Electronic Supplementary Material (ESI) for Molecular BioSystems.

Patch formation of a viral channel forming protein within a lipid membrane – Vpu of HIV-1.

Supporting Material

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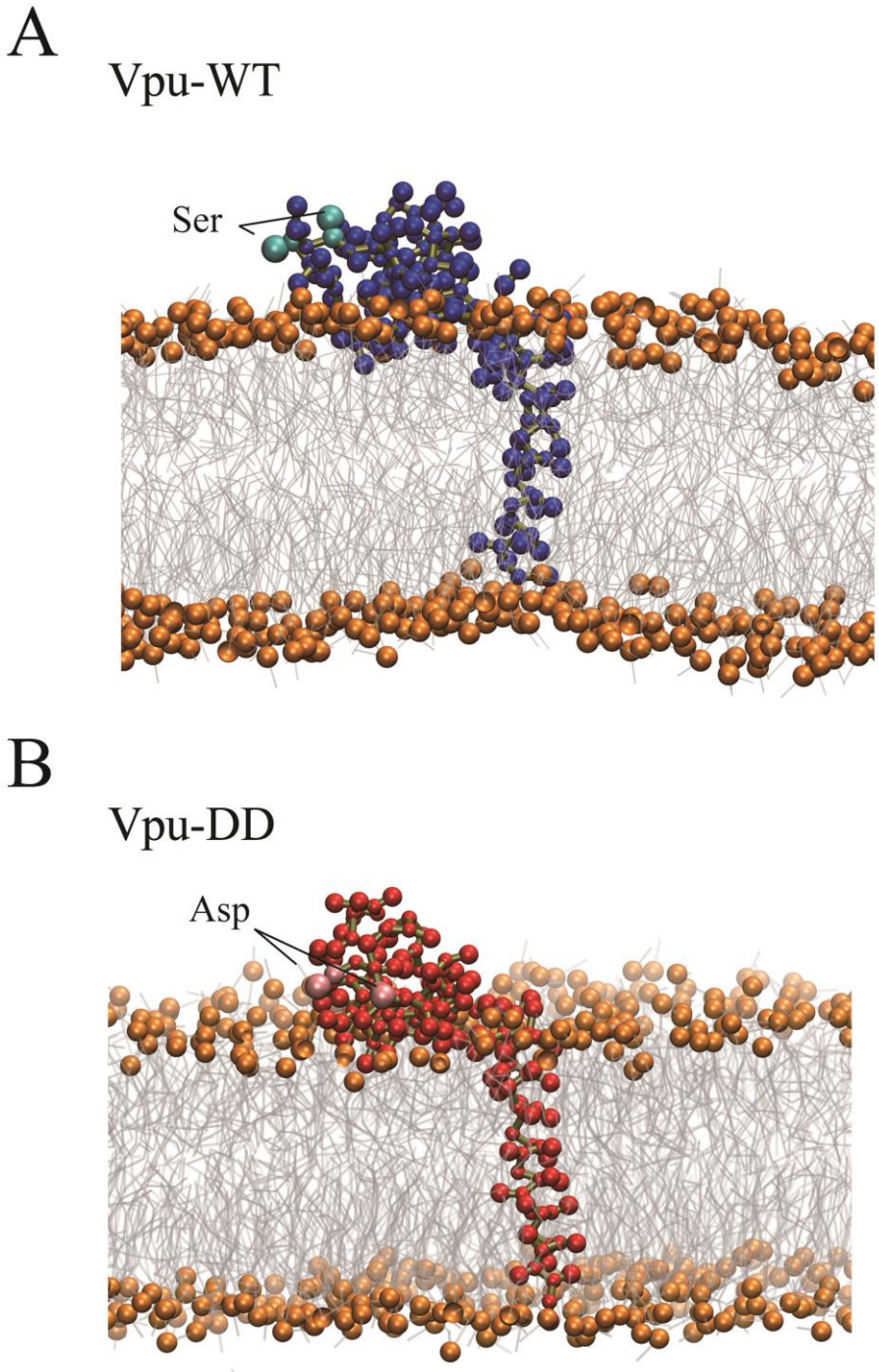
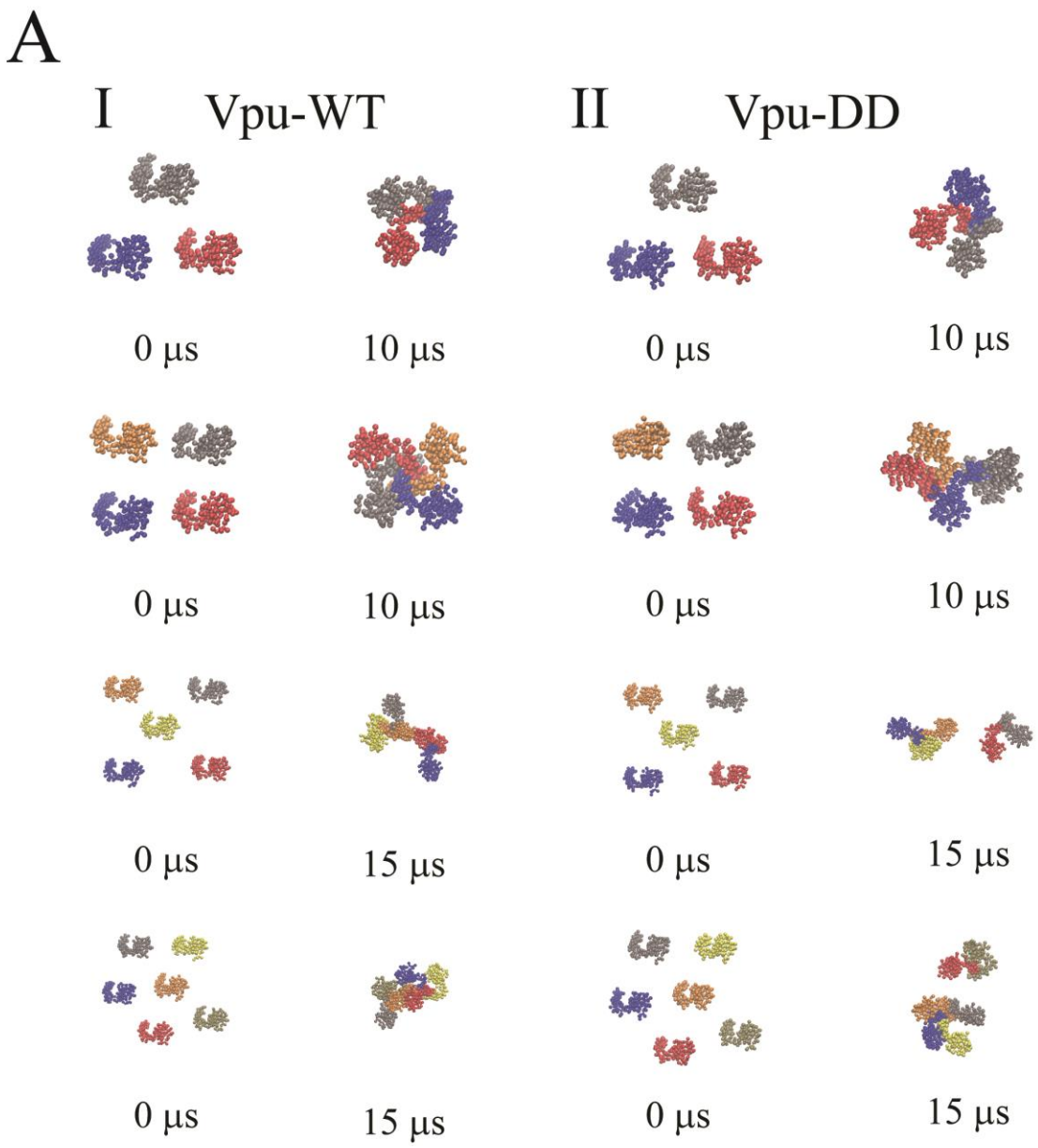
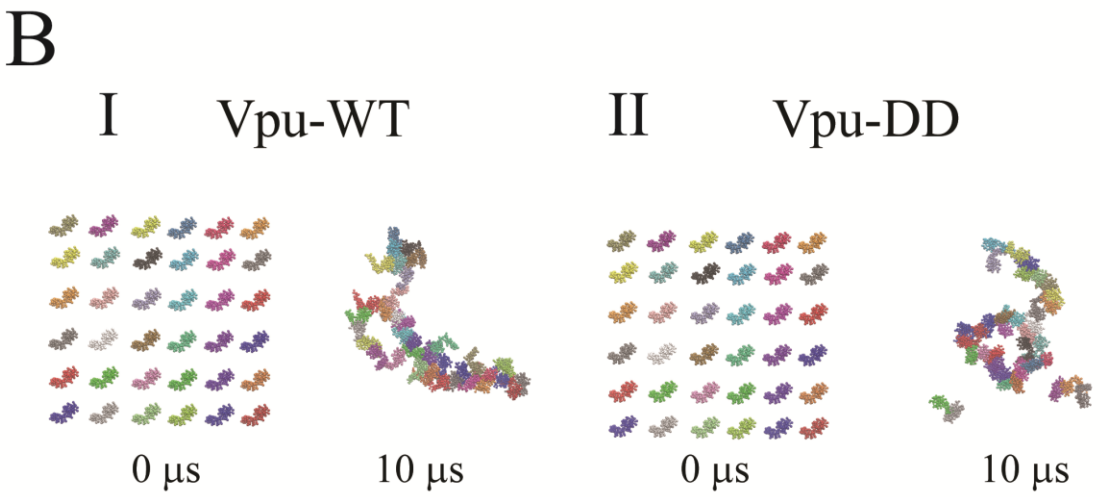


