Supporting Information

Molecular Dynamics Simulations of KirBac1.1 Mutants Reveal Global Gating Changes of Kir Channels

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Figure S1

Overview of the KirBac1.1 channel (3 subunits are shown) embedded in a POPC lipid bilayer (grey lines). The mutated G143E residues are shown in orange, the arginine 153 positions are shown in blue. 2 K^+ ions in the filter are shown as pale blue spheres.

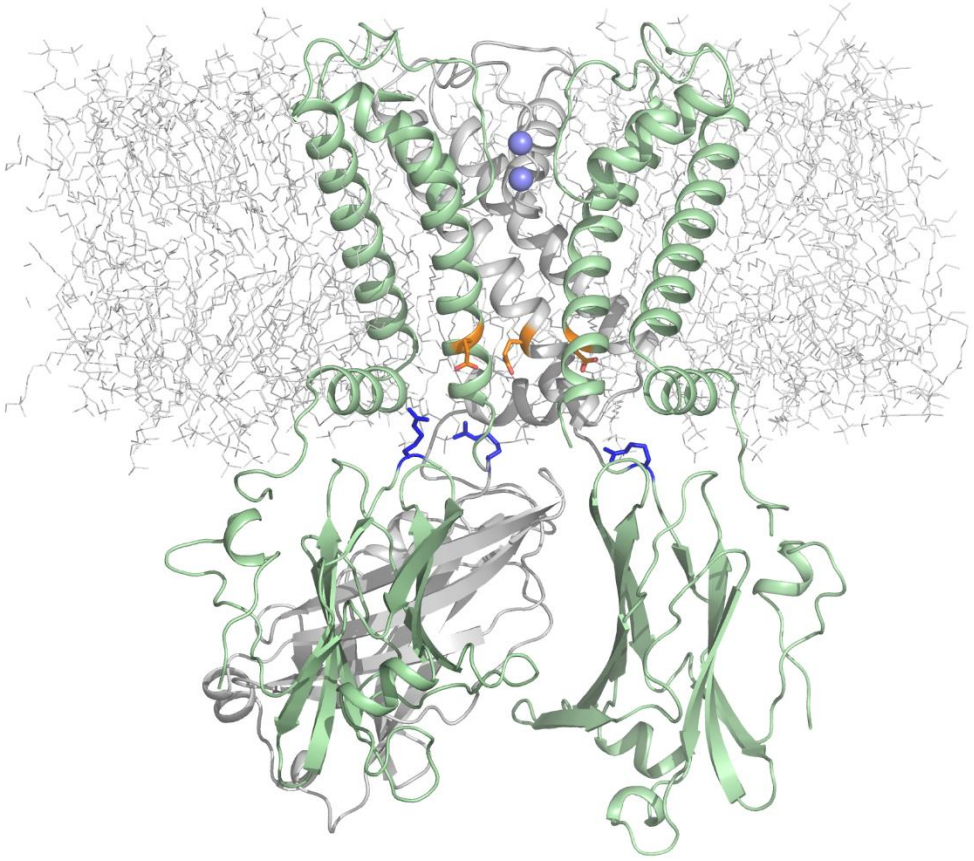
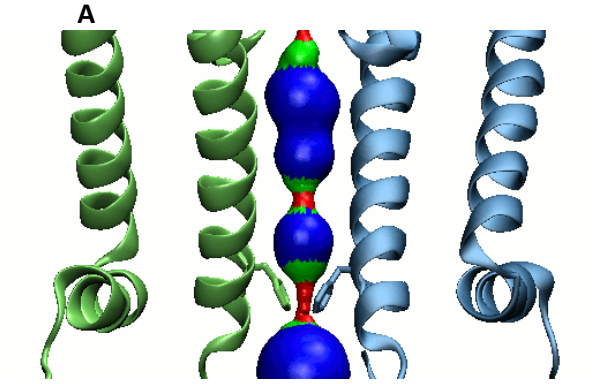
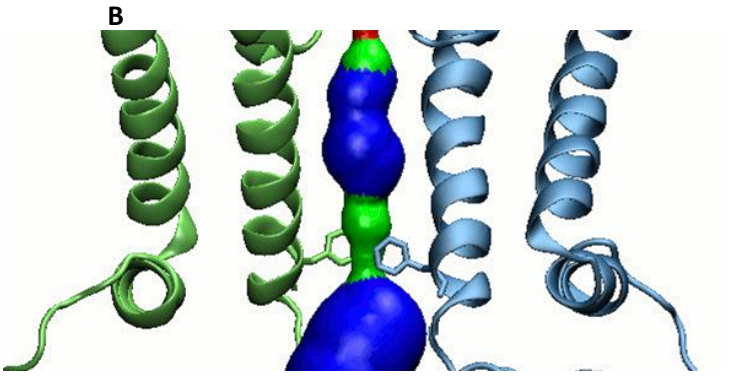


Figure S2

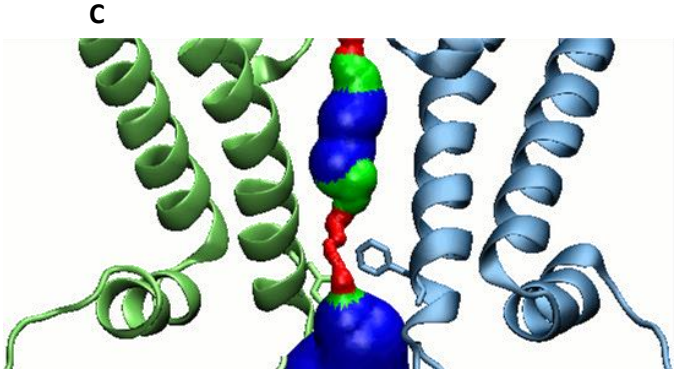
Hole analysis of Kirbac1.1 WT and mutant channels revealing conformational changes at the HBC gate.



Kirbac1.1 WT



Kirbac1.1 G143Ed (200ns)



Kirbac1.1 G143Ep (200ns)

References

O. S. Smart, J. G. Neduvelil, X. Wang , B. A. Wallace, M. S. Sansom, HOLE: A program for the analysis of the pore dimensions of ion channel structural models. J. Mol. Graph. 14, 354–360, 376 (1996).