Atomistic molecular dynamics simulations enable prediction of the arginine permeation pathway through OccD1 from *Pseudomonas aeruginosa.*

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Supplementary Information

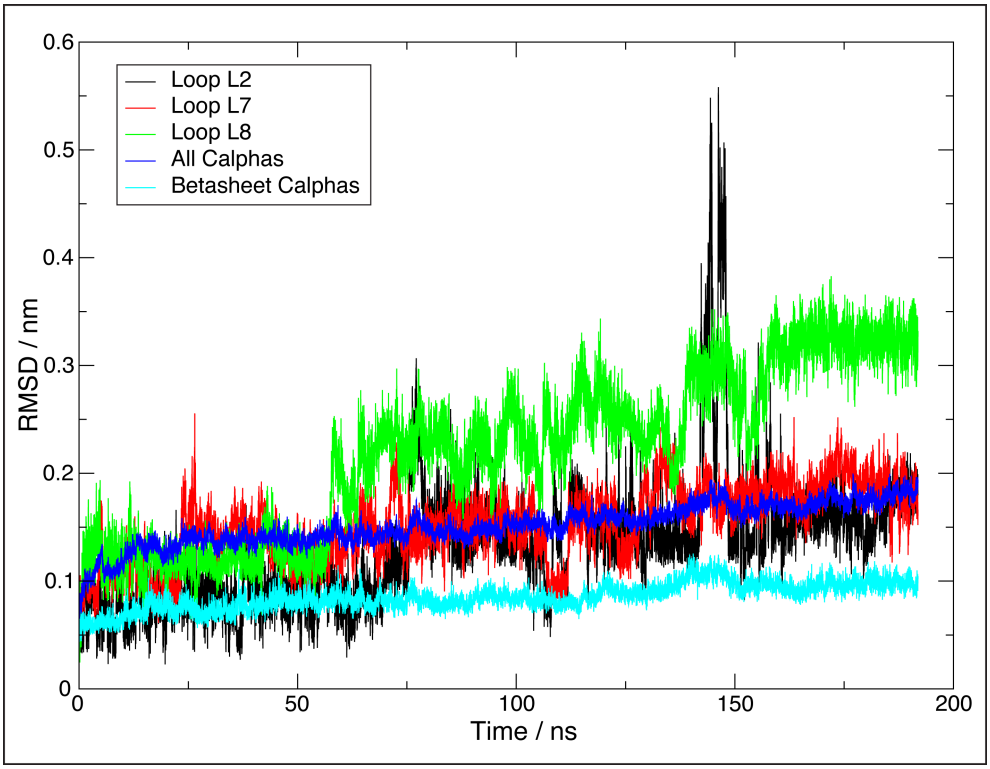

Figure S1: RMSD data generated from *SMD_WT_b*. The backbone Cα shown in cyan show a stable structure, with a plateau RMSD of ~ 0.1 nm. The entire protein is shown in blue, with an RMSD of ~ 1.5 nm.

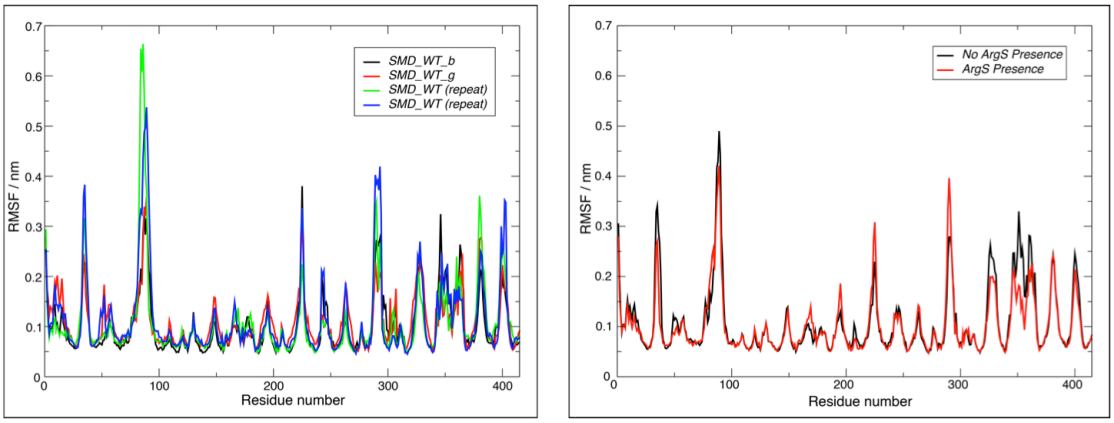

Figure S2: RMSF plots showing the conformational flexibility of OccD1. The left panel shows SMD data for each simulation incorporating successful permeation of ArgS through OccD1. The right panel shows data averaged over all equilibrium simulations.

