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

Supplementary data

The Effects of Implicit Modeling of Nonpolar Solvation on Protein Folding Simulation

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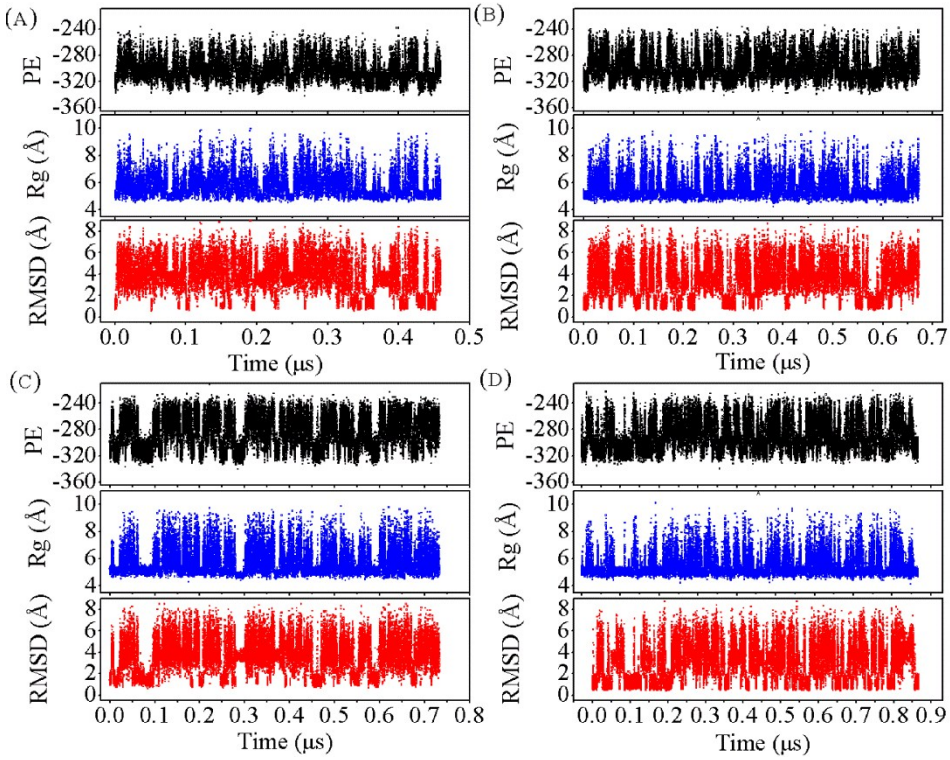

Figure S1. Time series of the potential energy (black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in the trajectories of implicit solvent simulations of CLN025 with γ of (A) 0, (B) 0.0025, (C) 0.0050, and (D) 0.0075 kcal/mol/Å^2, respectively.

