SUPPORTING INFORMATION

Identification and structural characterization of an intermediate in the folding of the measles virus X domain

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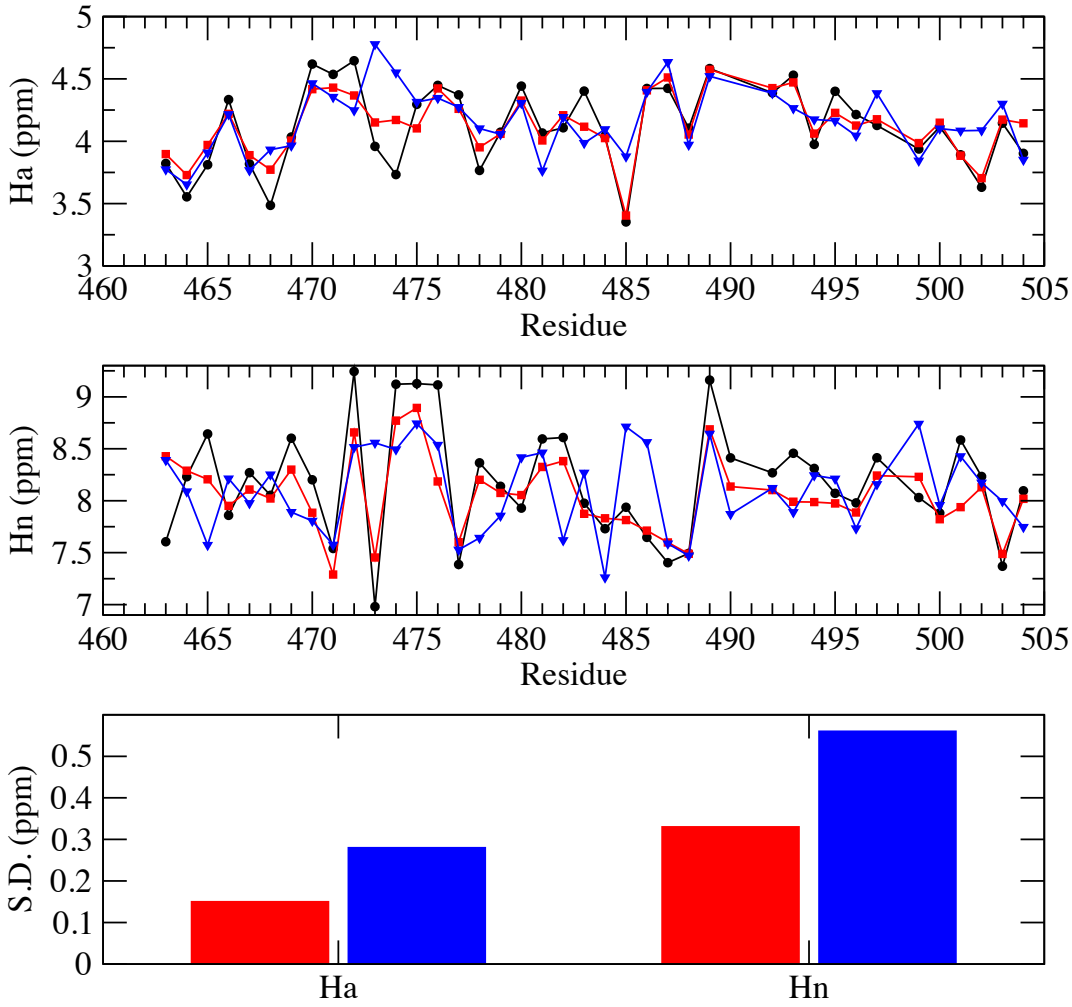

Figure S1. Comparison of the NMR chemical shifts of the XD domain from the ensemble generated by metadynamics (red), from the crystal structure (blue) and measured experimentally by NMR spectroscopy (black). The top panel refers to the Hα atoms, whereas the middle panel refers to the H_N atoms. The standard deviation of the experimental chemical shifts from the model generated by metadynamics (red) and those calculated from the crystal structure (blue) is reported in the bottom panel. The values obtained from the RAM simulations resemble very closely those obtained by NMR experiments and are significantly improved compared to those calculated from the crystal structure, indicating that some effects of the dynamics of the ensemble are lost in the crystal state.

