Supplementary Data

Counterion Effects on the Denaturing Activity of Guanidinium Cation to Protein

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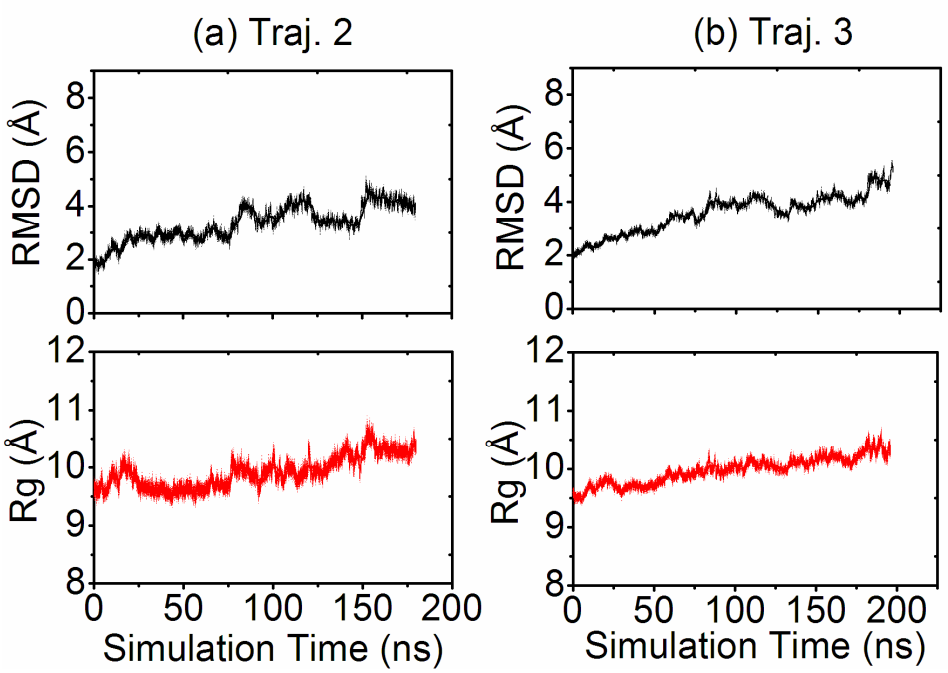

Figure S1. RMSD (top panel), and R_g (bottom panel) of BdpA as a function of simulation time from (a) the second and (b) the third independent simulation trajectories of GdmSCN solution.

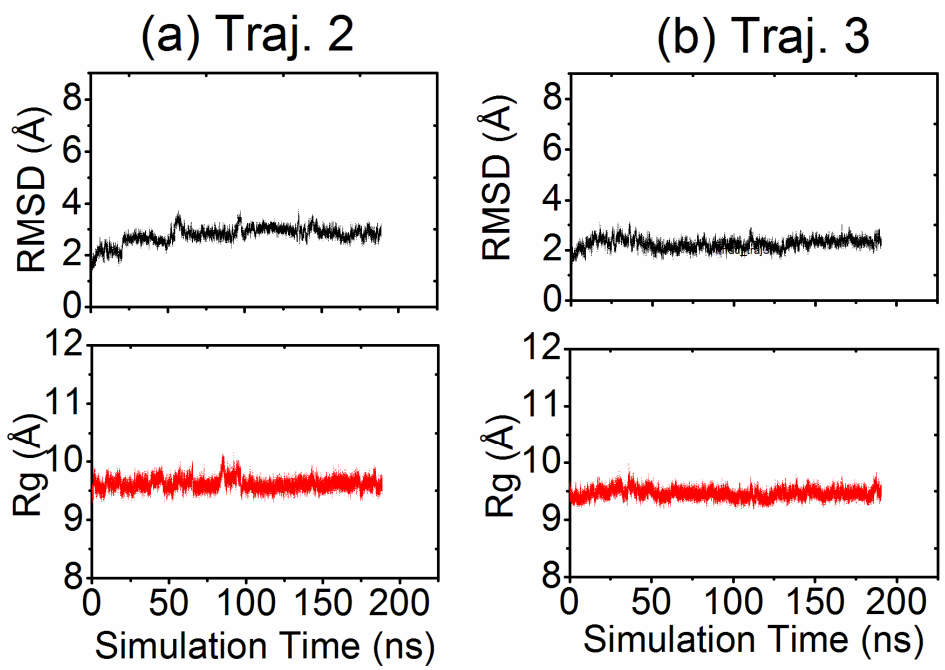

Figure S2. RMSD (top panel), and R_g (bottom panel) of BdpA as a function of simulation time from (a) the second and (b) the third independent simulation trajectories of GdmCl solution.

