Supporting Information for

A Molecular Dynamics Study on the Resilience of Sec61 Channel from Open to Closed State

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Fig. S1 The initial and final snapshots of independent 0.1 μs simulations. (A) The structure at 1.9 μs in SA is set as the initial structure for three independent 0.1 μs simulations; (B), (C) and (D) show the final structures of three independent 0.1 μs simulations respectively; (E) The structure at 2.1 μs in SA. Three independent 0.1 μs simulations (B, C and D) obtained similar pyramidal shape structures. Additional 0.1 μs simulation (E) shows that the pyramidal shape structure remains stable in at least 0.2 μs simulation.

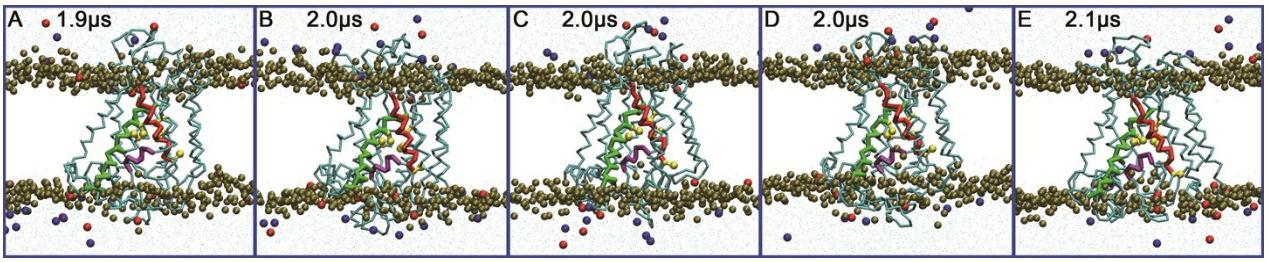

Fig. S2 The time evolution of angle between TM2 and TM7. The angle is measured by the vector of V85-I90 and I292-L297.

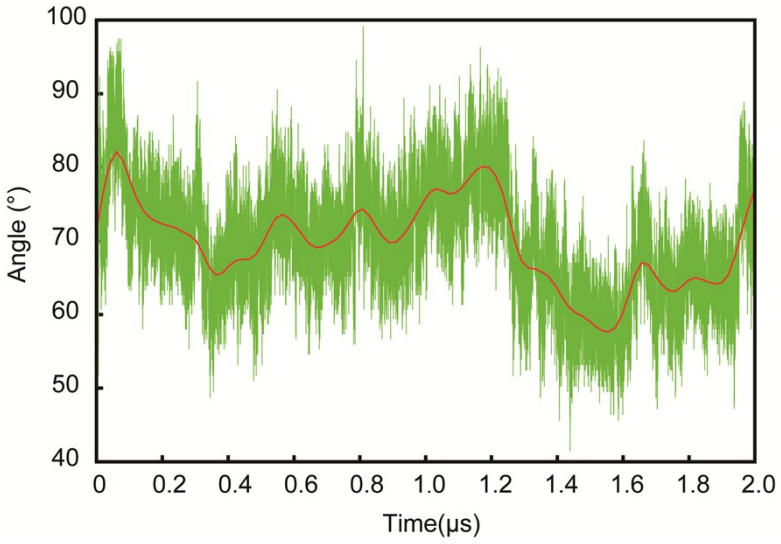

Fig. S3 The coordinates of plug as a function of time. The origin is set at the center of mass of the channel, Z axis is perpendicular to the bilayer from external to cytoplasmic side, Y is parallel to the bilayer, and the lateral gate faces to the positive direction. The point color of SA and SB become darker and darker as time goes on that shows the trajectories of plug during simulations.