

**Figure S4. Analysis of binding free energy components and per-residue decomposition from the first molecular dynamics (MD) trajectory of PmrB-ATP interaction.** The left panel (A-D) represents energetic components contributing to the total binding free energy (ΔG), which were calculated using the MMGBSA method for *A. baumannii* (A), *E. coli* (B), *K. pneumoniae* (C), and *P. aeruginosa* (D). Energy components include van der Waals (VDWAALS), electrostatic (EEL), polar solvation (EGB), and nonpolar solvation (ESURF) energies. The right panel (E-H) displays per-residue decomposition analysis of the PmrB-ATP binding free energy for *A. baumannii* (E), *E. coli* (F), *K. pneumoniae* (G), and *P. aeruginosa* (H) highlighting individual residues' energetic contribution to the PmrB-ATP interaction, where the residues with negative values contribute favorably to the binding.