Soft Matter

SUPPORTING INFORMATION

pH response of sequence-controlled polyampholyte brushes

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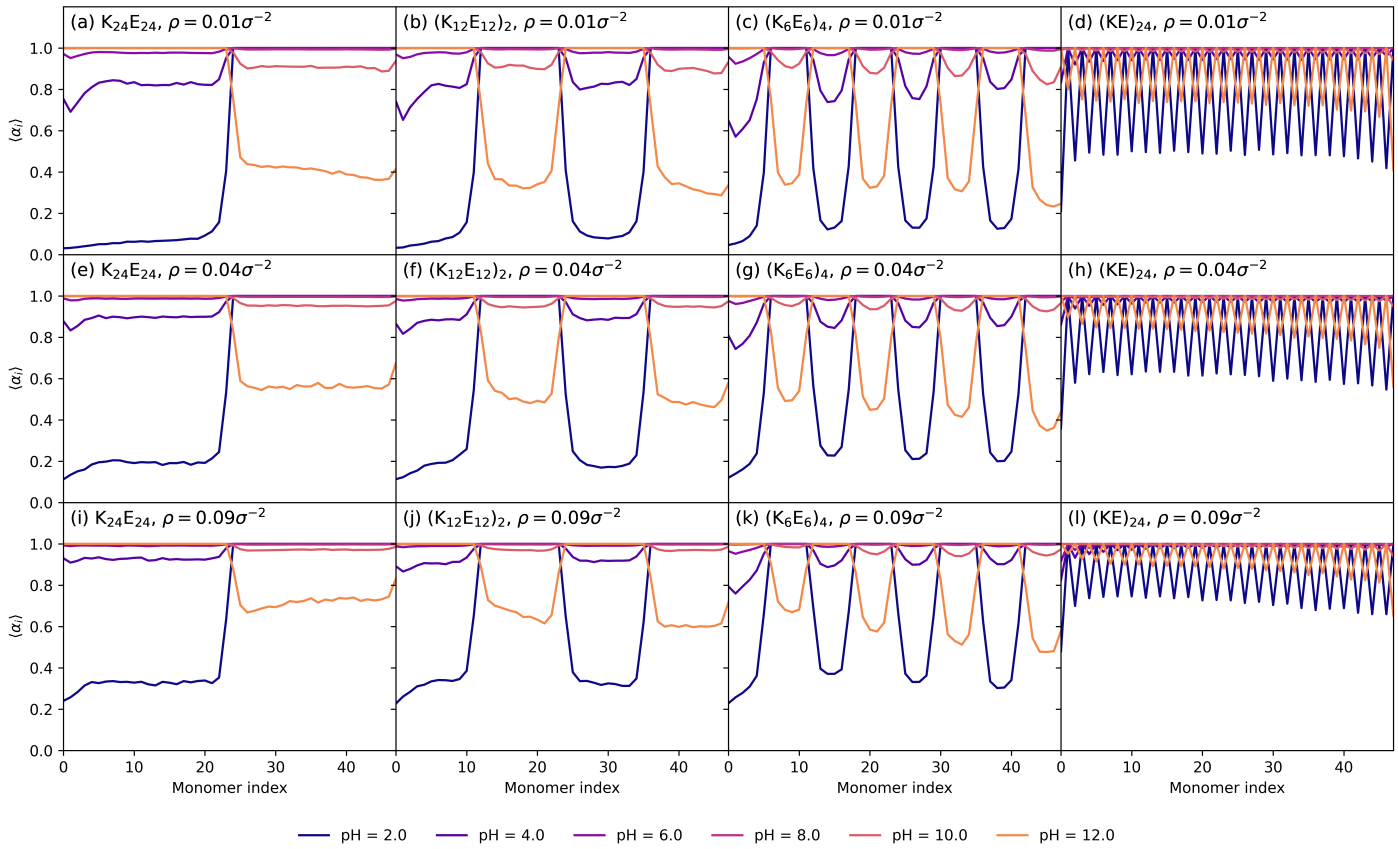

Fig. S1 The average degree of ionization $\langle \alpha_i \rangle$ as a function of monomer index i for brushes with different monomer sequences and grafting densities.

