SUPPORTING MATERIAL

Molecular Mechanism of Depolarization-Dependent Inactivation in W366F Mutant of Kv1.2

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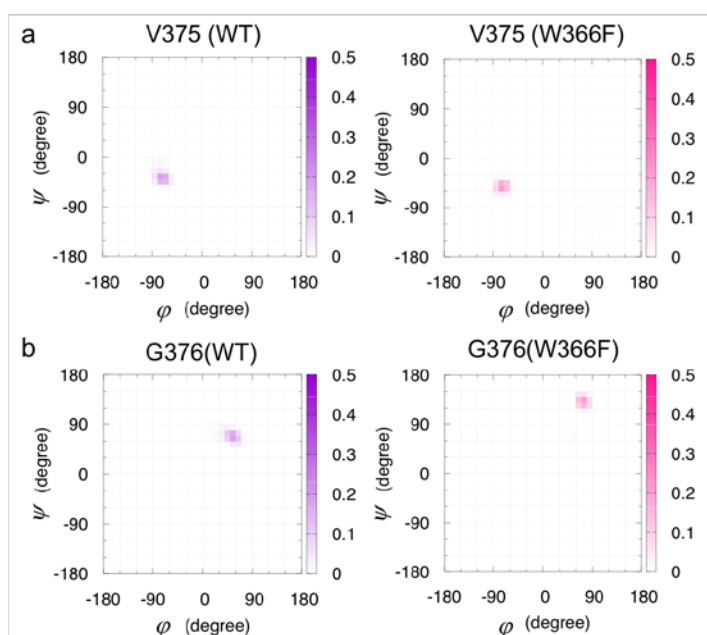
Figure S1

Figure S1. Probability distributions of dihedral angles (φ and ψ) of V375 (a) and G376 (b). The left and right panels show the distribution of WT and W366F, respectively.
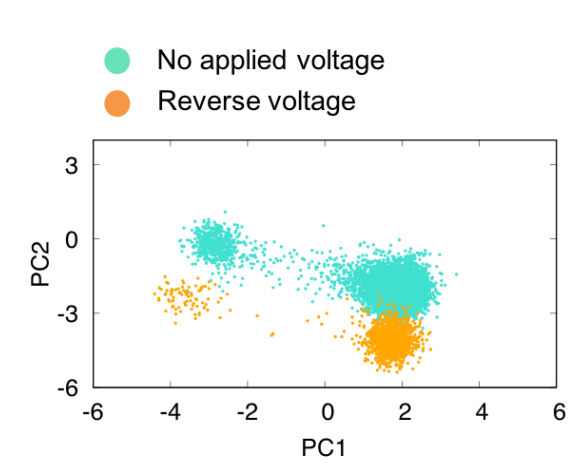
Figure S2

Figure S2. The projection of trajectories with no-applied voltage and reverse voltage onto the first and second principal component axis (PC1 and PC2 values) obtained from PCA of SF conformations of WT and W366F mutant.
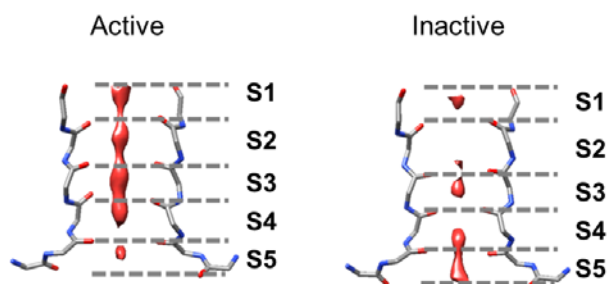
Figure S3

Figure S3. Comparison of the distributions of K^+ ions of W366F mutant with PC1 values of larger than 2.5 (left, active) and less than -2.5 (right, inactive, same as Fig. 3d). These distributions are the average of 10 snapshots. The main-chain atoms of SF (T374–G378) are shown in stick representation. The regions represented as red surface are those with high probability distributions of K^+ ions ($g(r) > 15.5$). Only chain 1 and chain 2 are shown. Five peaks were observed around S1–S5 in the active state.