SUPPLEMENTARIE FIGURES

"Alterations of nonconserved residues affect protein stability and folding dynamics through charge-charge interactions" ***Swarnendu Tripathi, Angel E. Garcìa, and George I. Makhatadze***

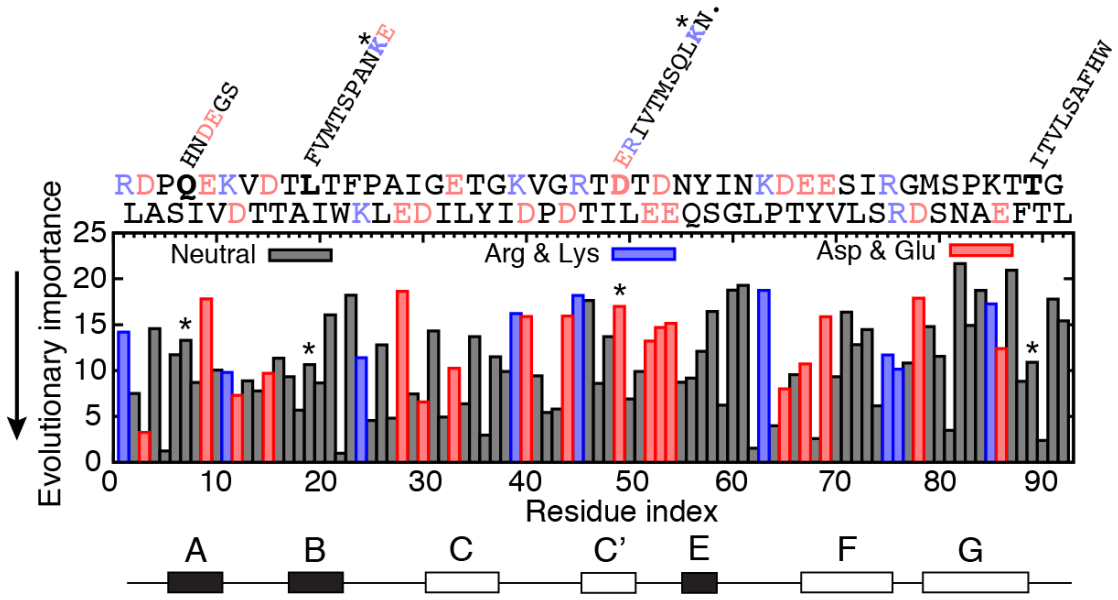

Figure S1. Evolutionary trace (ET) analysis of WT TNfn3. Real value evolutionary trace (rvET) score of WT TNfn3 is plotted for each residue along the sequence. Low value of rvET score indicates evolutionary important residues. Positively charged (Arg and Lys), negatively charged (Asp and Glu) and neutral residues are represented in blue, red and black color, respectively. The four residues (Q7, L19, D49 and T89) that were mutated to Lys in the MUT TNfn3 are indicated by the * symbol and the corresponding sequences are shown in the bold letters above the plot. Variations in these four residues from multiple sequence alignment based on the ET analysis are also shown above the sequence of WT TNfn3. Secondary structure of TNfn3 is shown below the plot.

