Figure S17. Comparison of WPD loop conformational transitions in TMD simulations with different spring constants on the reduced PC planes. Projection of WPD loop transitions on (A) PC1-PC2, and (B) PC1-PC3 planes. Black and blue circles represent TMD simulations with spring constant equal to 3000 $kcal \cdot mol^{-1} \cdot Å^{-2}$ and 500 $kcal \cdot mol^{-1} \cdot Å^{-2}$, respectively. (C) Transition of WPD loop in the first cycle of both simulations on PC1-PC2 plane. Black (TMD_1) and blue lines (TMD') represent the WPD loop trajectory during the first loop closing, while red (TMD_1) and green (TMD') represent the first loop opening.