ASSOCIATED CONTENT

NMR and Computation Reveal a Pressure-Sensitive Folded Conformation of Trp-Cage

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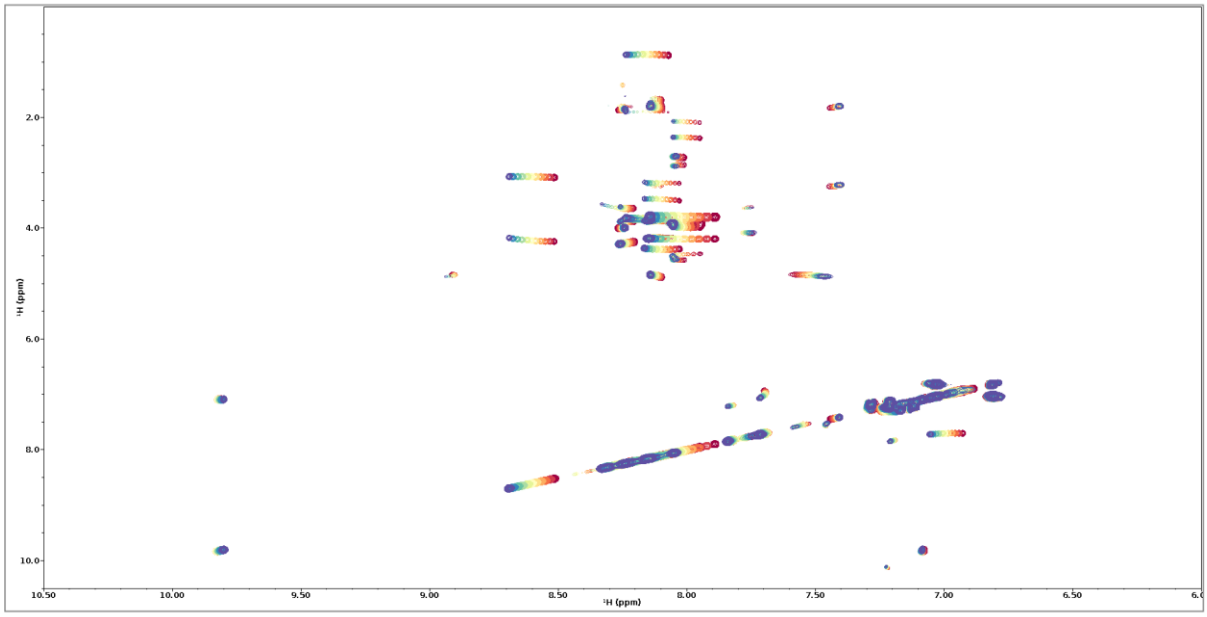

Figure S1. Pressure titration spectra for the 298K pH 7 conditions. Lowest pressure is displayed in red. Highest pressure is displayed in blue.

