

Force fields for simulating intrinsically disordered proteins: Assessing conformational sampling and structural dynamics

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Supplementary Figures

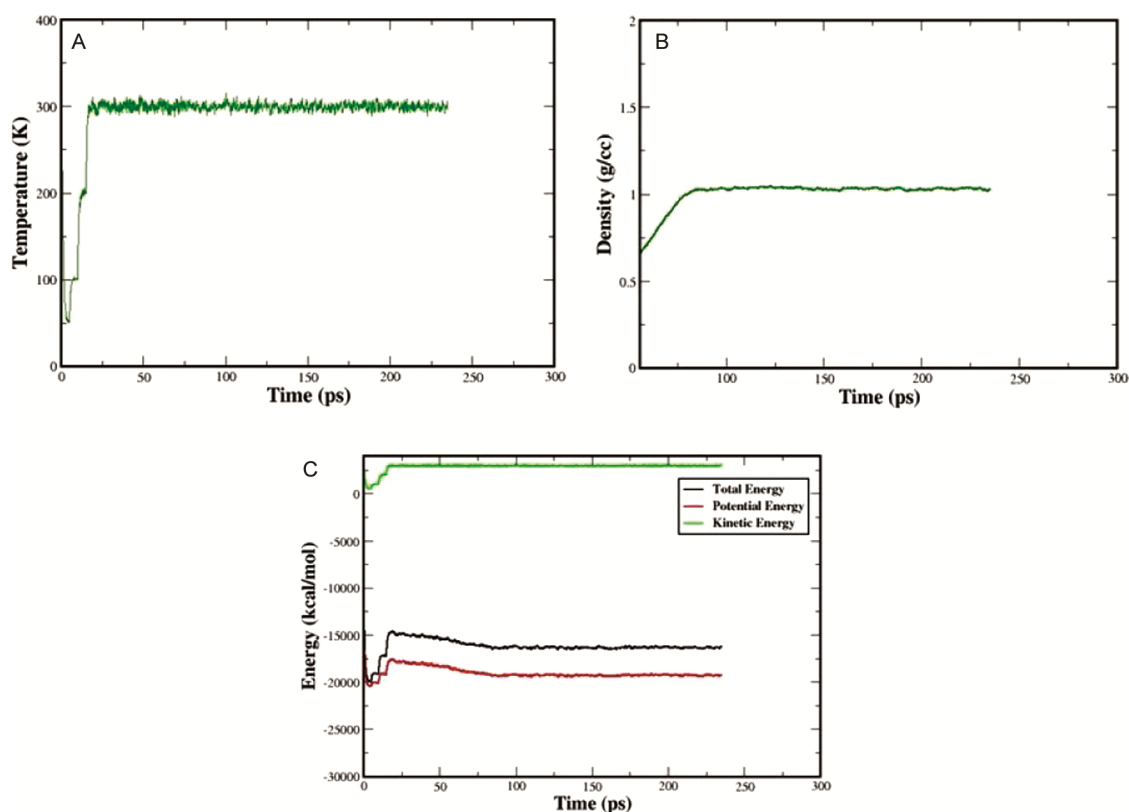


Fig. 1 — (A) Temperature, (B) Density and (C) Energy plots of Histatin 5 simulated with ff19SB-OPC water model as a function of simulation time

