Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The regulation mechanism of phosphorylation and mutations on the intrinsically disordered protein 4E-BP2

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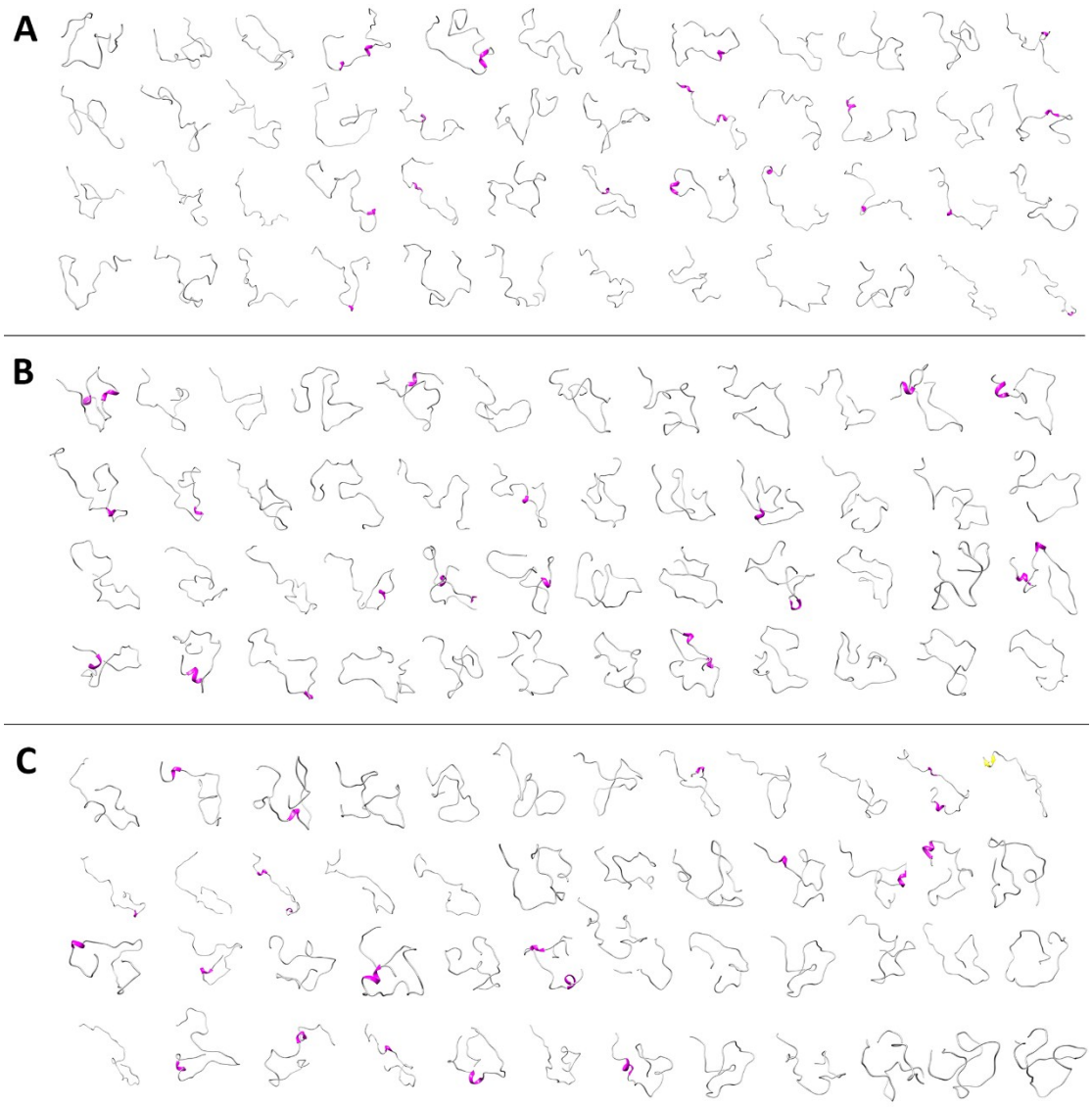

Figure S1. The initial structures for the REMD simulations. (A) The 48 initial structures for WT 4E-BP2. (B) The 48 initial structures for pWT 4E-BP2. (C) The 48 initial structures for pMT 4E-BP2.