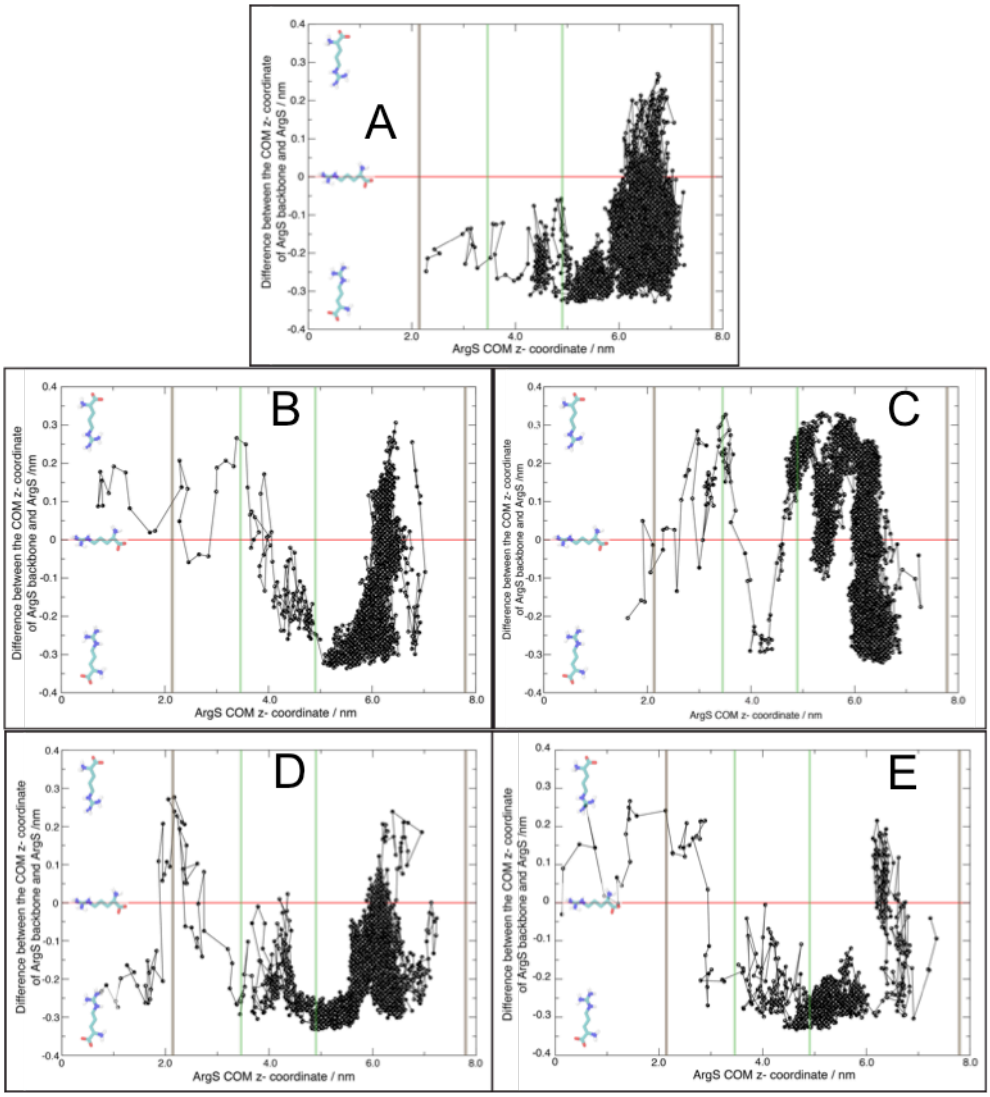

Figure S3: A – E: Graphs showing the orientation of the ArgS during SMD transport through OccD1. *Figures A, B and E* are from repeat simulations with only the pull force, 25 kJ mol^{-1}, acting perpendicular to the bilayer, *SMD_WT*.

Figure C & *E* are from *SMD_WT_b* and *SMD_WT_g* respectively. The red line indicates that ArgS is horizontal with respect to the plane of the bilayer. The green lines indicate a region in which the substrate is required to be in a specific orientation, namely for the backbone carboxylate group to be pointing towards the periplasmic mouth of the protein. The brown lines indicate the periplasmic, ~2.1 nm, and extracellular, ~7.8 nm, ends of the protein.

