

**Figure S6. Comparison of initial and equilibrated PmrB homology models from MD simulations.** The equilibrated structure corresponds to the frame with the lowest ΔG after 50 ns equilibration. (A) *A. baumannii*. (B) *E. coli*. (C) *K. pneumoniae*. (D) *P. aeruginosa*. Left panel: initial structure (green); Middle panel: lowest ΔG structure (white); Right panel: superimposition. This figure demonstrates the stability of the PmrB models and highlights conformational changes upon equilibration, particularly in loop regions and the ATP-binding site. The close agreement between structures supports the reliability of the models for further investigations.