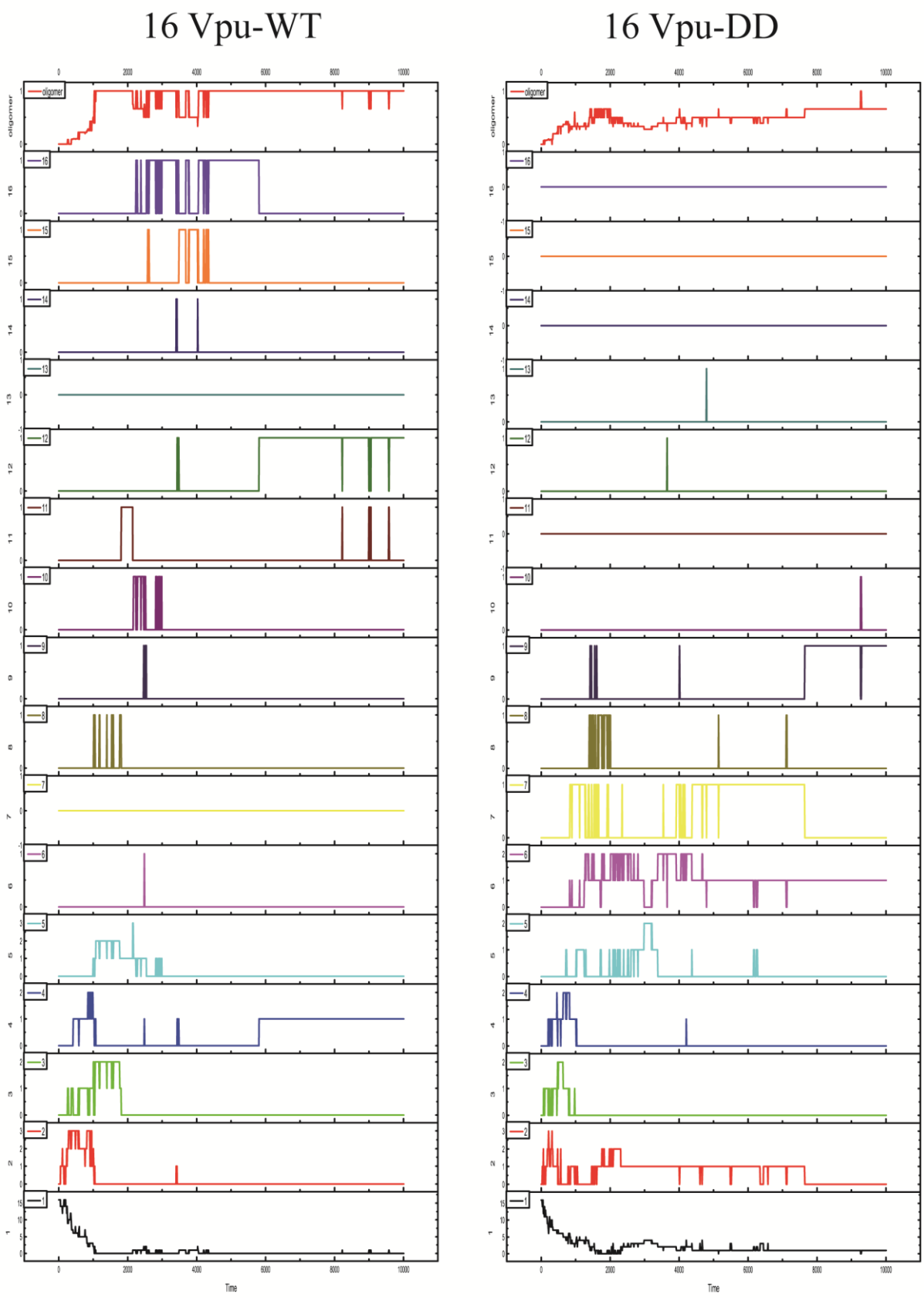
Suppl. Fig. 1: Snapshot taken at 200 ns of one out of two Vpu-WT in blue (A) and Vpu-DD in red (B) during the CGMD simulation. The structures are shown in a side view within the hydrated lipid bilayer with the serines, Ser-52 and -56 (shown in light blue spheres) and aspartic acids, Asp-52 and -56 (shown in light red spheres) highlighted. The phosphate moieties of the lipid bilayer are shown in orange to indicate the approximate dimension of the lipid bilayer. The hydrophobic tails are indicated by light grey lines. Spheres representing the water molecules are omitted for clarity. There are two proteins, 449 POPCs, 8346 CG-Waters and 12 sodium ions in the system.



