# Supplementary material for the paper ‘Dynamic stability of salt stable cowpea chlorotic mottle virus capsid protein dimers and pentamers of dimers’

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## Supplementary Data

### Trajectories

The supplementary data file contains trajectories for four dimer structures in Amber crd format: 4 parallel runs of the four dimer types each at 350 K in implicit solvent, one run of the four dimer types each at 350 K in explicit solvent, 2 µs simulations for the four dimer types and the pentamer of dimers at 300 K in explicit solvent.

### Movies

**Supplementary Movie 1:** Animation of the 2 µs NPT ensemble molecular dynamics simulations at 300 K for the T1 dimer.
**Supplementary Movie 2:** Animation of the 2 µs NPT ensemble molecular dynamics simulations at 300 K for the T2 dimer.
**Supplementary Movie 3:** Animation of the 2 µs NPT ensemble molecular dynamics simulations at 300 K for the T3 dimer.
**Supplementary Movie 4:** Animation of the 2 µs NPT ensemble molecular dynamics simulations at 300 K for the TX dimer.
**Supplementary Movie 5:** Animation showing the dissociation of the T2 dimer in implicit solvent molecular dynamics simulations at 350 K.
**Supplementary Movie 6:** Animation of the 2 µs NPT ensemble molecular dynamics simulations at 300 K for the pentamer of dimers.

The supplementary data can be downloaded from https://szilard.ro/files/ccmv-supplementary.zip.

## Supplementary Figures

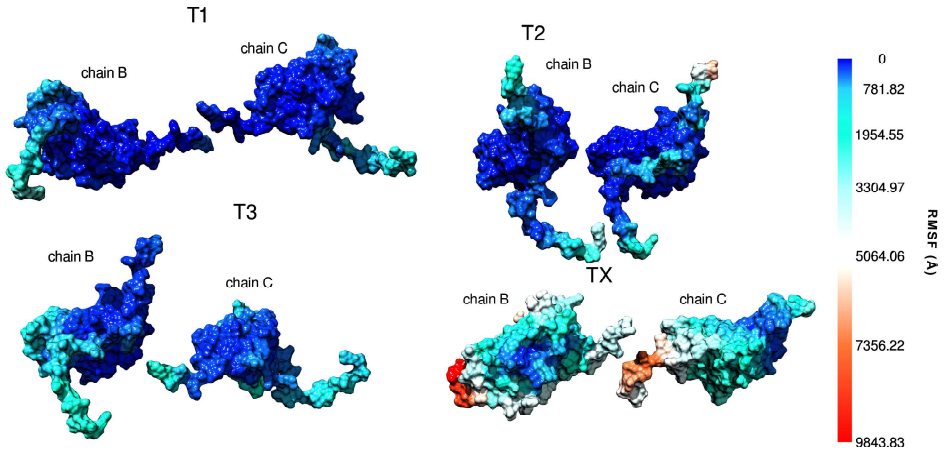


**Figure S1.** T1, T2, T3 and TX dimers with surface representations coloured by overall residue mobility during the long timescale simulations. The dimers are separated for a better view.

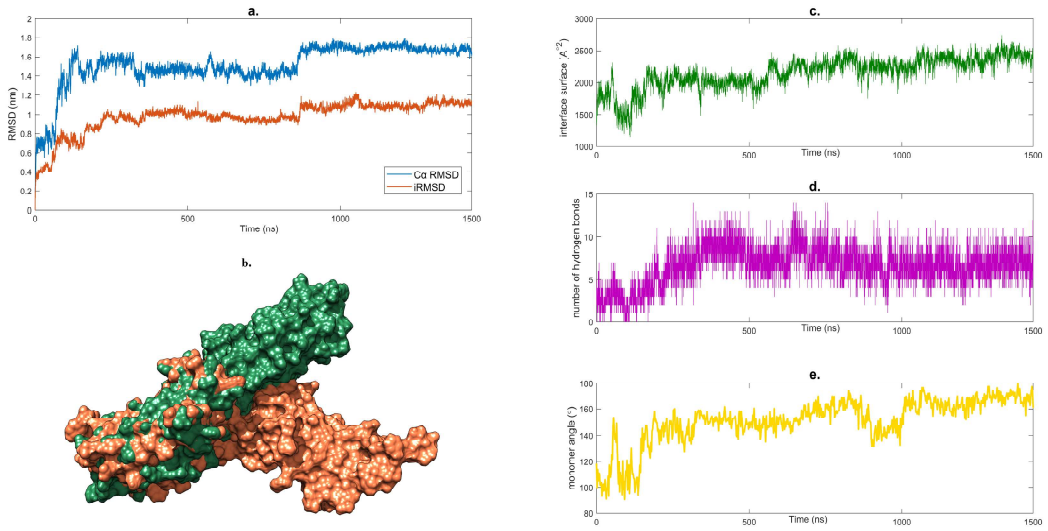


**Figure S2.** Analysis of the 1.5 µs NPT, explicit solvent simulation for the TX interface: **a.** C$\alpha$ RMSD and iRMSD; **b.** initial (red) and final (green) structures of TX superimposed with surface representation; **c.** change in the interface surface; **d.** number of hydrogen bonds; **e.** variation of the angle between the monomers of the protein.

