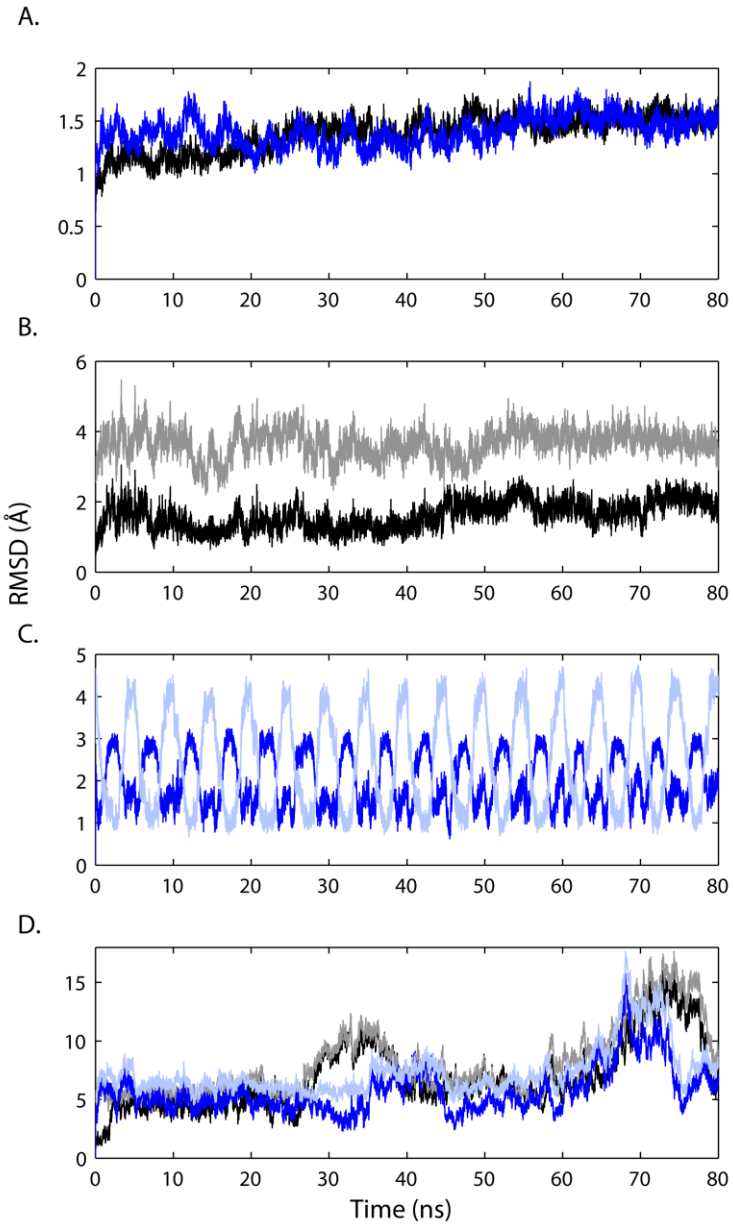

Figure S2. RMSD of various structural elements of PTP1B in EMD and TMD_1 simulations from crystal structures. (A) RMSD of PTP1B in MD (black) and TMD_1 (blue) simulations from the WPD_{open} crystal structure (PDB ID: 2F6F). (B) RMSD of the WPD loop in EMD simulation from WPD_{open} (black) and WPD_{closed} (gray, PDB ID: 1SUG) crystal structures. (C) RMSD of the WPD loop in TMD_1 simulation from WPD_{open} (dark blue) and WPD_{closed} (light blue) crystal structures. (D) RMSD of α7 (residues 281 to 298) in EMD simulation from WPD_{open} (black) and WPD_{closed} (gray) crystal structures. RMSD of the same region in TMD_1 simulation from WPD_{open} (dark blue) and WPD_{closed} (light blue) crystal structures. Disordered nature of α7 is confirmed by EMD and TMD simulations.