

Charge pattern affects the structure and dynamics of polyampholyte condensates

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Supporting Material

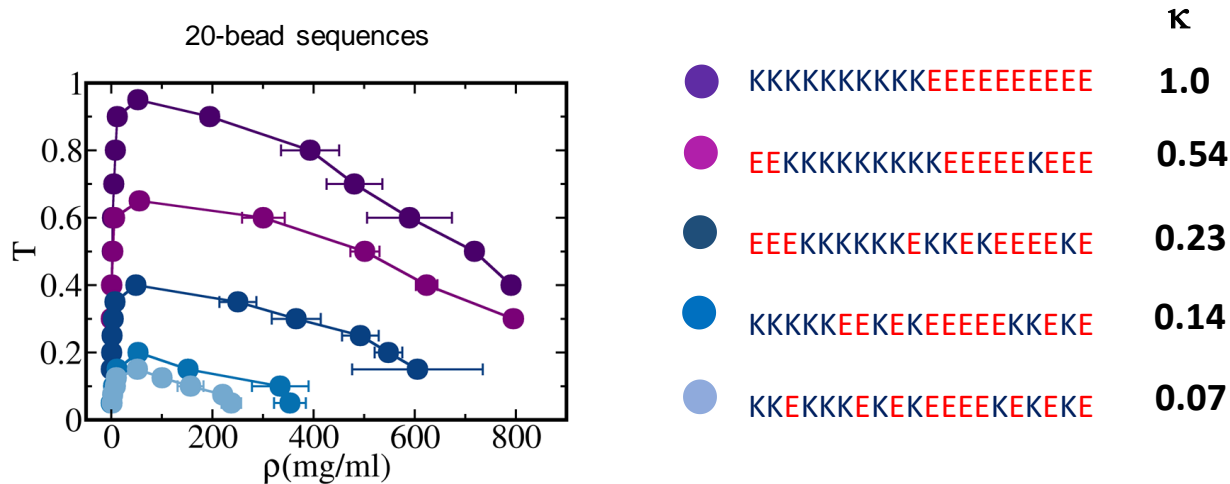


Figure S1. Temperature-density phase diagram of model 20-bead polyampholyte sequences. The critical temperature has been evaluated from the following relation of universal scaling of density near critical point, $\rho_{Dense\ phase} - \rho_{Dilute\ phase} = A \left(1 - \frac{T}{T_c}\right)^\beta$. Coloring scheme represents sequence charge pattern (κ) in model IDP sequences as shown on the right.

