Supplementary Information

# Residual structures and transient long-range interactions of p53 transactivation domain: Assessment of explicit solvent protein force fields

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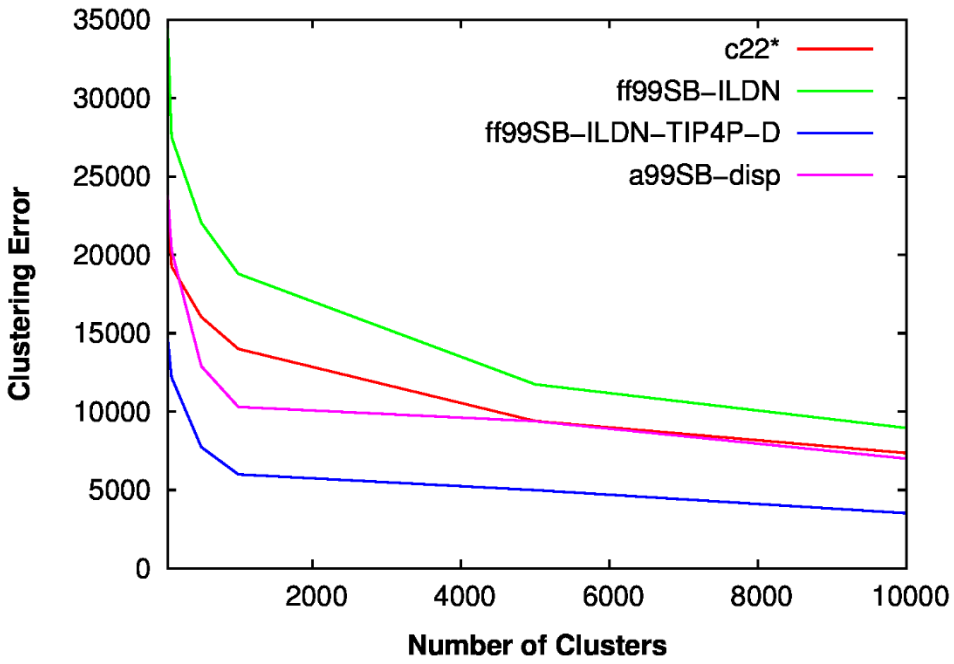


**Figure S1.** Clustering error (i.e., sum of squared distances of samples to their closest cluster center) as a function of number of clusters for the structural ensembles obtained using four force fields.

