Rotation triggers nucleotide-independent conformational transition of the empty β subunit of F_1-ATPase

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SUPPORTING INFORMATION

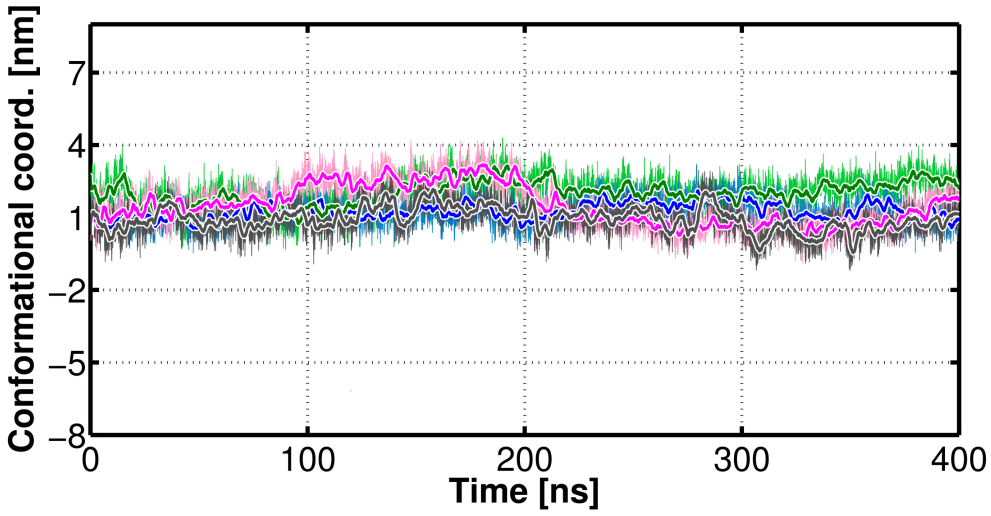

Figure S1: Conformational dynamics of the empty β subunit during four additional simulations in which the γ-shaft was stopped at $+80°$, presumably corresponding to the so-called ATP-dependent dwell of the motor.