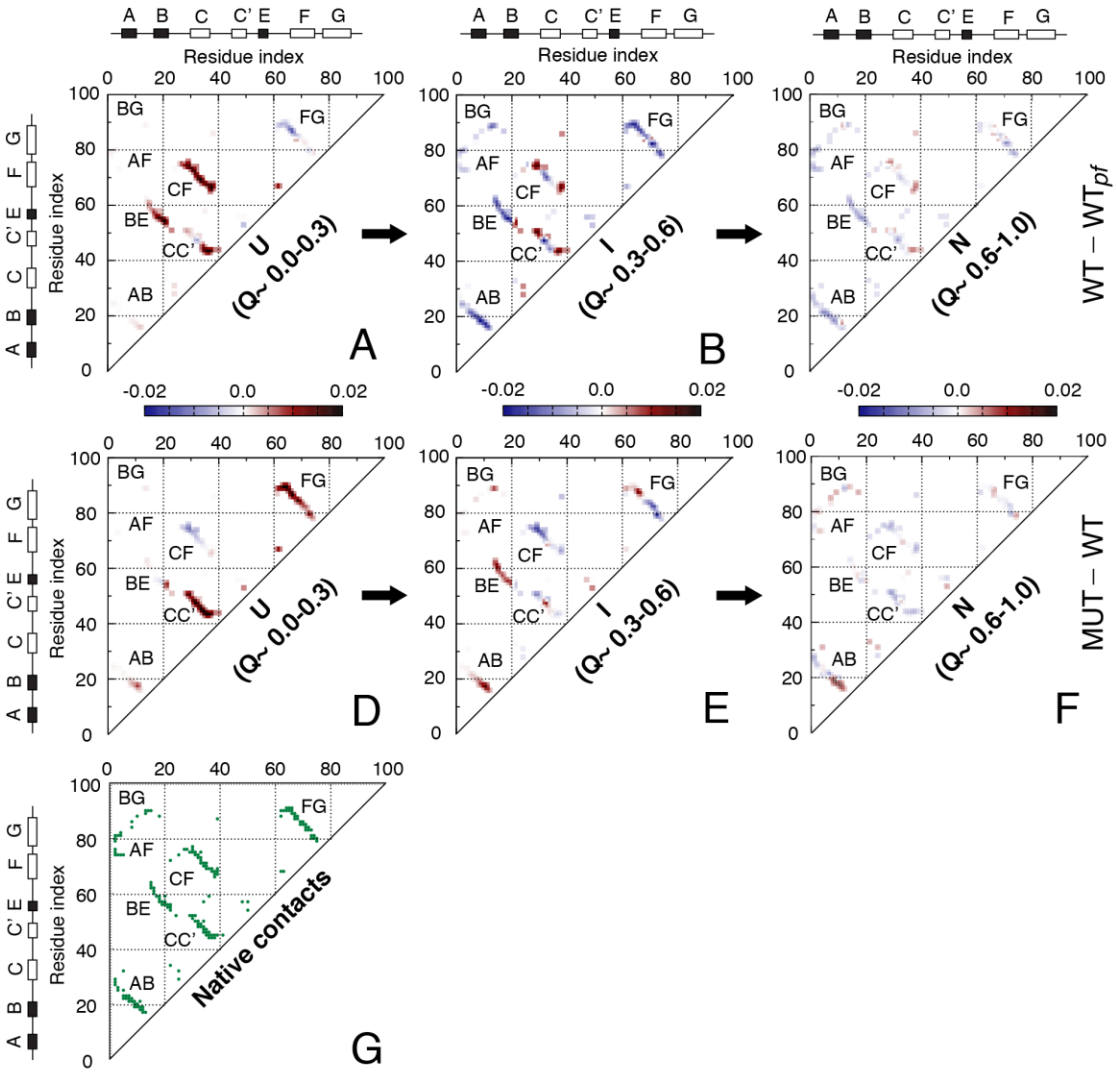

Figure S2. Probability of native contact formation of TNfn3. Panels A-C illustrate the deference in the probability of native contact formation, $\langle \Delta Q_i \rangle^{WT-WTpf}$ between the WT and WT_{pf} proteins for the unfolded (U), intermediate (I) and native (N) state ensembles. Similarly, panels D-F illustrate the $\langle Q_i \rangle^{MUT-WT}$ between the MUT and WT proteins for the U, I and N state ensembles. In the color bars red indicates higher probability of the contacts to form and blue indicates lower probability to form the contacts in the WT or MUT relative to the WT_{pf} or WT, respectively. Panel G shows the native contact map of TNfn3 which is the same for all three systems.