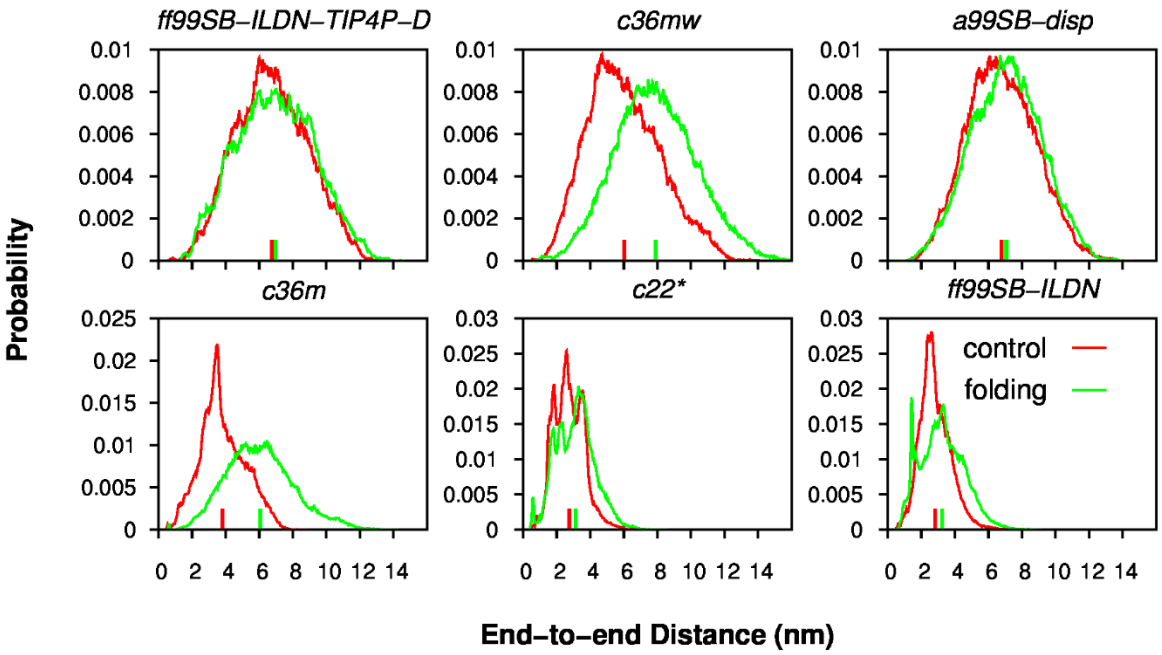


**Figure S2.** Probability distributions of the p53-TAD end-to-end distance calculated from independent control (red lines) and folding (green lines) simulations using six force fields. The corresponding ensemble averaged values are indicated using vertical bars.

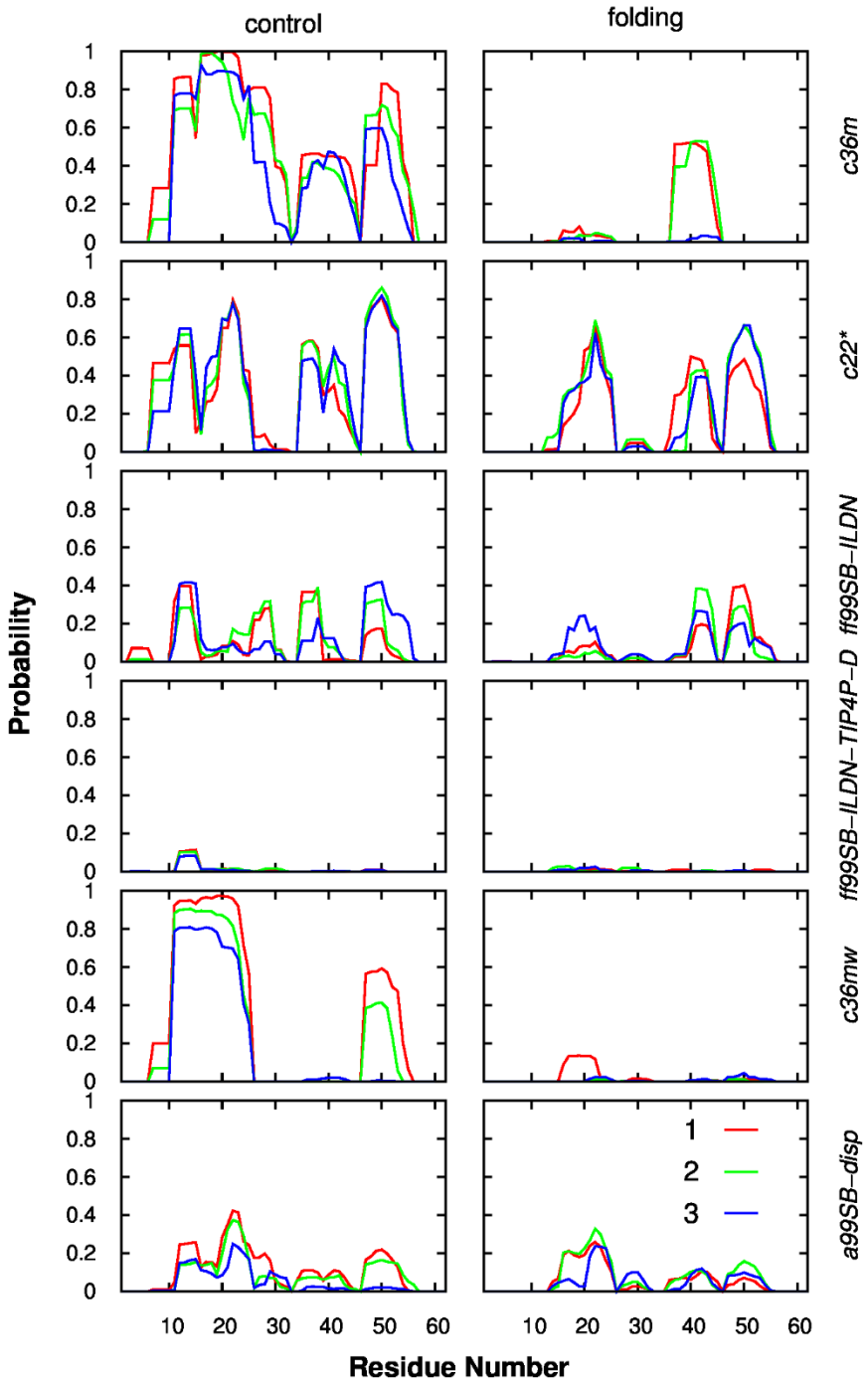


**Figure S3.** Averaged residue helicity profiles of p53-TAD calculated from the equally divided three portions of each trajectory using six force fields.