Suppl. Fig. 2: description see next page.

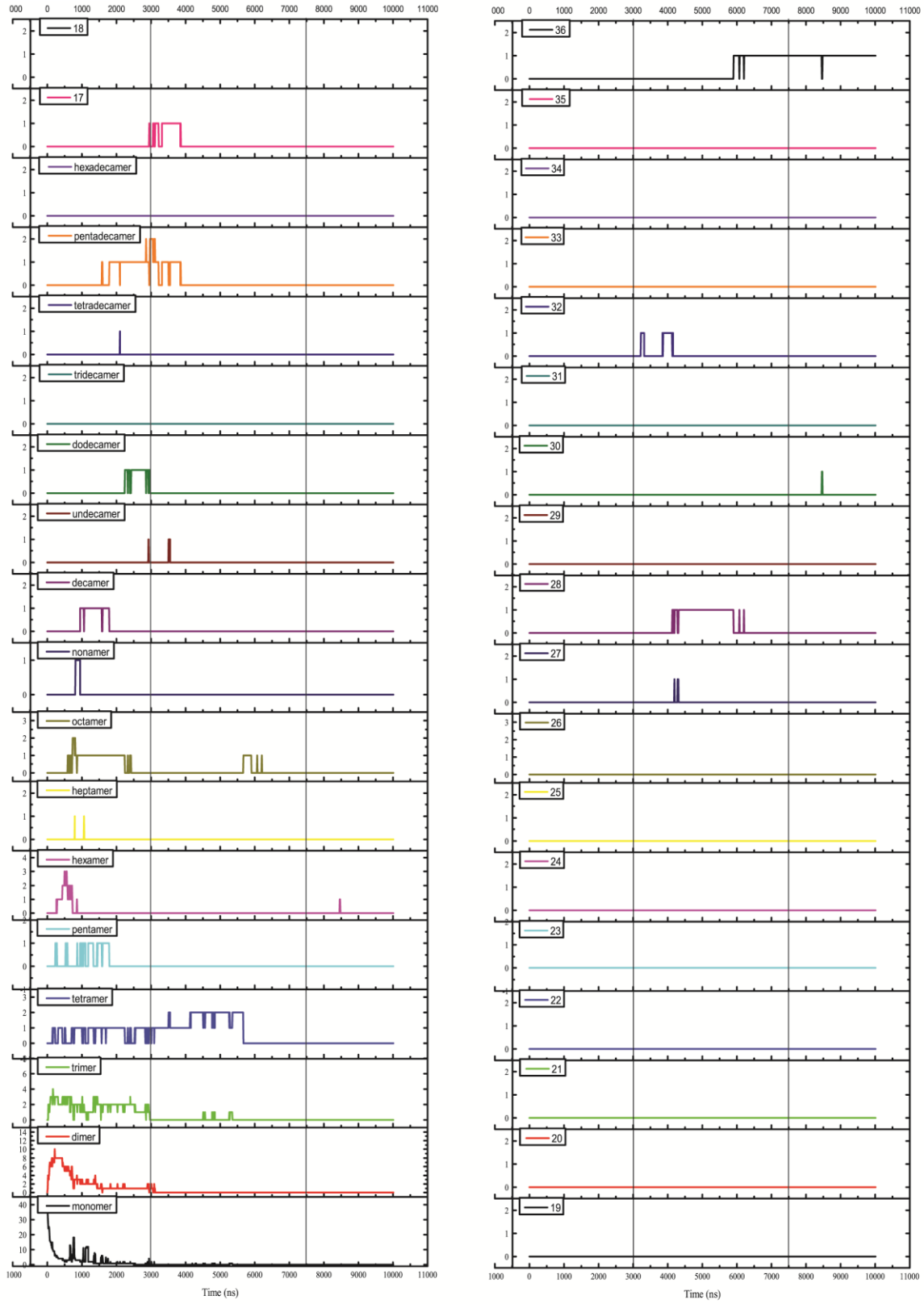


Suppl. Fig. 2: Top view (towards the membrane normal seeing the cytoplasmic domain) of three to six Vpu-WT (I) and Vpu-DD (II) from top to bottom (A) as well as representations of the respective simulations with 36 proteins (top to bottom) (B) in a in their starting configuration (0 µs) and at the final conformation at the end of each of the simulations. The 36 proteins