Supporting Information

Molecular complementarity and structural heterogeneity within co-assembled King-Webb β-sheet nanofibers

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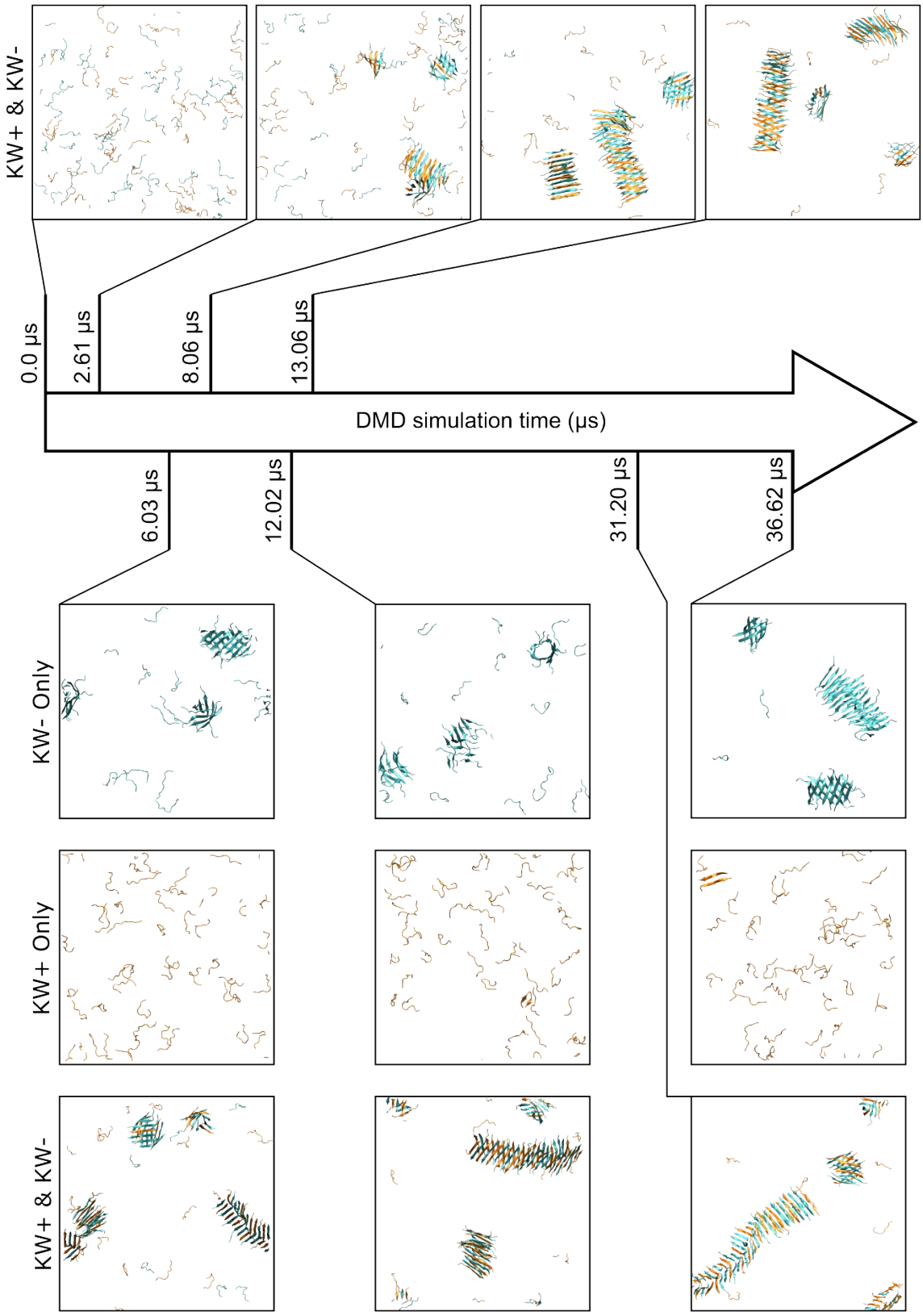

Figure S1. Snapshots of coarse-grained discontinuous molecular dynamics (DMD) simulations of King-Webb peptides at specified times.

