



**Figure S16. Structural analysis of WPD loop in TMD' simulation.** (A) RMSD of the WPD loop from its conformation in  $WPD_{open}$  (dark blue) and  $WPD_{closed}$  (light blue) crystal structures. (B) Trajectory of  $\phi_{182}$  dihedral angle. Lines and coloring are identical to those in Figure S13. (C) Histogram of the backbone dihedral angles of Phe182.