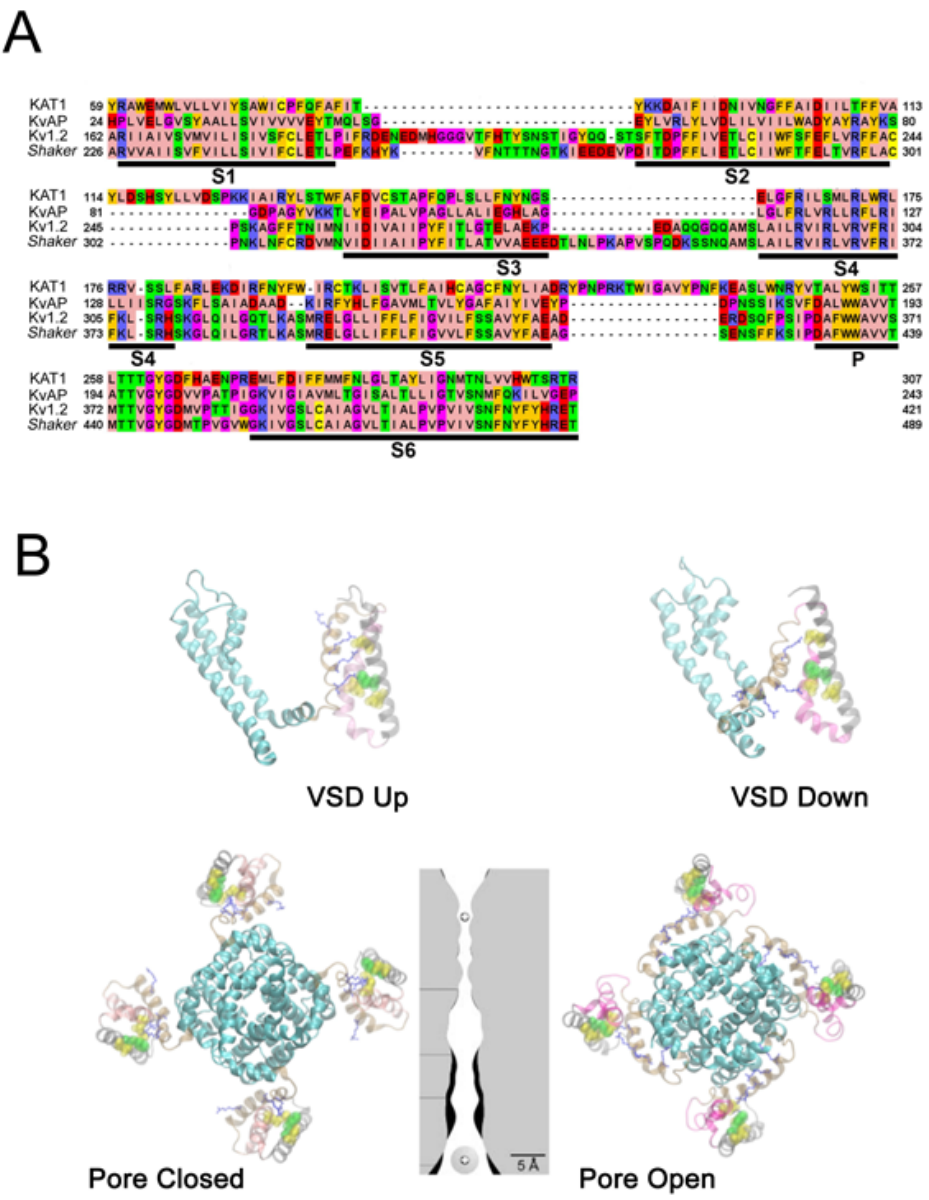
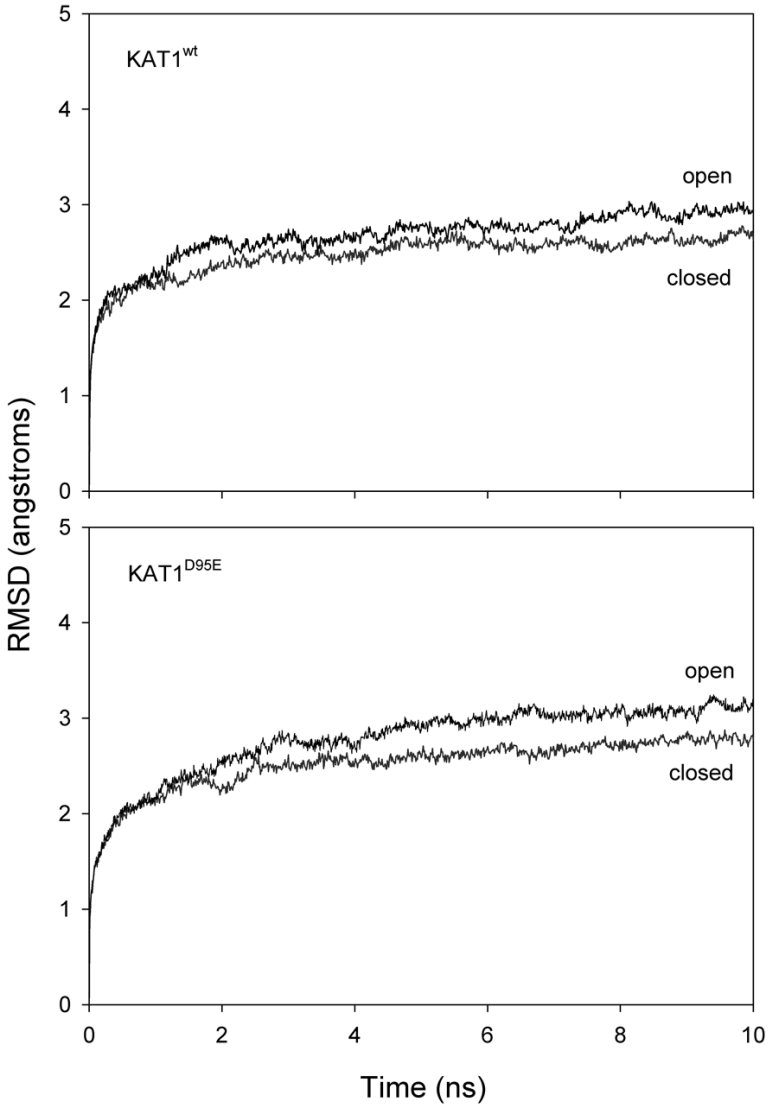