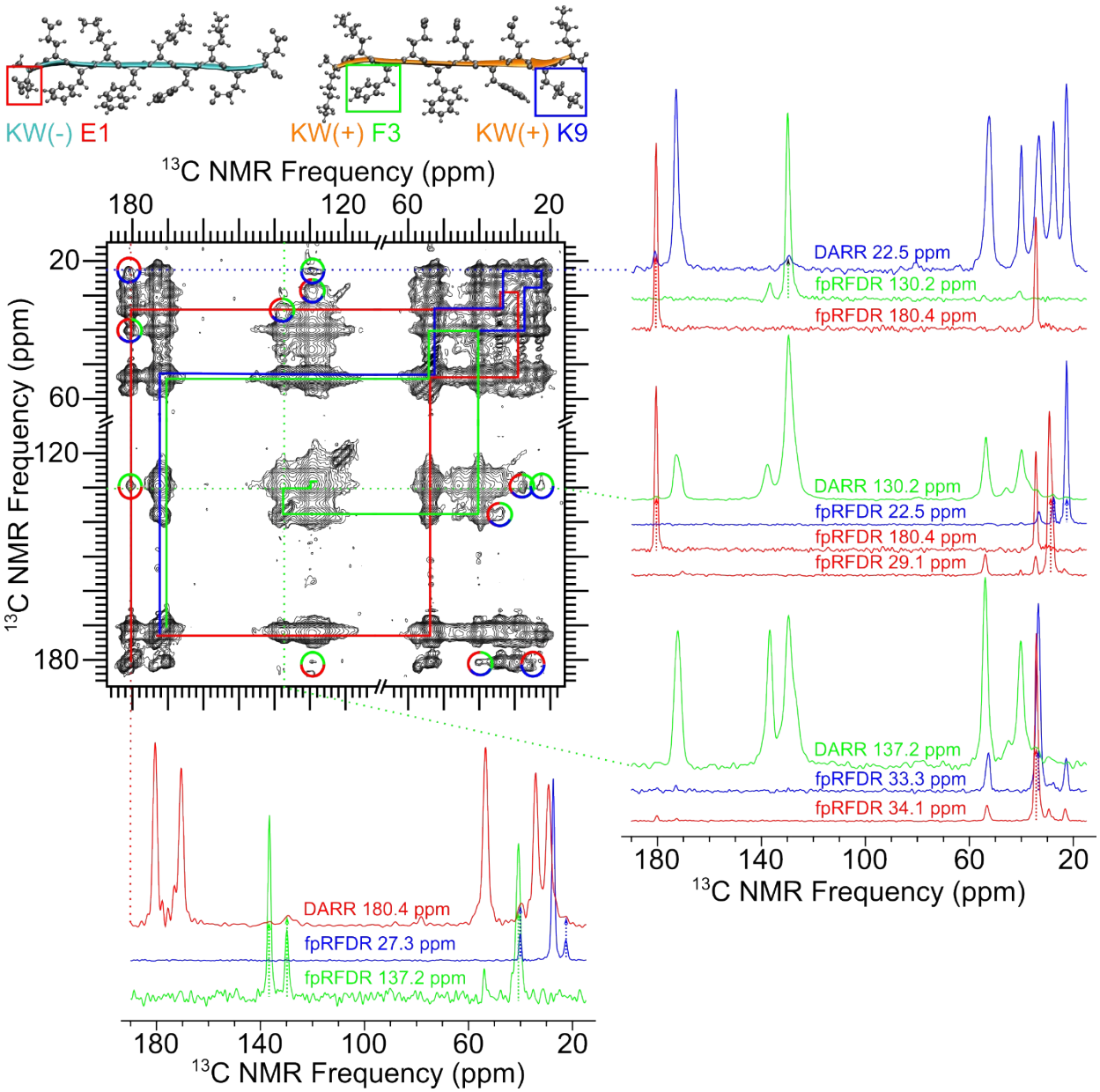

Figure S2. 2D ^{13}C-^{13}C 500ms dipolar assisted rotational resonance (DARR) spectrum of an isotopically labeled KW peptide nanofiber sample (Sample A). Colored lines indicate spectral assignments for isotopically labeled residues determined by 2D fpRFDR. Bi-colored circles highlight off-diagonal crosspeaks resulting from interresidue ^{13}C-^{13}C couplings. Tri-colored circles indicate overlapping crosspeaks with signal contributions from 3 residues. 1D slices are shown to illustrate analysis of interresidue ^{13}C-^{13}C couplings at indicated frequencies.