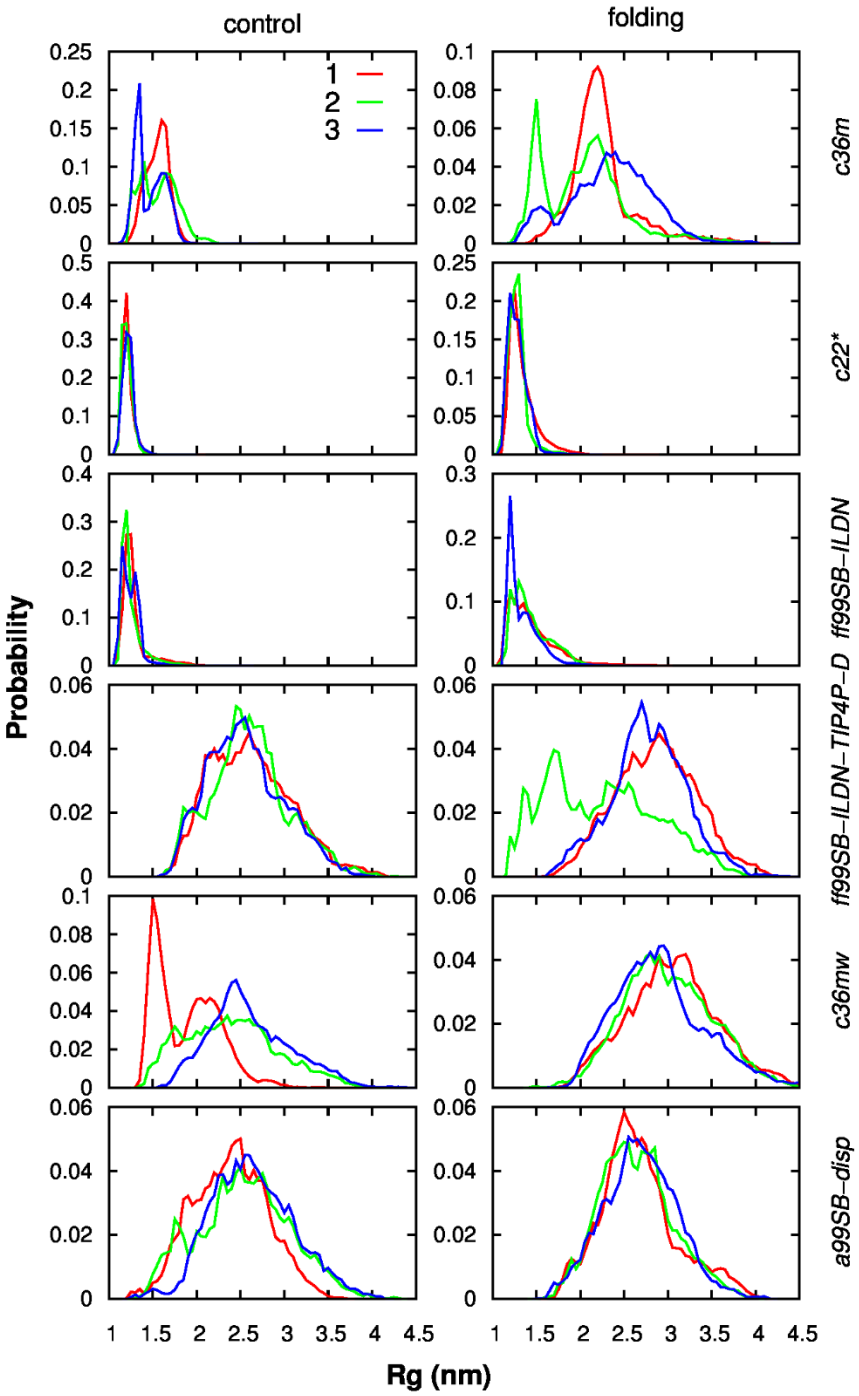


**Figure S4.** Probability distributions of $R_g$ of p53-TAD calculated from the equally divided three portions of each trajectory using six force fields.