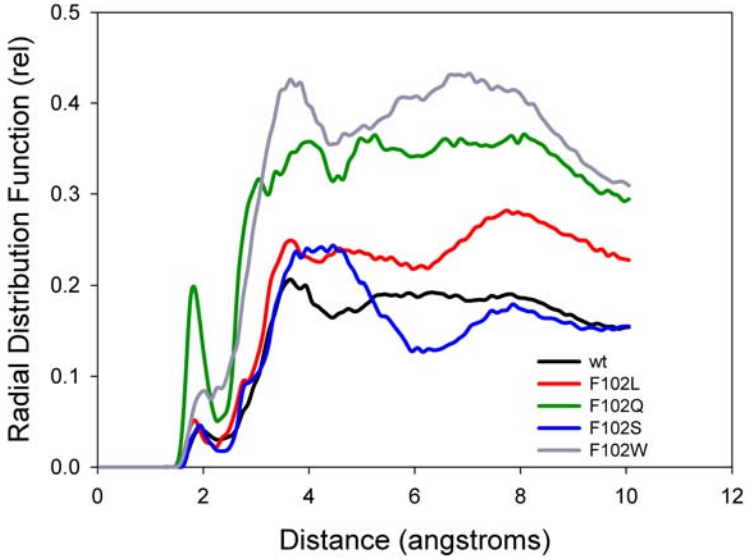
Supplemental Fig. S1. KAT1 model template and resolved conformations in the 'up' (closed) and 'down' (open) states of the channel VSD and its pore.

(A) Alignment of the transmembrane regions of KAT1 with *Aeropyrum pernix* KvAP channel (PDB 1ORQ), the mammalian Kv1.2 channel (PDB 2A79) and the *Shaker* K^+ channel (PDB 3LUT) used to map interacting residues identified by Grabe, et al. (2007). Sequence alignment and figure modified from Pathak, et al. (2007).

(B) KAT1 conformations in the 'up' (closed, *left*) and 'down' (open, *right*) states. Images above are projections within the plane of the membrane and correspond with the projections in Fig. 1B and include the S5 and S6 α-helices that line the pore (in aquamarine). Projections below show all four subunits assembled to form the pore as viewed from below the membrane. The grey cross section (*center*) illustrates the permeation pathway through the membrane as viewed from the side in the closed (black) and open (grey) states. Potassium ions (+, black spheres) in the dehydrated form within the selectivity filter (above) and surrounded by a hydration shell (grey sphere, below) in the internal mouth of the pore. Scale, 5 Å. Figure adapted from Gajdanowicz, et al. (2009).



Supplemental Fig. S2. Equilibration of molecular dynamic simulations for $KAT1^{wt}$ (above) and the $KAT1^{D95E}$ mutant (below). Root mean squared deviation (RMSD) calculated using the α-C atoms to confirm equilibration over a 10 ns period.



Supplemental Fig. S3. Radial Distribution Function (RDF) for water around KAT1 residue at position 102 as a function of distance from this residue. An RDF value of 1.0 corresponds to a distribution of water in free solution. Data derived from molecular dynamic simulations as described in the text.

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