

Figure S4. Transformation of reconstructed trajectories to reconstructed in-phase trajectories using PCA. (A) Reconstructed trajectories of three-Cartesian components of WPD loop  $C_{\alpha}$  atoms. (B) In-phase components obtained by employing PCA on the trajectories shown in (A). (C) In-phase components obtained by employing PCA on the reconstructed trajectories of  $C_{\alpha}$  atoms between residues 2 to 278.