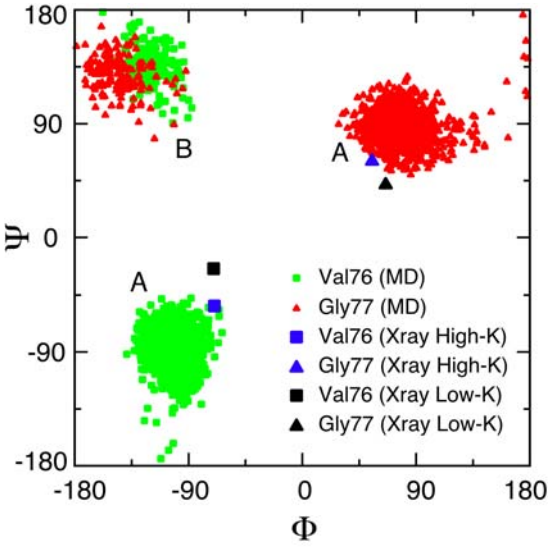
Supplemental Data

Coordinate File in PDB Format

The file kcsa_inac.pdb contains the atomic coordinates of the non-conducting conformational state of broken symmetry that is shown in Fig. 1d in the article. Ions are present in the binding site S_1 and S_3; there is an additional ion in the cavity. Coordinates will be deposited in the PDB.

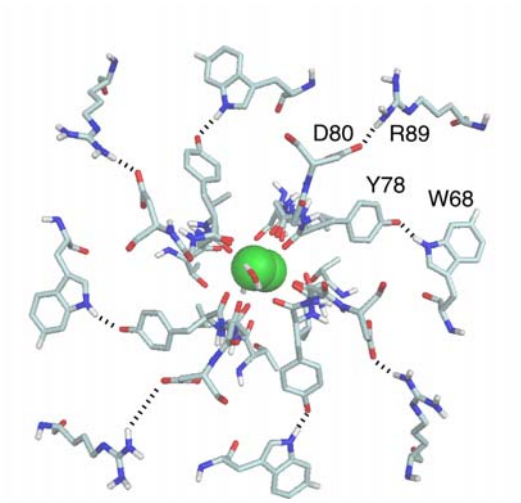
Quick Time Animation

Illustration of the complete transition from the symmetric ion-conducting conformation to the non-conducting conformation of broken symmetry. A targeted MD trajectory was generated using a RMSD energy restraint applied to all non-hydrogen atoms of residues 72 to 77 (Young et al., 2001, Yang et al., 2002). The full KcsA system (channel, solvent and lipid bilayer) was simulated for 10 ps with a force constant of 500 kcal/mol/Å^2.



Supplemental Figure S1. Backbone Dihedral Angles in the Selectivity Filter

Φ-Ψ map of the Val76-Gly77 amide plane. The MD data were extracted from a simulation of 1.5 ns in which a backbone transition occurred (Bernèche and Roux, 2000). The conformations of the amide plane corresponding to the conducting and non-conducting states are respectively identified by the letter A and B. The conformation of these residues as observed in the X-ray structure determined in presence of 2 mM KCl and 148 mM NaCl (pdb id 1K4D) (Zhou et al., 2001) is also plotted. The structure corresponds only to a slight deviation from the high K conducting structure (pdb id 1K4C) (Zhou et al., 2001).



Supplemental Figure S2. Hydrogen Bonding Network Surrounding the Selectivity Filter

View from the extra-cellular side showing the inter-subunit interactions involving residues Tyr78-Trp68 and Asp80-Arg89.

References

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