are run at a lipid : protein ratio of 9 : 1. Lipid and water molecules are omitted for clarity.

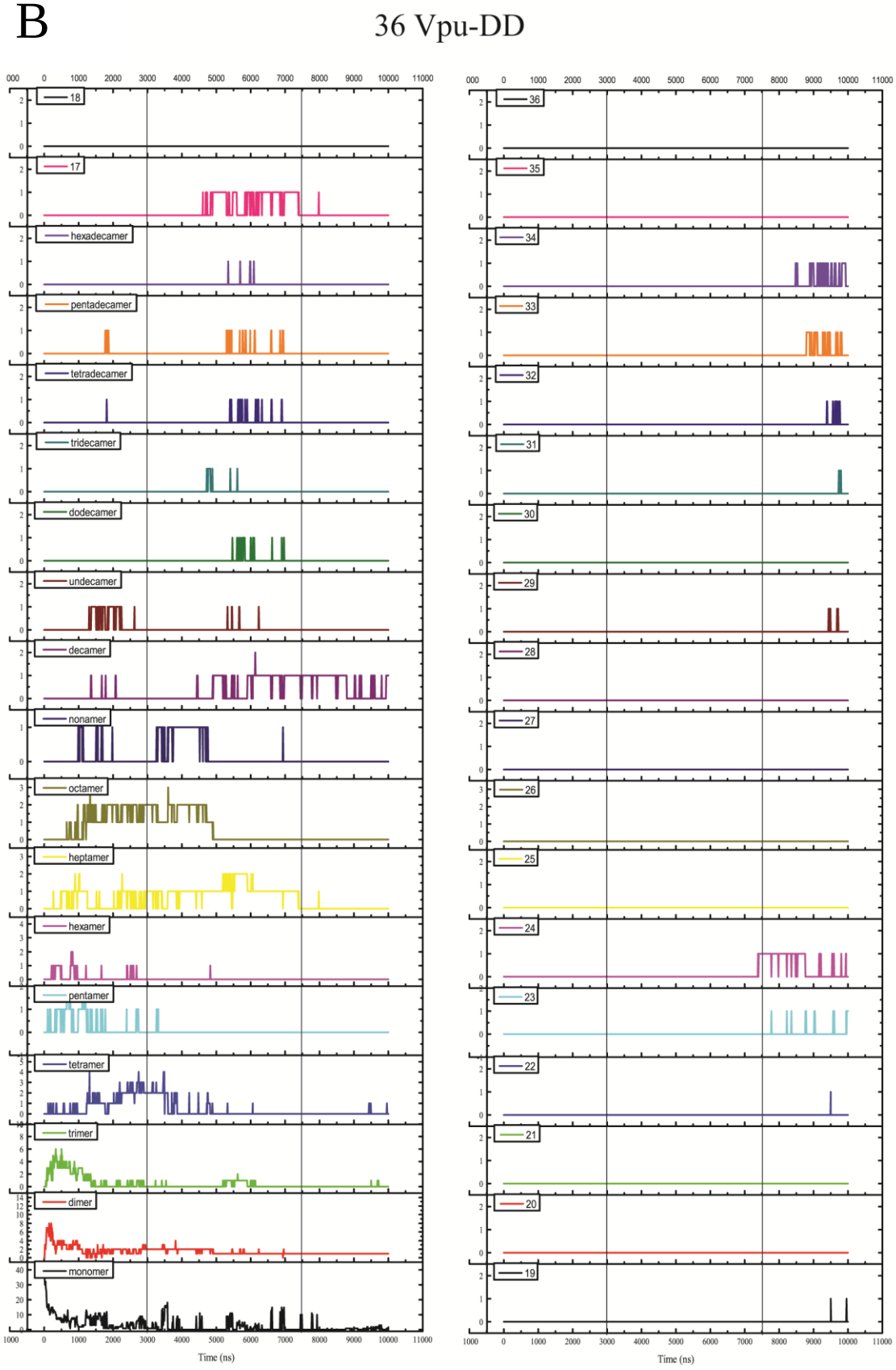


Suppl. Fig. 3: Time-resolved numbers of oligomers and total oligomerization ratio of the individual protein assemblies from a simulation with 16 Vpu-WT proteins (left) and Vpu-DD (right). Values for oligomers and monomers are shown in individual colours. The total oligomerization ratio is shown on top of the graphs.