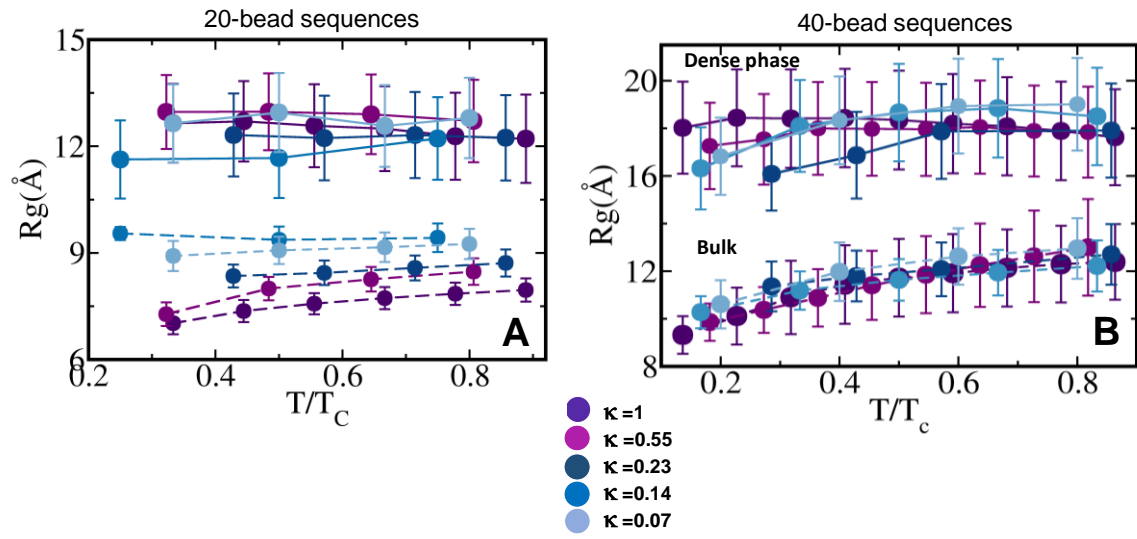


Figure S2. Dimension of polyampholytes in dense and bulk. Average R_g of dense phase (solid lines) and bulk (dashed lines) as a function of temperature for (A) 20-bead polymers and (B) 40-bead polymers.

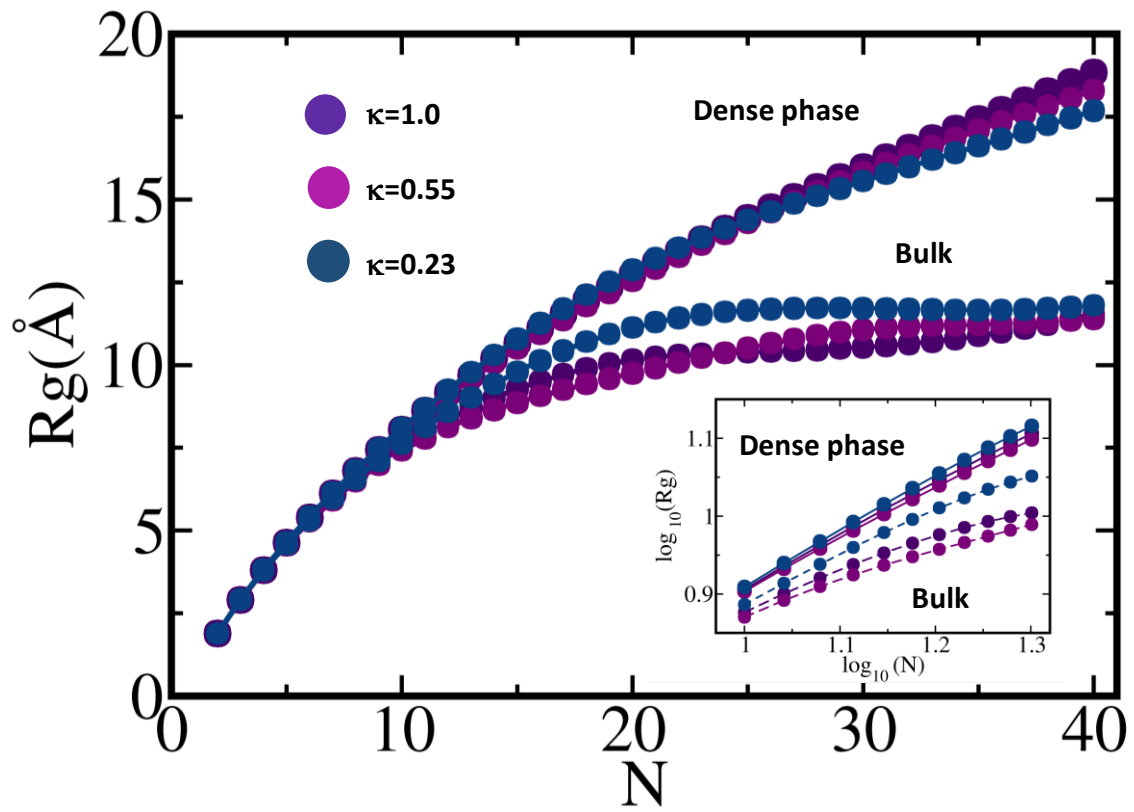


Figure S3. Average radius of gyration (R_g) as a function of polymer size (N) in dense phase (Circle with solid line) and bulk (Circle with dashed line) calculated from trajectories of polymers consisting 40 amino acid beads. Polymers in dense phase have predominantly extended conformations. While fitted with the following relation $\log R_g = A_0 + \nu \log N$, the Flory exponent (ν) turns out to be 0.69 and almost independent of sequence charge distribution in dense phase. In bulk, Flory exponent of polymers varies between 0.3-0.55 depending on sequence κ . For sequence $\kappa=1$, Flory exponent is higher than $\kappa=0.55$ in bulk, owing to its unique nature of charge distribution which let the polymers to adopt a hairpin like conformation.