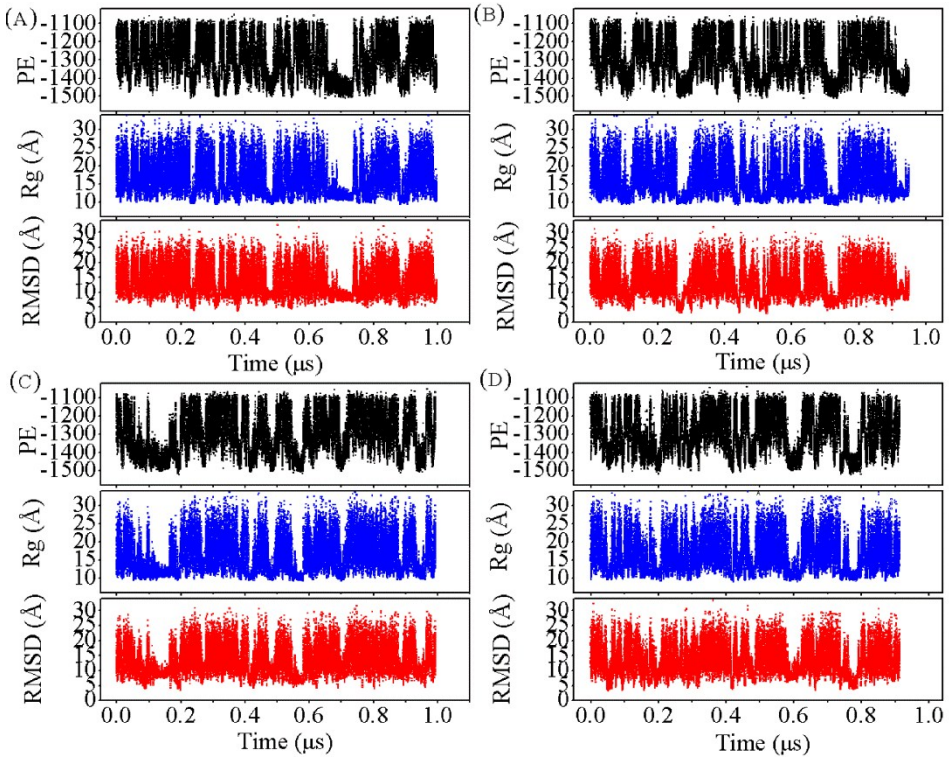

Figure S2. Time series of the potential energy (black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in individual trajectories (A-D) of implicit solvent simulations of BdpA with $\gamma = 0$ kcal/mol/Å^2.

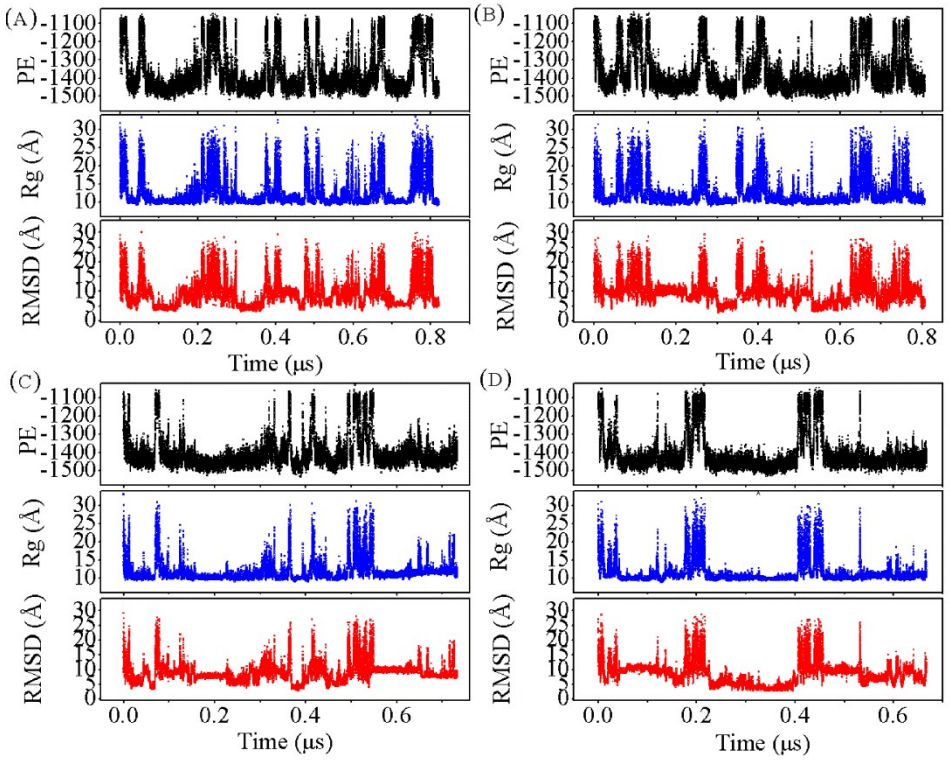

Figure S3. Time series of the potential energy (black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in individual trajectories (A-D) of implicit solvent simulations of BdpA with $\gamma = 0.0025$ kcal/mol/Å^2.