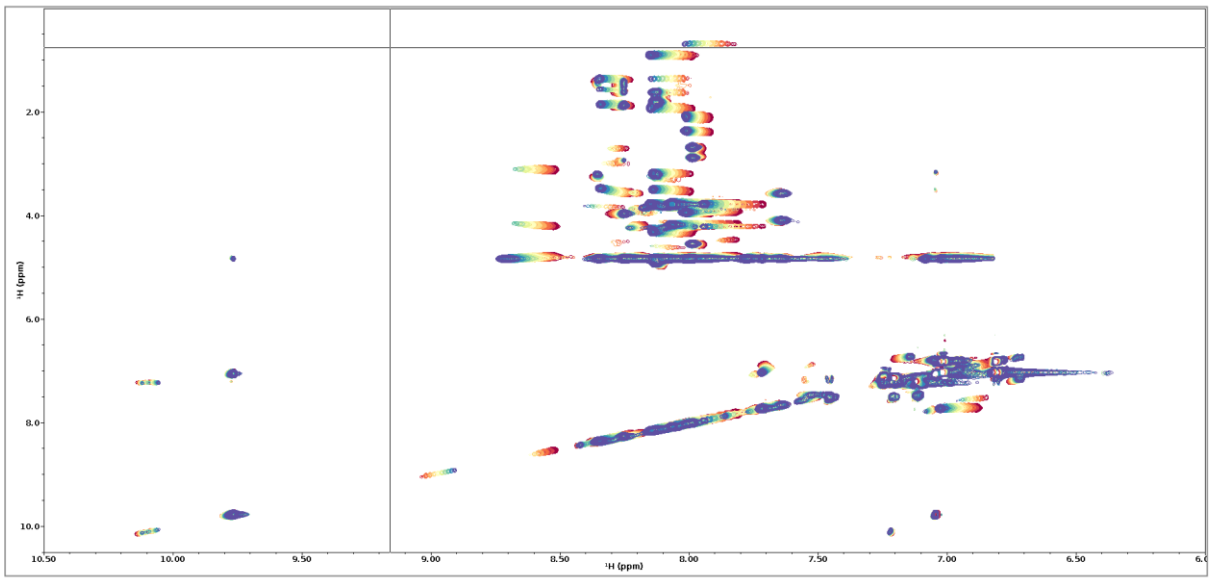

Figure S2. Pressure titration spectra for the 285K pH 5 conditions. Lowest pressure is displayed in red. Highest pressure is displayed in blue.

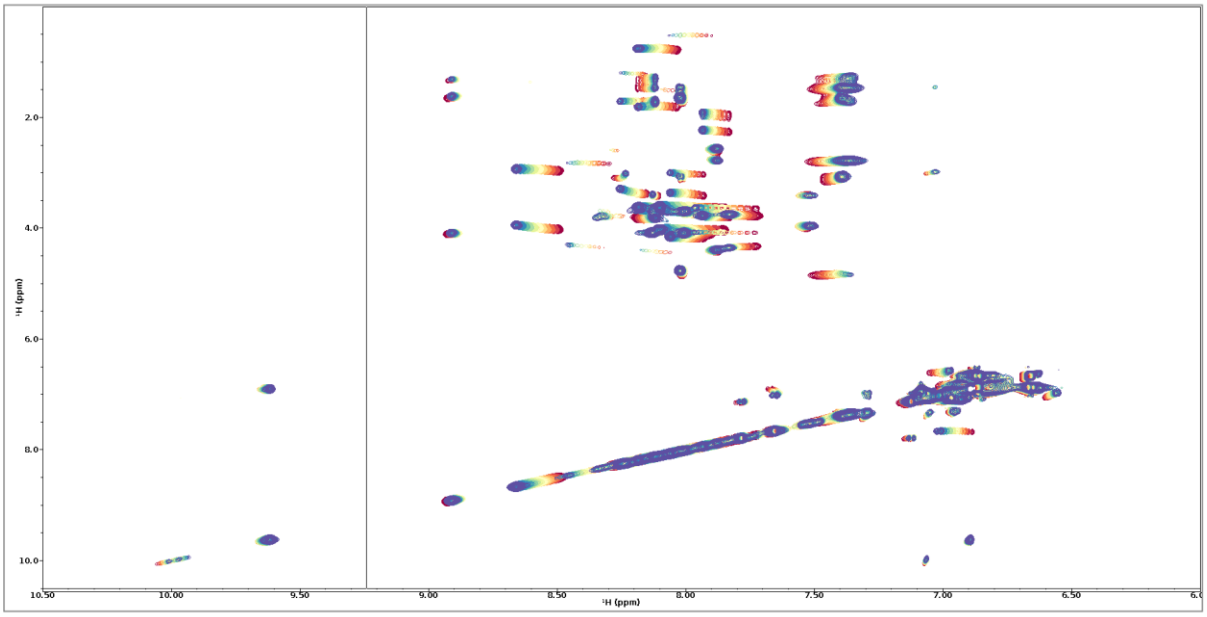

Figure S3. Pressure titration spectra for the 282K pH 5 conditions. Lowest pressure is displayed in red. Highest pressure is displayed in blue.

