

## Understanding the conformational dynamics of an intrinsically disordered protein bound to a small molecule

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### Supplementary data

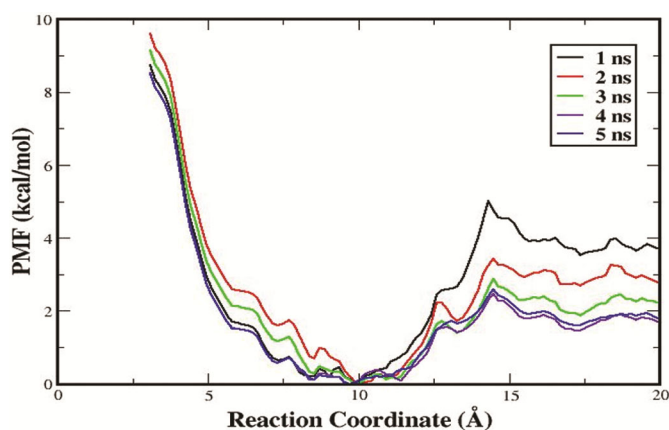


Fig. 1 — Assessment of convergence of the PMFs calculated by umbrella sampling (US) for the NUPR1-ZZW-115 complex with 5 ns US simulations performed for each window

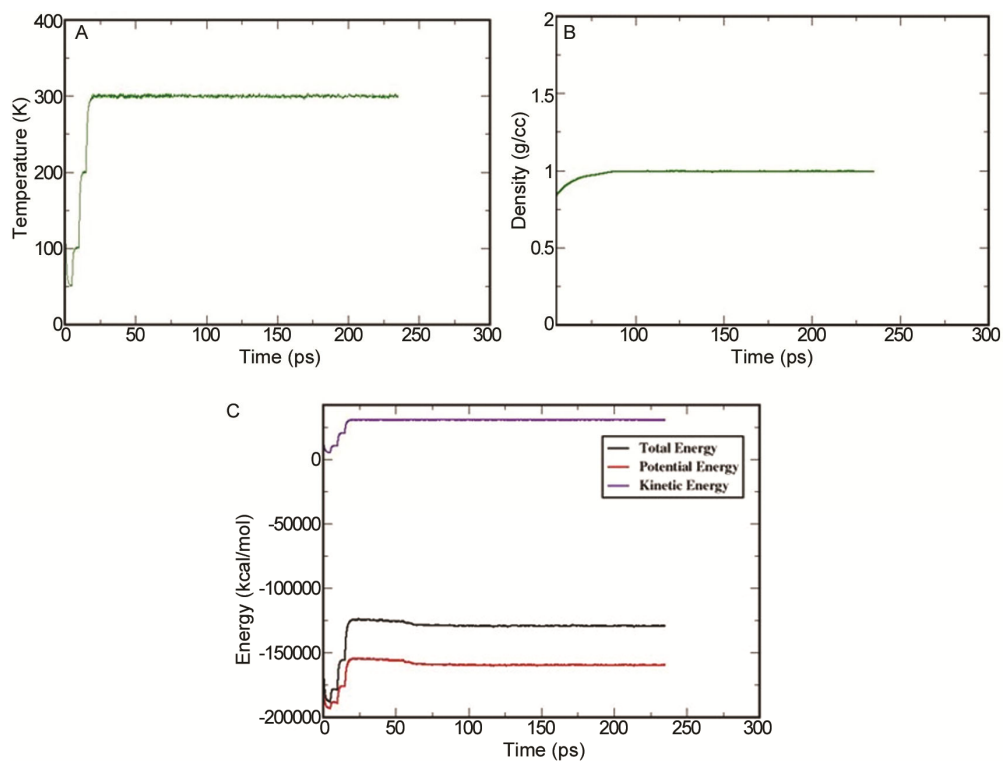


Fig. 2 — (A) Temperature, (B) Density; and (C) Energy plots of NUPR1ZZW-115 complex system as a function of simulation time in unbound state

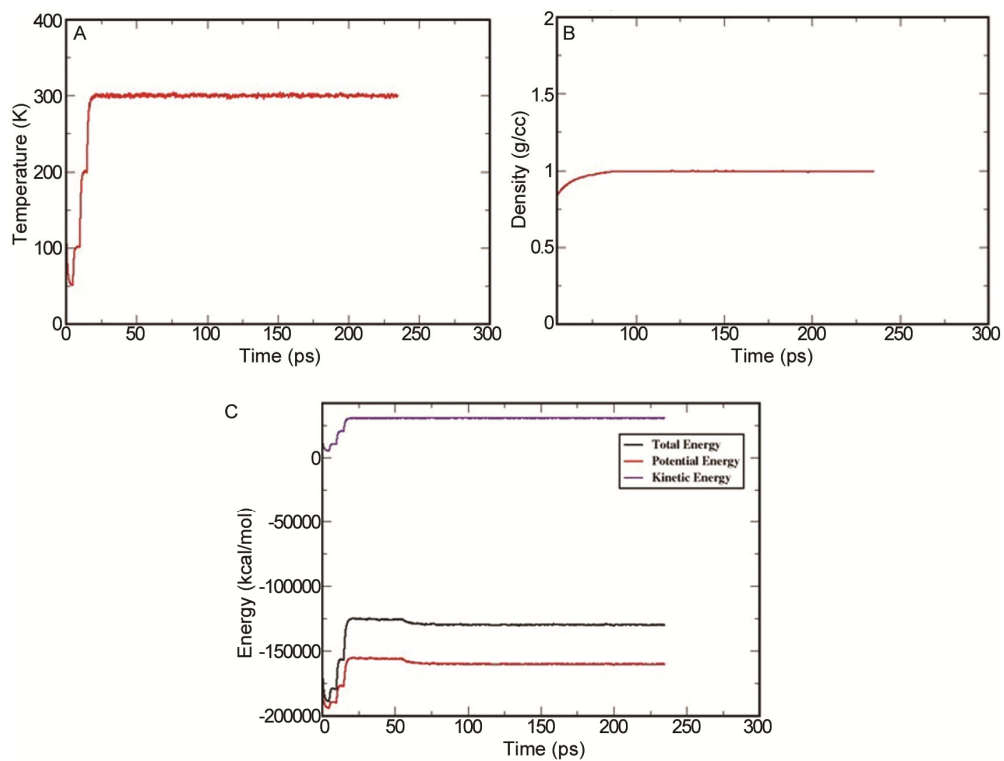


Fig. 3 — (A) Temperature, (B) Density; and (C) Energy plots of NUPR1 as a function of simulation time in bound state