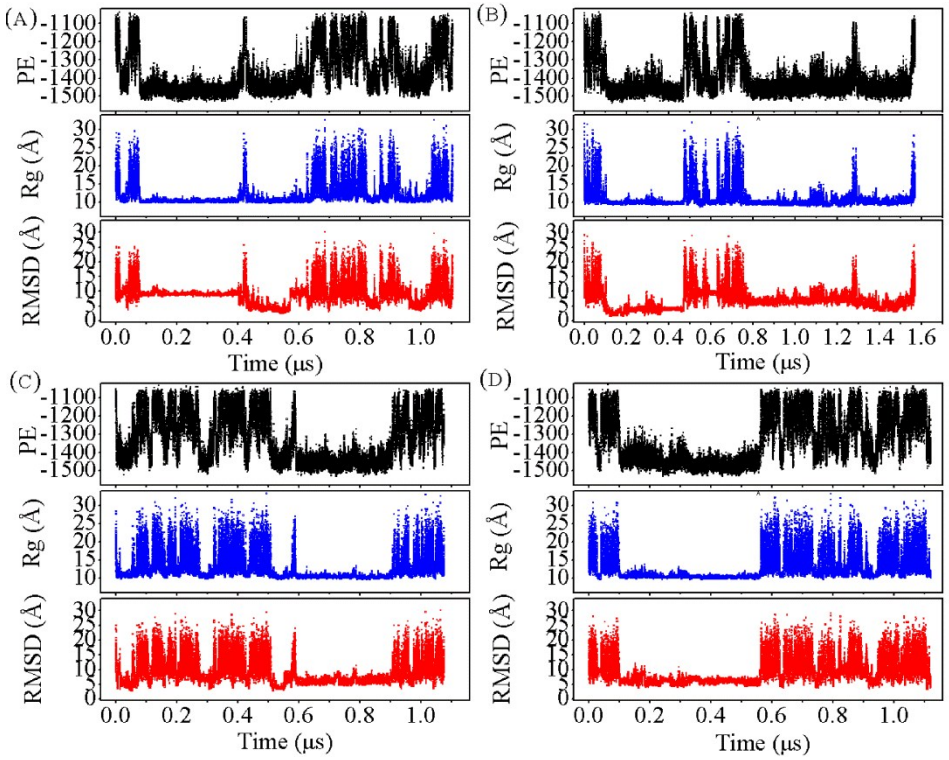

Figure S4. Time series of the potential energy (black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in individual trajectories (A-D) of implicit solvent simulations of BdpA with $\gamma = 0.0050$ kcal/mol/Å^2.

