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**Supplemental Information**

**H95 Is a pH-Dependent Gate in Aquaporin 4**

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## Supplementary data.

### Supplementary Figures: Legends

**Figure S1, related to the Molecular Dynamics section of the experimental procedures.** The typical simulation system is shown. The protein AQP4 is shown in cartoon representation. The DMPC lipids are shown as sticks. The water molecules are shown as transparent spheres. Water molecules inside the channel pore are shown as van der Waals spheres.

**Figure S2, Distance of the E41 from H95, related to figure 4.** The distance of the E41 residue from the H95 residue along the H95 gate mode. The distance decreases monotonously along close-open axis of the mode, reaching a minimum near the open state.

### Supplementary Table.

**Table S1 related to figure 2 and figure 5.** The calculated and observed permeabilities of AQP4 proteins in simulations and experiments respectively.

AQP4 protein	Simulation Permeability in $10^{-14}$ cm <sup>3</sup> /second
H95ND	$1.72 \pm 0.26$
H95+	$2.62 \pm 0.37$
H95A	$1.35 \pm 0.19$
H95+ (Open)	$3.02 \pm 0.55$
H95+ (Closed)	$1.78 \pm 0.25$

Supplementary Figures

Figure S1.

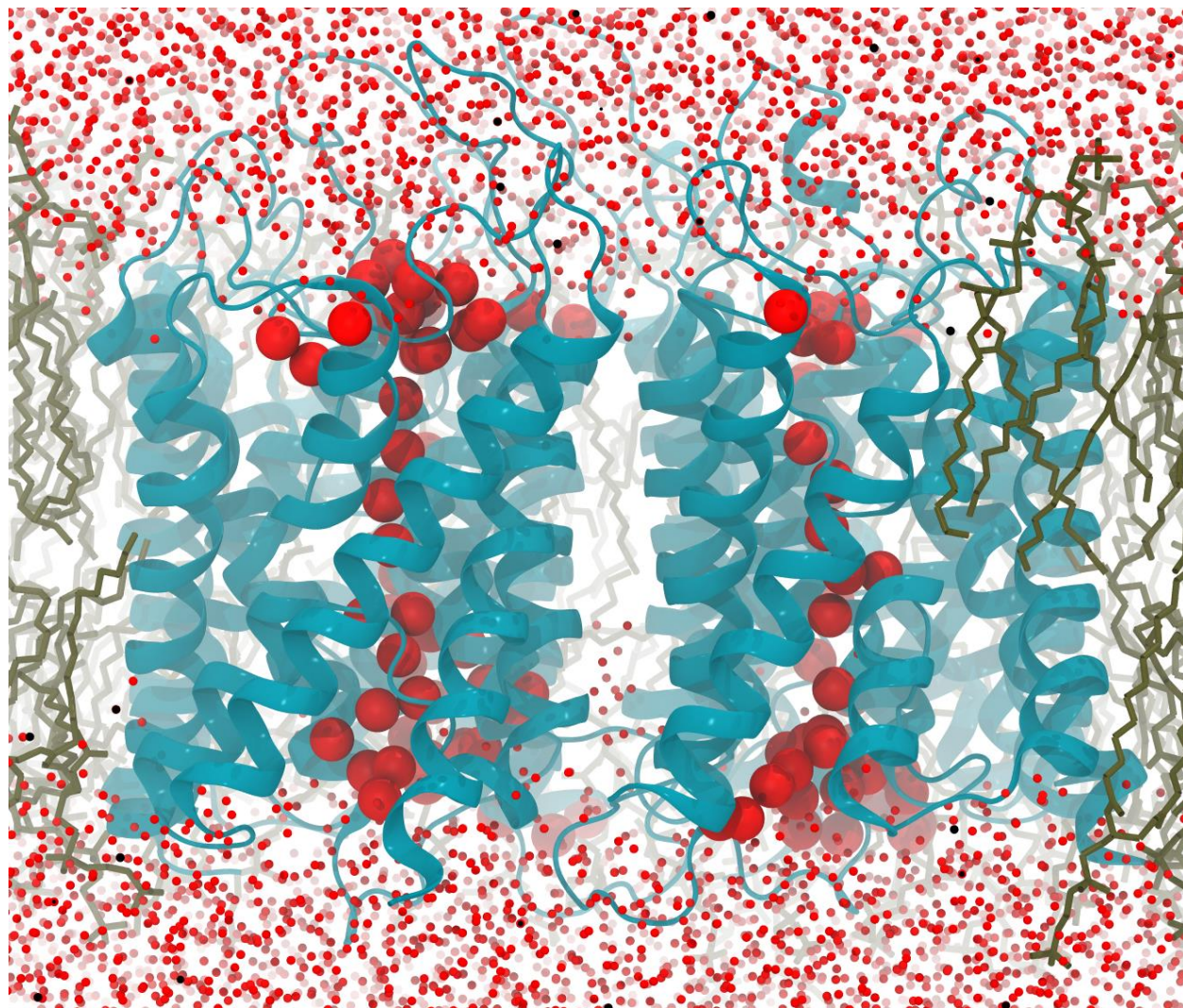


Figure S2.