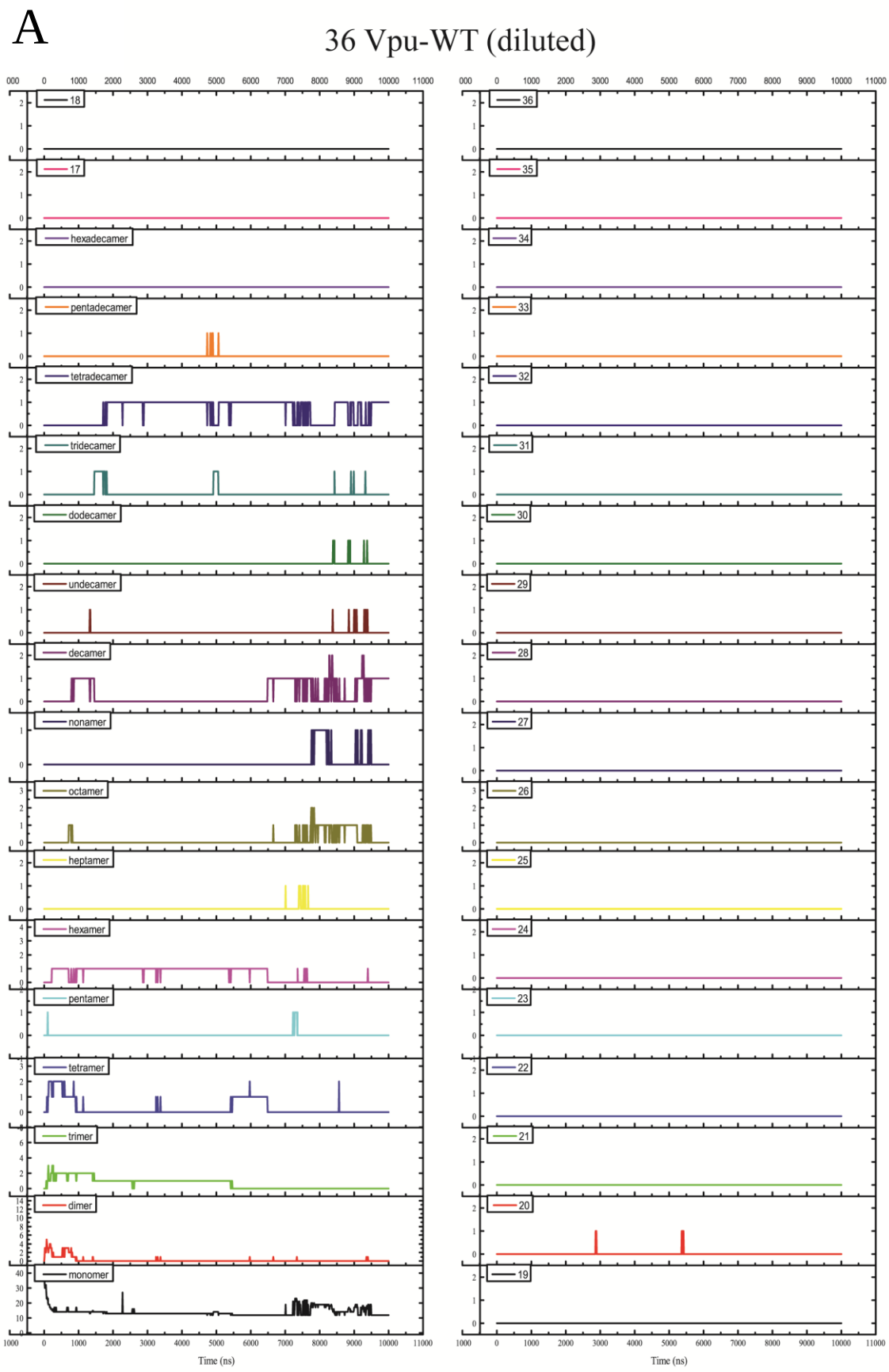
A