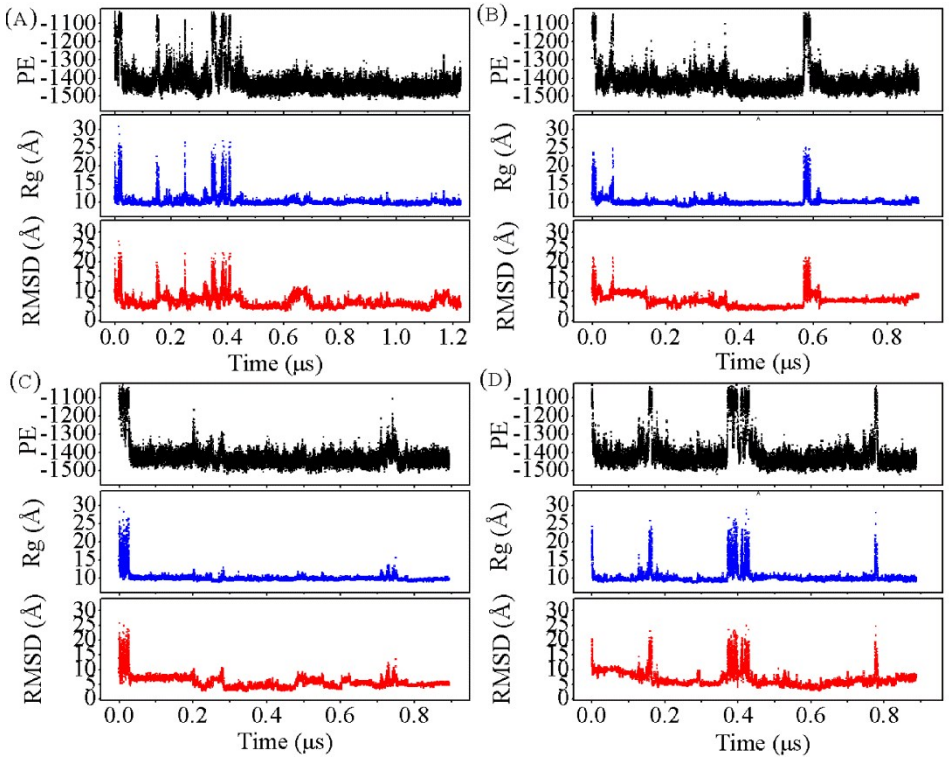

Figure S5. Time series of the potential energy (black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in individual trajectories (A-D) of implicit solvent simulations of BdpA with $\gamma = 0.0075$ kcal/mol/Å^2.

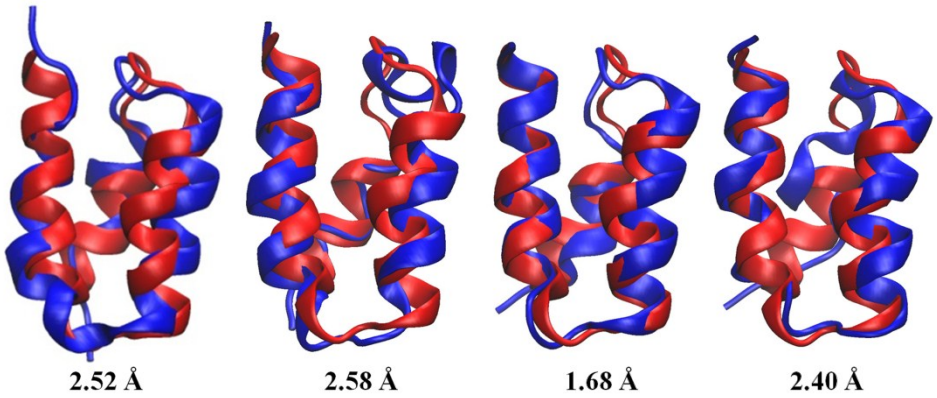

Figure S6. Comparison of the simulated structures with lowest RMSDs (blue) to the experimental native structure of BdpA (red). Under each structure is shown the backbone RMSD value. From left to right are the results from the simulations with γ = 0, 0.0025, 0.0050, and 0.0075 kcal/mol/Å^2, respectively.

