Figure S2. Time evolution of the number of clusters during molecular dynamics simulations.

Shorter segments of MD trajectories were analyzed in order to find out what is the shortest MD simulation necessary to discriminate between the functional and nonfunctional forms of p53 mutants. Number of clusters for the p53 mutants calculated at each of 5, 10, 20, 25 and 30 ns of MD simulations are graphed separately in the form of column graphs. Functionally active p53 mutants are grouped and designated with a green arrow while nonfunctional p53 mutants were designated with a red arrow.The clustering results at RMSD cutoff of 1.15 Å indicates that at least 30 ns of MD simulation is required.

Number of clusters — First 5 ns

Number of clusters — First 10 ns

Number of clusters — First 20 ns

Number of clusters — First 25 ns

Number of clusters — First 30 ns