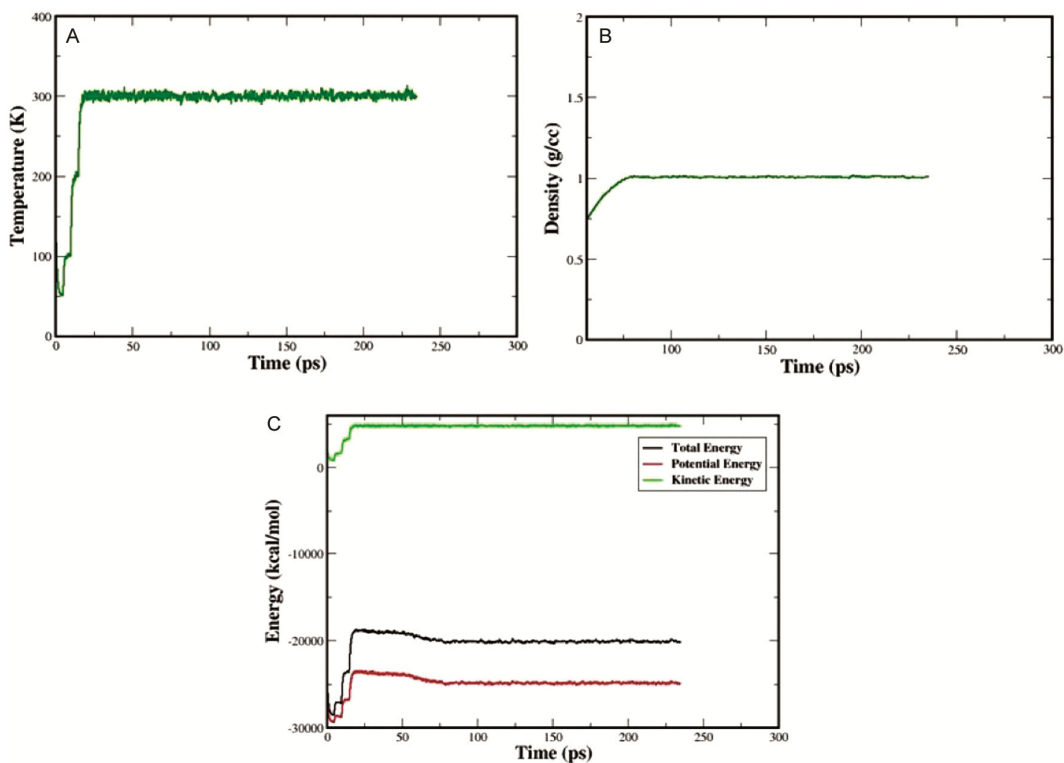


Fig. 2 — (A) Temperature, (B) Density and (C) Energy plots of Histatin 5 simulated with ff99SBildn-TIP3P water model as a function of simulation time

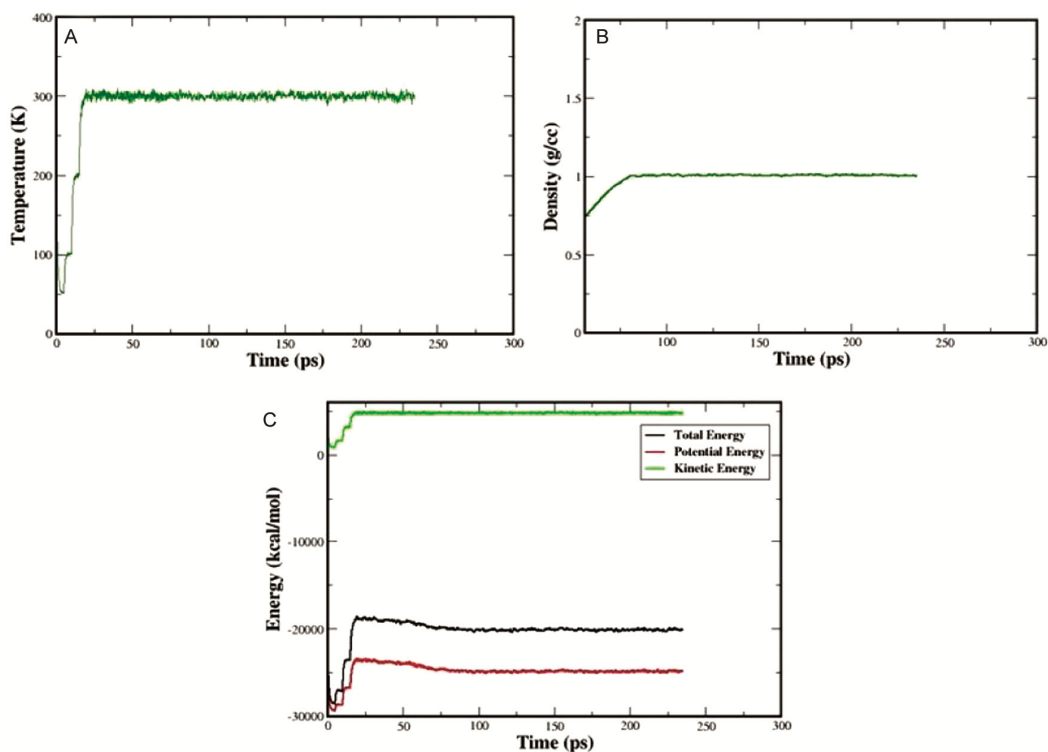


Fig. 3 — (A) Temperature, (B) Density and (C) Energy plots of Histatin 5 simulated with ff99SB-TIP3P water model as a function of simulation time