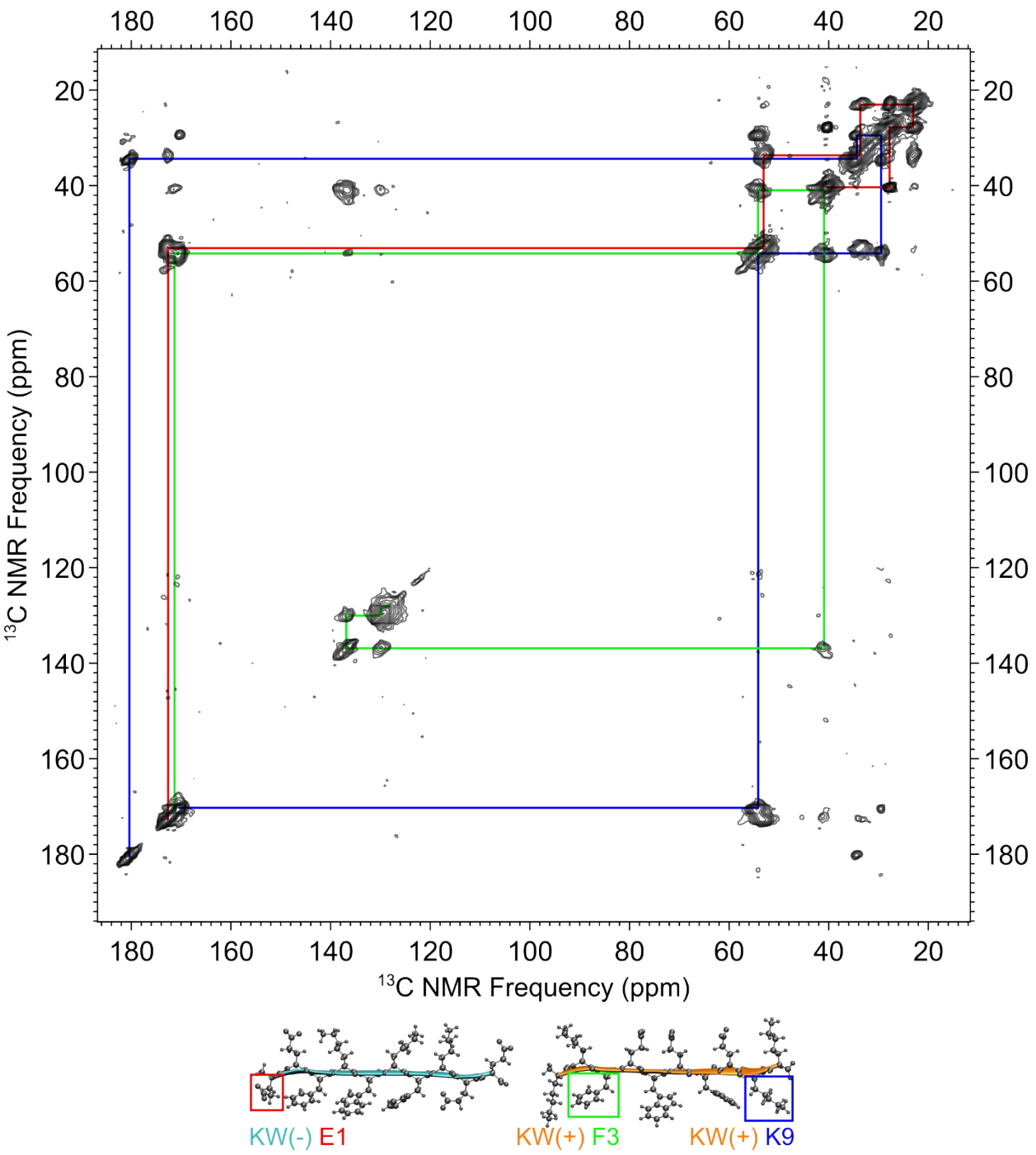

Figure S3. 2D ^{13}C-^{13}C finite-pulse radio-frequency driven recoupling (fpRFDR) NMR spectrum of Sample A. Solid lines indicate spectral assignments determined by analysis of peak positions with random coil values from the BMRB.