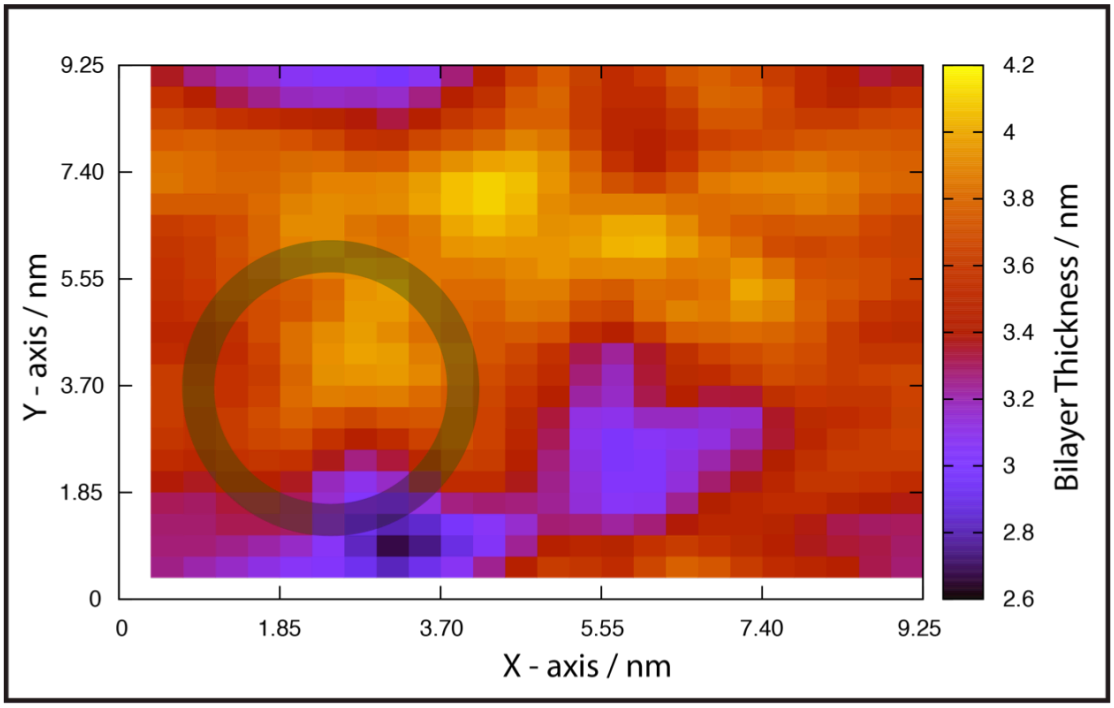

Figure S4: Representative plot showing the effect of OccD1 on membrane thickness (*Sim_WT_*A) site of pinching at ~ 2.7 x 1.0 nm caused by interactions at the extracellular end of strands S5 and S6, where L3 is connected to the beta-barrel.

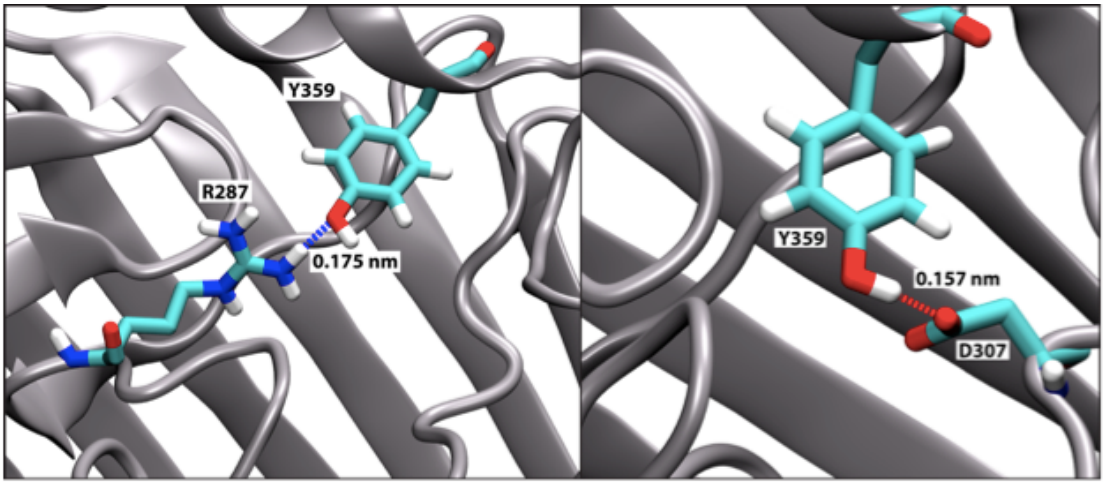

Figure S5: Typical hydrogen bonding between Y359 and R287/D307. Atoms are colored by atom, with nitrogen in blue, carbon in cyan, oxygen in red and hydrogen in white.