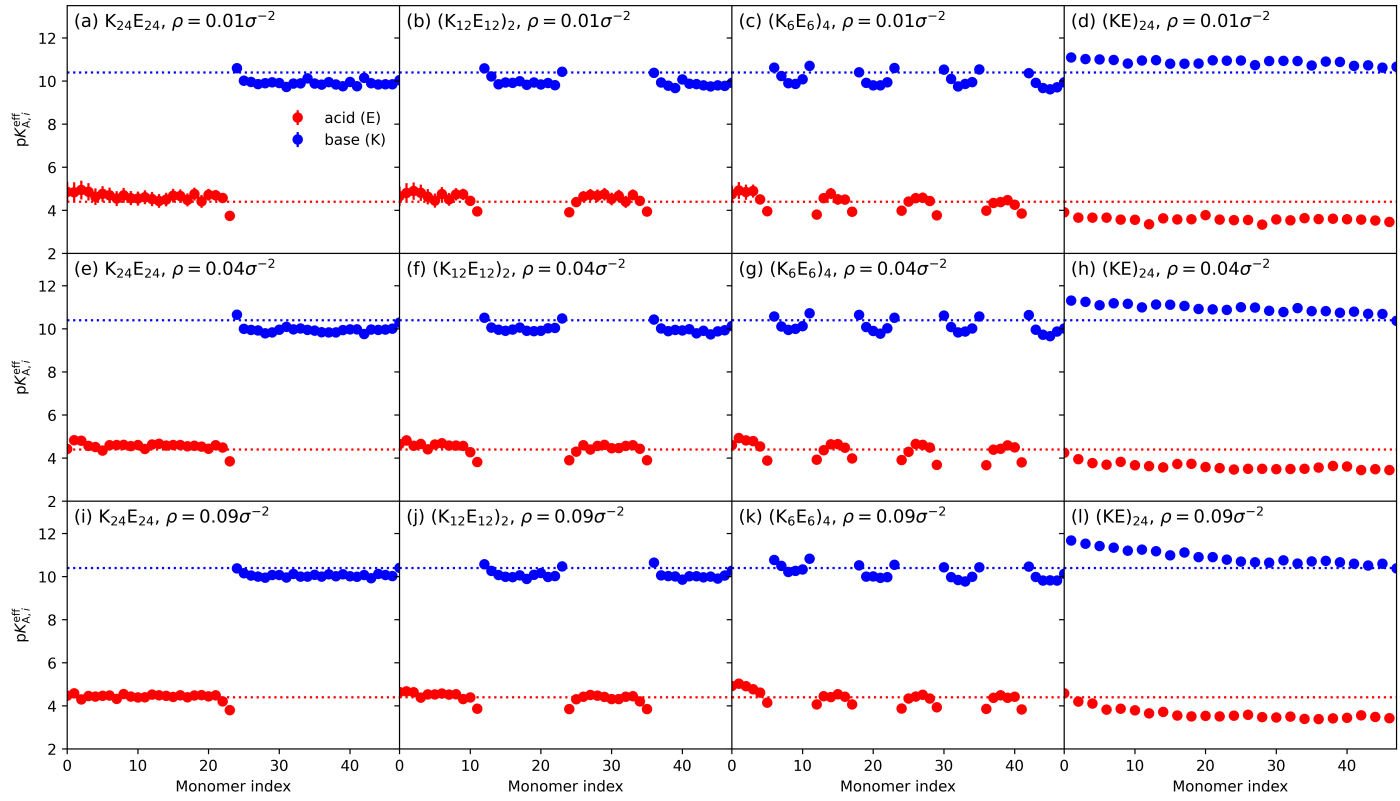

Fig. S2 The effective disassociation constants $pK_{A,i}^{eff}$ as a function of monomer index i for brushes with different monomer sequences and grafting densities. For acidic monomers, $pK_{A,i}^{acid,eff} = pH^{res} + \log_{10} \frac{1-\langle\alpha_i\rangle}{\langle\alpha_i\rangle}$, whereas $pK_{A,i}^{base,eff} = pH^{res} - \log_{10} \frac{1-\langle\alpha_i\rangle}{\langle\alpha_i\rangle}$ for basic monomers. The dotted lines show the intrinsic disassociation constant values of $pK_A^{acid} = 4.4$ and $pK_A^{base} = 10.4$