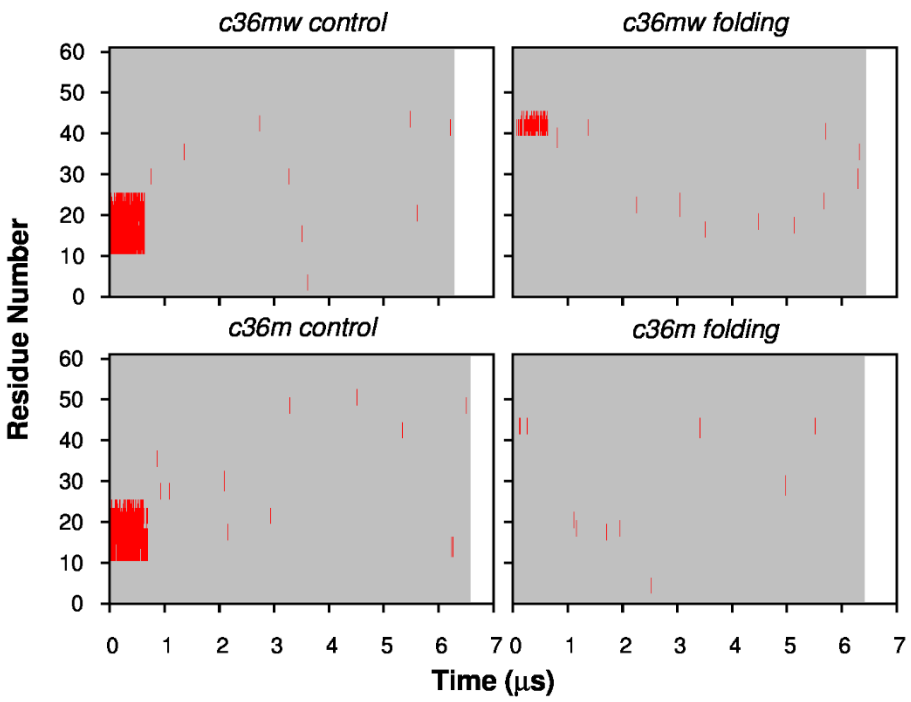


**Figure S5.** Evolution of the secondary structure of each residue in p53-TAD during standard MD simulations at 298 K. Red indicates helical state, and grey indicates non-helical state.