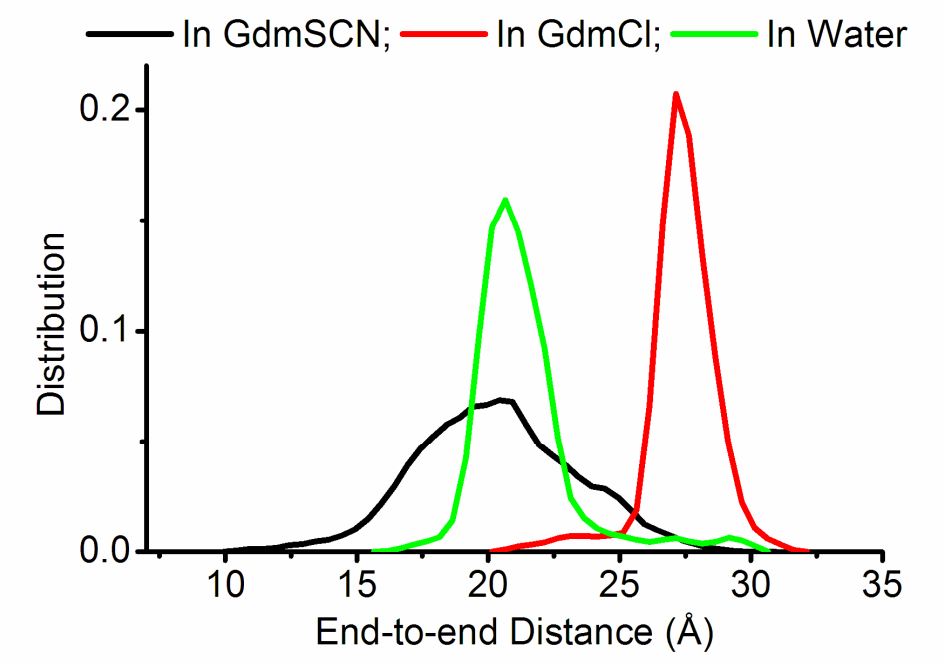

Figure S3. The end-to-end distance distribution of BdpA in three solutions (GdmSCN, GdmCl, and pure water).

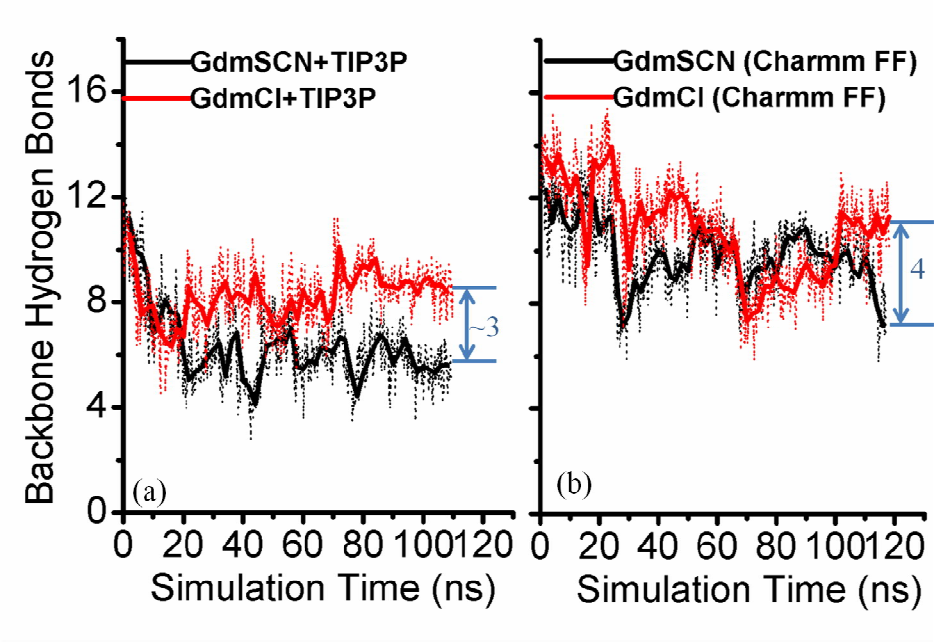

Figure S4. The total number of backbone hydrogen bonds formed in BdpA as a function of simulation time in (a) GdmSCN and GdmCl solutions using Gdm^+ force field of Jorgensen et al. (Ref.1) and TIP3P explicit solvent model, (b) GdmSCN and GdmCl solutions using Gdm^+ force field of MacKerell et al. (Ref.2) and SPC/E explicit solvent model, respectively.