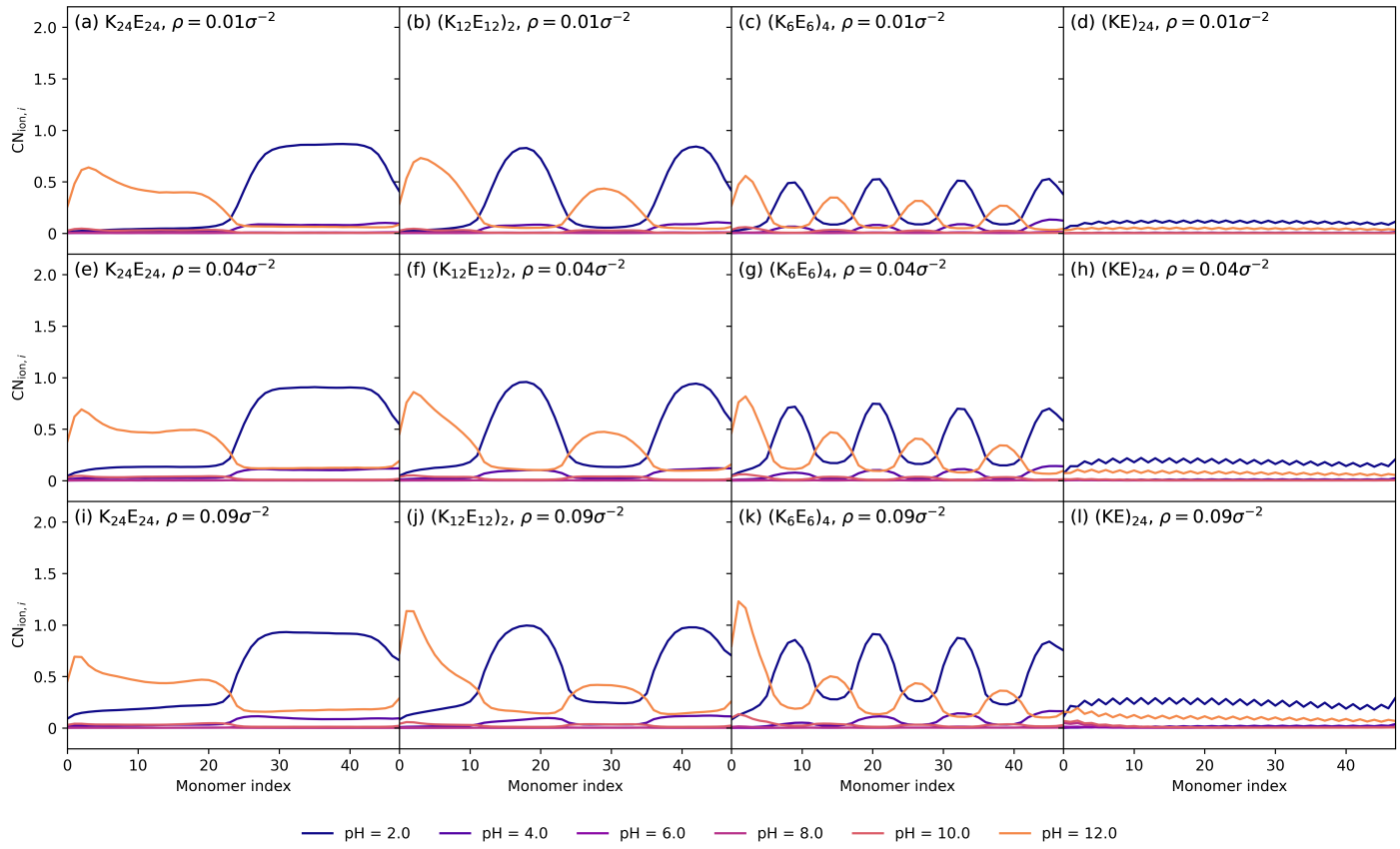

Fig. S3 The free ion coordination number (number of free solution ions near each monomer) $\mathrm{CN}_{\mathrm{ion},i}$ as a function of monomer index i for brushes with different monomer sequences and grafting densities. The coordination number was calculated using a cutoff radius of 1.5σ.

