Supporting Information:

Predictive Atomic Resolution Descriptions of Intrinsically Disordered hTau40 and α -Synuclein in Solution from NMR and Small Angle Scattering

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FIGURE LEGENDS

S1. Reproduction of htau40 RDCs by the ensemble selected against ${}^{13}C^{\alpha}$, ${}^{13}C^{\beta}$, ${}^{13}C^{\circ}$, ${}^{15}N$ and ${}^{1}H^{N}$ chemical shifts (CSs), SAXS and paramagnetic relaxation enhancements (PREs) from 12 different cysteine mutants were combined in a single ensemble selection. Top – Five independent selections showing the reproducibility of the RDC prediction. Red – experimental, blue - predicted. Middle – reproduction of experimental data (red) by RDCs calculated using the local alignment window approach combined with a generic baseline modulation assuming no long-range contacts (black line). Bottom - reproduction of experimental data (red) by RDCs calculated using the local alignment window approach combined with the baseline modulation calculated directly from the ensemble of structures (black line). See also figure 6.

S2. Dependence of the reduced χ^2 for cross-validated ${}^{1}D_{HN}$ RDCs on the conformational differences between the statistical coil (black points) and ASTEROIDS selection (red points) based on CSs, SAXS and PREs. When all residues are included in the comparison the cross-validated χ^2 is approximately twice as good for the ASTEROIDS selection compared to statistical coil. This improvement increases when only amino acids deviating from the statistical coil are included in the comparison. $\Delta_{Rama,thresh}$ defines a measure of the difference in local backbone potentials between the statistical coil and selected ensemble for each amino acid. N is the number of amino acids fulfilling this criterion and therefore retained in the average. See also table 1.





Figure S2

