Supporting Information

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Movie S1. Gating and dynamics of water transport across AQP0. The movie represents \approx 100 ns of simulated time, with snapshots separated by 6 ps. It shows water diffusing through a single AQP0 monomer, taken from a simulation of tetrameric, lipid-embedded AQP0⁴. Water is shown in red and white, residues 128–179 of helices IV and V and loop D are in green, and the aquaporin half helices B and E with lumen-exposed carbonyl groups are in gray. The backbone carbonyl group of Val-160, located in helix V, is shown for reference. The remainder of the protein has been omitted for clarity. Side chains of key channel-lining residues are shown in stick representation: Arg-187, His-172, and Phe-48 of the ar/R region near the extracellular end of the channel; the centrally located NPA motifs; the highly conserved tyrosine residues Tyr-23 and Tyr-149; and His-66 near the extracellular end of the channel.

Movie S1 (MPG)



Movie 52. Complete permeation event across AQP0. The movie shows \approx 30 ns of simulated time, with snapshots separated by 12 ps. It shows water diffusing through a single AQP0 monomer, taken from a simulation of octameric, lipid-embedded AQP0⁸_J. A water molecule completely permeating the channel is indicated in yellow. See the Movie S1 legend for more details.

Movie S2 (MPG)

Other Supporting Information Files

SI Appendix (PDF)