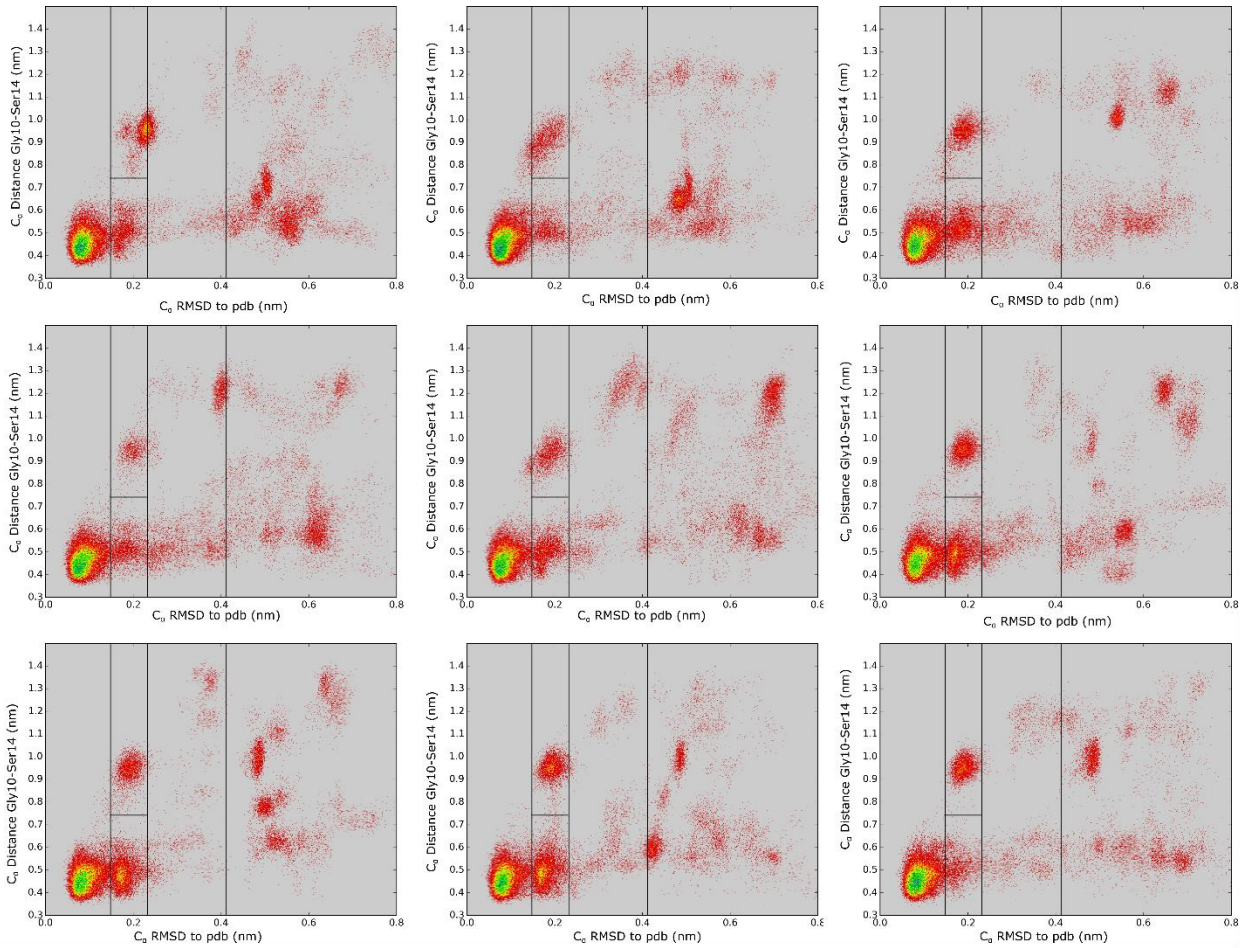

Figure S4. Block averaging of the Low density replica 1 simulation run. Each block is 50ns long.