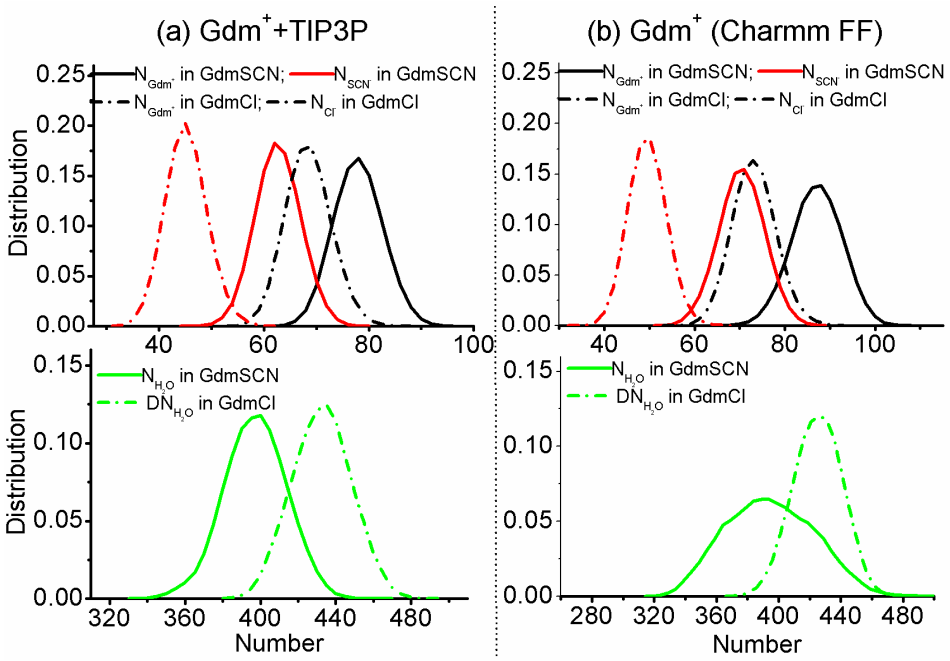

Figure S5. The distribution of the number of Gdm^+ cations, SCN^- (Cl^-) anions, and water molecules within 6 Å of protein surface in GdmSCN (GdmCl) solutions using Gdm^+ force field of Jorgensen et al. (Ref.1) and TIP3P explicit solvent model, and using Gdm^+ force field of MacKerell et al. (Ref.2) and SPC/E explicit solvent model, respectively.