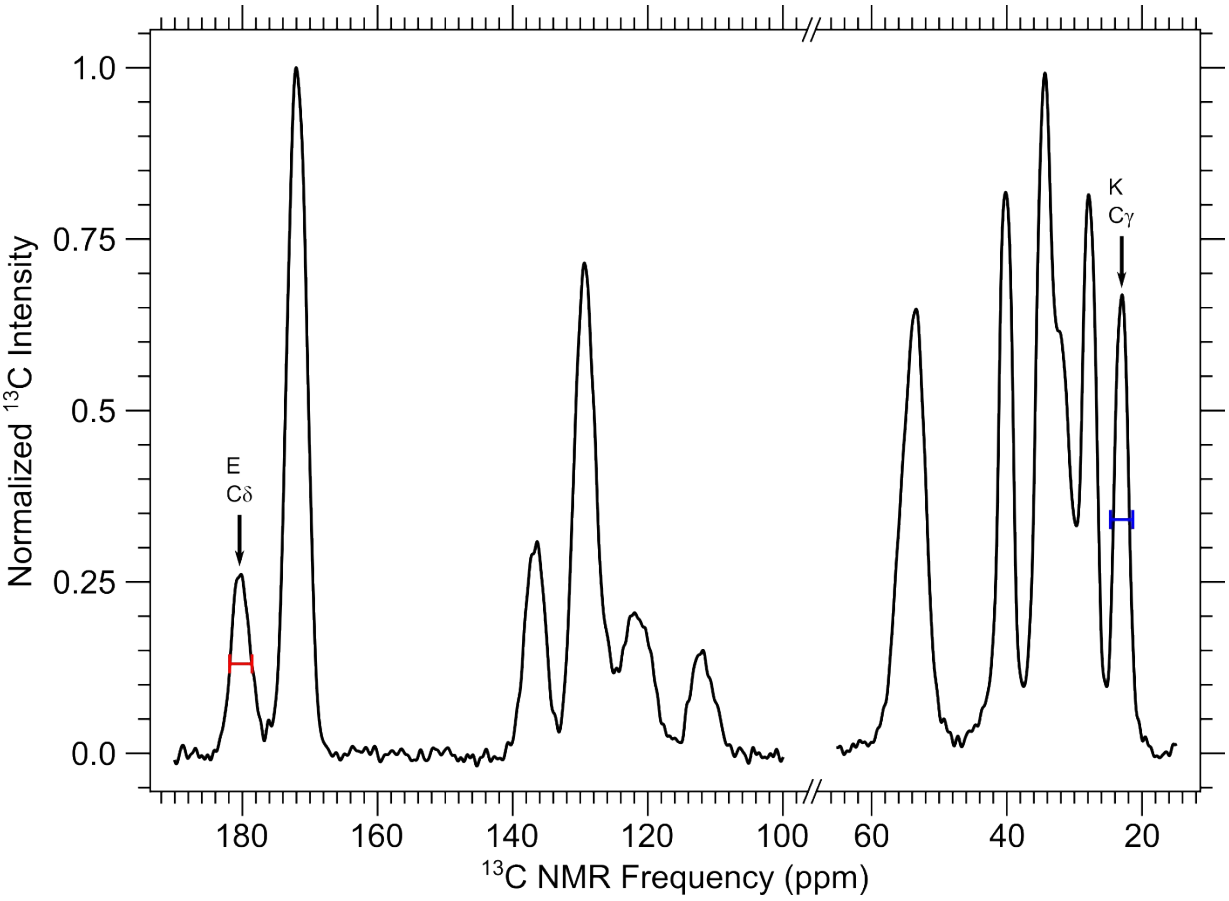

Figure S4. 1D ^{13}C NMR spectrum of Sample D where signal intensity represents naturally abundant ^{13}C. NMR linewidths of glutamic acid δ-carbon and lysine γ-carbon are highlighted for reference.