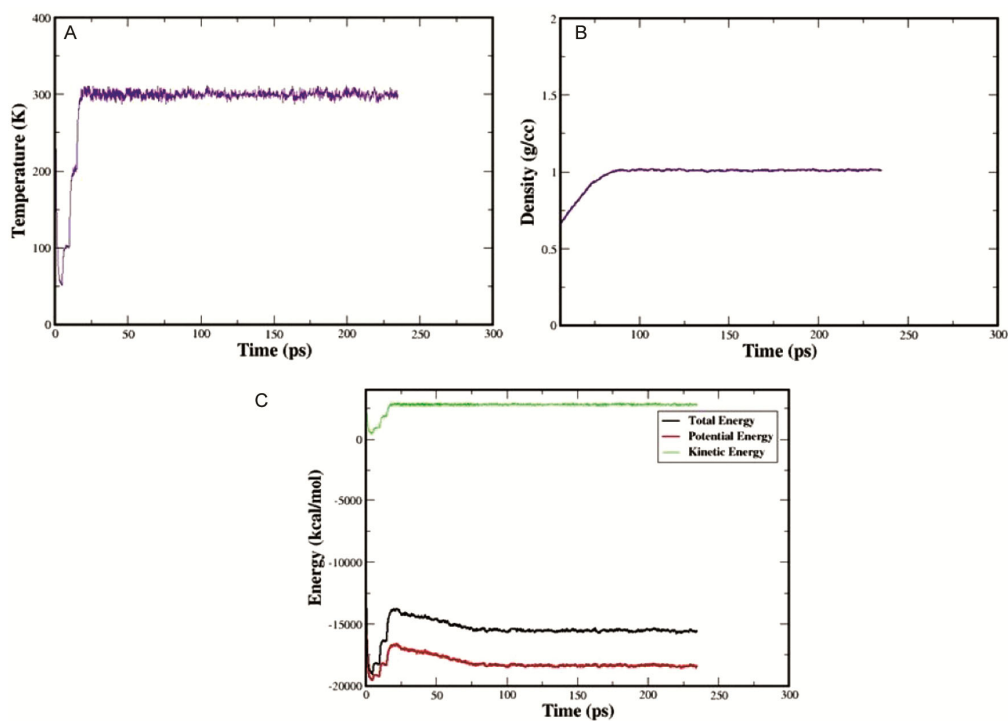


Fig. 4 — (A) Temperature, (B) Density and (C) Energy plots of Trp-cage simulated with ff19SB-OPC water model as a function of simulation time