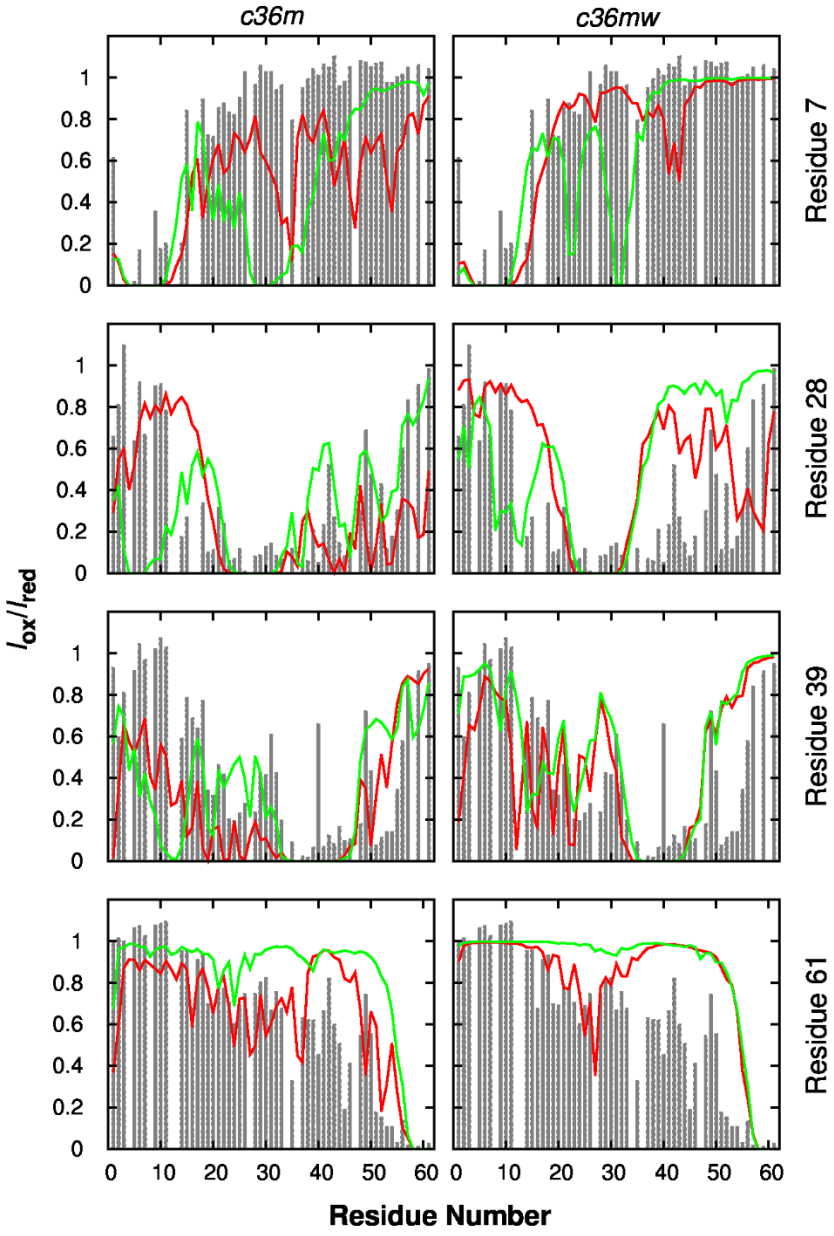


**Figure S6.** Calculated (lines) and experimental (grey bars) PRE effects induced by paramagnetic spin labelling at residues 7, 28, 39, and 61. Red and green traces are calculated from independent control and folding simulations, respectively, using c36m and c36mw force fields.

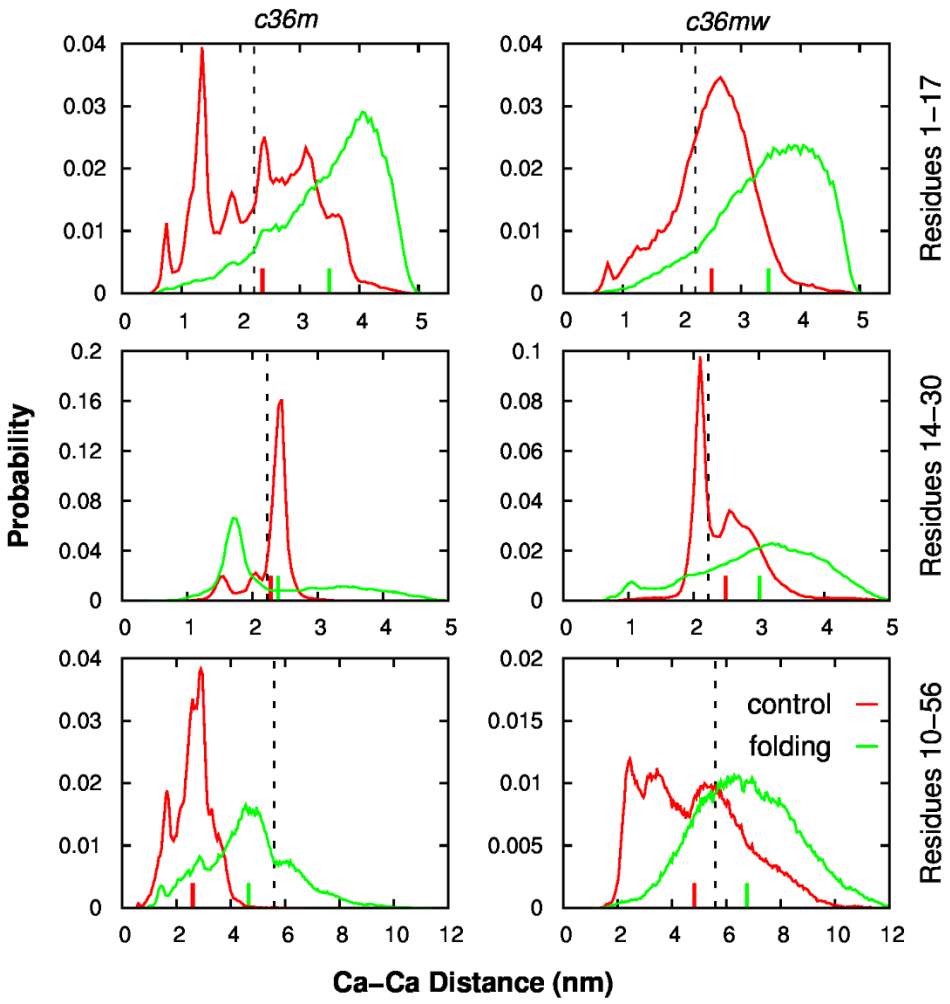


**Figure S7.** Probability distributions of distances between three pairs of residues, 1 and 17 (top row), 14 and 30 (middle row), and 10 and 56 (bottom row), calculated from independent control (red) and folding (green) simulations using c36m and c36mw force fields. The corresponding ensemble averages were indicated as vertical bars. The vertical black line indicated experimental values from smFRET and TR-FRET measurements.

