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Supplemental Information

Microtubule Simulations Provide Insight into the Molecular Mechanism Underlying Dynamic Instability

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Supporting Figure S1:

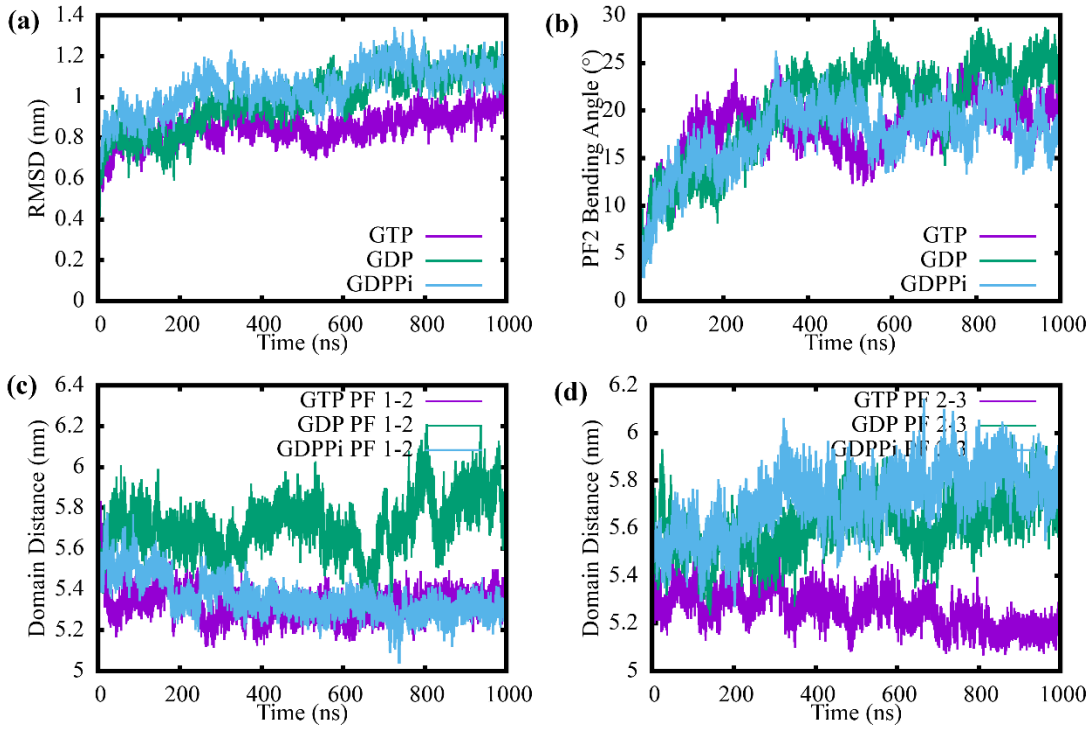

Figure S1: Convergence analysis of 1 μs 3-PF MT patch simulations in different nucleotide states. Shown are the time evolution of (a) Cα RMSD value, (b) The bending angle of the middle PF in the MT patch, (c) The COM distance between β tubulin domains at the top of PF 1 and 2, (d) The COM distance between β tubulin domains at the top of PF 2 and 3.

Supporting Figure S2:

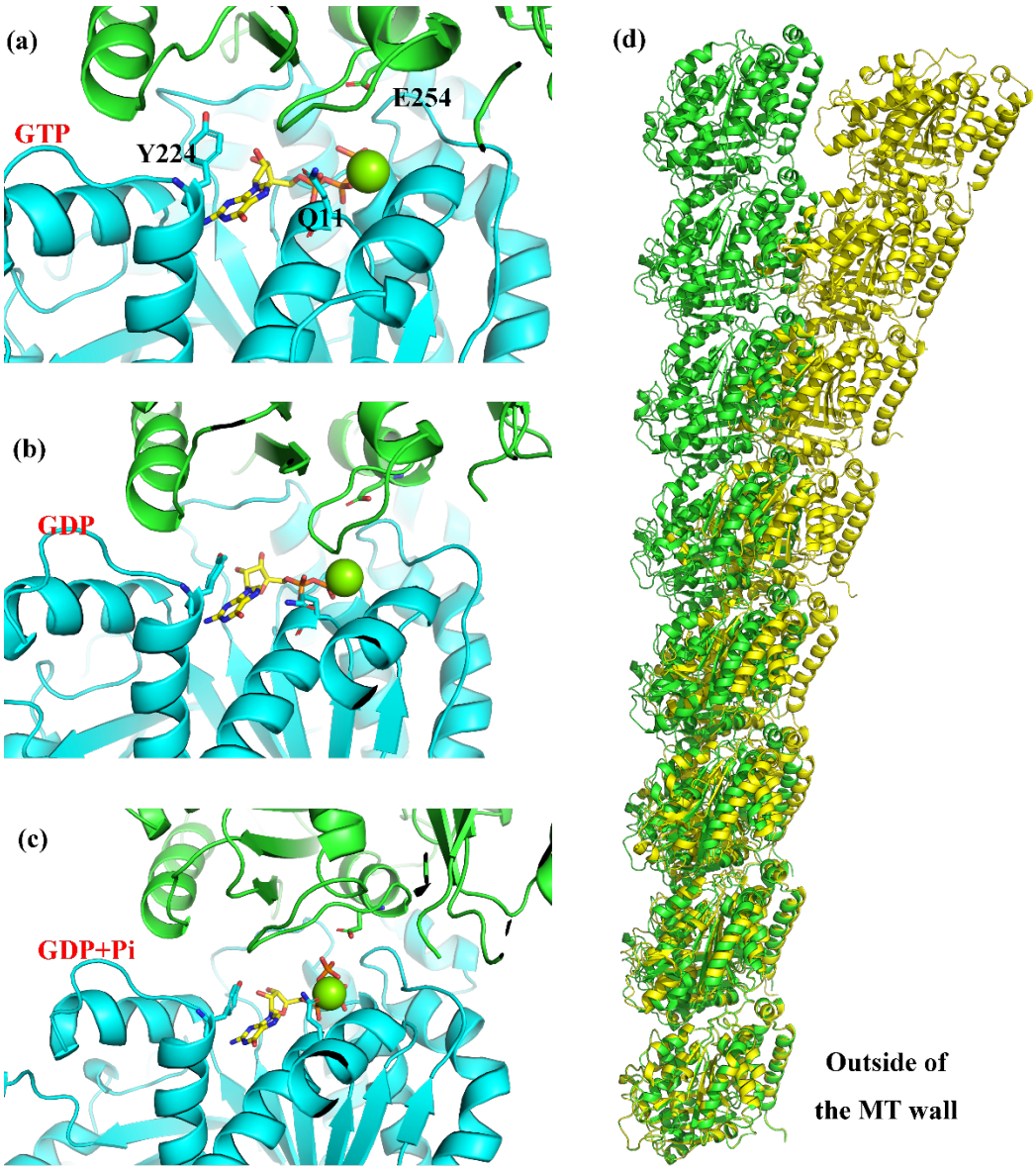

Figure S2: Snapshot view of the last frame simulation structure. (a-c) The exchangeable nucleotide binding site in the top of the middle PF, with the binding of (a) GTP, (b) GDP, (c) GDP+Pi. The β tubulin is colored in cyan and α tubulin domain is colored in green. The bound nucleotide and residue E254 (α), Q11(β) and Y224 (β) is represented by sticks. (d) The outward bending of middle PF in GTP state simulation. The cryo-EM structure with straight PF is colored in green, while the structure in simulation is colored in yellow.

Supporting Figure S3:

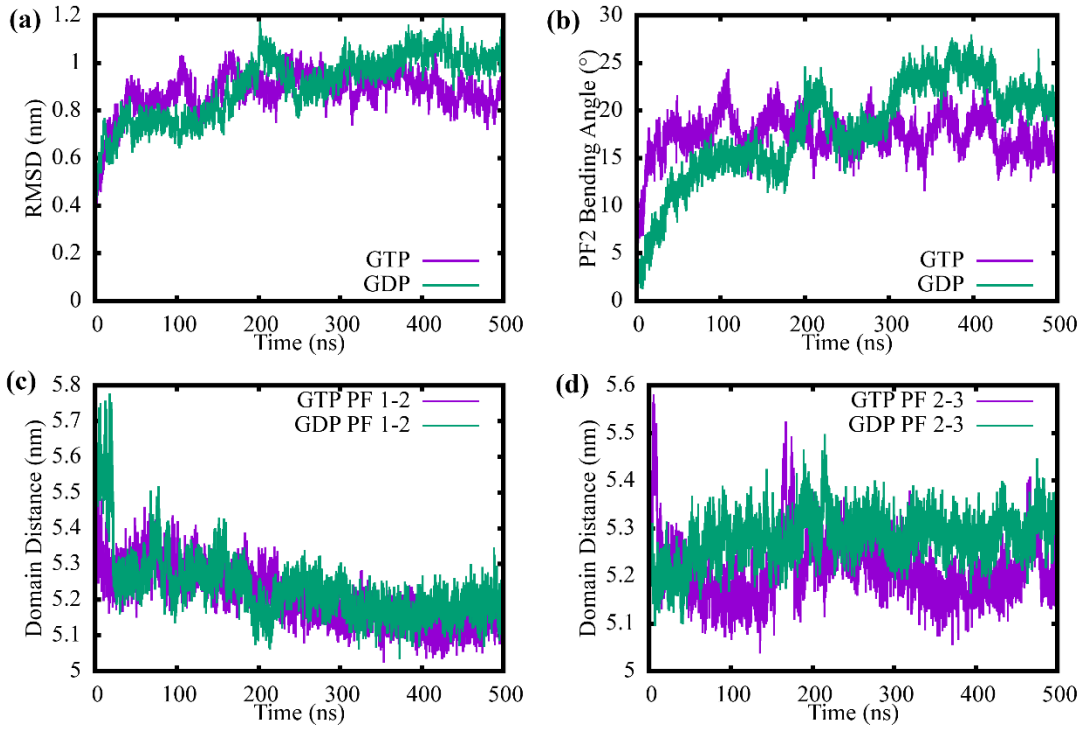

Figure S3: Convergence analysis of 500 ns 3-PF MT patch simulations in different nucleotide states starting from alternative structures with PDB IDs: 3JAT (GTP) and 3JAS (GDP). Shown are the time evolution of (a) Cα RMSD value, (b) The bending angle of the middle PF in the MT patch, (c) The COM distance between β tubulin domains at the top of PF 1 and 2, (d) The COM distance between β tubulin domains at the top of PF 2 and 3.

Supporting Figure S4:

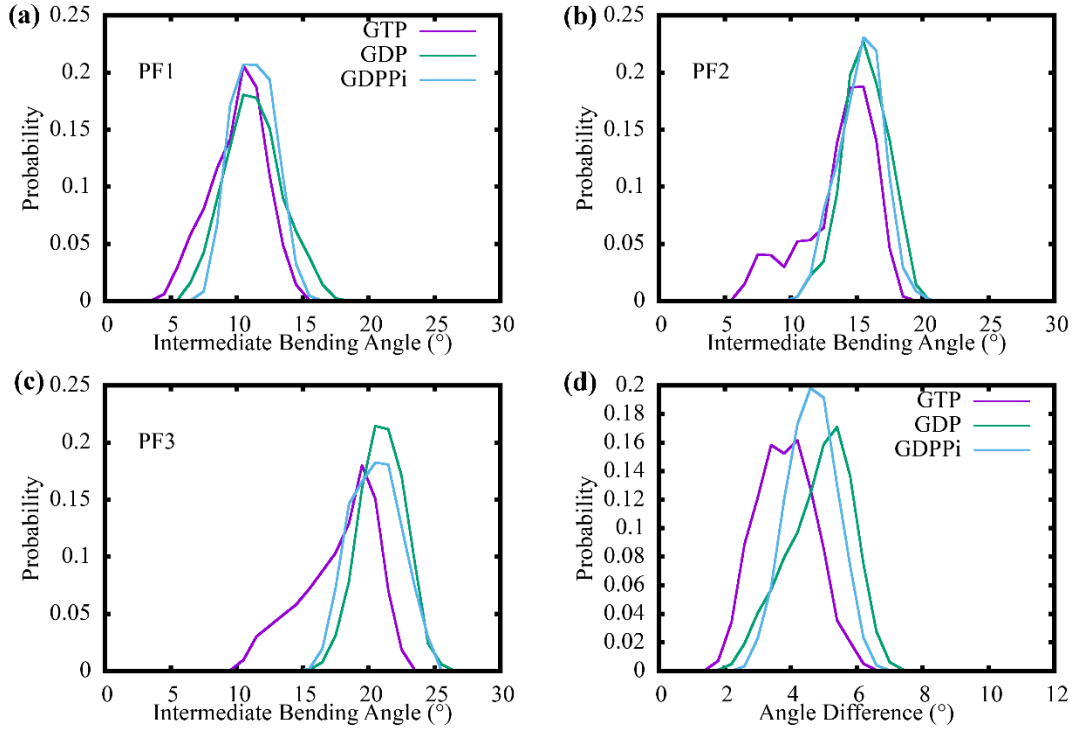

Figure S4: The bending angle distributions of intermediate tubulin dimers. Shown here are the results from third tubulin dimer numbering from the PF bottom. (a-c) Comparison of bending angle distributions of the MT PFs in the GTP (purple), GDP (green), and GDP+Pi (cyan) states. (d) The probability distributions of bending angle differences between neighboring PFs in three different nucleotide states.

Supporting Figure S5:

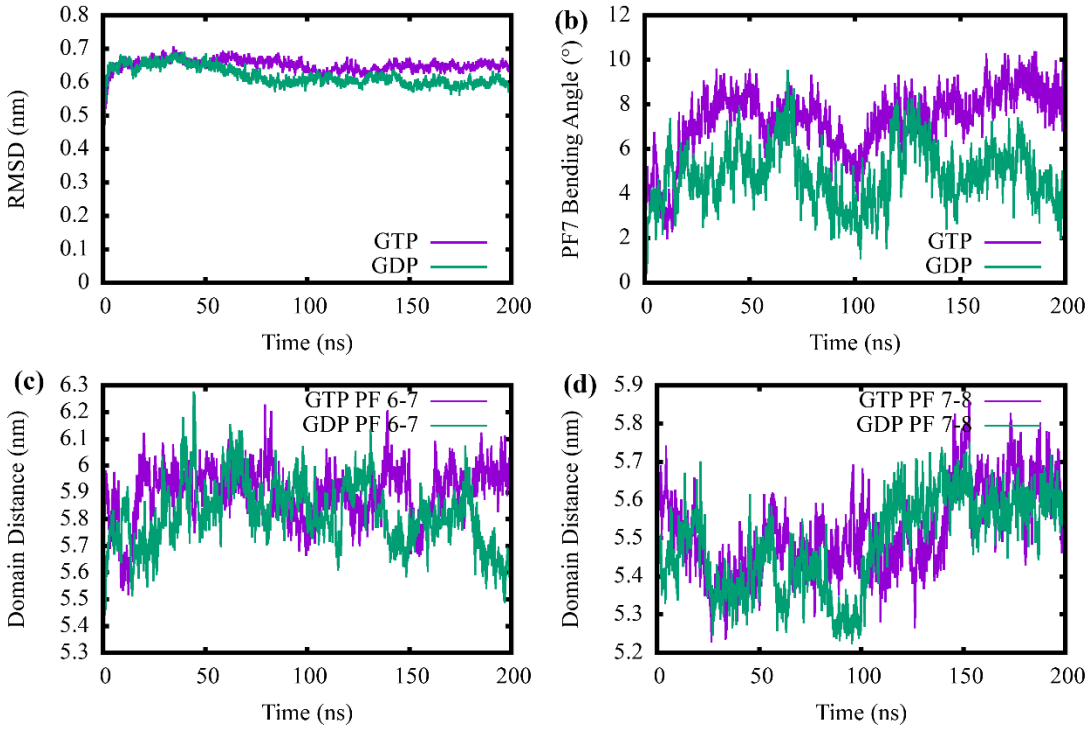

Figure S5: Convergence analysis of 200 ns closed MT segment simulations in different nucleotide states. Shown are the time evolution of (a) Cα RMSD value, (b) The bending angle of the middle PF in the closed MT segment, (c) The COM distance between β tubulin domains at the top of the middle PF 6 and 7, (d) The COM distance between β tubulin domains at the top of the middle PF 7 and 8.