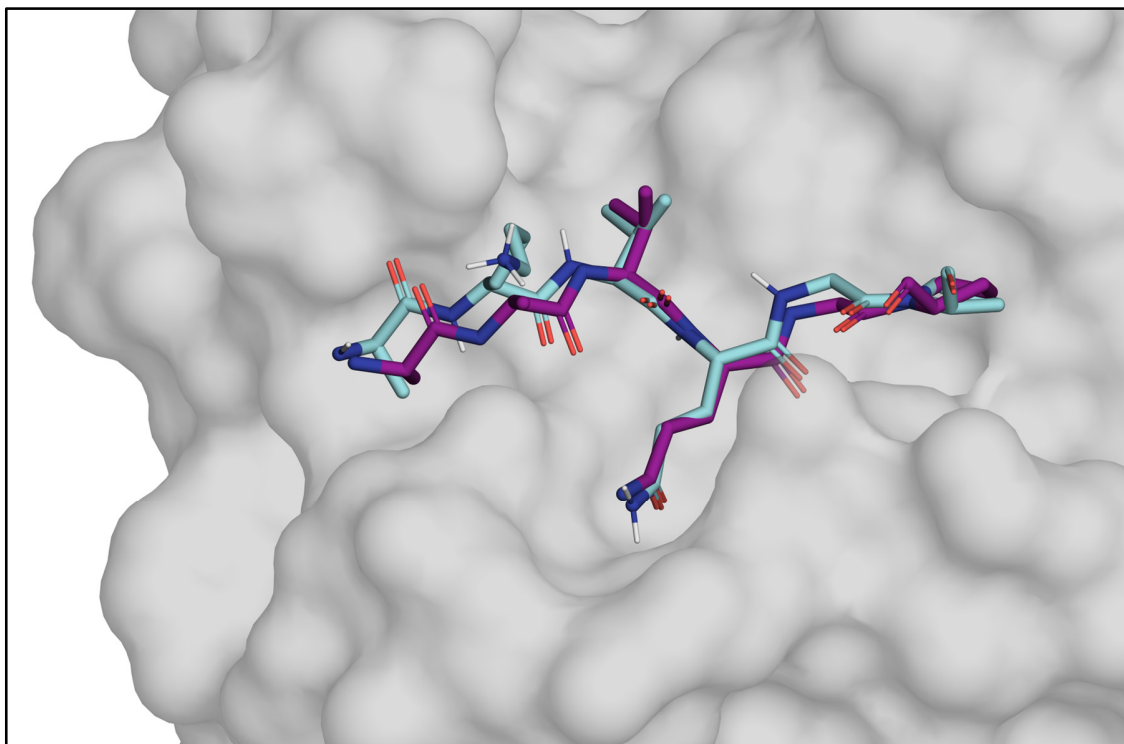


Figure S2. EV68-3C protease bound to the 3B3C peptide from the molecular model (cyan) compared with the experimental co-crystal structure (purple). The agreement between the two structures further supports and validates the molecular modeling approach. The protease is shown in gray surface representation.