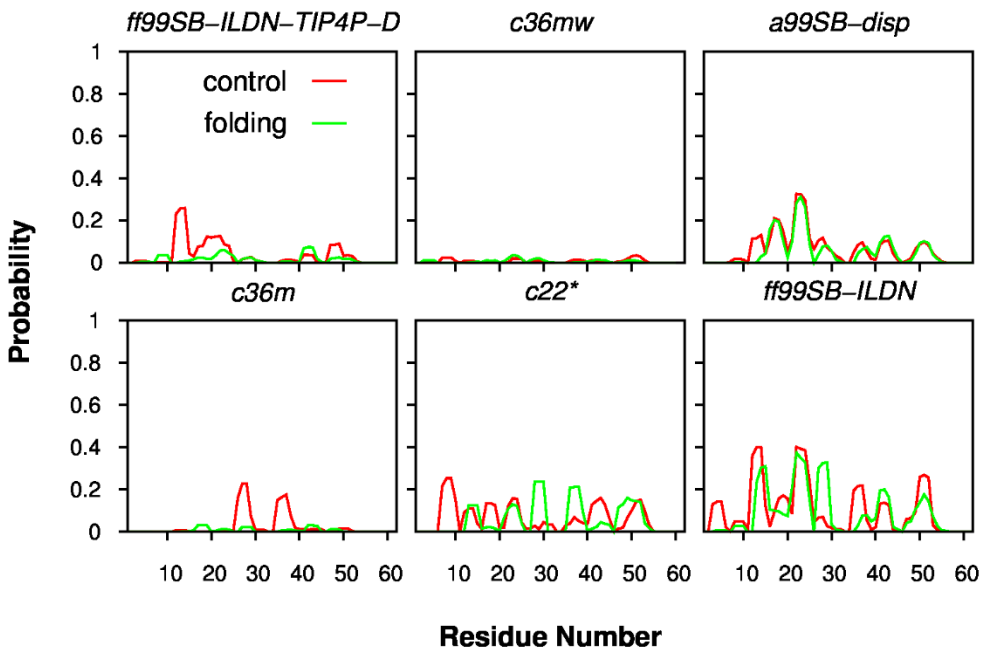


**Figure S8.** Probability of forming $3_{10}$ helices for each residue of p53-TAD calculated from independent control (red) and folding (green) simulations using six force fields.

