Supporting Information:

Investigation of the Polymeric Properties of α-Synuclein and Comparison with NMR Experiments: A Replica Exchange Molecular Dynamics Study

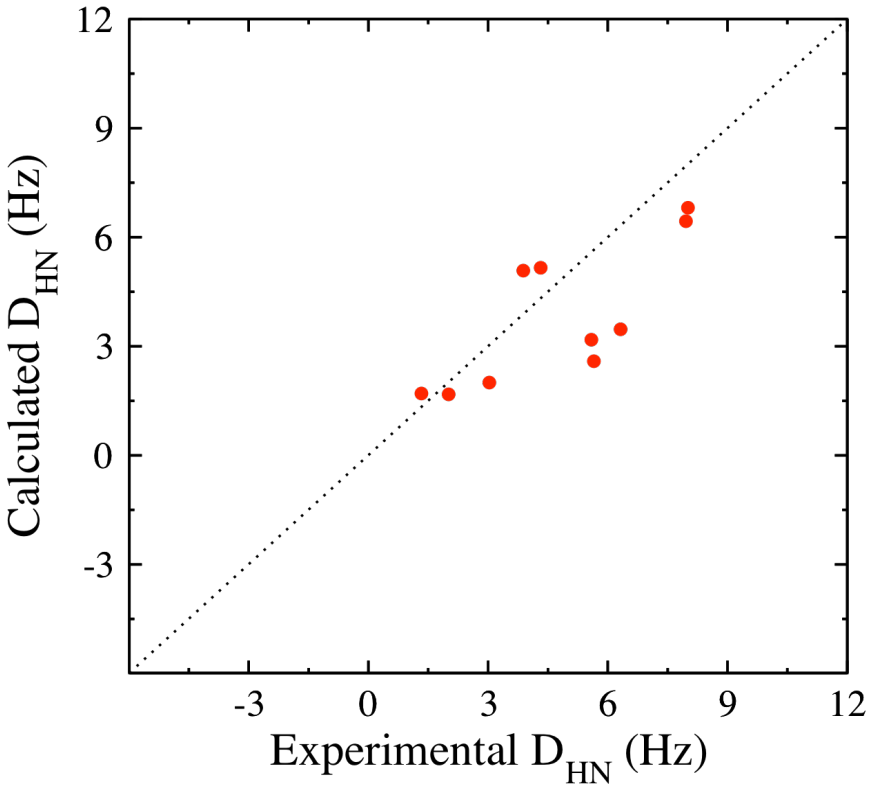

Figure S1

Comparison of the calculated HN RDCs not used in the fitting procedure. Red dots correspond to the back-calculated RDCs not used in the fitting procedure used for the selection of ensembles fitting the experiment.

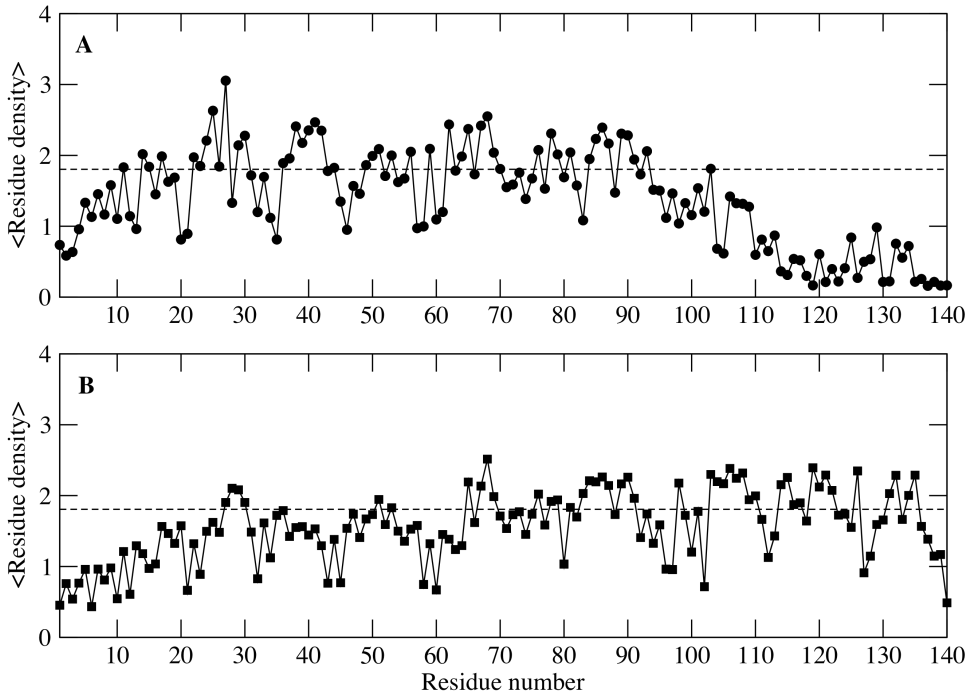

Figure S2

Comparison of residue densities of α-synuclein at neutral (A) and low pH (B) conditions.

