Supplementary File S1 for Conformational effects of multisite phosphorylation of disordered peptides

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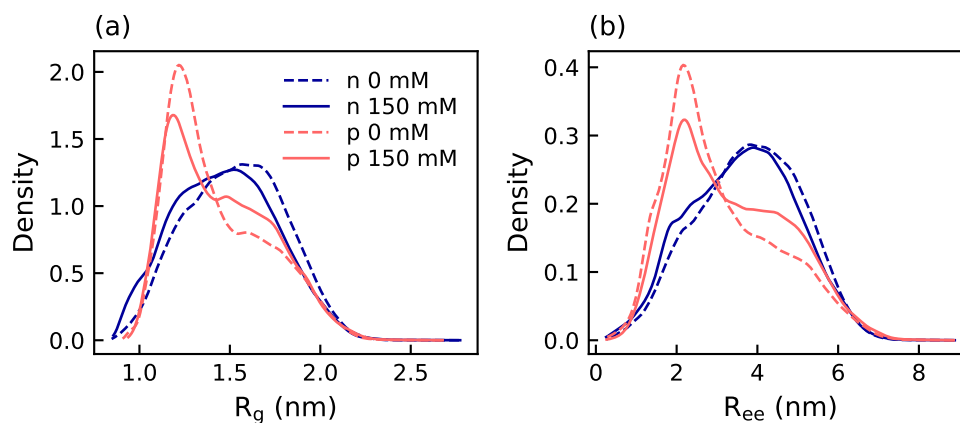
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Figure S1: Distribution of a) radius of gyration and b) end-to-end distance of non-phosphorylated (n) and phosphorylated (p) bCPP simulated with 0 or 150 mM NaCl. The data for the phosphorylated peptide are taken from ref. [1].
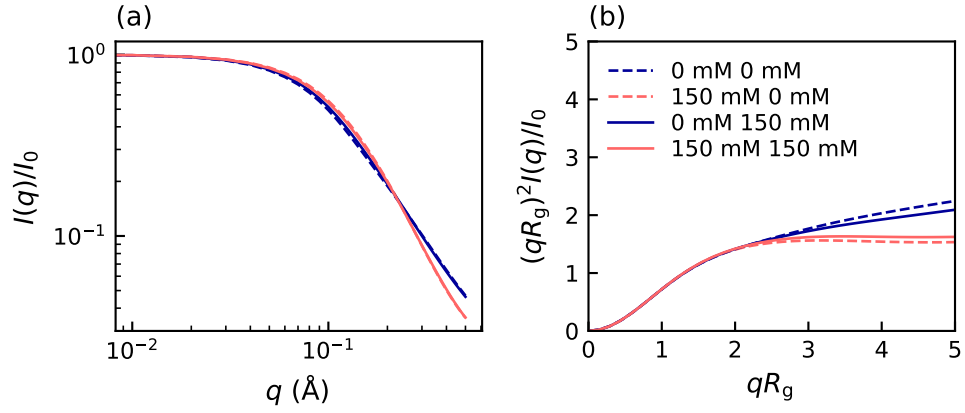
Figure S2: a) Calculated form factor and b) dimensionless Kratky plot of non-phosphorylated (n) and phosphorylated (p) bCPP simulated with 0 or 150 mM NaCl. The data for the phosphorylated peptide are taken from ref. [1].
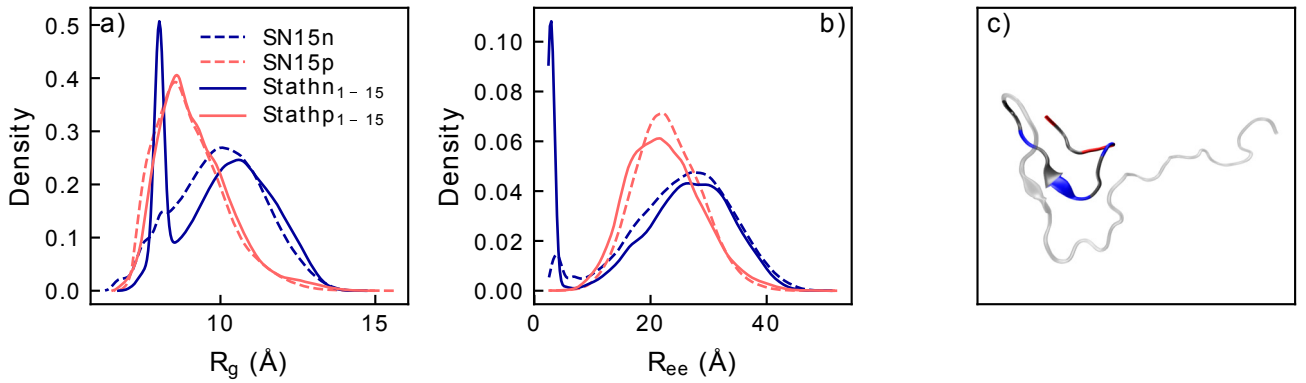

Figure S3: a) Radius of gyration and b) end-to-end distance distributions of non-phosphorylated (n) and phosphorylated (p) Stath$_{1-15}$ and SN15. c) Snapshot of the type of conformation giving rise to the sharp peak in the Stathn$_{1-15}$ distributions, where residue 16-43 is traced in light gray. The SN15 data are taken from ref. [2].
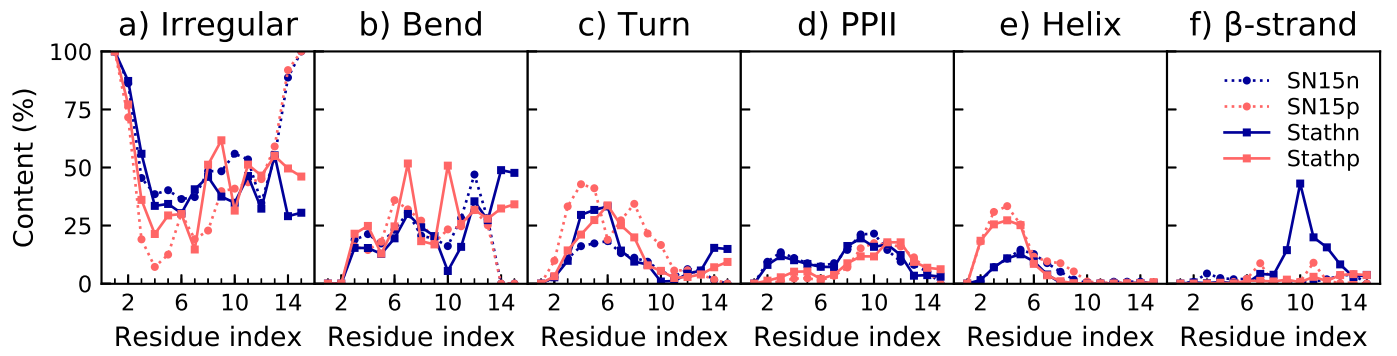
Figure S4: Secondary structure content along the sequence in non-phosphorylated (n) and phosphorylated (p) Stath$_{1\text{-}15}$ and SN15. Helix includes α-helix and 3$_{10}$-helix. β-strand also includes β-bridge. The SN15 data are taken from ref. [2].

References

[1] Ellen Rieloff and Marie Skepö. Molecular dynamics simulations of phosphorylated intrinsically disordered proteins: A force field comparison. *Int. J. Mol. Sci.*, 22(18), 2021.

[2] Ellen Rieloff and Marie Skepö. Phosphorylation of a disordered peptide—structural effects and force field inconsistencies. *Journal of Chemical Theory and Computation*, 16(3):1924–1935, 2020.