

Description of Additional Supplementary Files

File name: Supplementary Movie 1

Description: Representation of the segmented cryoEM map of Rnf and its corresponding model.

File name: Supplementary Movie 2

Description: Sodium binding from the intracellular and extracellular sides.

File name: Supplementary Movie 3

Description: Inward/outward transition from MD simulations.

File name: Supplementary Movie 4

Description: Dominant normal modes from MD simulations of the NADH-reduced structures.

File name: Supplementary Movie 5

Description: Dominant normal modes from MD simulations of the Fd-reduced structures.

File name: Supplementary Movie 6

Description: Inward/outward pathway explored by SMD simulations.

File name: Supplementary Movie 7

Description: Free energy simulations of the inward/outward transition coupled to Na⁺ transport.