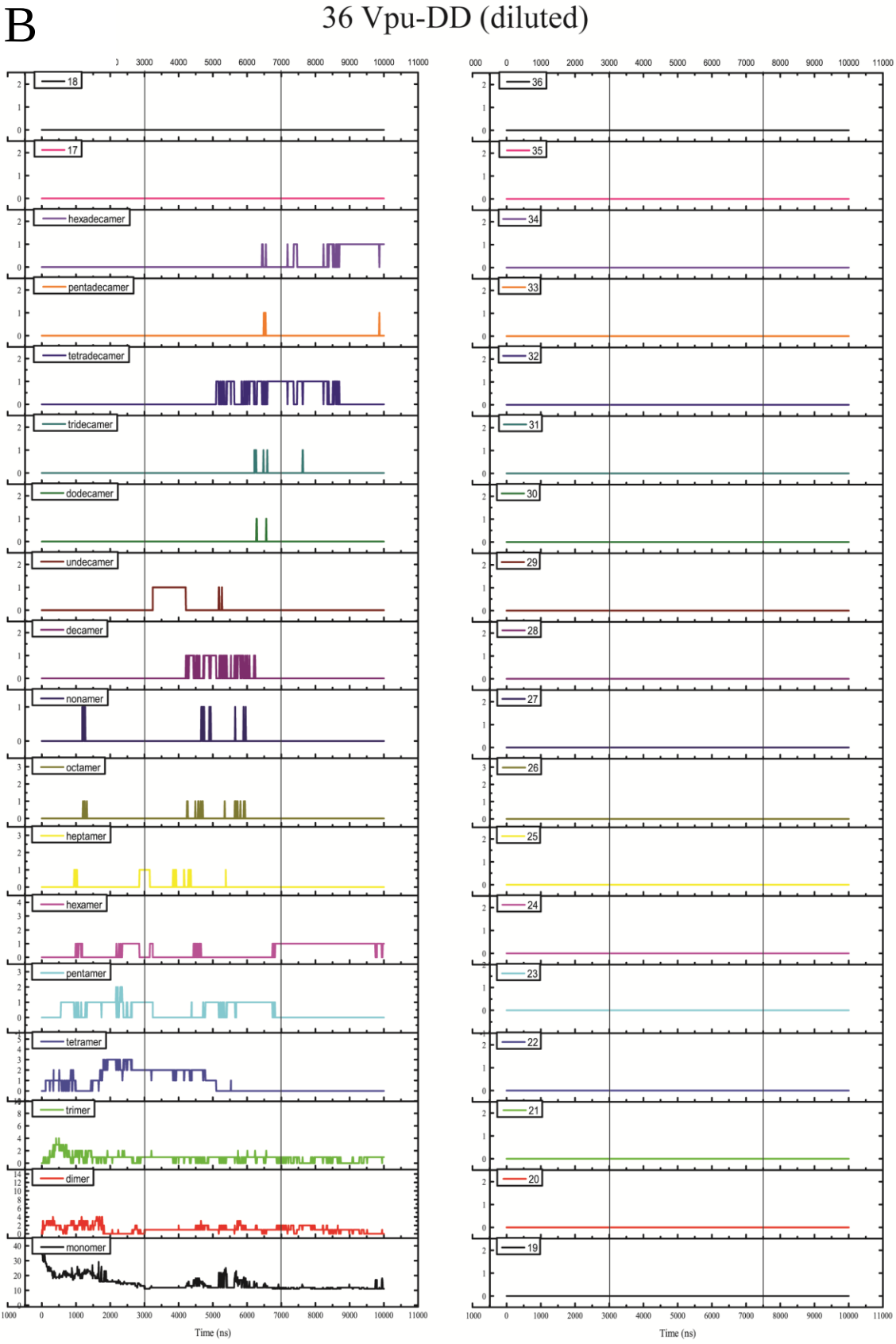
Suppl. Fig. 4: description see next page.



