Supporting Information for: Single-Protein Collapse Determines Phase Equilibria of a Biological Condensate

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Figure S1: MD simulation of FUS θ temperature. (a) Simulated radii of gyration of FUS protein fragments as a function of the fragment length, |i − j|, where i and j indicate the indices of the fragment’s terminal beads. Each $R_g(|i − j|)$ value was obtained by averaging over all (i, j) pairs of the same index difference. (b) The scaling exponent $\nu$ that best describes the asymptotic relation $\langle R_g(i − j) \rangle \sim |i − j|^{\nu}$ when the difference of the bead indices $|i − j| \rightarrow \infty$. The horizontal dashed line indicates the $\nu = 0.5$ value that corresponds to the θ temperature.
Figure S2: The ratio of the averaged bond length, $l_0$ and averaged the bond angle, $\psi$ at different temperatures to the values at 290 K. Each data point was extracted from the last 3 $\mu$s fragment of a 5 $\mu$s MD trajectory of a single FUS protein.
Figure S3: Determination of virial coefficient parameters. Open and solid symbols show the values of $\sigma$ and $q$, respectively, obtained directly from MD simulations of individual FUS proteins at specified temperature. Red circles plot the right-hand side of Eq. (5) evaluated using the $\sigma$ and $q$ obtained from the MD simulations. Blue squares show the values of the left-hand side of Eq. (5) evaluated using the best fit values for $B$ and $K$. The residue of the fitting, i.e., the difference between the right-hand side and the left-hand side of Eq. (5), is 0.04, which corresponds to a relative error of $\sim 7\%$. 
Movie 1: Animation illustrating a CG MD simulation of 64 WT FUS proteins at 292 K, forming a liquid-like droplet after ~ 1μs.
Movie 2: Animation illustrating a CG MD simulation of 64 (R→K) FUS mutants at 292 K, remaining disperse state after ~ 1μs.
Movie 3: Animation illustrating three CG MD simulations of a slab FUS system performed at different temperatures. Each system contains 125 FUS proteins.