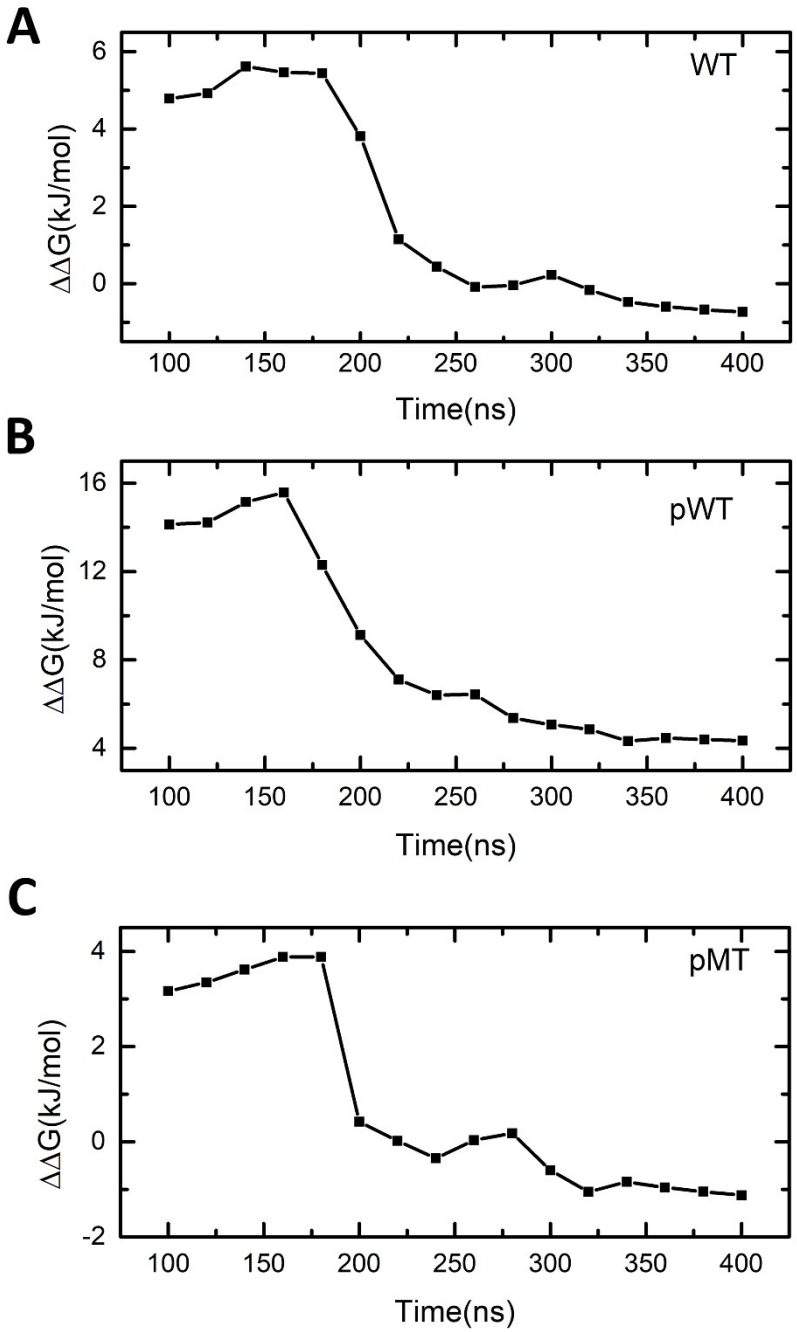

Figure S2. The convergence tests of REMD. (A) Free energy differences between the minima U1 and U3 of WT 4E-BP2 as a function of simulation time; (B) Free energy differences between the minima U2 and F of pWT 4E-BP2 as a function of simulation time; (C) Free energy differences between the minima U1 and U4 of pMT 4E-BP2 as a function of simulation time.