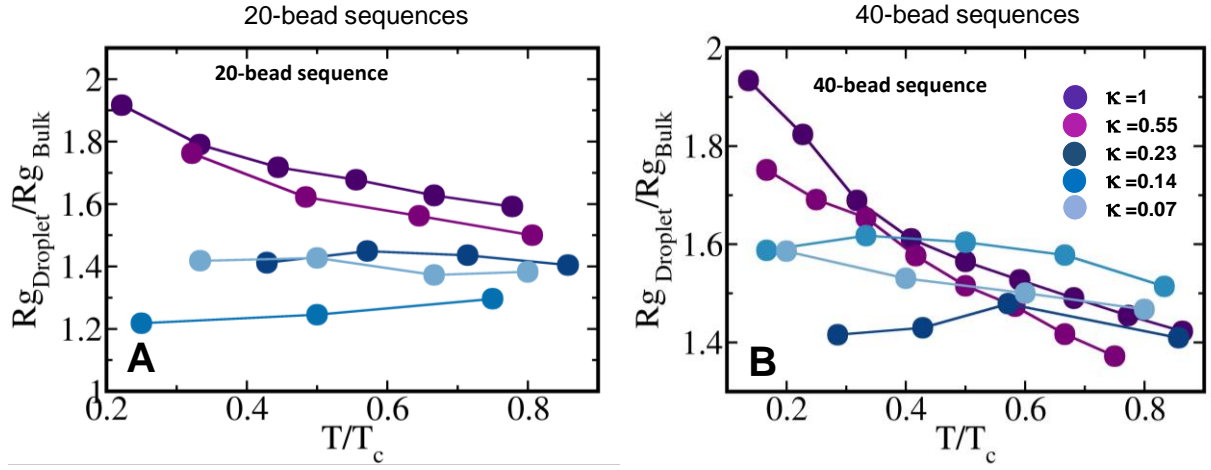


Figure S4. Ratio of average R_g of polymers in droplet and bulk. The ratio of R_g is plotted as a function of scaled temperature with regard to the critical point for (A) 20-bead polymers and (B) 40-bead polymers. For similar distance from criticality, the ratio tends to increase with increase in sequence κ (prominent in high- κ regime). When sequence κ is large, the ratio tends to decrease with temperature. But for low sequence κ the ratio does not show such trend.