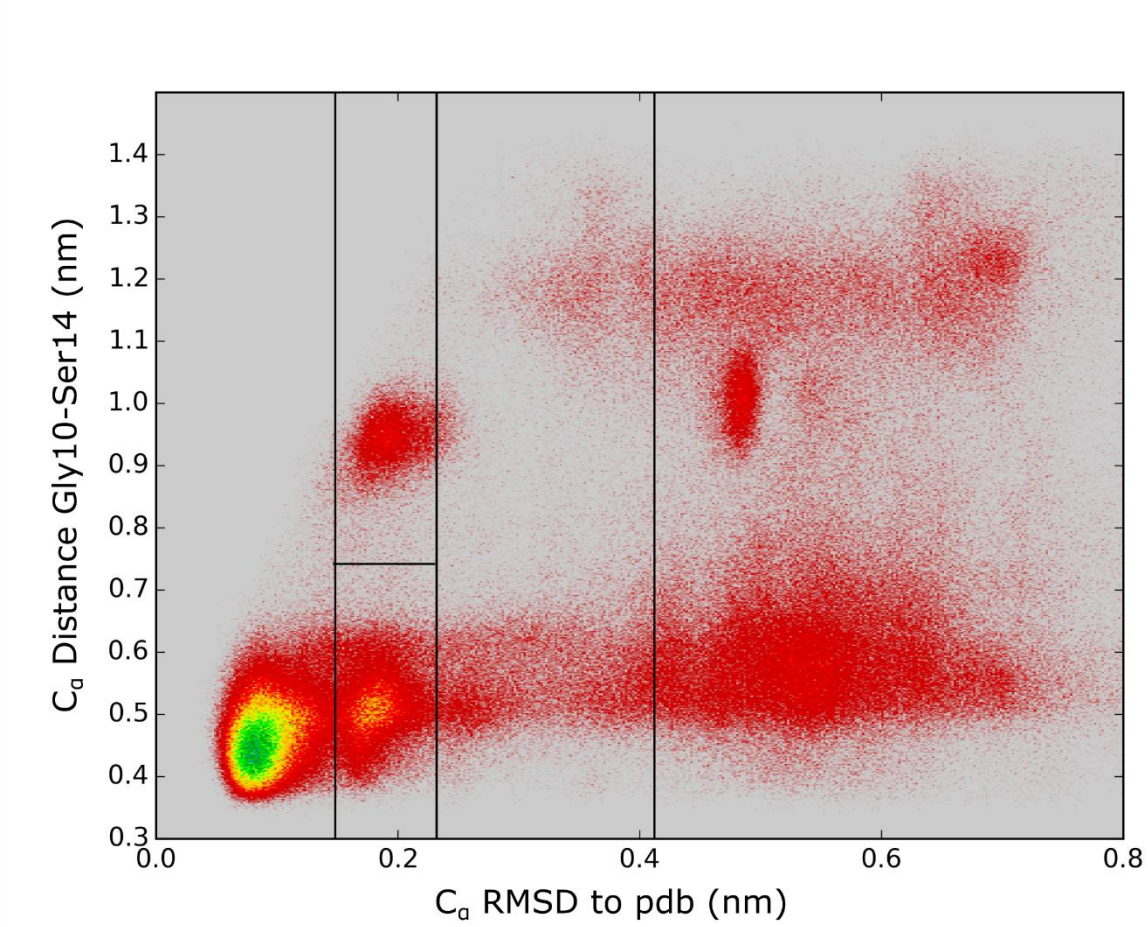

Figure S5. C_α distance Gly10H_N-Ser15H_N vs C_αRMSD to pdb structure (pdb 1l2y) for replica 11 yielding a pressure of 0 bar and a temperature of 330K. Black lines represent the boundaries chosen for RMSD based discrimination of structures at RMSDs of 0.147nm, 0.23 nm and 0.44 nm for the vertical lines and Gly10H_N-Ser15H_N distance of 0.75 nm for the horizontal lines.

