**Figure S2. Chemical shifts prediction for 1** µs DriFREE **simulation.** Chemical shifts were predicted from the 1 µs DriFREE simulation by the PPM webserver [12] and compared to experimental chemical shifts of 1C20 PDB entry. Rmsd values for the different atom types (Cα, Cβ, C’, HN and N) have been plotted as a function of the simulation time. The green dotted line corresponds to the rmsd value calculated by PPM for the starting structure of the simulation (first conformer in 1C20 PDB entry).

****