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

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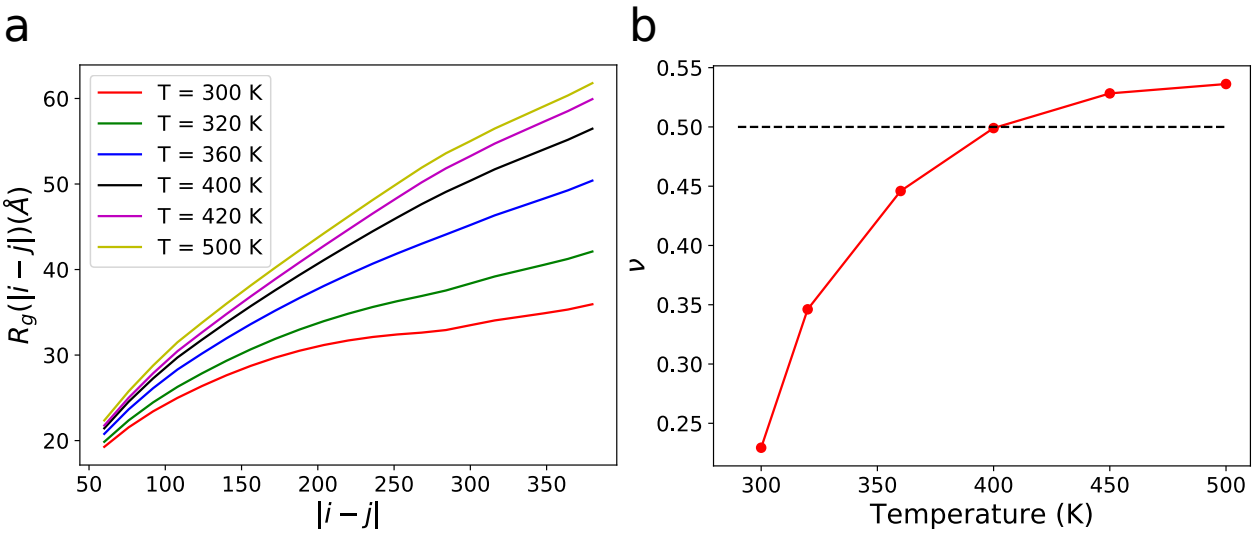


Figure S1: MD simulation of FUS θ temperature. (a) Simulated radii of gyration of FUS protein fragments as a function of the fragment length, $|i-j|$, where i and j indicate the indices of the fragment's terminal beads. Each $R_g(|i-j|)$ value was obtained by averaging over all (i,j) pairs of the same index difference. (b) The scaling exponent ν that best describes the asymptotic relation $\langle R_g(i-j)\rangle \sim |i-j|^{\nu}$ when the difference of the bead indices $|i-j| \to \infty$. The horizontal dashed line indicates the $\nu = 0.5$ value that corresponds to the θ temperature.

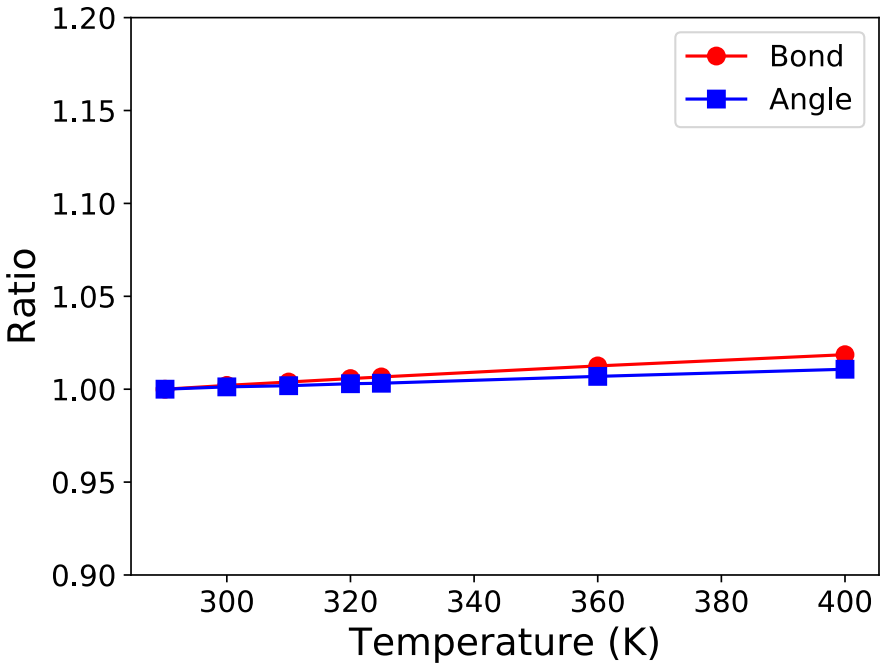


Figure S2: The ratio of the averaged bond length, l_0 and averaged the bond angle, ψ at different temperatures to the values at 290 K. Each data point was extracted from the last 3 μs fragment of a 5 μs MD trajectory of a single FUS protein.