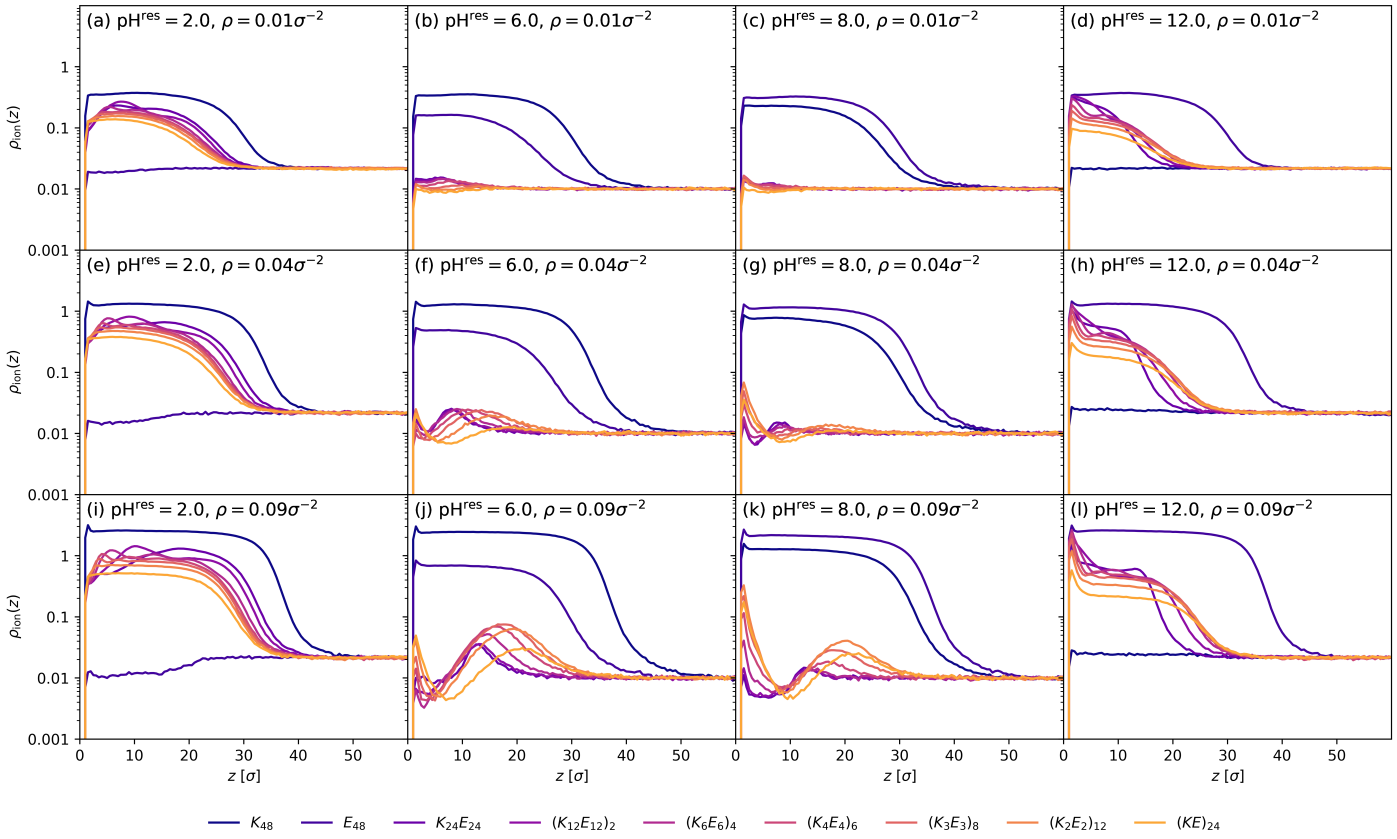

Fig. S4 The free ion number density $\rho_{\mathrm{ion}}(z)$ as a function of the distance from the grafting surface z for brushes with different monomer sequences and grafting densities.