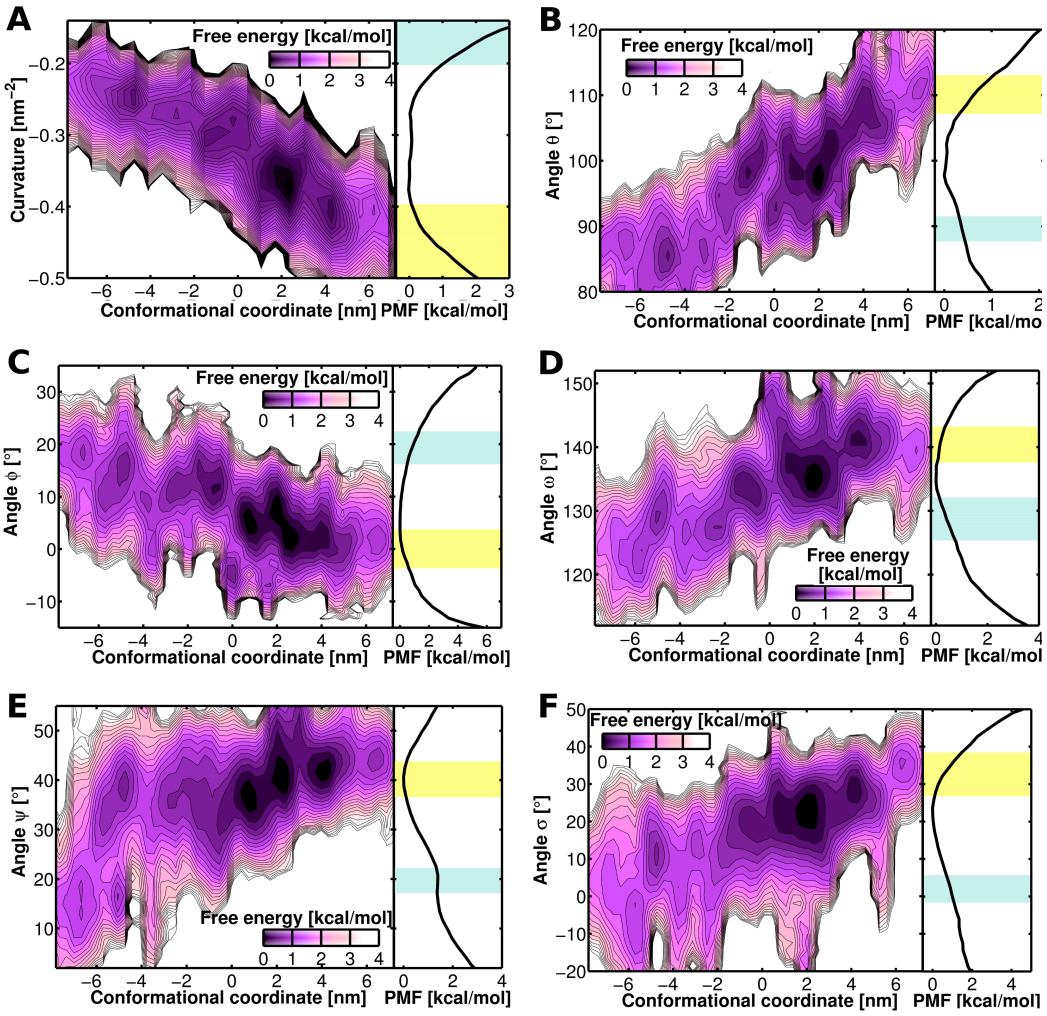

Figure S2: Two-dimensional free energy surfaces describing the conformational equilibrium of the isolated nucleotide-free β subunit. Conformational coordinate, bending angle θ and the curvature of the central domain β-sheet are defined as in the main text; ϕ is the C-terminal domain twist angle with respect to the longest principal axis of the entire β subunit; ω is the bending angle defined as in Yagi et al. (JACS (2004) 126, 16632–16638); ψ is the H1/H2 bend angle. The surfaces were obtained by reweighting the biased two-dimensional histograms from the umbrella sampling trajectories by a factor of $\exp\left[\left(V_i(\xi) - F_i\right)/k_BT\right]$, where $V_i(\xi)$ and F_i denote the biasing potential and the WHAM free energy constant, respectively, corresponding to the i-th US window.

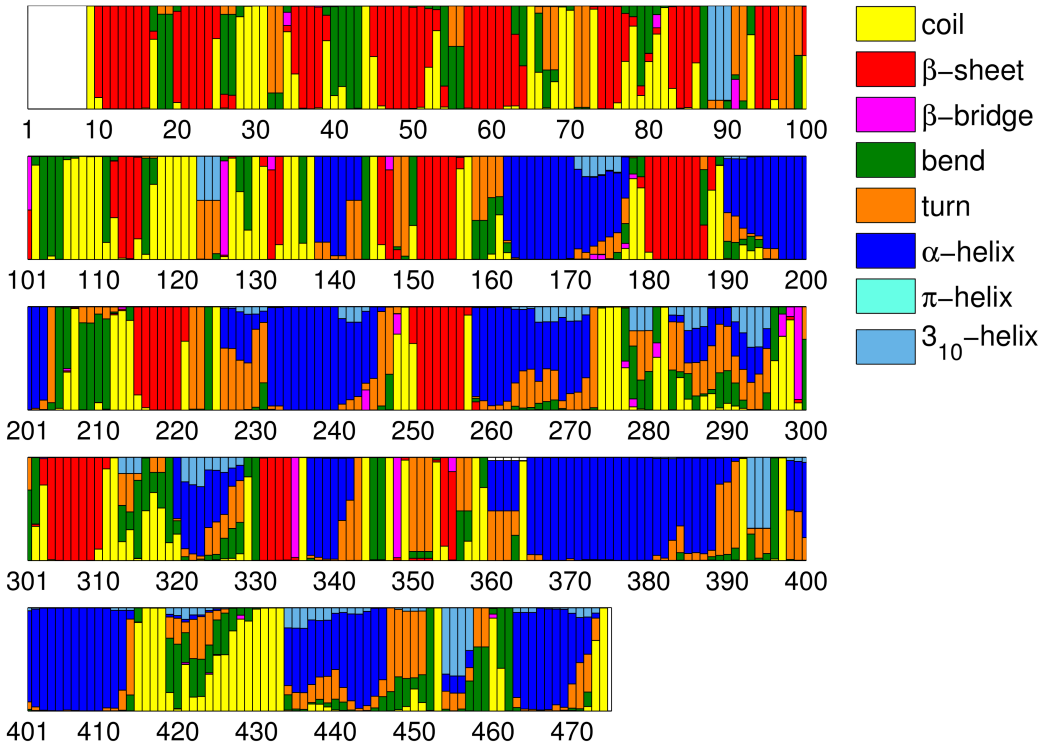

Figure S3: Equilibrium populations of different secondary structures along the β chain for the isolated nucleotide-free subunit.