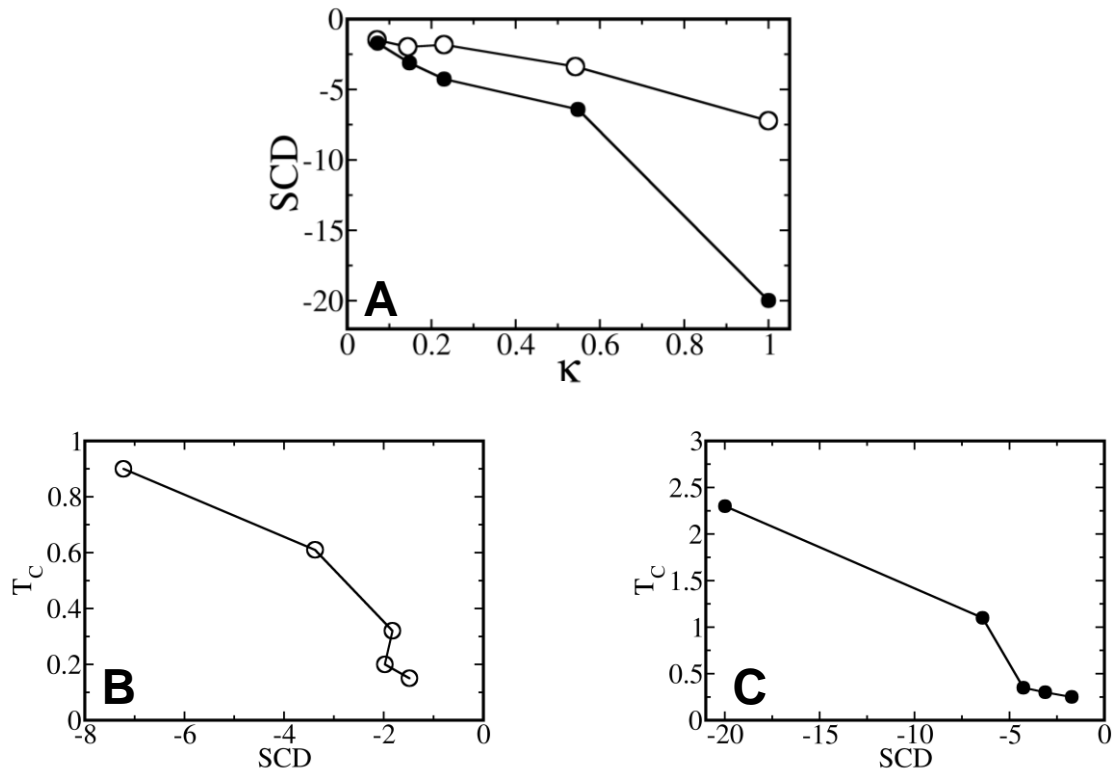


Figure S5. Sequence properties of the studied polyampholytes. A). Sequence charge decoration (SCD) metric of Sawle and Ghosh² plotted against the sequence charge pattern order parameter introduced by Das and Pappu¹ for 20-bead (void circles) and 40-bead sequences (filled circles) used in the present work. The dependence of the critical temperature of the 20- (B) and 40-bead (C) sequences on SCD. These figures complement the correlation between the critical temperature and κ (Figure 1, inset).

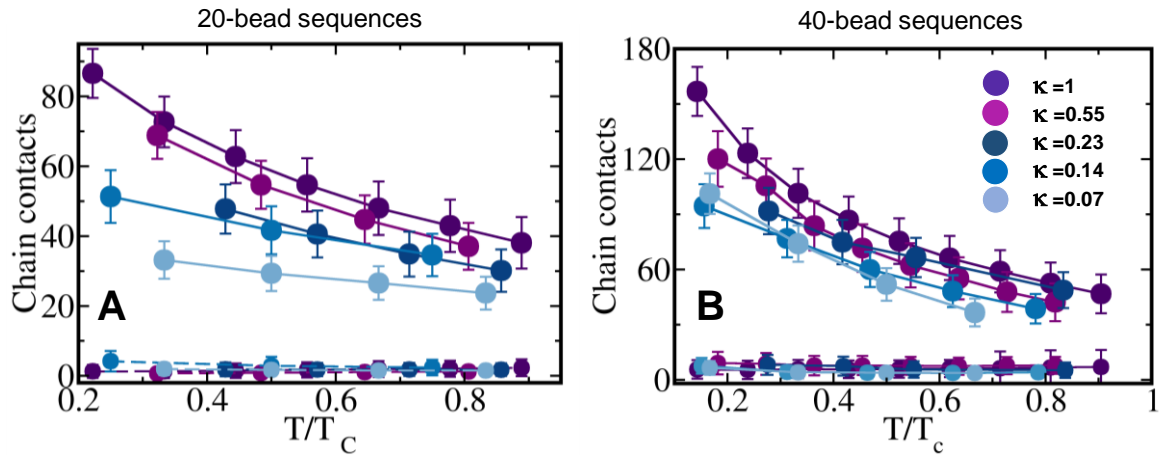


Figure S6. Average inter-chain and intra-chain contacts for each polymer in the dense phase plotted against temperature. The number of inter and inter contacts in dense phase is plotted for (A) 20-bead polymers and (B) 40-bead polymers. For same distance from criticality, the inter-chain contacts tend to decrease as sequence κ decreases. The same effect is observed when one tends to increase the temperature for a specific sequence.

