Supplementary Figures to the manuscript "Common patterns of hydrolysis initiation in P-loop fold nucleoside triphosphatases - united in diversity" by

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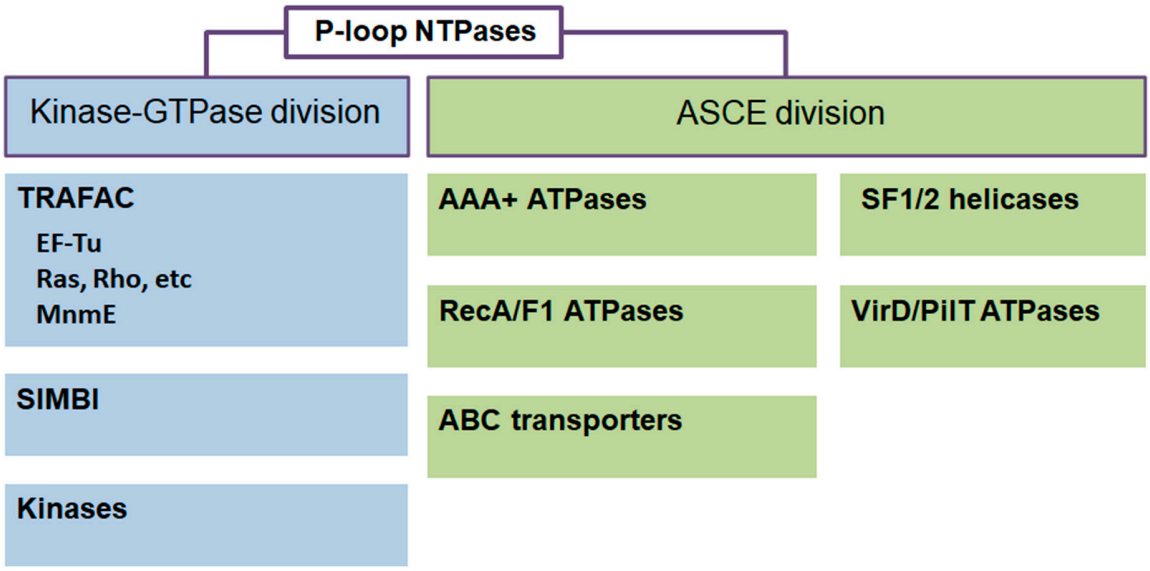


Figure S1. Major classes of P-loop fold NTPases according to [1-5].

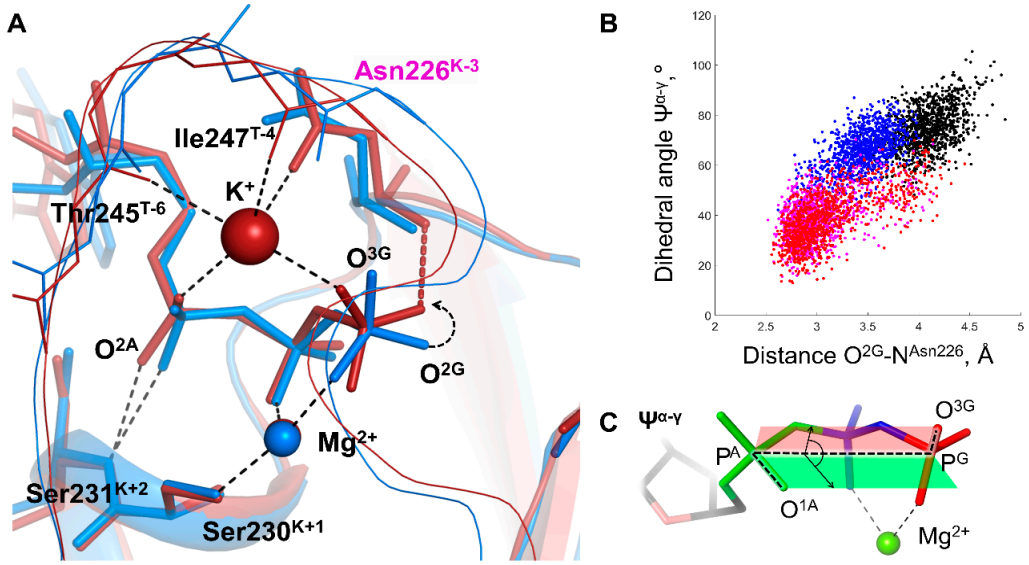


Figure S2. Molecular dynamics of the MnmE GTPase (The figure is taken from [6] and modified).

A. Superposition of the GTP-binding sites of the inactive, monomeric G-domain of MnmE (blue) and active, K^+-bound G-domain in a dimer (red); the representative structures were sampled from 100 ns simulations as described in [6]. The protein backbones are shown as cartoons; GTP and surrounding amino acid residues are shown as sticks; Mg^{2+} and K^+ ions are shown as spheres. Black dashed lines indicate hydrogen bonds and coordination bonds for cations that are present in both structures; the red dashed line indicates the H-bond between **NH**$^{K-3}$ and O^{2G} that is present only in the K^+-containing dimer.

B. Conformational space of GTP in different states of MnmE GTPase. Scatter plot of the $\Psi^{\alpha-\gamma}$ dihedral angle (Y-axis) against the distance between the O^{2G} atom and **NH** of Asn226^{K-3} (X-axis) as sampled from the MD simulations of three systems: (1) active dimer of G-domains with K^+ ions bound (red and magenta for individual monomers); (2) monomeric G-domain of MnmE with the K^+ ion replaced by a water molecule, blue; and (3) inactive monomer G-domain of MnmE without a full-fledged K-loop, black.

C. The dihedral angle $\Psi^{\alpha-\gamma}$ in the phosphate chain of GTP as measured for the plot on panel B.

References

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