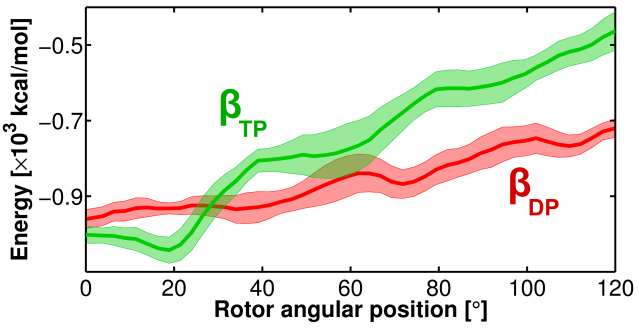

Figure S4: The interaction energy between the γ subunit and the C-terminal domains of β_{TP} and β_{DP} as a function of the angular position of the γ-shaft.

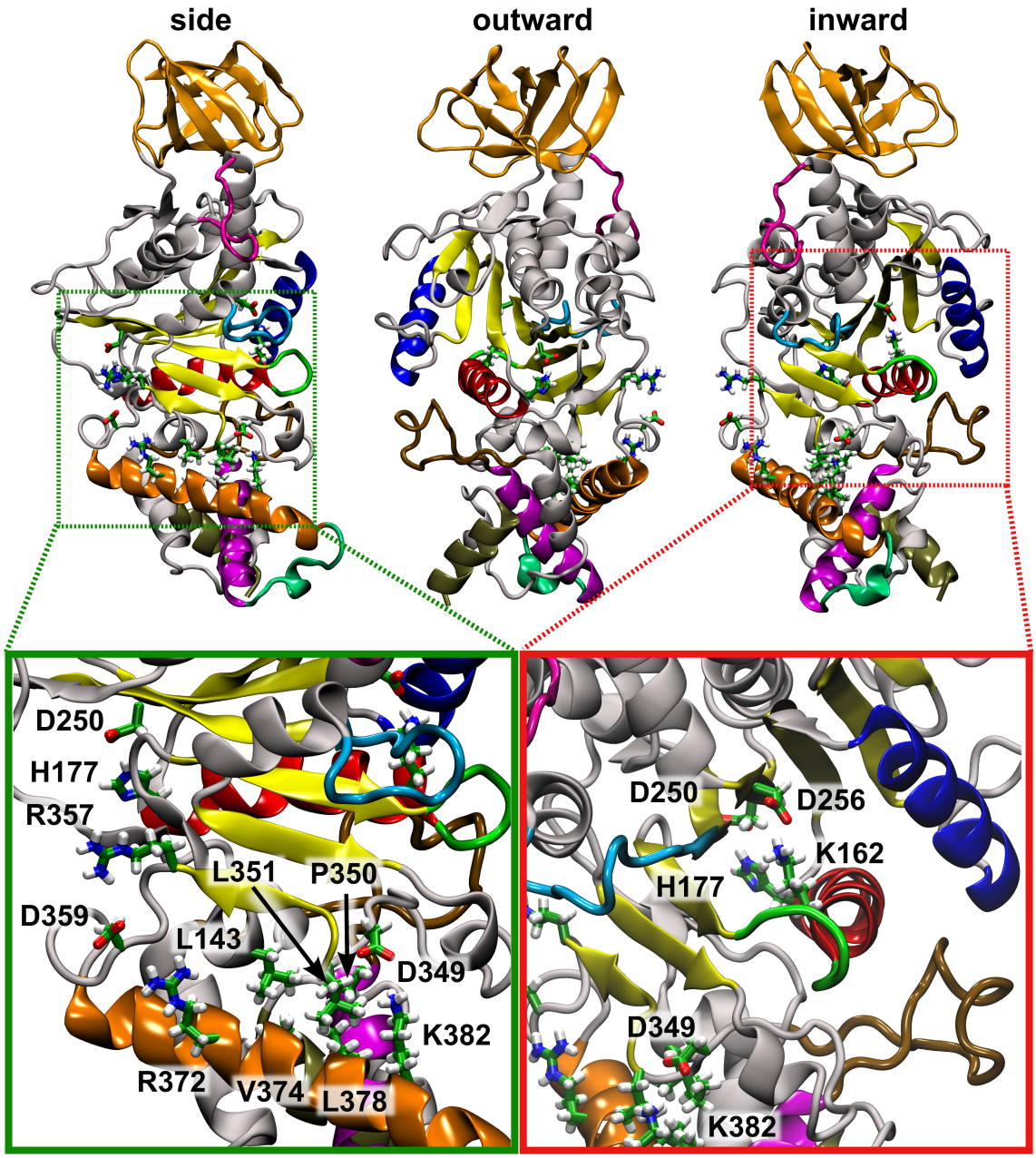

Figure S5: Residues participating in the propagation of the γ-induced strain from the C-terminal domain to the active site of the β_{E} subunit in the putative catalytic dwell of F_1-ATPase (0°). Top panel shows three different views of the β_{E} subunit: the interface with α_{TP}(side), the outward surface exposed to the aqueous environment (outward) and the inward surface facing the γ subunit (inward). Color-coding the structural elements of β_{E} is consistent with Fig. 1.

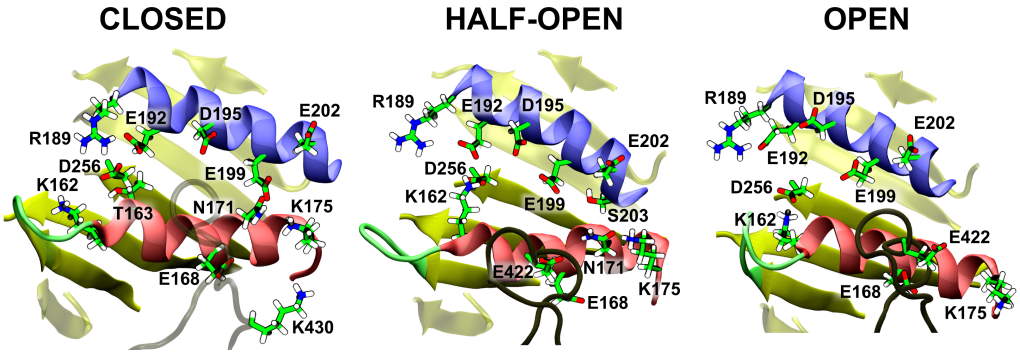

Figure S6: Three conformations of the nucleotide-binding site of the empty β subunit. Helices H1 and H2 are shown in red and blue, respectively, and P-loop is shown in green.