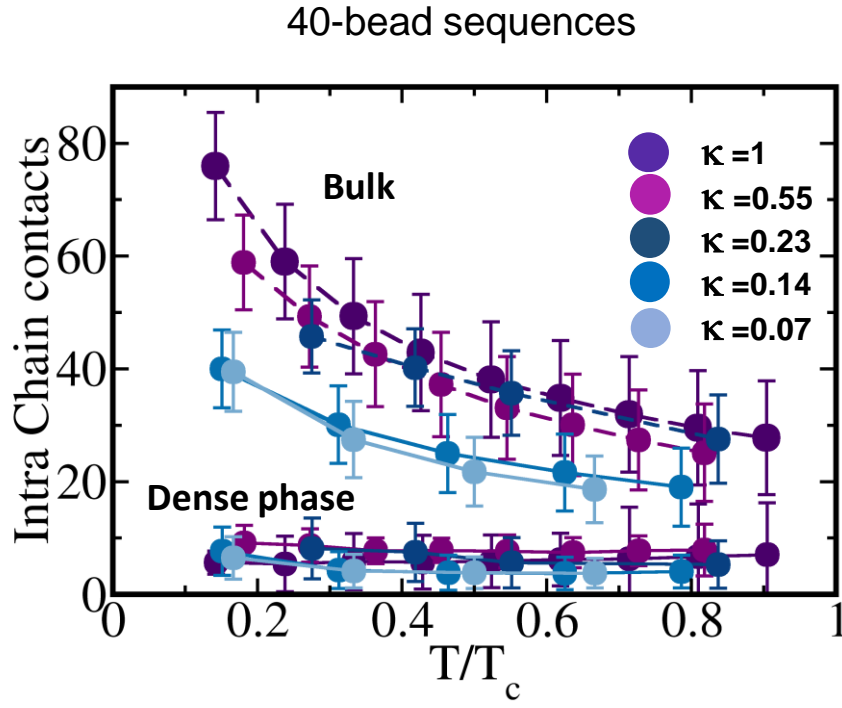


Figure S7. Average intra-chain contact per chain in dense phase and bulk as a function of temperature for κ for 40-bead sequences. Intra-chain contact increases 10-fold in bulk than that of droplet phase for a chain. With increase in temperature, intra-chain contacts show a pronounced decrease in bulk. Decrease in sequence charge pattern order parameter also has the same effect in bulk at the same distance from criticality.