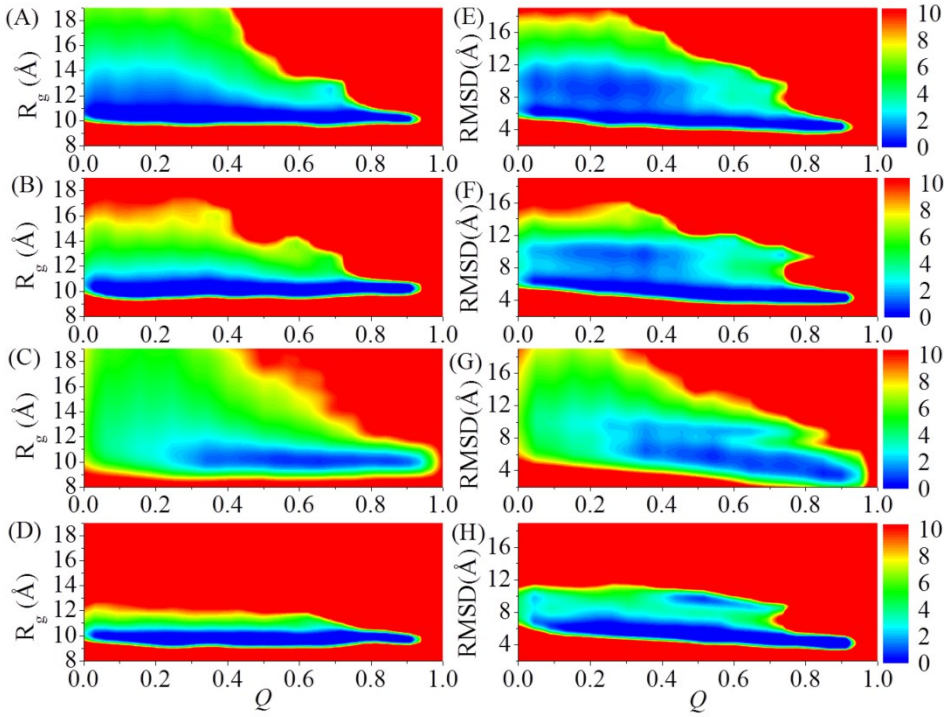

Figure S7. Two-dimensional free-energy profiles as the function of the fraction of native contacts (Q) and (A-D) R_g or (E-H) RMSD for the folding of BdpA in implicit solvent simulations with γ = 0, 0.0025, 0.0050, and 0.0075 kcal/mol/Å^2 (from top to bottom).

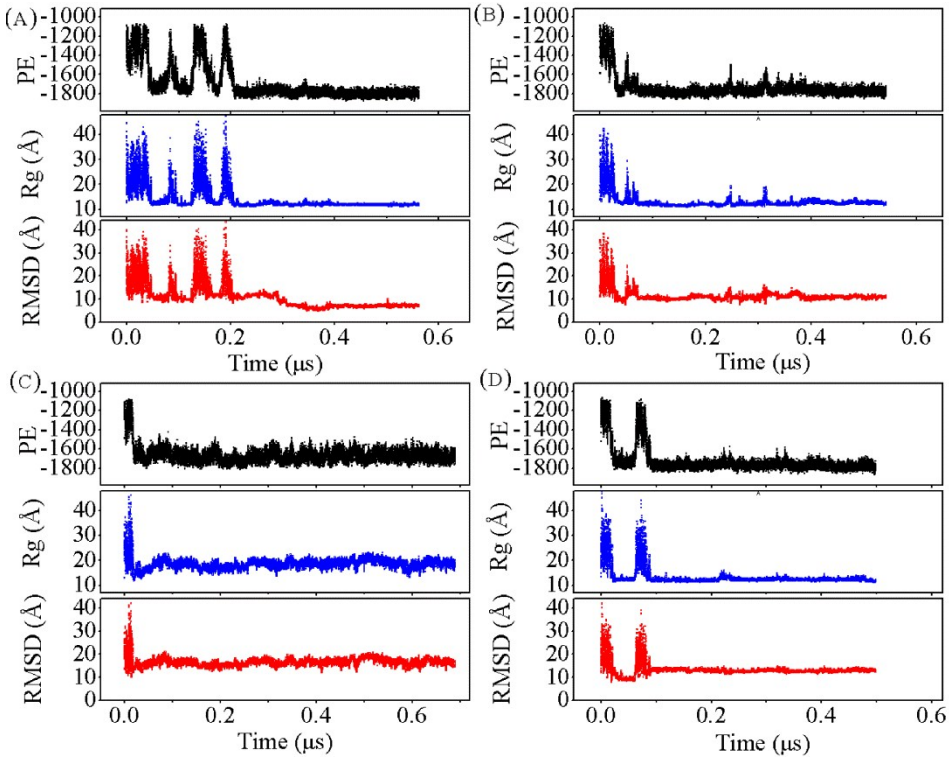

Figure S8. Time series of the potential energy (black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in individual trajectories (A-D) of implicit solvent simulations of λ-repressor with $\gamma = 0$ kcal/mol/Å^2.