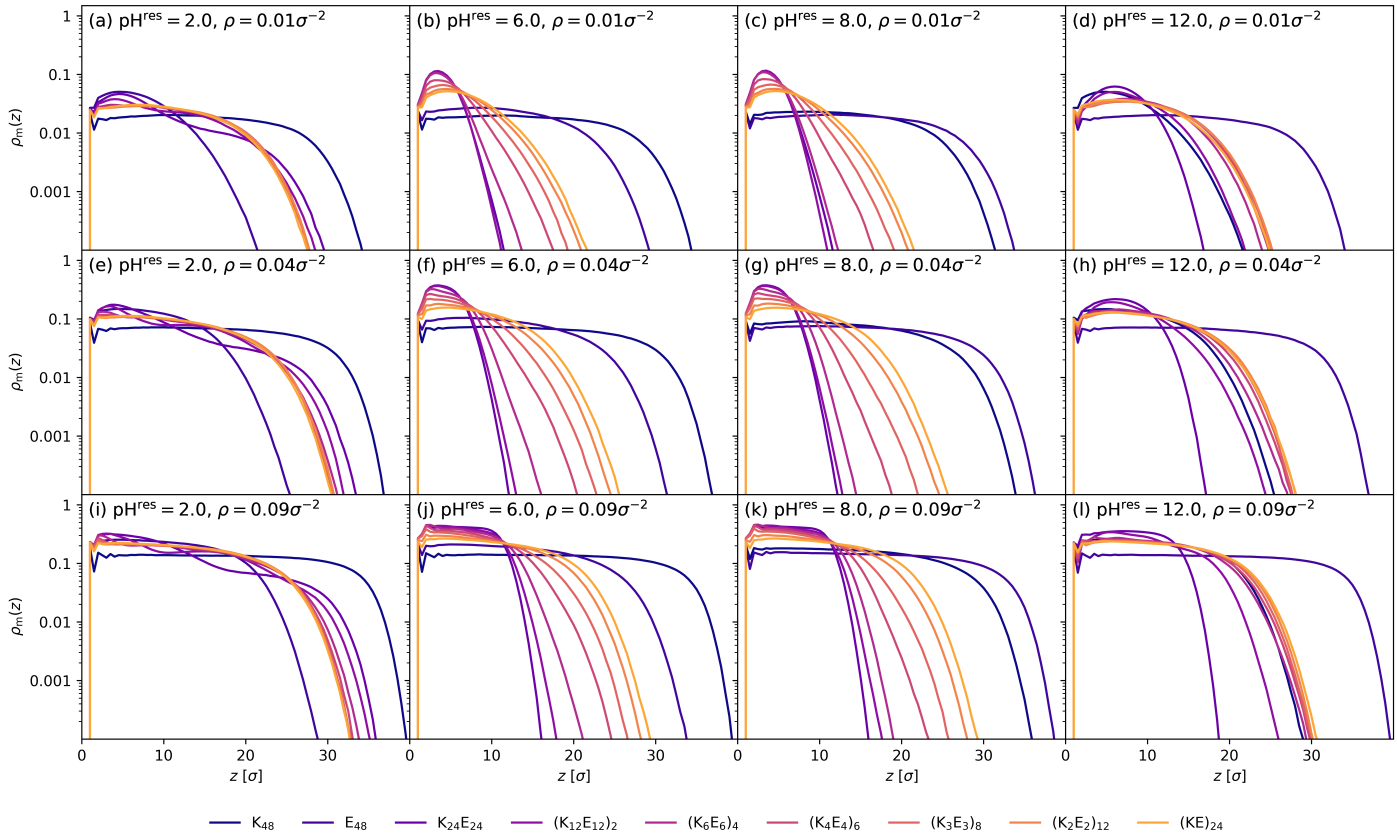

Fig. S5 The monomer number density $\rho_m(z)$ as a function of the distance from the grafting surface z for brushes with different monomer sequences and grafting densities.

