

Supplementary information, Figure S9

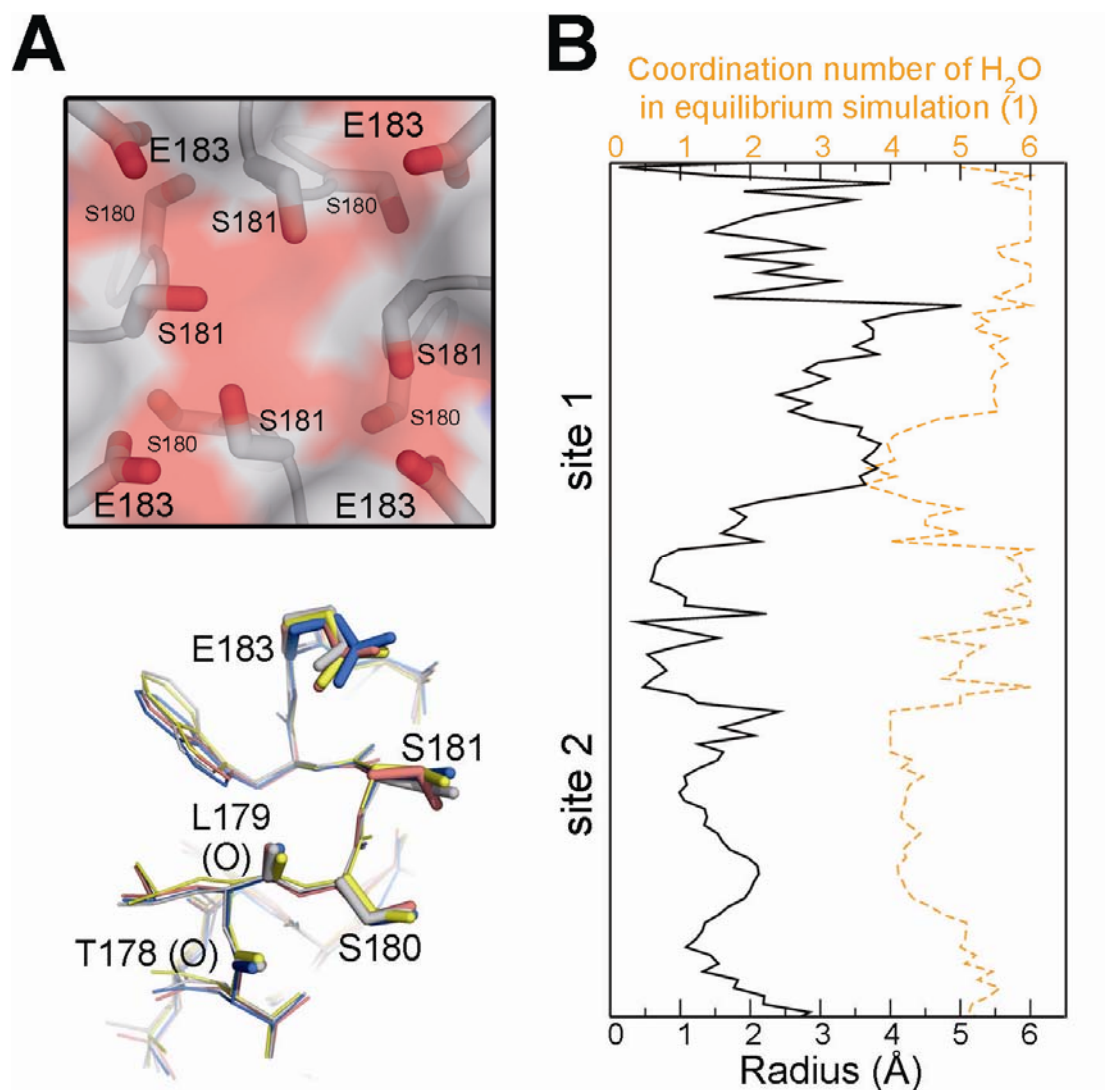


Figure S9 Na^+ penetrates Na_vRh away from the axial center of SF. **(A)** The SF of Na_vRh in the crystal structure (PDB code: 4DXW) is asymmetric. A semi-transparent surface illustration of periplasmic entrance to SF (*upper panel*) and superposition of SF from the four protomers (*lower panel*) indicate the structural heterogeneity among the SFs of Na_vRh subunits. Oxygen atoms are colored red. **(B)** The radial distribution (black solid line) of Na^+ anti-correlates with water coordination number (orange dashed line). The radii from the center in XY plane are shown as a function of the SF axis (Z). The data are derived from simulation 1 (*right panel*).