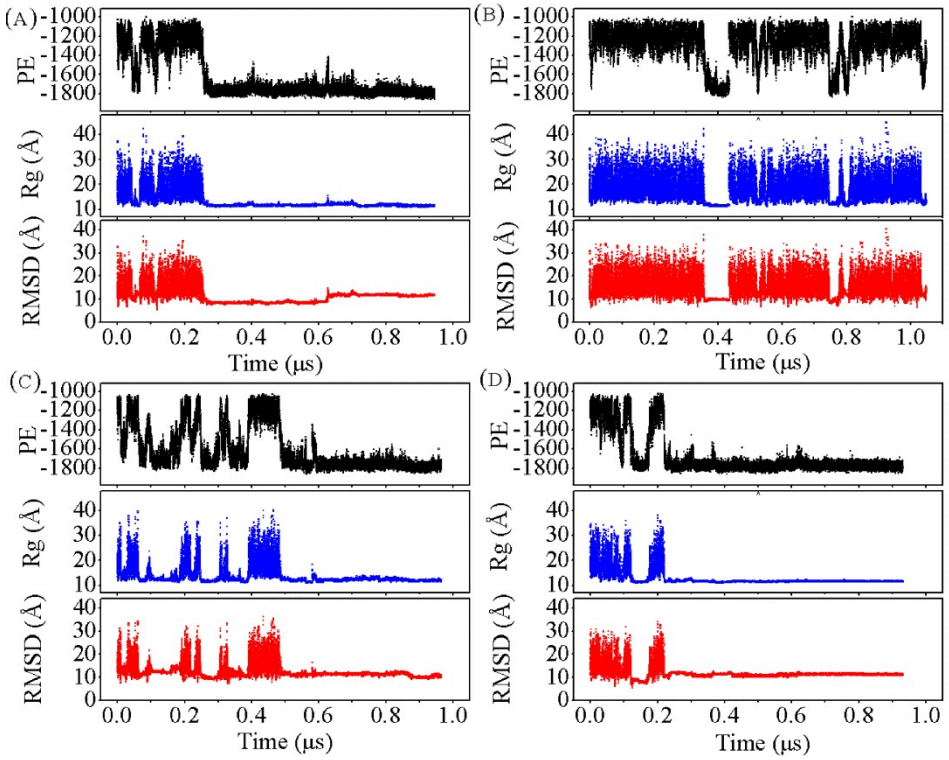

Figure S9. Time series of the potential energy (black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in individual trajectories (A-D) of implicit solvent simulations of λ-repressor with $\gamma = 0.0050$ kcal/mol/Å^2.