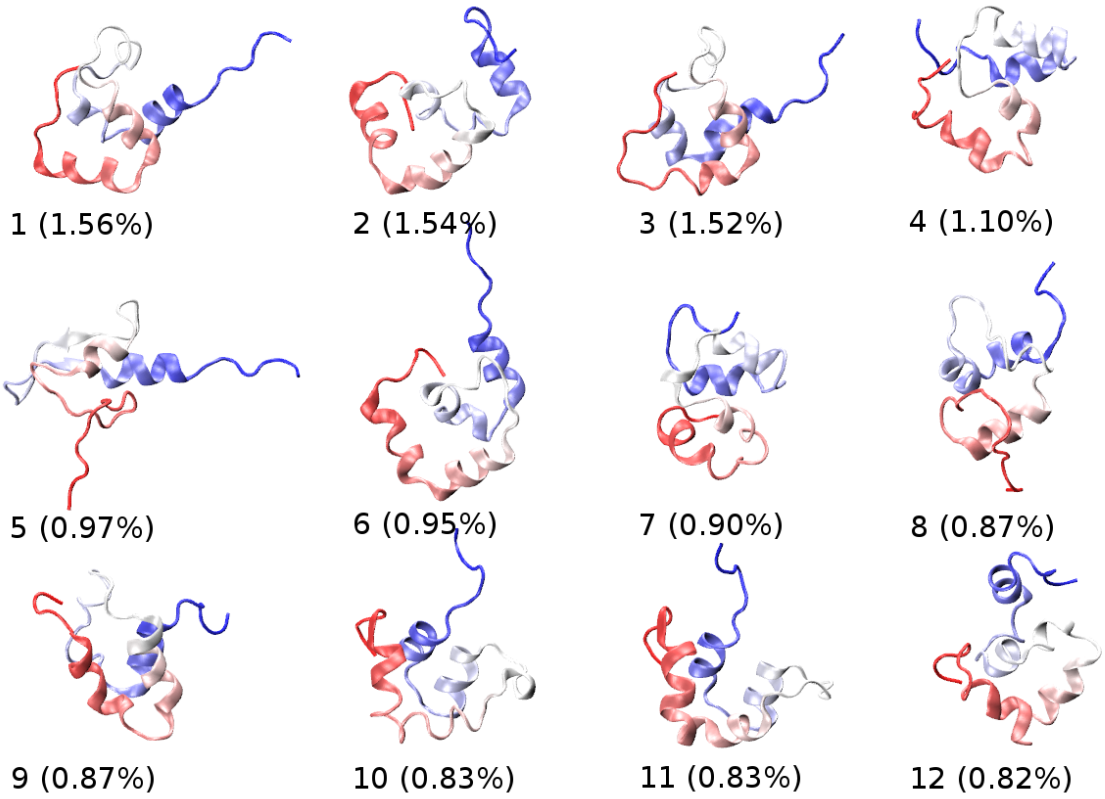


**Figure S9.** Center structures and populations of top 12 most populated clusters for the structural ensemble derived from c22* simulations. The p53-TAD peptide is shown in Cartoon, with the color changing from red (at N-terminus) to blue (at C-terminus).

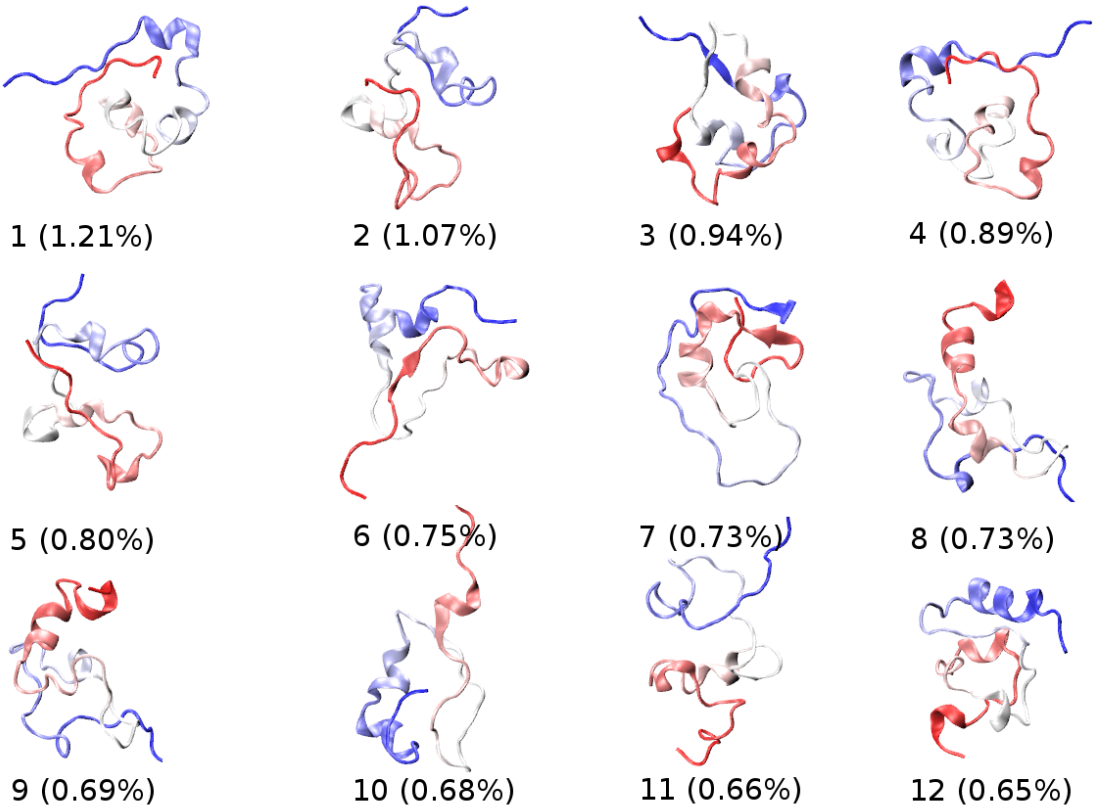


**Figure S10.** Center structures and populations of top 12 most populated clusters for the structural ensemble derived from ff99SB-ILDN simulations. The p53-TAD peptide is shown in Cartoon, with the color changing from red (at N-terminus) to blue (at C-terminus).