The low pH simulation ensembles were generated for a study published previously [1]. The N and C terminal regions of α-synuclein show significant changes in the residue density with change in pH. With shift in pH from low to neutral pH, the total charge in the N-terminus increases significantly while the net charge is low. This region adopts a more collapsed conformation with increased charge density, as predicted from theory of polyampholyte chains. The C-terminal region is observed to also show an increase in charge density with increasing pH, although net charge also increases significantly in this case, leading to charge repulsion resulting in an expanded conformation of this region with increase in pH. The behavior of the C-terminal region at neutral pH is consistent with that expected for a polyelectrolyte chain.

Convergence of Simulations:

To assess the convergence of simulations, we calculated the standard errors of the means for the scaling of internal distances. Fig. S3 shows the scaling of internal distances plotted as a function of sequence separation for the low, intermediate and high temperature ensembles. The error bars represent the calculated standard errors of the means. The low values of the calculated standard errors of the mean indicate that the simulations are well converged.

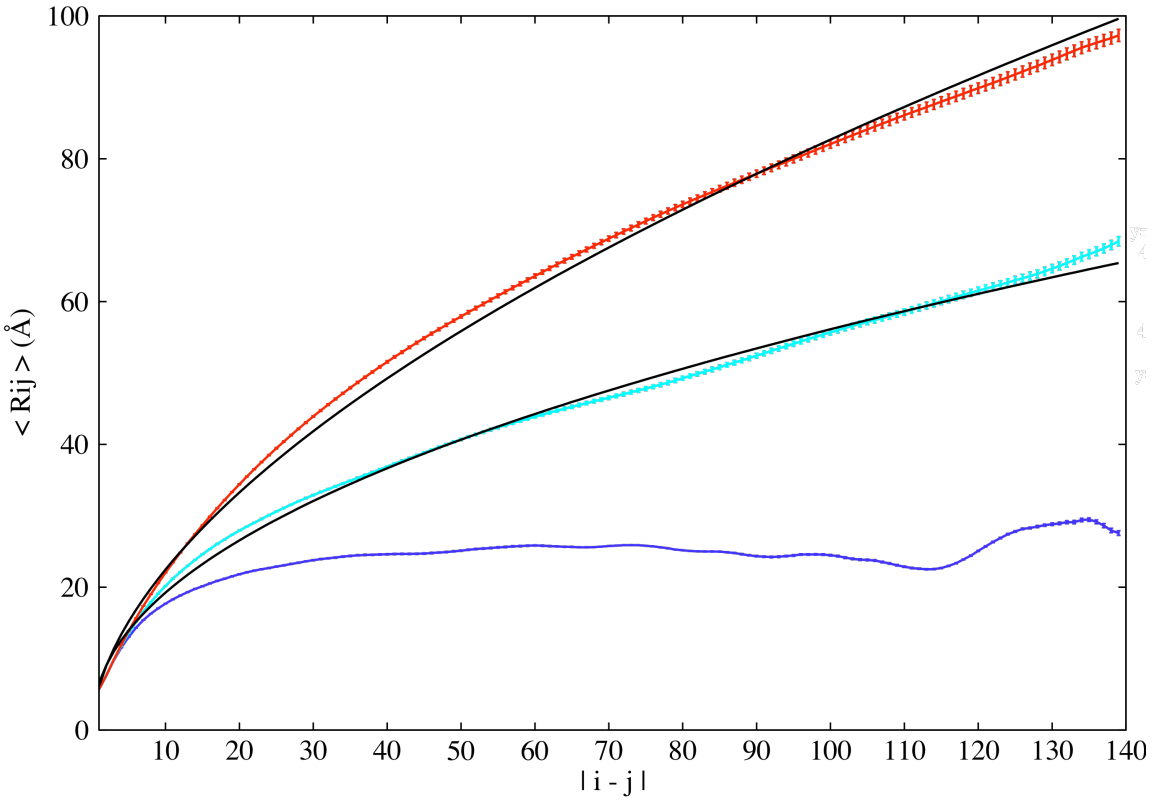

Figure S3

Scaling of internal distances as a function of sequence separation for the low (blue), intermediate (cyan) and high (red) temperature ensembles. Error bars represent the standard errors of the mean.

Supplemental References

(1) Wu, K.-P.; Weinstock, D. S.; Narayanan, C.; Levy, R. M.; Baum, J. *J Mol Biol* **2009**, *391*, 784.