Eris-aided structure pre-relaxation relieves backbone strains of the α-spectrin initial structure. (a) The scatter plot of the calculated and experimental ΔΔG values obtained using NMR-determined structure (PDB ID 1aj3). The Pearson correlation coefficient between the computed and experimental ΔΔG values is 0.66 for surface mutants (●) and only 0.28 for core mutants (∗). (b) The scatter plot of the calculated and experimental ΔΔG values obtained using the Eris pre-relaxed structure. Significant correlations are obtained for both surface (●; r = 0.60) and core mutations (∗; r = 0.70). The lines are the linear regression fits.