

**Supplementary materials**

**for**

**Host-virus interactions in**

**Japanese encephalitis virus**

*Urmi Roy\**

Department of Chemistry & Biomolecular Science

Clarkson University

8 Clarkson Avenue, Potsdam, NY 13699-5820, United States

\*To whom correspondence should be addressed. E-mail: [urmi@clarkson.edu](mailto:urmi@clarkson.edu)

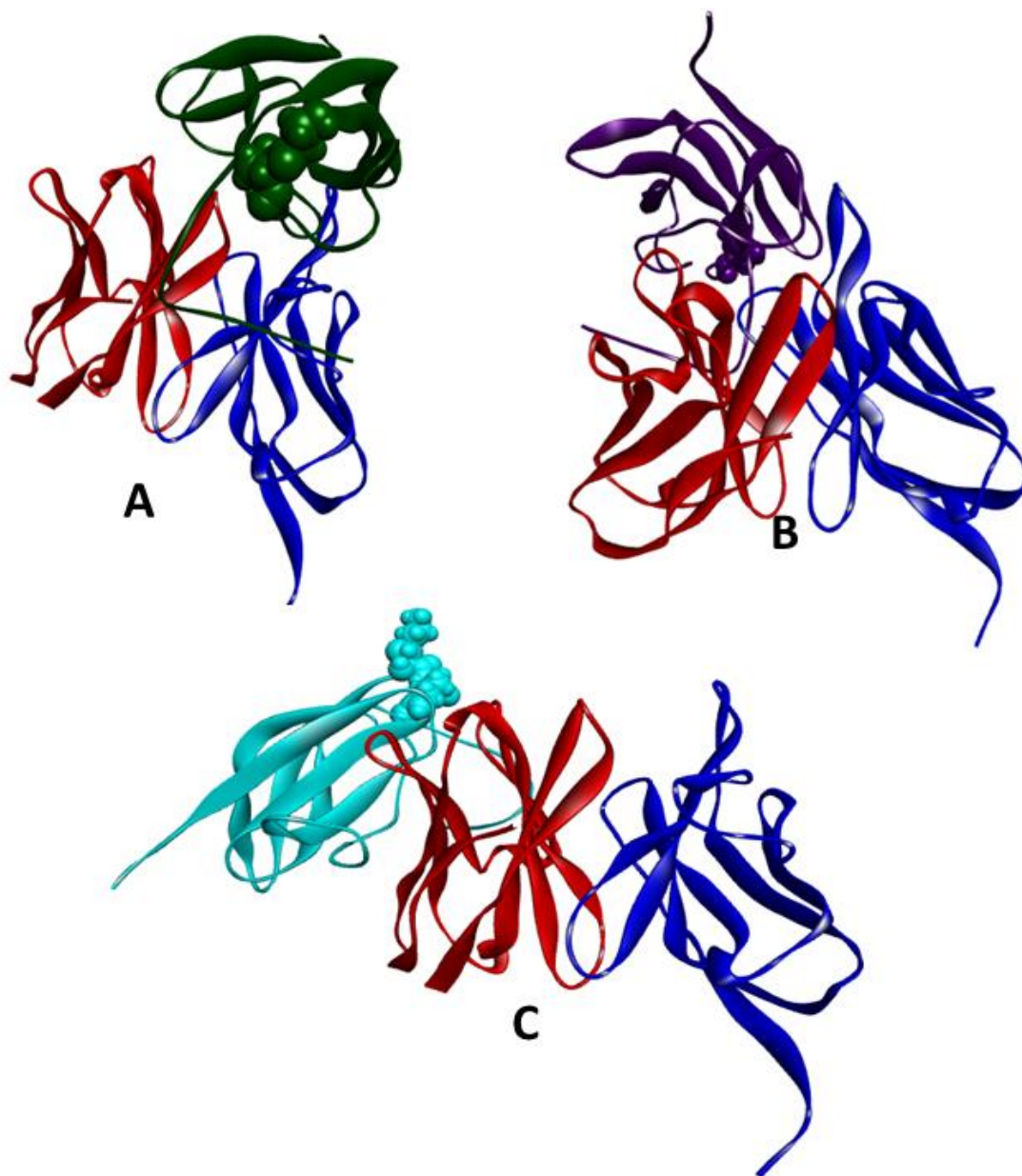
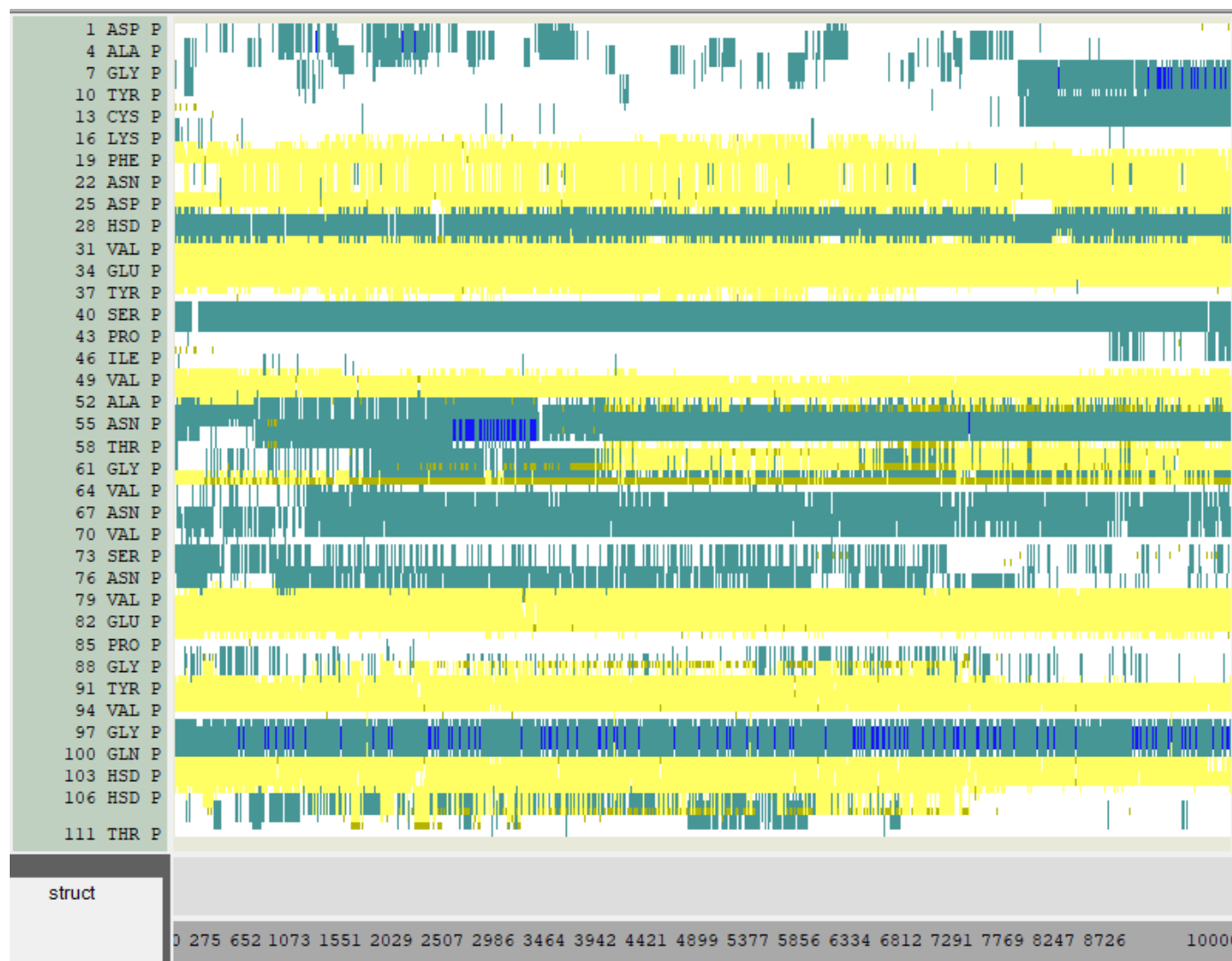


Figure S1. The wt and mutant JEV-ED3/mAb-Fab complexes using Pathdock and Firedock server. A. The wt JEV-ED3/receptor complex. The global energy value for this complex is -20.64 energy unit. B. The mutant 2 (Asp41Arg)/receptor complex, with global energy value -9.49 energy unit. C. Double mutant/receptor complex with a different ligand binding mode is displayed. The global energy value for this complex is -8.39 energy unit. These values may change during the simulation process.



A



**B**



C



D

Figure S2. Secondary structure changes of wt and mutant ligand proteins with time. A. Secondary structure changes of wt 1PJW-ED3 ligand in JEV-ED3/mAb Fab complex (This plot refers to the configuration shown in Fig. 1B of the main article). B. Secondary structure changes of mutant2 ligand protein in mutant2/mAb

Fab complex (This plot refers to the configuration shown in Fig. 2B2 of the main article). C. Secondary structure changes of double mutant ligand protein in double-mutant/mAb Fab complex (This plot refers to the configuration shown in Fig. 2C2 of the main article). D. The scheme of the color codes used in this figure is described. Default color codes are used. The X axis represents the frames corresponding to the simulation time. On this scale the 20ns correspond to 10000 frames. The Y axis denotes the proteins' residue numbers.