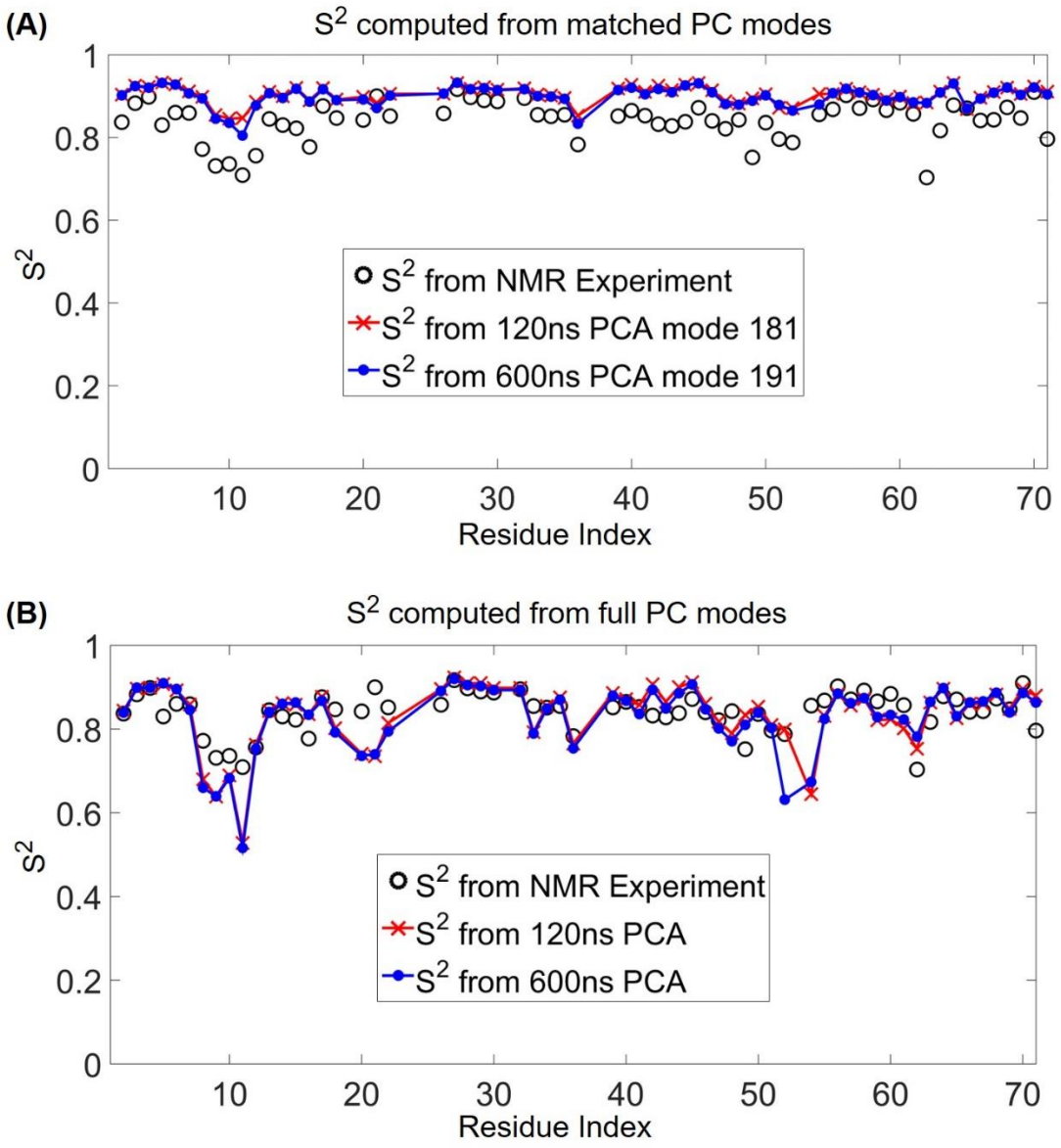

Fig S3. NMR order parameters (S^2) estimated from the 120 ns and 600 ns MD trajectories. **(A)** The profiles are the order parameters derived from PC modes (k=181 and 191 for 120 and 600ns simulations, respectively) that best-match the experimental data. One can obtain the time scales of 1.0 ns and 2.3 ns for the NMR-characterized S^2 profile from the best-matched mode 181 and 191, respectively. **(B)** The profiles are order parameters derived from full PC modes (k=1 in **Eq S9**). It is readily understandable that the longer the simulation is, the wider the spatial distribution (and therefore less order) of an atom would result.