Supplemental Information

Exploring the Dynamics of the TWIK-1 Channel

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SUPPLEMENTARY INFORMATION

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Figure S1. Root mean square deviation (RMSD) of the backbone of the transmembrane helices of TWIK-1 in simulations: (A) HSE, (B) HSEP, (C) HSD, (D) HSDP, (E) HSP and (F) HSPP.
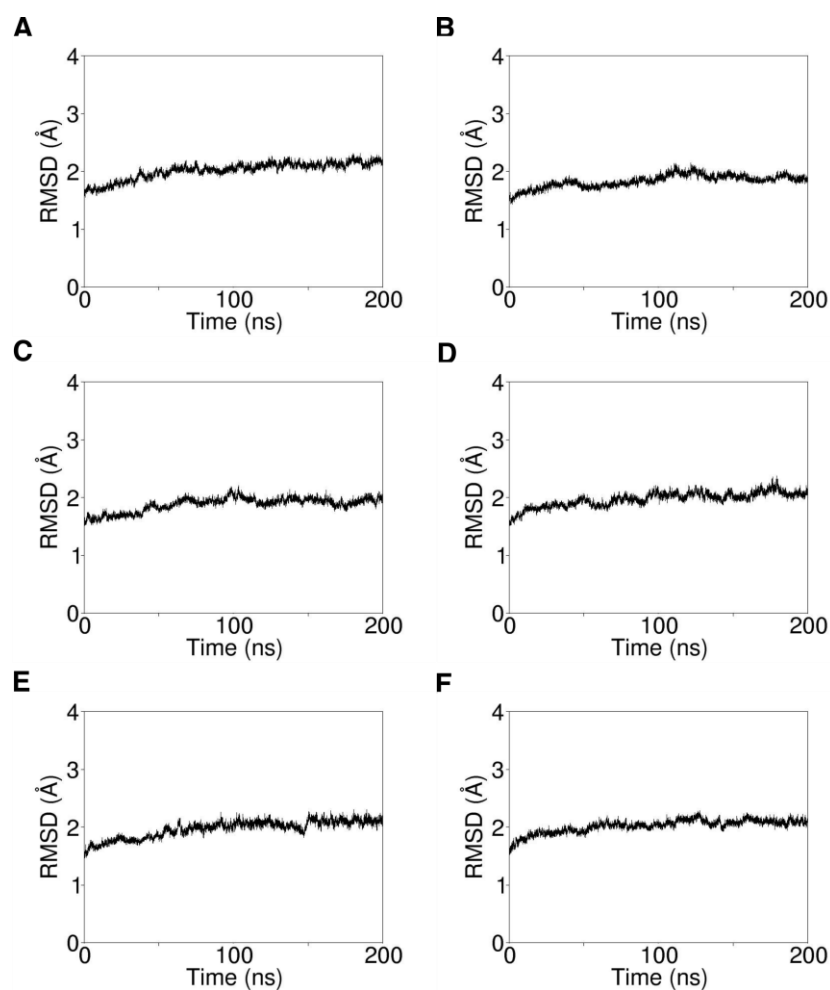
Figure S2. Root mean square deviation (RMSD) of the extracellular cap corresponding to residues S80 to D103 in simulations: (A) HSE, (B) HSEP, (C) HSD, (D) HSDP, (E) HSP and (F) HSPP.
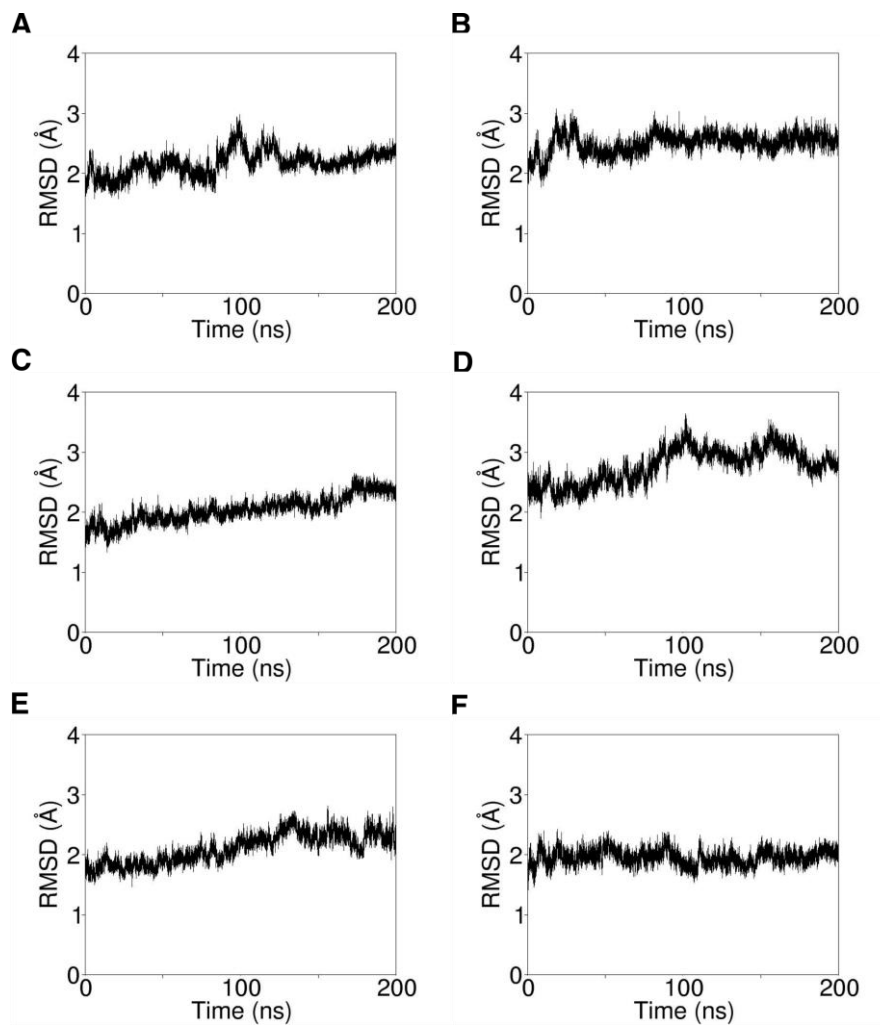
Figure S3. Representative snapshots of each ion configuration throughout simulations (A) HSE, (B) HSEP, (C) HSD, (D) HSDP, (E) HSP and (F) HSPP. The selectivity filter residues T117 to G121 and T225 to G229 are displayed in licorice representation, with Van der Waals spheres representing ions and water molecules, with oxygen, nitrogen, carbon, sodium and potassium atoms shown in red, blue, cyan, yellow and orange respectively.