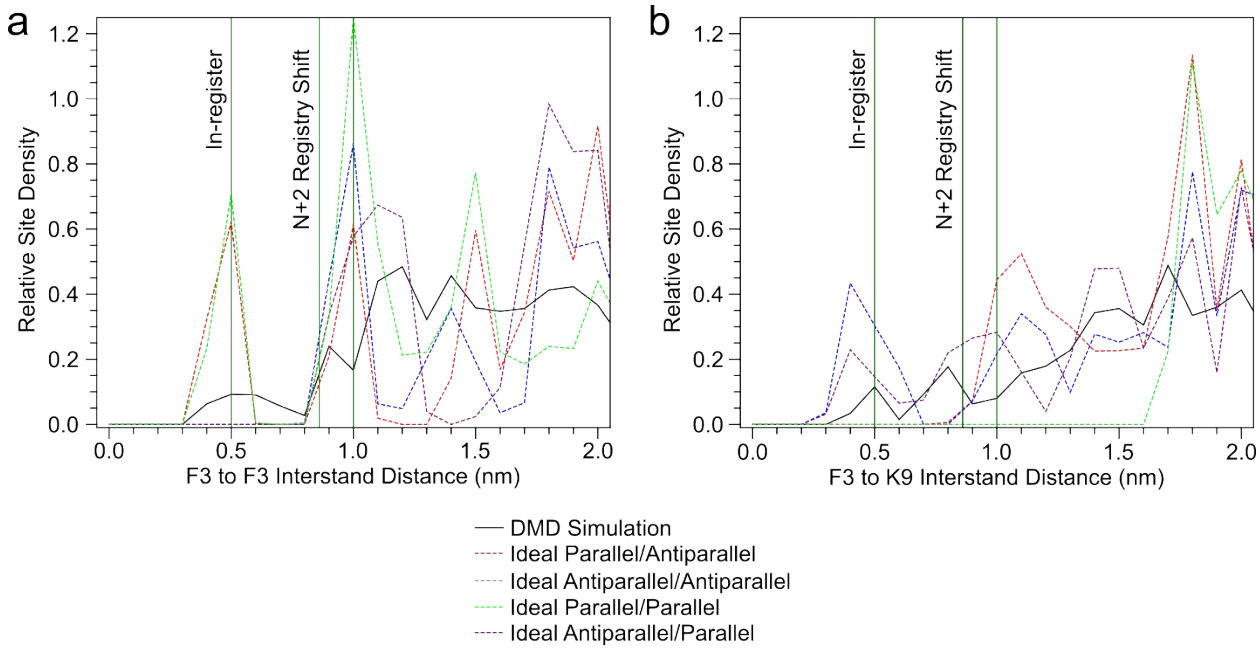

Figure S5. Analysis of parallel and antiparallel β-sheet content averaged over 6 coarse-grained DMD simulations. a) Distance distribution between F3 carbonyl sites as analyzed from the cg DMD simulation. b) Distance distribution between F3 carbonyl and K9 backbone nitrogen sites evaluated from the cg DMD simulation shown in Figure 1d.

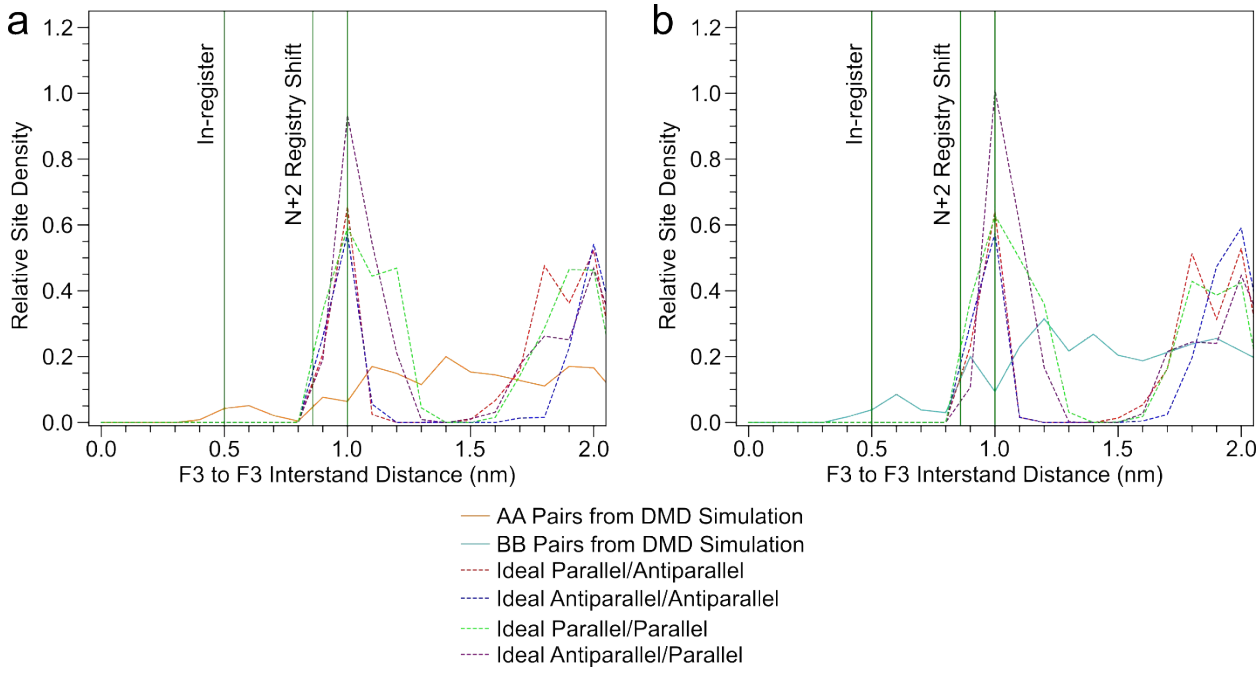

Figure S6. Analysis of self-association of King-Webb peptides averaged over 6 coarse-grained DMD simulations. a) Distance distribution of KW+ to KW+ (orange) peptides and b) distance distribution of KW- to KW- (cyan) peptides. Calculations are based on F3 carbonyl sites on KW+ and KW- peptides.