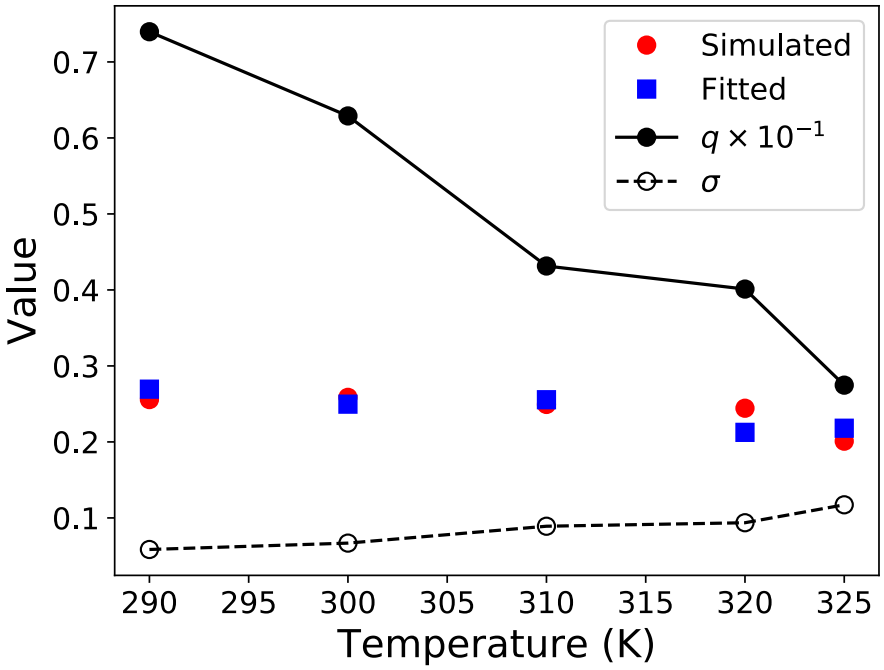
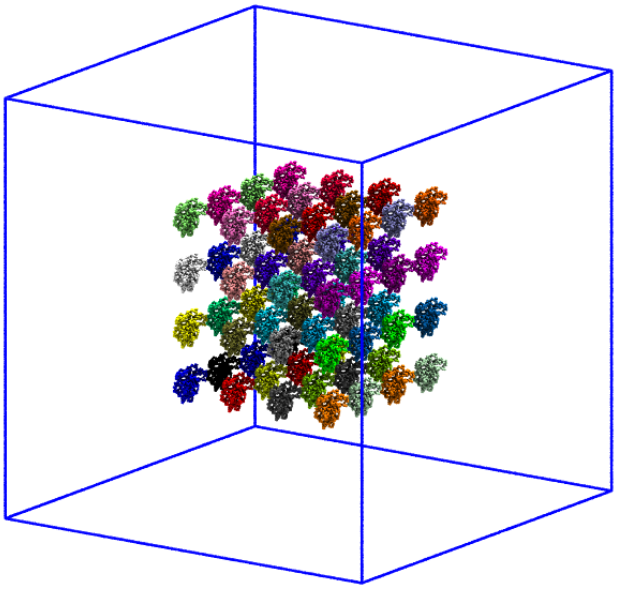
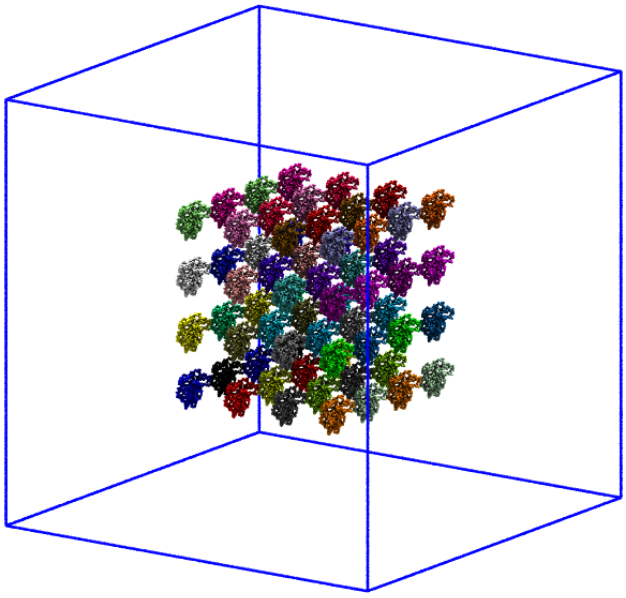


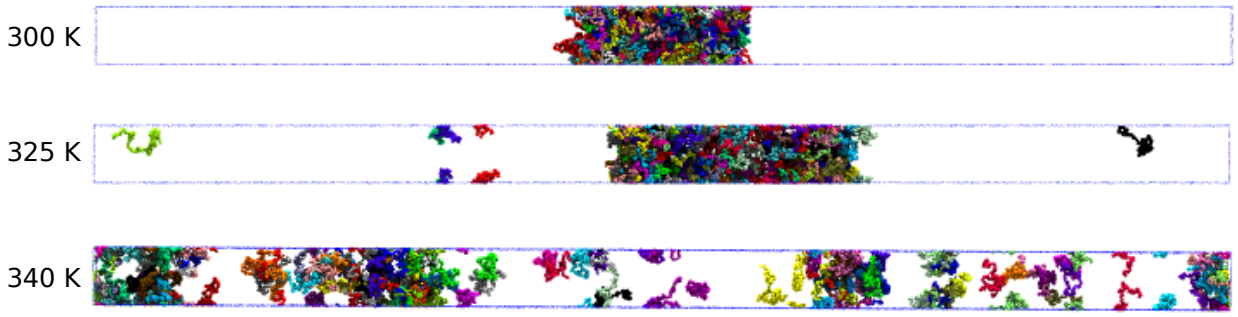
Figure S3: Determination of virial coefficient parameters. Open and solid symbols show the values of σ and q, respectively, obtained directly from MD simulations of individual FUS proteins at specified temperature. Red circles plot the right-hand side of Eq. (5) evaluated using the σ and q obtained form 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 ~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.