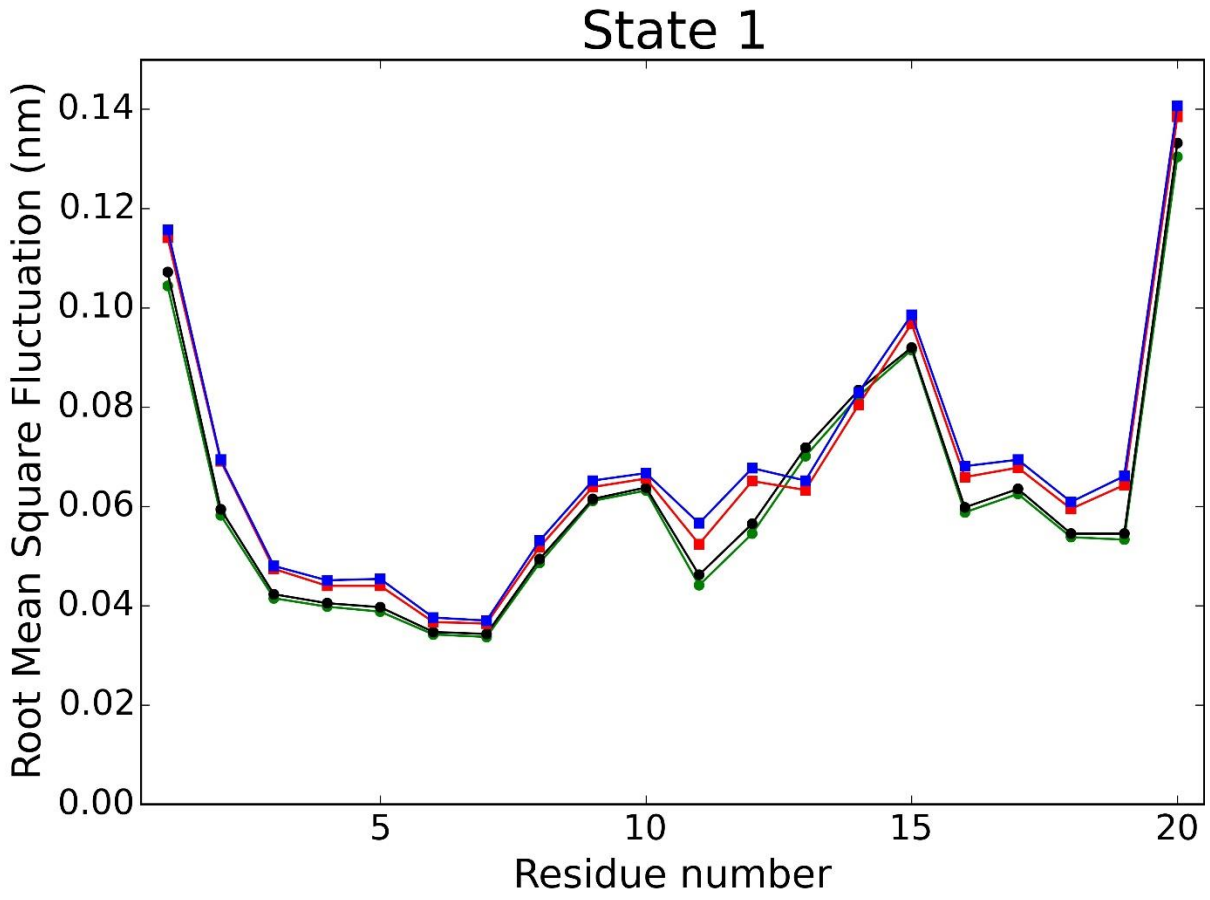

Figure S6. Root Mean Square Fluctuation for state 1. Green, and black correspond to high density runs at 285K and 297.6K, respectively, and red, and blue correspond to low density runs at 285K and 297.6K, respectively.

