Carvacho et al, http://www.jgp.org/cgi/doi/10.1085/jgp.200709862

PDB of the Molecular Model for the BK Pore

The model for the human BK pore was built using the crystallographic data for KcsA channel (PDB:1K4C) and MthK channel (PDB:1LNQ) as structural references. Inner and outer helices of KcsA were displaced until the backbone atoms superimposed with the equivalent residues of MthK. The result is an open KcsA structure. A homology model of the BK pore was obtained using the program ICM (Abagyan, R., M. Trotov, and D. Kuznetsov. 1994. *J. Comp. Chem.* 15:488–506) using the open KcsA x-ray structure as template. The extracellular loop of BK is sampling using ICM program. Two K^+ ions were associated to the model in positions S1 and S3 of the selectivity filter and a water molecule was placed in site S2. All molecular dynamic simulation was performed using the NAMD program (Phillips, J.C., R. Braun, W. Wang, J. Gumbart, E. Tajkhorshid, E. Villa, C. Chipot, R. D. Skeel, L. Kale, and K. Schulten. 2005. *J. Compu. Chem.* 26:1781–1802.).