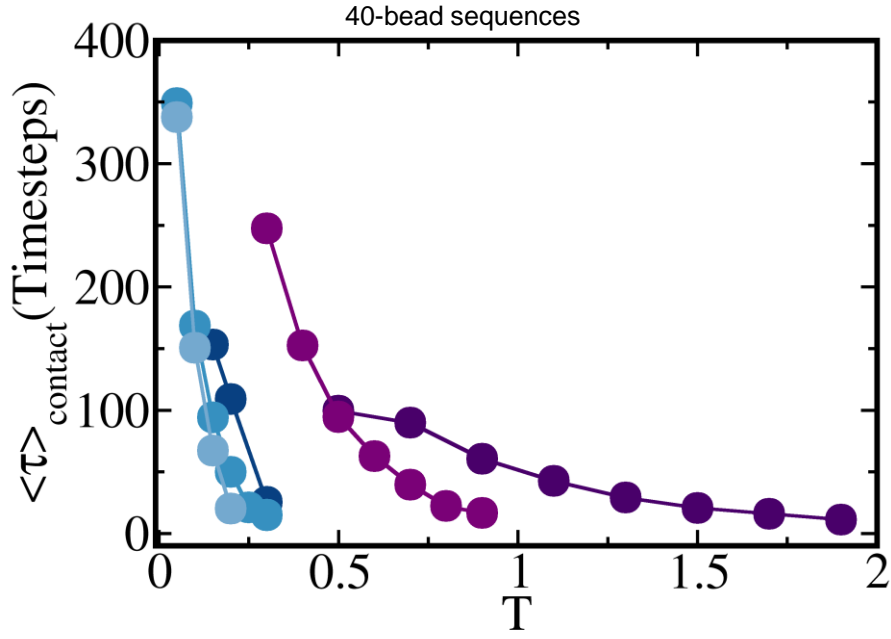


Figure S8. Average timescale of nearest neighbor contact flip plotted against temperature for 40-bead polymers. In order to obtain the time scales we define the correlation function, $c(t) = \frac{\langle h(0)h(t) \rangle}{\langle h(0)h(0) \rangle}$; where $h(t)$ is a step function. $h(t)$ is 1 as long as a nearest neighbor contact stays continuously in the dense phase, when the contact breaks $h(t)=0$. The timescales are obtained from a bi-exponential fit to the correlation function $c(t)$.

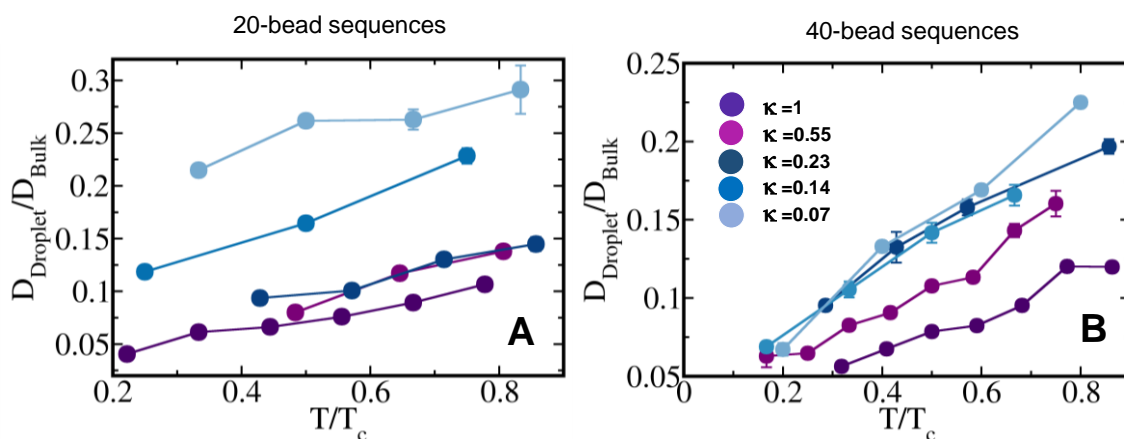


Figure S9. Ratio of translational diffusion constant in dense phase and bulk. The ratio is plotted against temperature for (A) 20-bead polymers and (B) 40-bead polymers. For same distance from criticality, we observe a prominent decrease in the ratio with increase in sequence κ due to the fact that inter-chain contacts tend to increase with sequence κ , hence the viscosity of the dense phase increases. As temperature breaks the inter-chain contacts of polymers in droplet, we observe a rise in the ratio for every sequence with increase in temperature.

- (1) Das, R. K.; Pappu, R. v. Conformations of Intrinsically Disordered Proteins Are Influenced by Linear Sequence Distributions of Oppositely Charged Residues. *Proceedings of the National Academy of Sciences of the United States of America* 2013, *110* (33), 13392–13397. <https://doi.org/10.1073/pnas.1304749110>.
- (2) Sawle, L.; Ghosh, K. A Theoretical Method to Compute Sequence Dependent Configurational Properties in Charged Polymers and Proteins. *Journal of Chemical Physics* 2015, *143* (8). <https://doi.org/10.1063/1.4929391>.