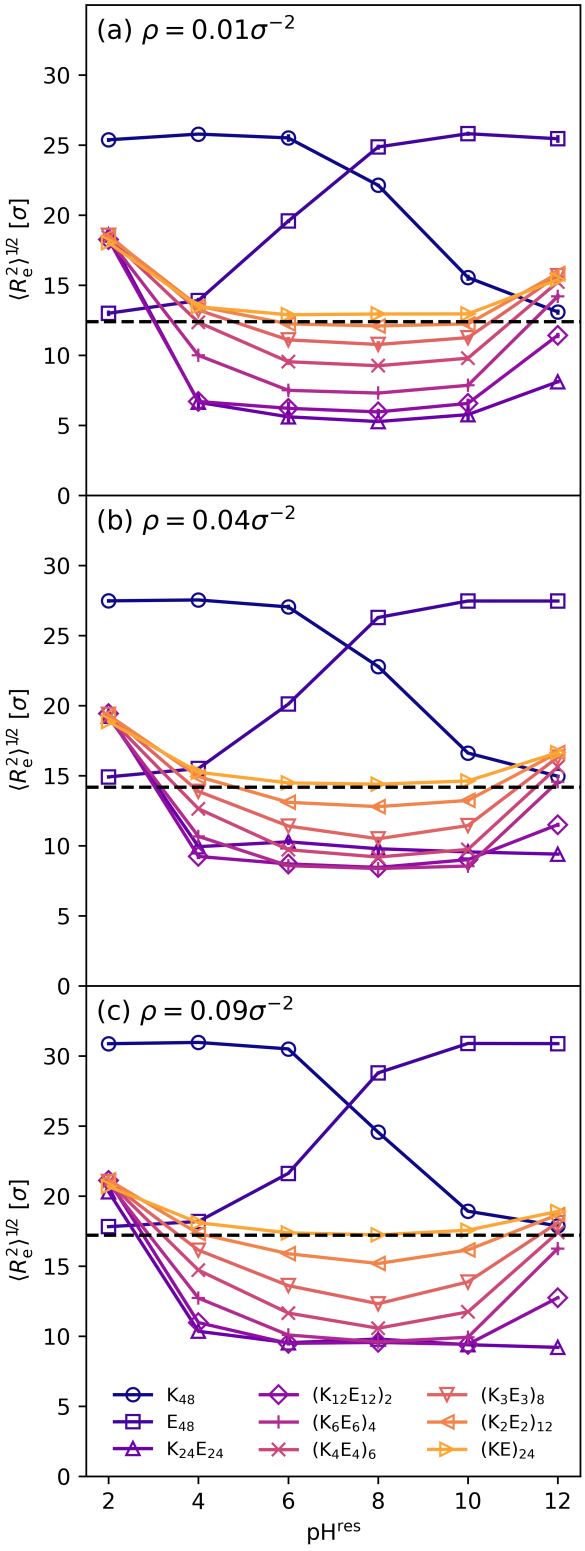

Fig. S6 Root-mean-squared chain end-to-end distance $\langle R_e^2 \rangle^{1/2}$ for brushes with different monomer sequences and grafting densities of $\rho =$ (a) 0.01, (b) 0.04, and (c) 0.09 σ^{-2}. The dashed line shows the reference value for a neutral brush with the same grafting density. Where not visible, uncertainties are smaller than symbol size.

