



**Figure S13. Trajectory of  $\phi_{182}$  backbone dihedral angle in TMD<sub>1</sub> simulation.** Black and maroon dashed lines represent the angles adopted by  $\phi_{182}$  in WPD<sub>open</sub> and WPD<sub>closed</sub> crystal structures. Yellow lines represent the trajectory of  $\phi_{182}$  from WPD<sub>open</sub> to WPD<sub>closed</sub> conformations, while blue lines represent the trajectory of  $\phi_{182}$  from WPD<sub>closed</sub> to WPD<sub>open</sub> conformations.