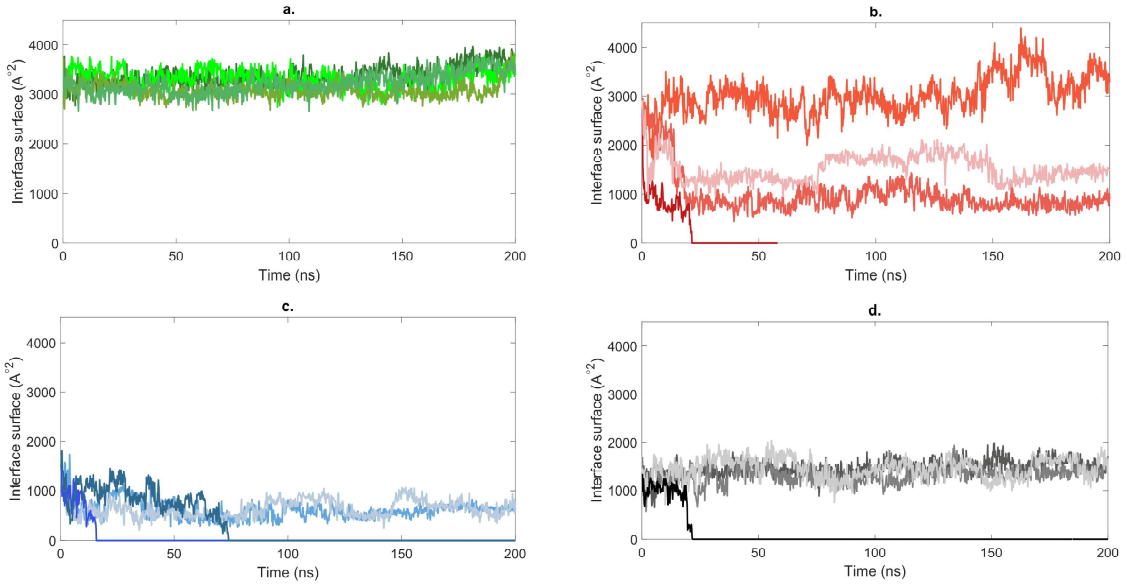


**Figure S3.** Variation of the interface surface for T1 (**a.**), T2 (**b.**), T3 (**c.**) and TX (**d.**) in 4 parallel runs for 200 ns implicit solvent simulation on 350 K

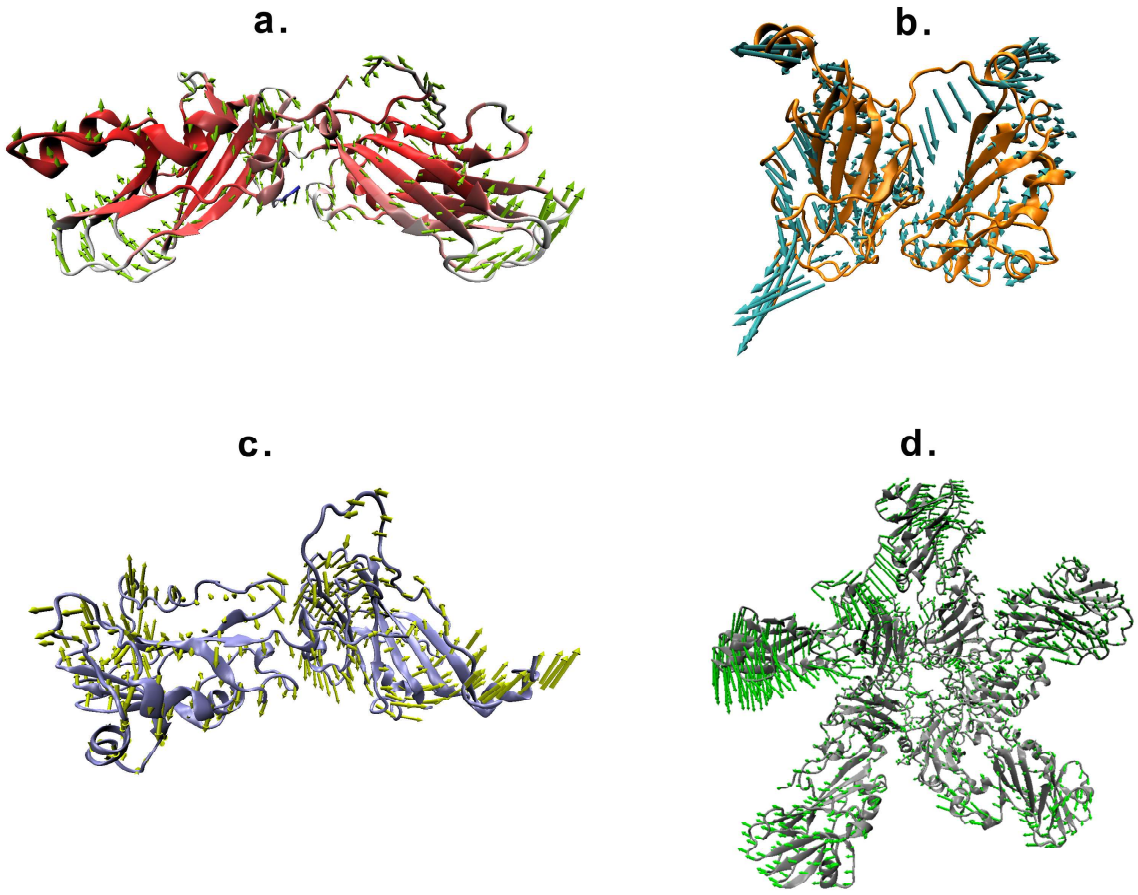


**Figure S4.** Relative motions of the Cα atoms shown as arrows aligned to the average structure of 2 μs NPT ensemble simulation for T1 (**a.**), T2 (**b.**), T3 (**c.**) and PD (**d.**).