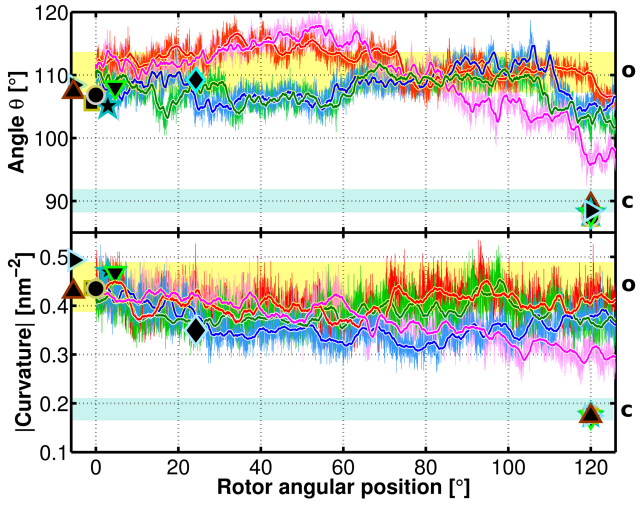

Figure S7: Conformational dynamics of the β_E mutant (all acidic residues in H2 replaced by Ala) during four independent 300-ns flexible-rotation cycles of F_1. the bend angle θ (middle) and the curvature of the central domain β-sheet (bottom) as a function of the γ-shaft angular position. Yellow and blue shaded areas show the extent of fluctuations of the analyzed parameters at the initial resting state (0°) for the open and closed conformation, respectively. The panel on the right show changes of the further evolution of the parameters during the additional 300 ns run with the γ-shaft kept at its final position (120°). The markers show values of the analyzed parameters for the open (0°), half-closed (24°) and closed (120°) conformations taken from several F_1 x-ray structures (♦ - 1H8E, ★ - 1BMF, ▼ - 2JIZ, ■ - 2WSS, ● - 1E79, ► - 2HLD, ▲ - 2V7Q)