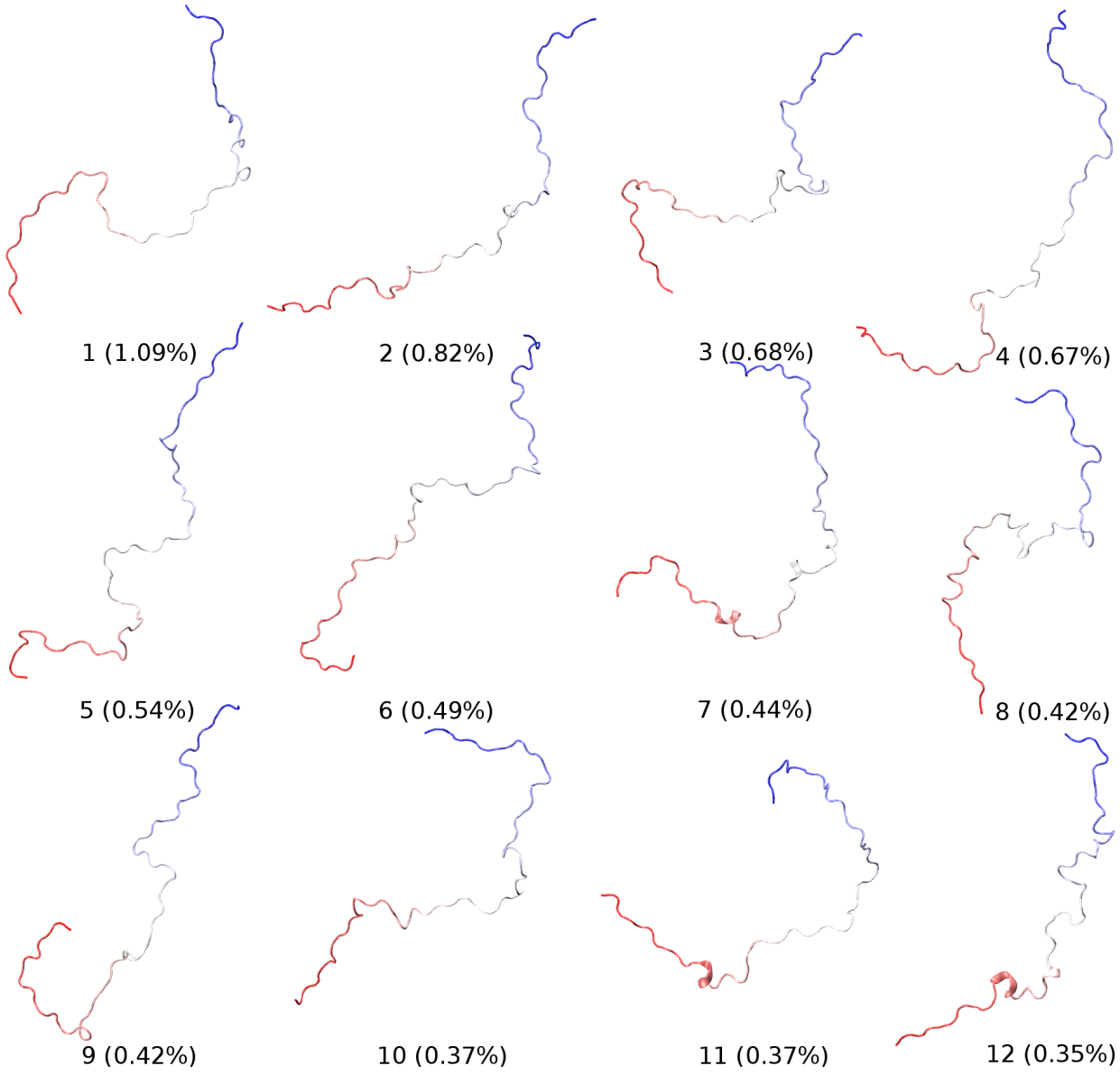


**Figure S11.** Center structures and populations of top 12 most populated clusters for the structural ensemble derived from ff99SB-ILDN-TIP4P-D simulations. The p53-TAD peptide is shown in Cartoon, with the color changing from red (at N-terminus) to blue (at C-terminus).