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

Supplementary materials for

Correction of Erroneously Packed Protein's Side Chain in NMR Structure Based on *Ab Initio* Chemical Shift Calculations

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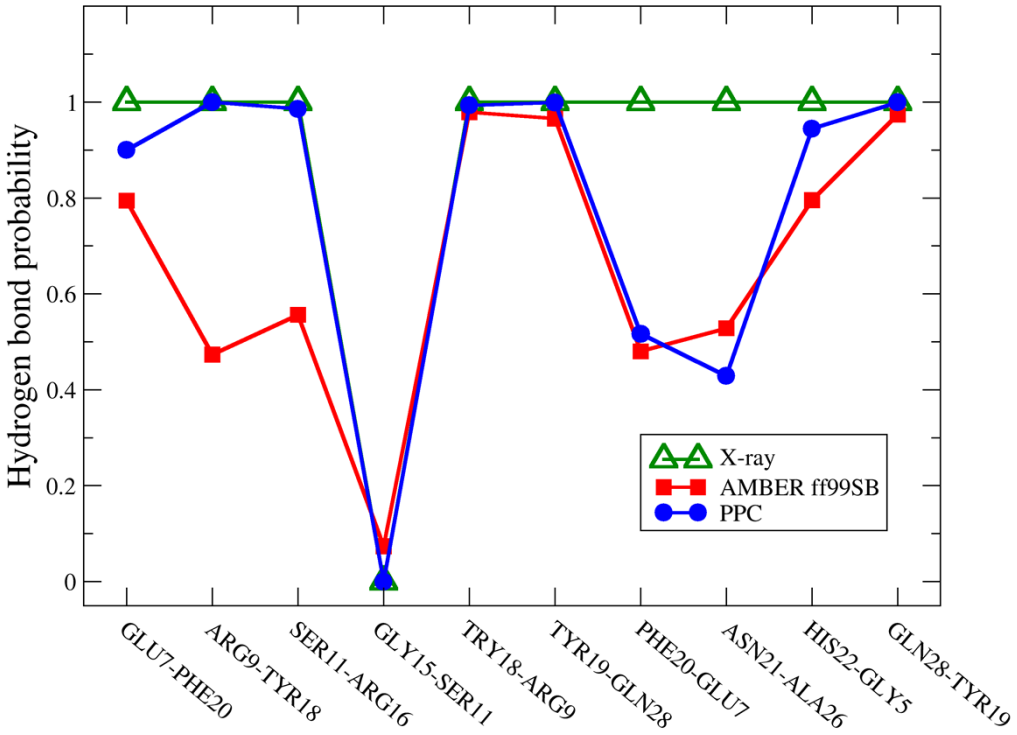

Figure S1. Hydrogen bond probabilities of several important hydrogen bonds in Pin1 WW domain during MD simulations using the Amber ff99SB and PPC charge models.

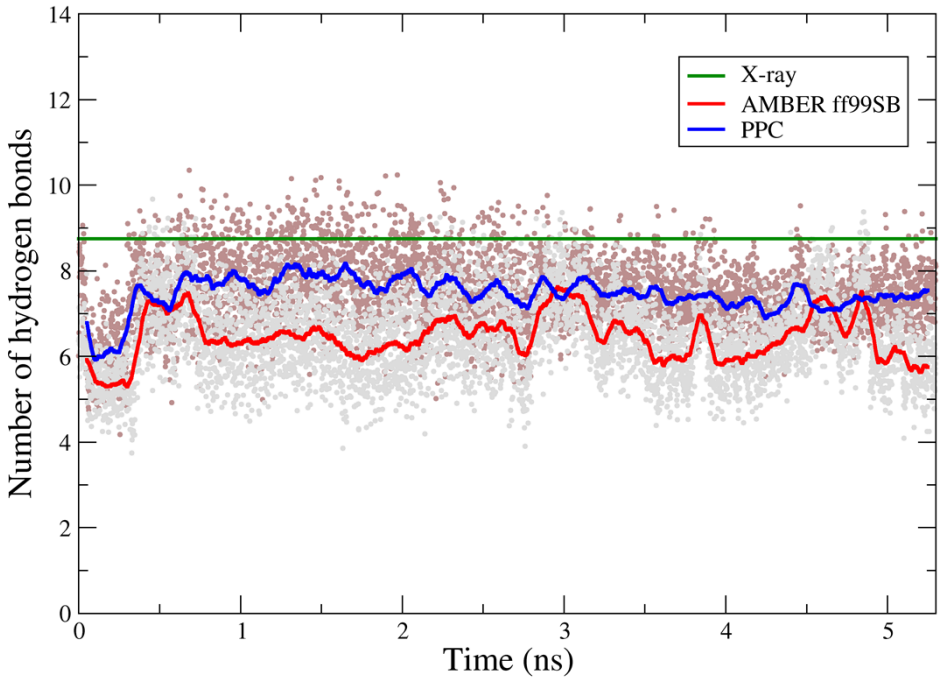

Figure S2. Number of hydrogen bonds in Pin1 WW domain as a function of MD simulation time for both Amber ff99SB and PPC trajectories. Red (Amber) and blue (PPC) lines are average values for every 100 ps. The hydrogen bonds were counted using a sigmoidal function of the donor-acceptor distance d as $f_{\mathrm{HB}}(d) = 1/(1+(d/2.6)^6)$ related to the strength of hydrogen bonds[1].

References:

1. Gao, Y.; Lu, X.; Duan, L. L.; Zhang, J. Z. H.; Mei, Y., Polarization of Intraprotein Hydrogen Bond Is Critical to Thermal Stability of Short Helix. *J. Phys. Chem. B* **2012**, 116, 549-554.