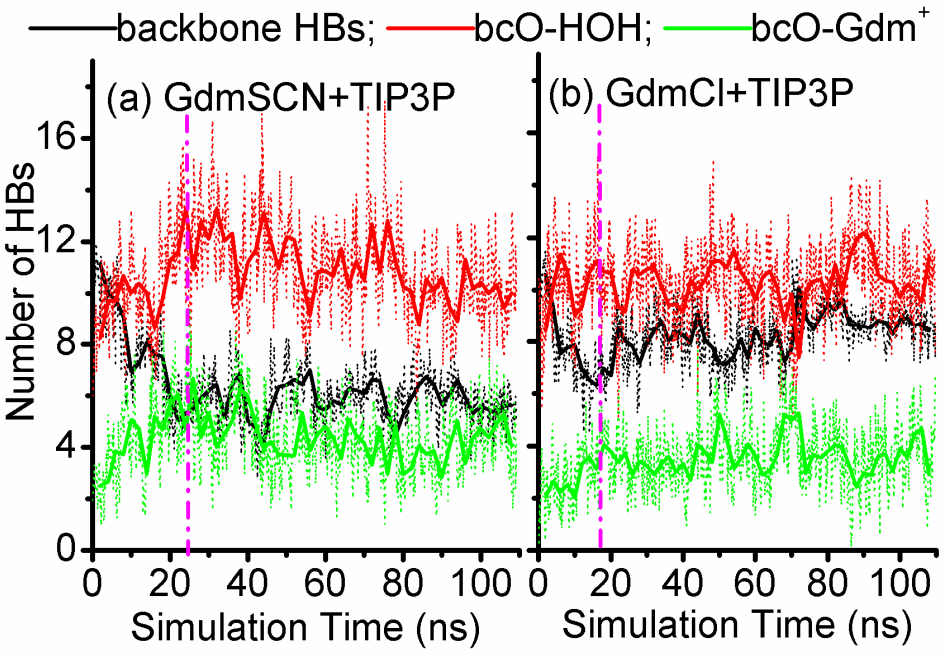

Figure S6. The breaking and formation of hydrogen bonds for residues involved in all backbone hydrogen bonds of BdpA in (a) GdmSCN and (b) GdmCl solutions using Gdm^+ force field of Jorgensen et al. (Ref.1) and TIP3P explicit solvent model. (Back line: the number of backbone hydrogen bonds; red line: the number of hydrogen bonds formed between carbonyl groups and water as hydrogen bonding donor; green line: the number of hydrogen bonds formed between carbonyl groups and Gdm^+ as hydrogen bonding donor).

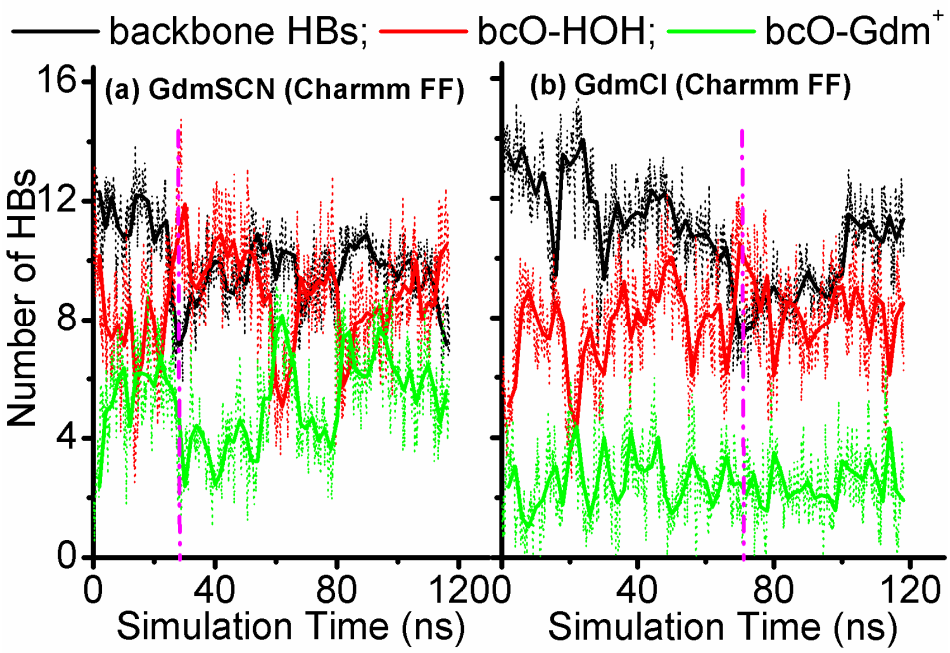

Figure S7. The breaking and formation of hydrogen bonds for residues involved in all backbone hydrogen bonds of BdpA in (a) GdmSCN and (b) GdmCl solutions using Gdm^+ force field of MacKerell et al. (Ref.2) and SPC/E explicit solvent model. (Back line: the number of backbone hydrogen bonds; red line: the number of hydrogen bonds formed between carbonyl groups and water as hydrogen bonding donor; green line: the number of hydrogen bonds formed between carbonyl groups and Gdm^+ as hydrogen bonding donor).

Reference

1. Jorgensen, W. L.; Tiradorives, J. *J. Am. Chem. Soc.* **1988,** 110, 1657-1666.
2. MacKerell, A. D.; Bashford, D.; Bellott, M.; Dunbrack, R. L.; Evanseck, J. D.; Field, M. J.; Fischer, S.; Gao, J.; Guo, H.; Ha, S.; Joseph-McCarthy, D.; Kuchnir, L.; Kuczera, K.; Lau, F. T. K.; Mattos, C.; Michnick, S.; Ngo, T.; Nguyen, D. T.; Prodhom, B.; Reiher, W. E.; Roux, B.; Schlenkrich, M.; Smith, J. C.; Stote, R.; Straub, J.; Watanabe, M.; Wiorkiewicz-Kuczera, J.; Yin, D.; Karplus, M. *J. Phys. Chem. B* **1998,** 102, 3586-3616.