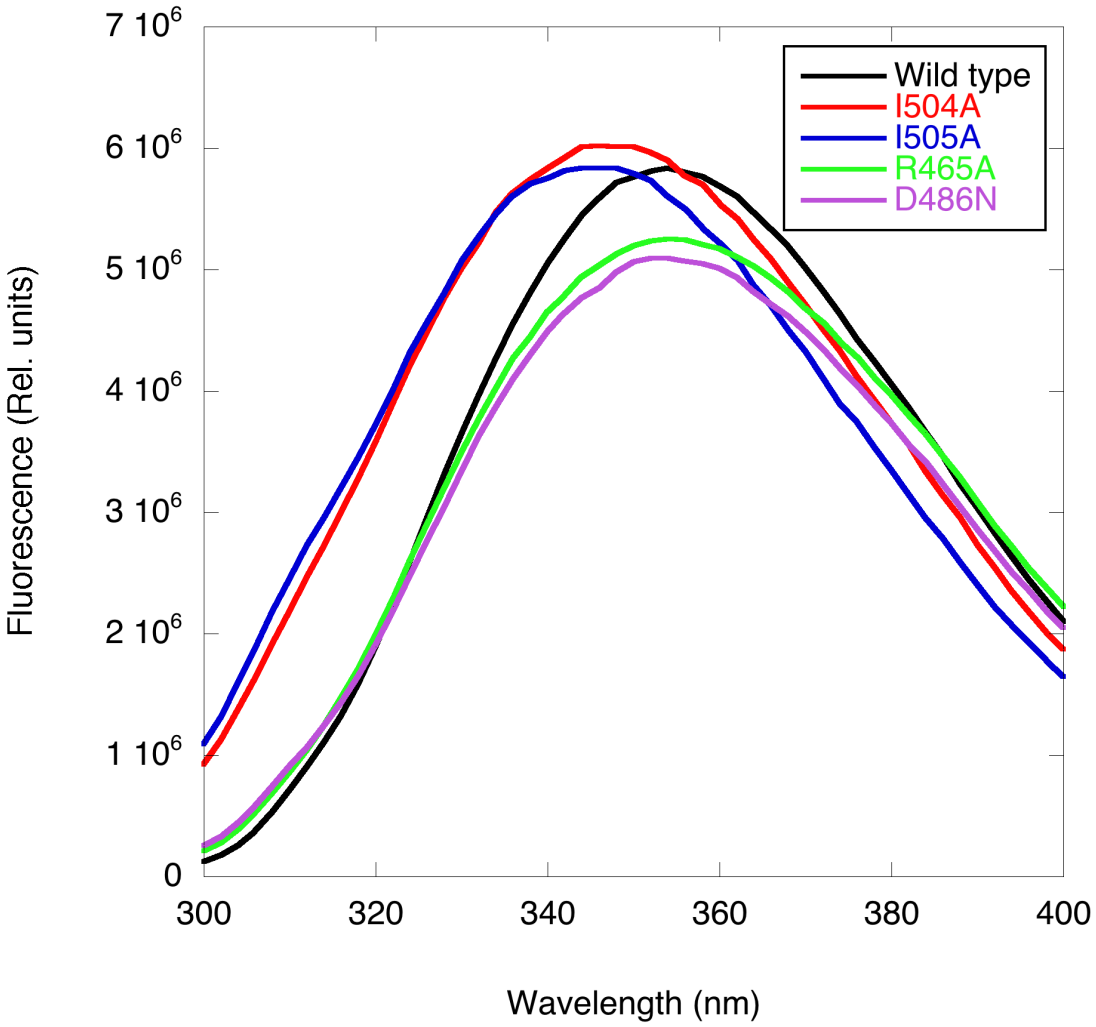

Figure S2. Emission spectra of XD and its site directed variants. Spectra were recorded by exciting the proteins at 280 nm, in the presence of 50 mM sodium phosphate, 300 mM NaCl at pH 7.2 and 25°C. It is evident that both the I504A and I505A mutants, which display a two-state folding transition (see text), display a blue-shifted λ_{max} compared to the other variants. This finding is consistent with a shift of population from a mixture of the native and intermediate states (as in the case of wild type XD, R465A and D486N), towards the native state only.