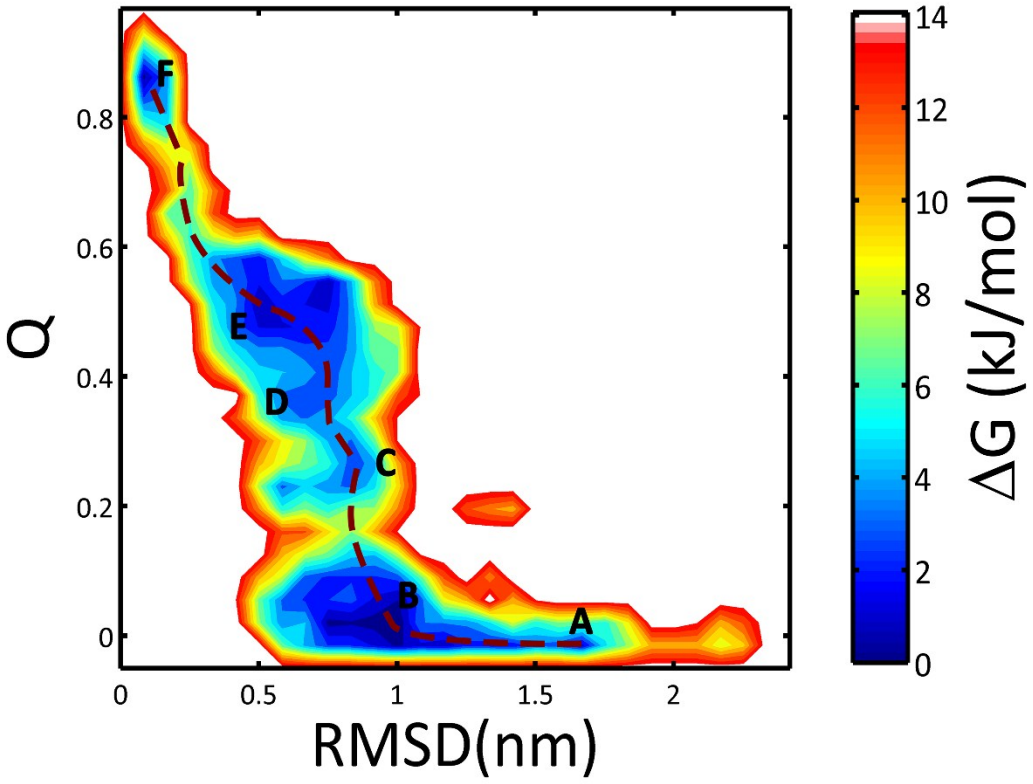

Figure S3. The folding pathway of pWT 4E-BP2. The red dash line indicates the folding pathway of pWT 4E-BP2, the intermediates on the pathway were labeled.