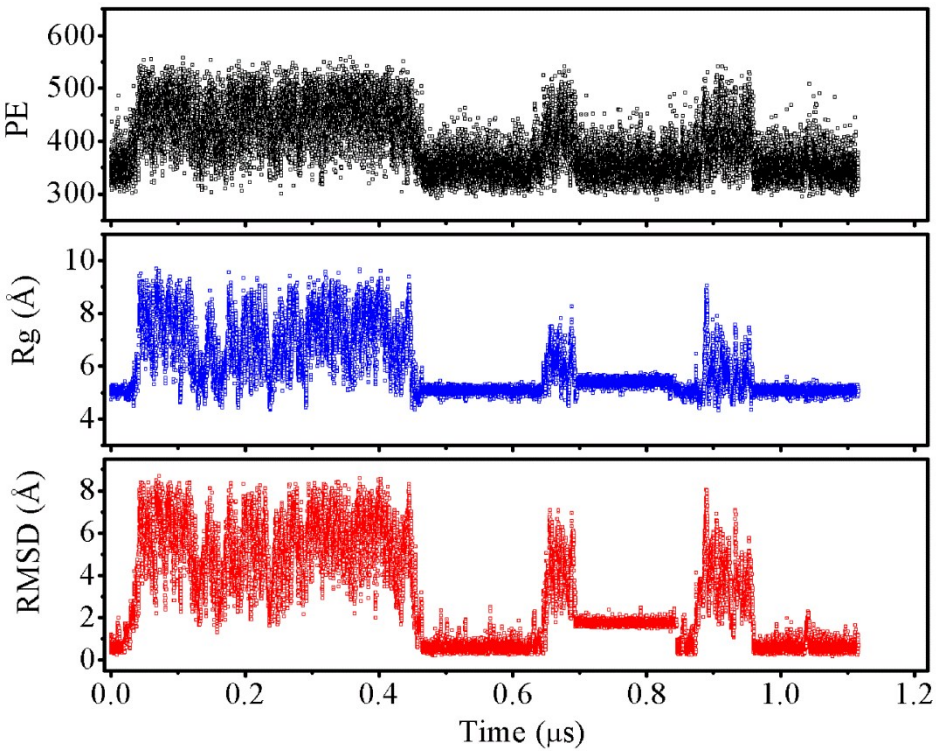

Figure S10. Time series of the protein relevant potential energy term (E_P+$0.5E_{PW}$, black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in the SITS-enhanced explicit solvent simulation trajectory of CLN025. The definition of the protein relevant potential energy term is indicated in the reference of (Yang and Gao, *J Chem Phys*, 2009, **131**, 214109).

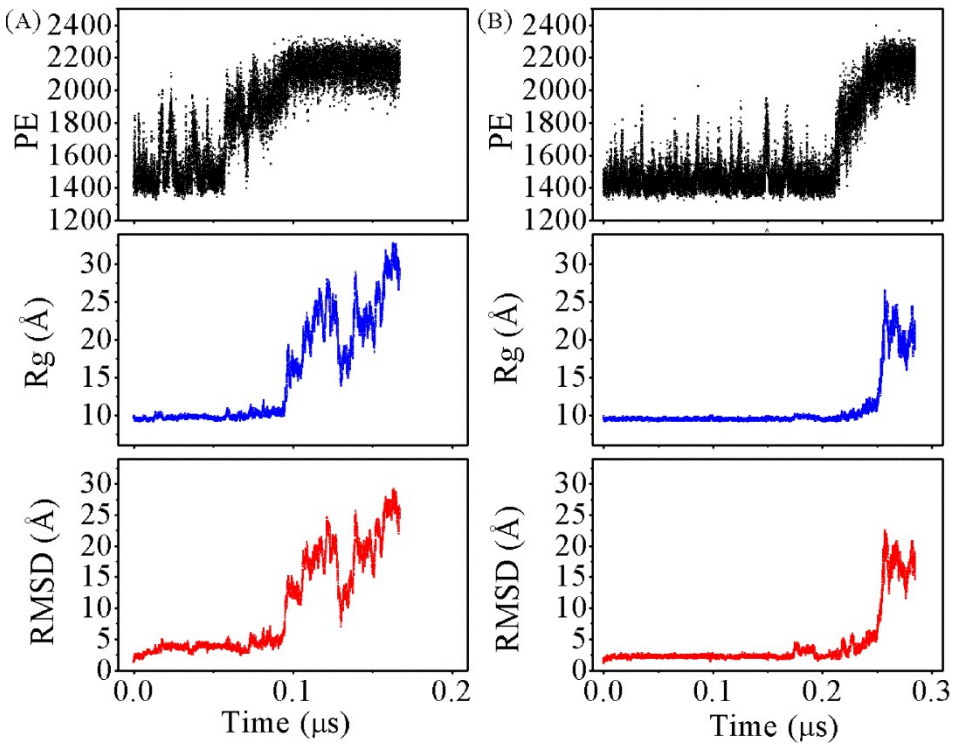

Figure S11. Time series of the protein relevant potential energy term (E_P+$0.5E_{PW}$, black line, unit: kcal/mol), the radius of gyration (Rg, blue line), and root-mean-square deviation (RMSD, red line) in two trajectories of SITS-enhanced explicit solvent simulations of BdpA.