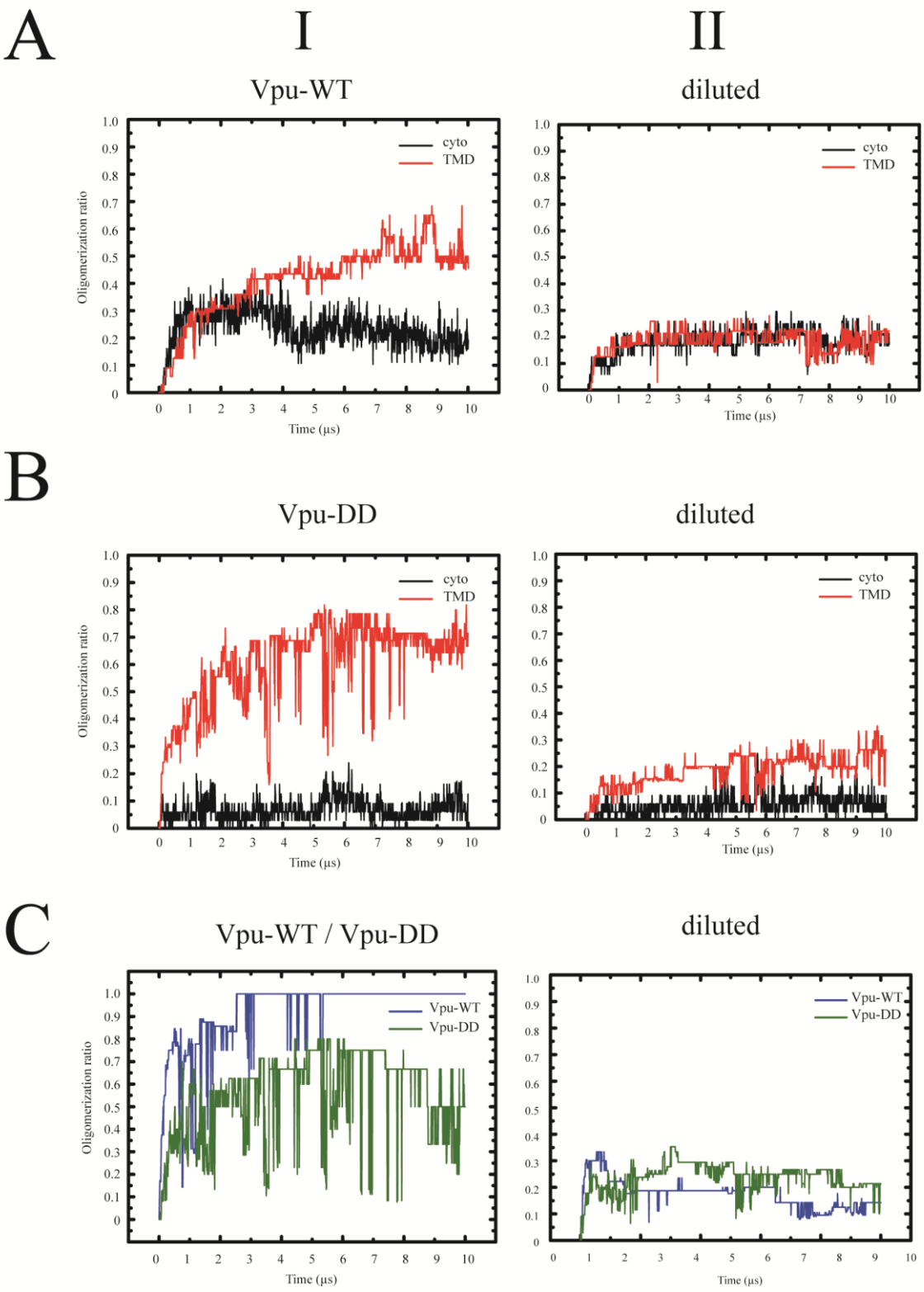
Suppl. Fig. 4: Time-resolved numbers of oligomers and total oligomerization ratio of the individual protein assemblies from a simulation with 36 Vpu-WT proteins (A) and mutant proteins Vpu-DD (B) at a lipid : protein ration of 9 : 1. Values for oligomers and monomers are shown in individual colours. The total oligomerization ratio is shown on top of the graphs.



Suppl. Fig. 5: description see next page.



Suppl. Fig. 5: Time-resolved numbers of oligomers and total oligomerization ratio of the individual protein assemblies from a simulation with 36 Vpu-WT (A) and Vpu-DD (B) at a lipid : protein ration of 20 : 1. Values for oligomers and monomers are shown in individual colours. The total oligomerization ratio is shown on top of the graphs.



Suppl. Fig. 6: Oligomerization ratio of from a simulation of 36 Vpu-WT (A) as well as 36 Vpu-DD (B). The ratio for the TMDs and the cytoplasmic (cyto) domains are shown in red and black, respectively. The total oligomerization ratio of Vpu-WT and Vpu-DD are shown in blue and green, respectively (C). Graphs in the right column show data from simulations at lipid : protein ratio of 9 : 1 whilst those graphs in the right column show data from those simulations at a lipid : protein ratio of 20 : 1.