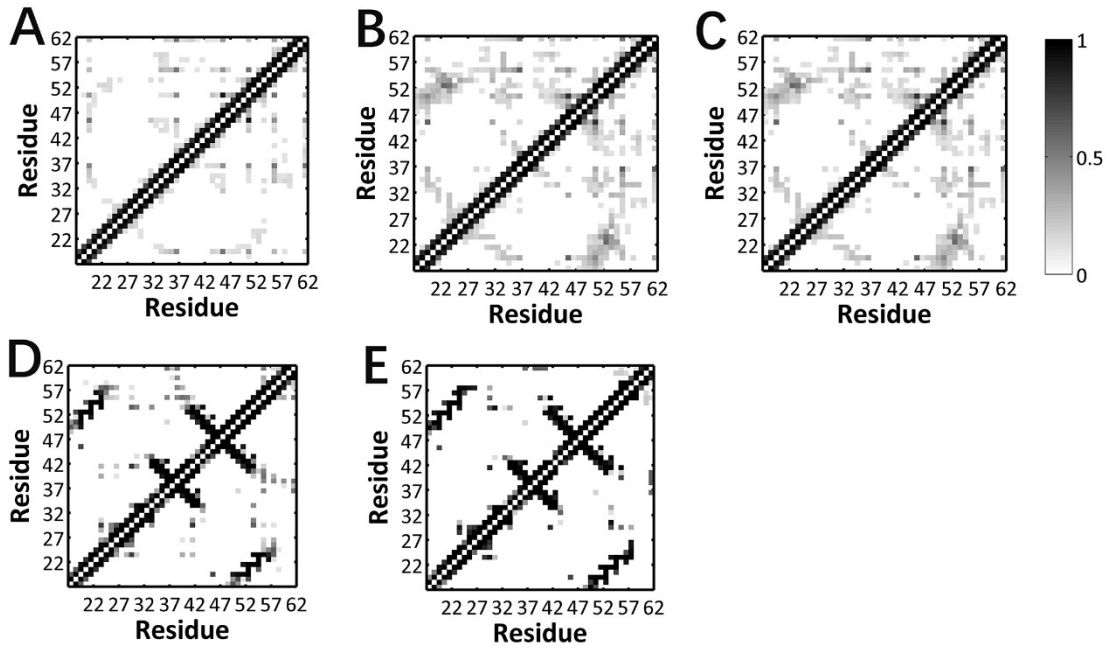

Figure S4: Residue-residue contact maps of pWT 4E-BP2 in different states. (A) Contact map of state with Q<0.13; (B) Contact map of state with 0.13<Q<0.2; (C) Contact map of state with 0.2<Q<0.73; (D) Contact map of state with 0.73<Q<0.8; (E) Contact map of state with Q>0.8. The criteria to divide the Q values are given in the legend of Figure 5.

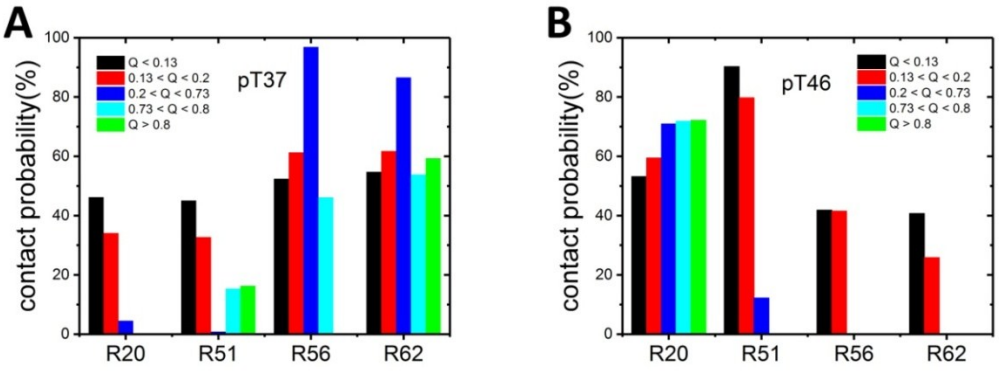

Figure S5. The contact probability of electrostatic interactions between phosphorylated residues and the positive charged residues in different states. (A) Contacts between pT37 and positive charged residues. (B) Contacts between pT46 and positive charged residues.

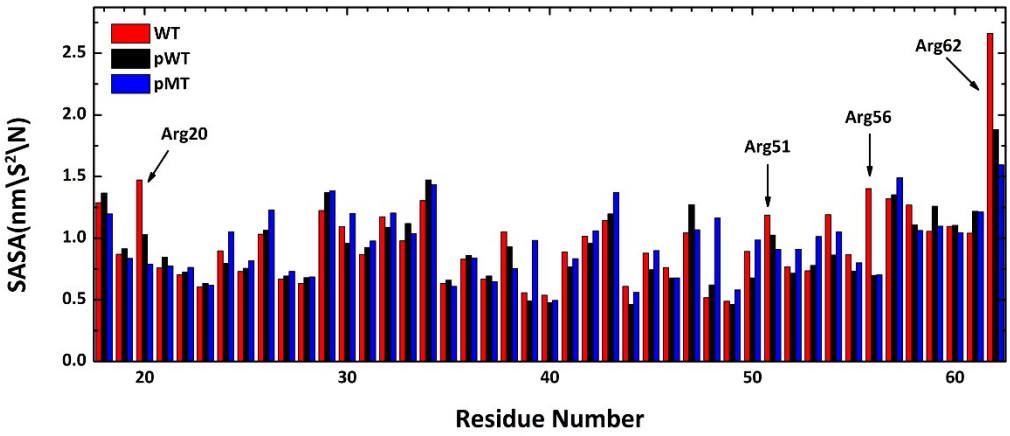

Figure S6. The residual solvent-accessible surface areas (SASA) of WT, pWT and pMT 4E-BP2.