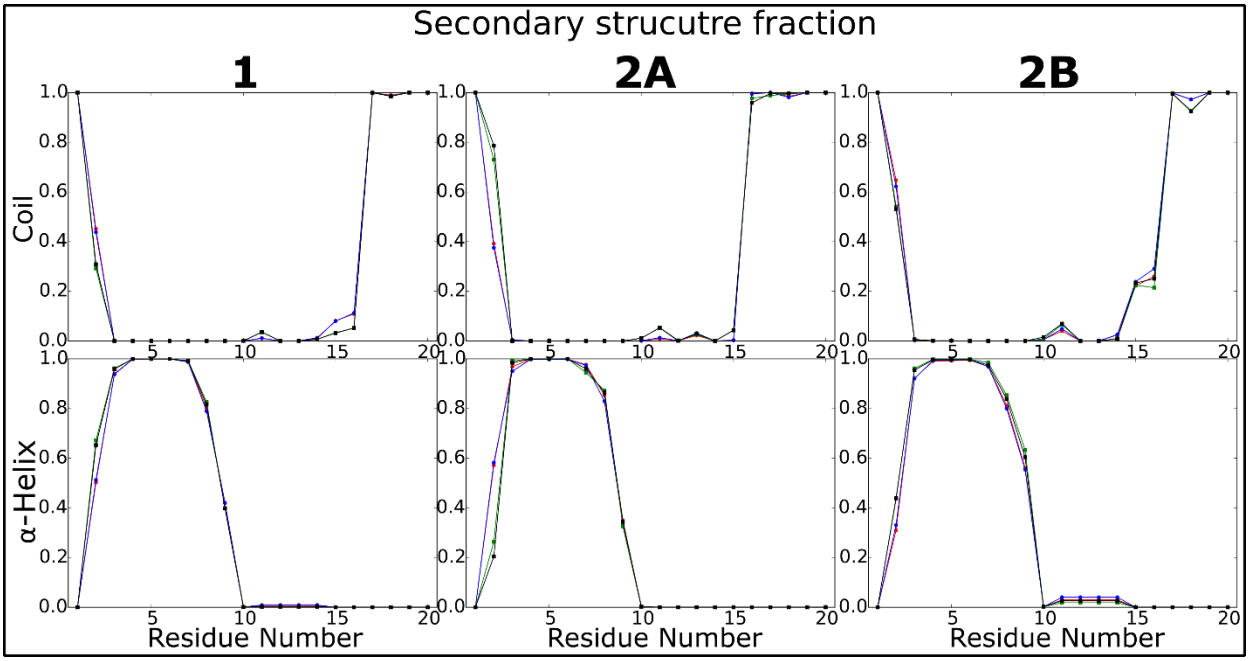

Figure S7. Fraction of secondary structure content by residue for each state as delimited in Figure 6, type of secondary structure is indicated on the left, points and line are colored by conditions, with blue, red, black, and green representing Low Density 297.6K, Low Density 285K, High Density 297.K and High Density 285K.