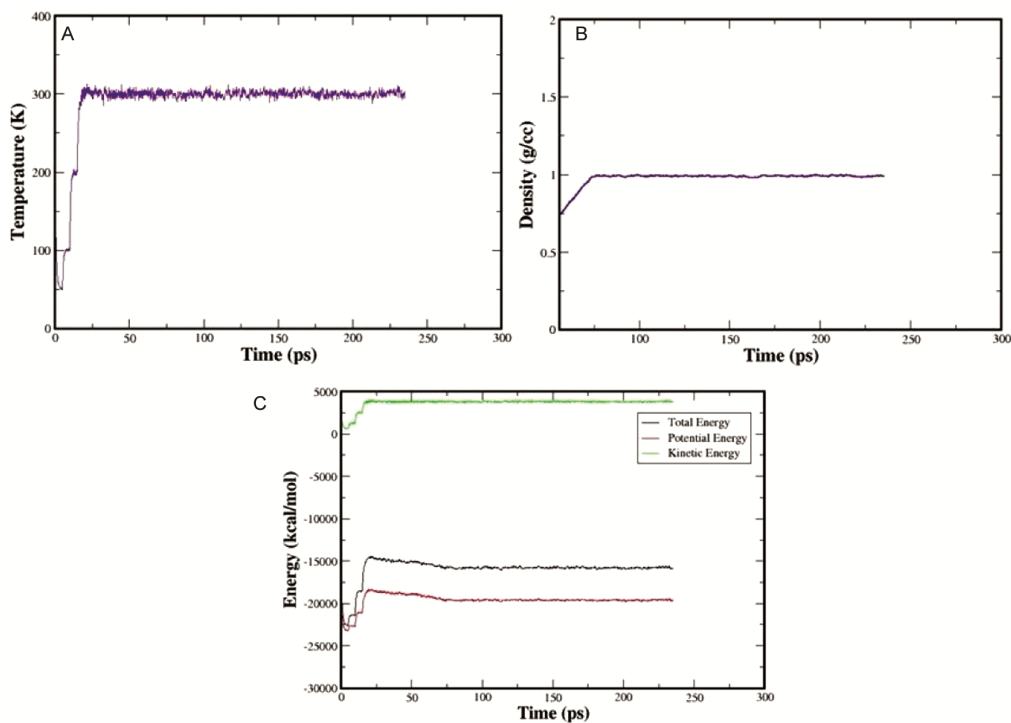


Fig. 5 — (A) Temperature, (B) Density and (C) Energy plots of Trp-cage simulated with ff99SBildn-TIP3P water model as a function of simulation time

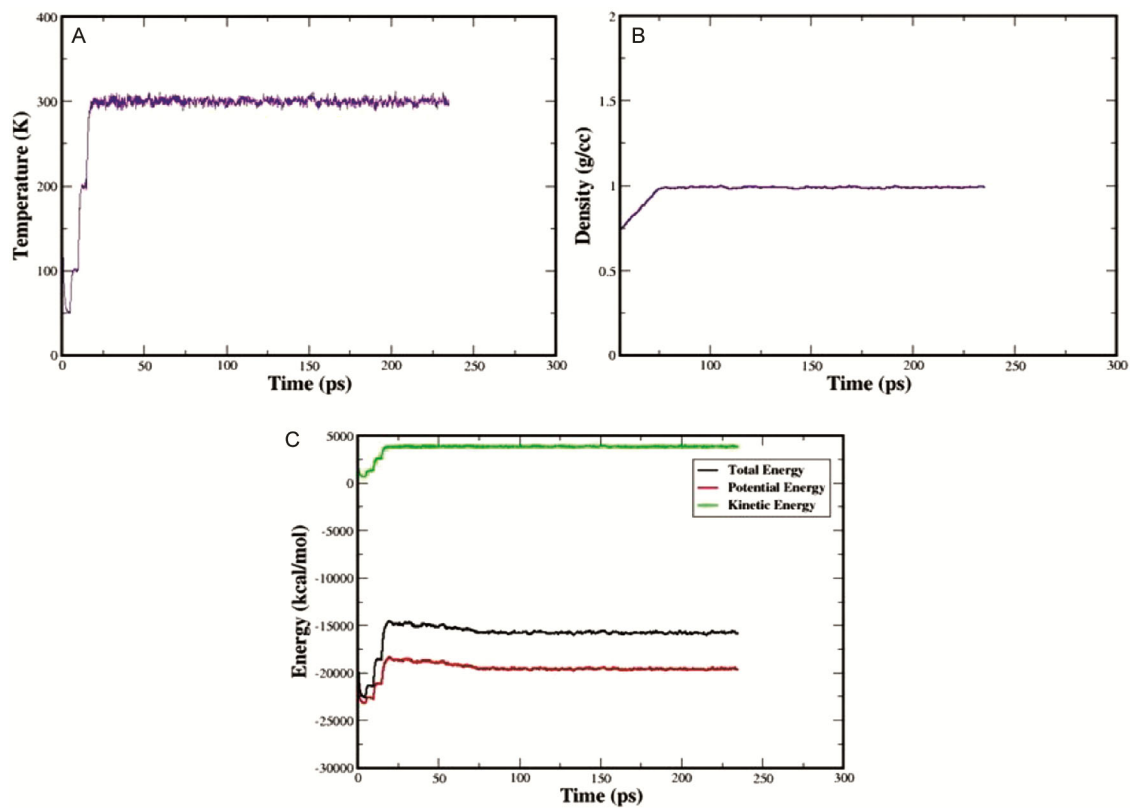


Fig. 6 — (A) Temperature, (B) Density and (C) Energy plots of Trp-cage simulated with ff99SB-TIP3P water model as a function of simulation time