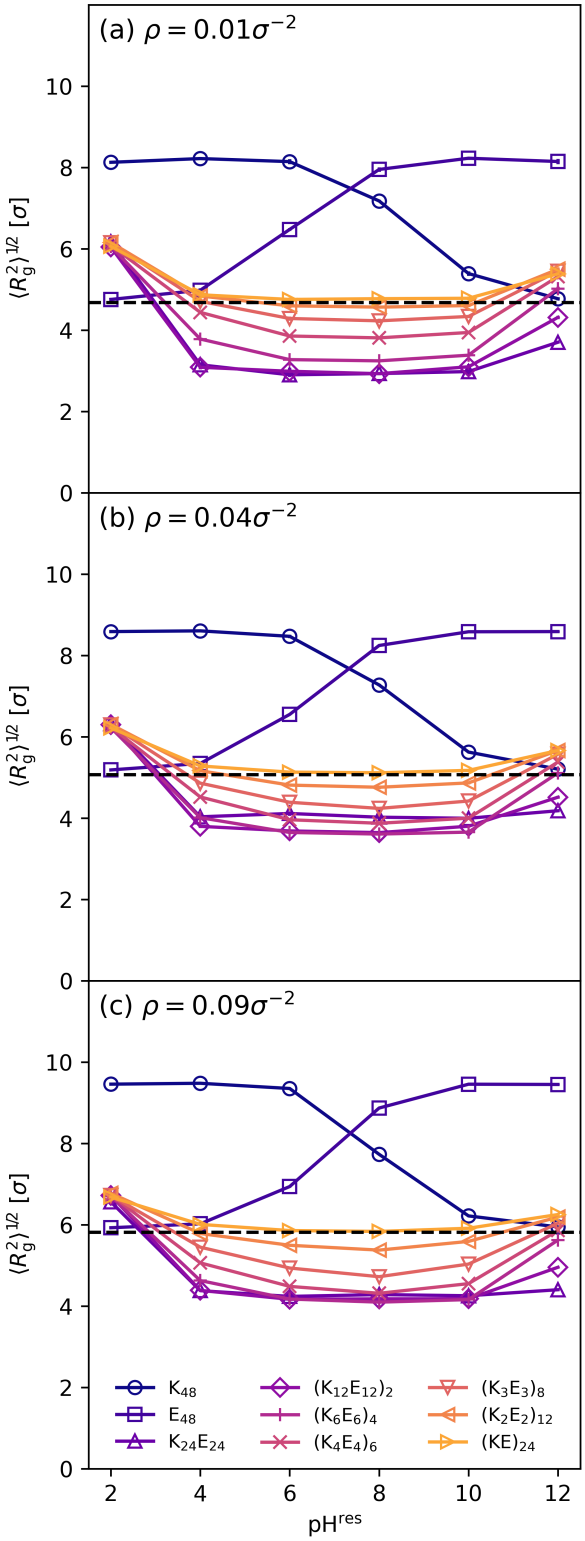

Fig. S7 Radius of gyration $\langle R_g^2 \rangle^{1/2}$ for brushes with different monomer sequences and grafting densities of $\rho =$ (a) 0.01, (b) 0.04, and (c) 0.09 σ^{-2}. The dashed line shows the reference value for a neutral brush with the same grafting density. Where not visible, uncertainties are smaller than symbol size.

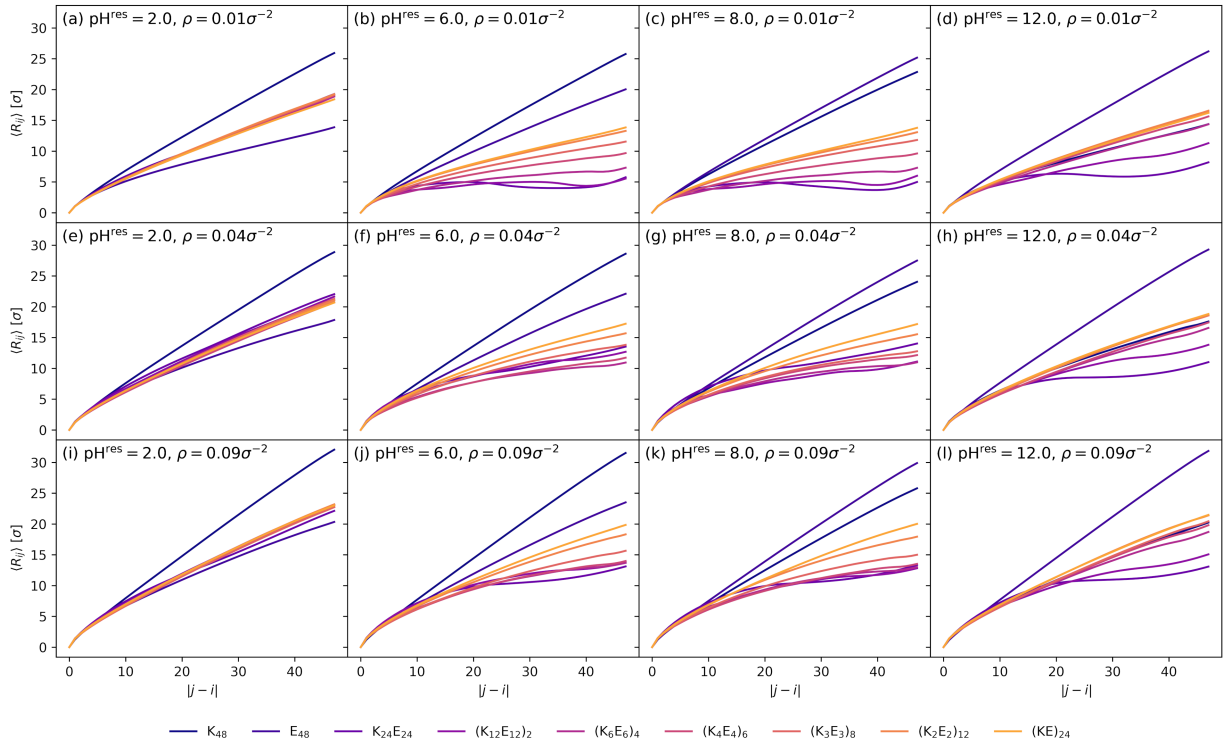

Fig. S8 The average intermonomer distance $\langle R_{ij} \rangle$ as a function of sequence separation in the chain $|j - i|$ for brushes with different monomer sequences and grafting densities. Non-monotonic behavior is observed near neutral pH^{res} for PABs with block sizes of 6, 12, and 24 ($(K_6E_6)_4$, $(K_{12}E_{12})_2$, and $K_{24}E_{24}$, respectively), indicating that the chains partially fold back on themselves due to attractive electrostatic interactions between oppositely charged blocks.