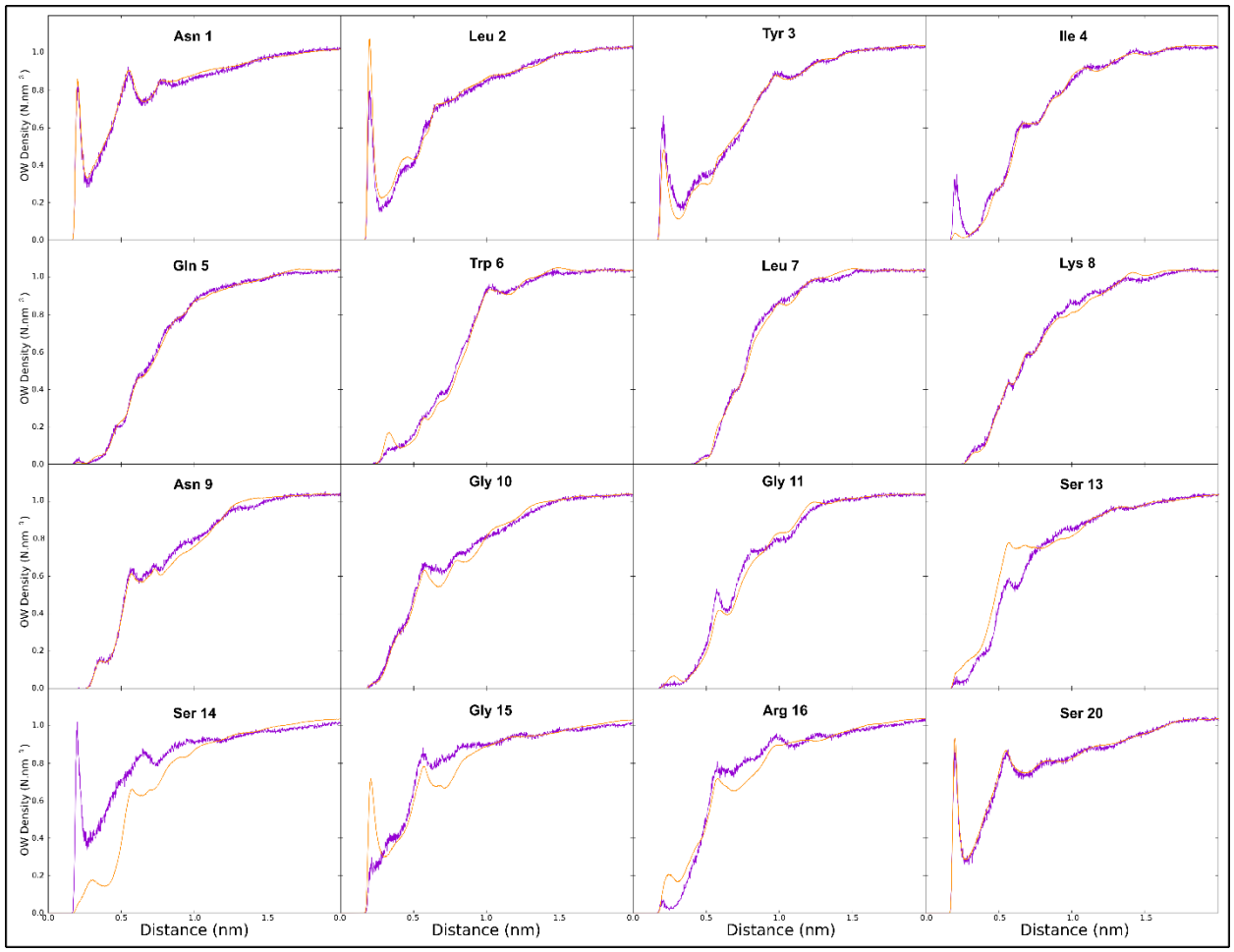

Figure S8. Radial Distribution Function of water oxygen around H_N of each residue averaged over all data sets for state 1 (orange) and state 2A (purple).

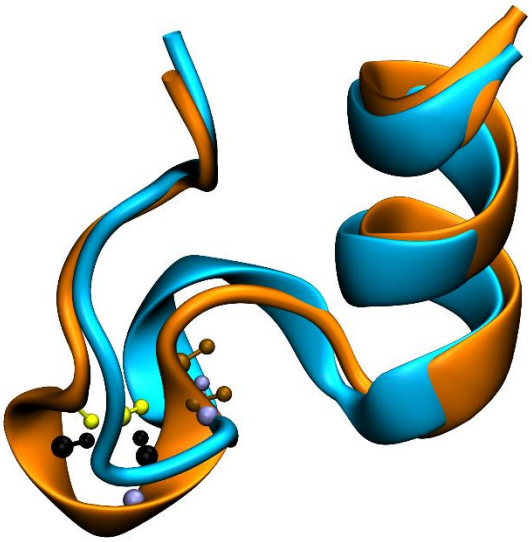

Figure S9. Difference in position of the amide hydrogen between state 1 (cyan) and state 2A (orange) for residue 13, 14, 15 and 16, displayed in brown, blue black and yellow, respectively. The smaller sphere is the amide hydrogen, the larger one the amide nitrogen.