pH-Dependent Conformational Changes Due to Ionizable Residues in a Hydrophobic Protein Interior: The Study of L25K and L125K Variants of SNase

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Supporting Information

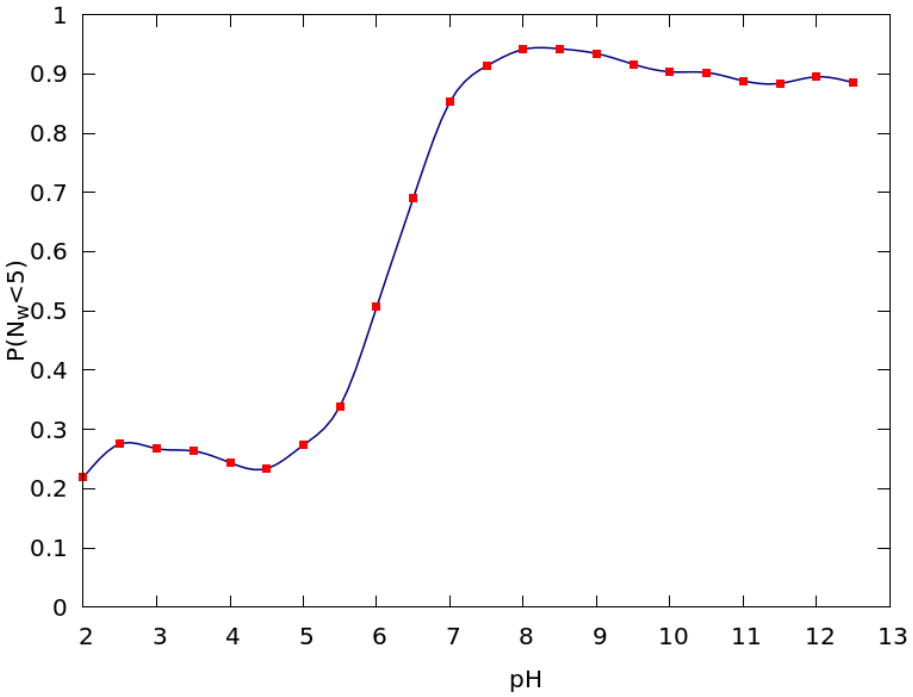

Figure S1. Probability of the occurrence of less than five water molecules within 3.4 Å of the NZ terminal of the Lys25 sidechain at different pH values. The solid line has been added to aid the eye.

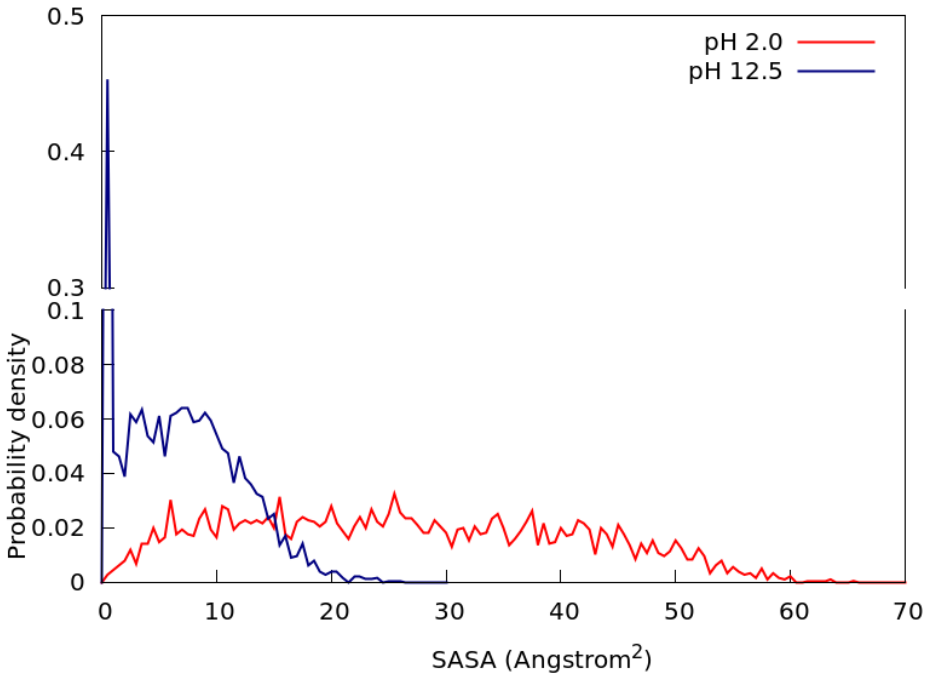

Figure S2. Normalized histogram of the solvent exposed surface area (SASA) of Lys25 at low pH (red) and high pH (blue). A SASA cut-off value of 15 Å was set to calculate the 'fraction of buried conformation' of Lys25 from the entire ensemble at different pH values.

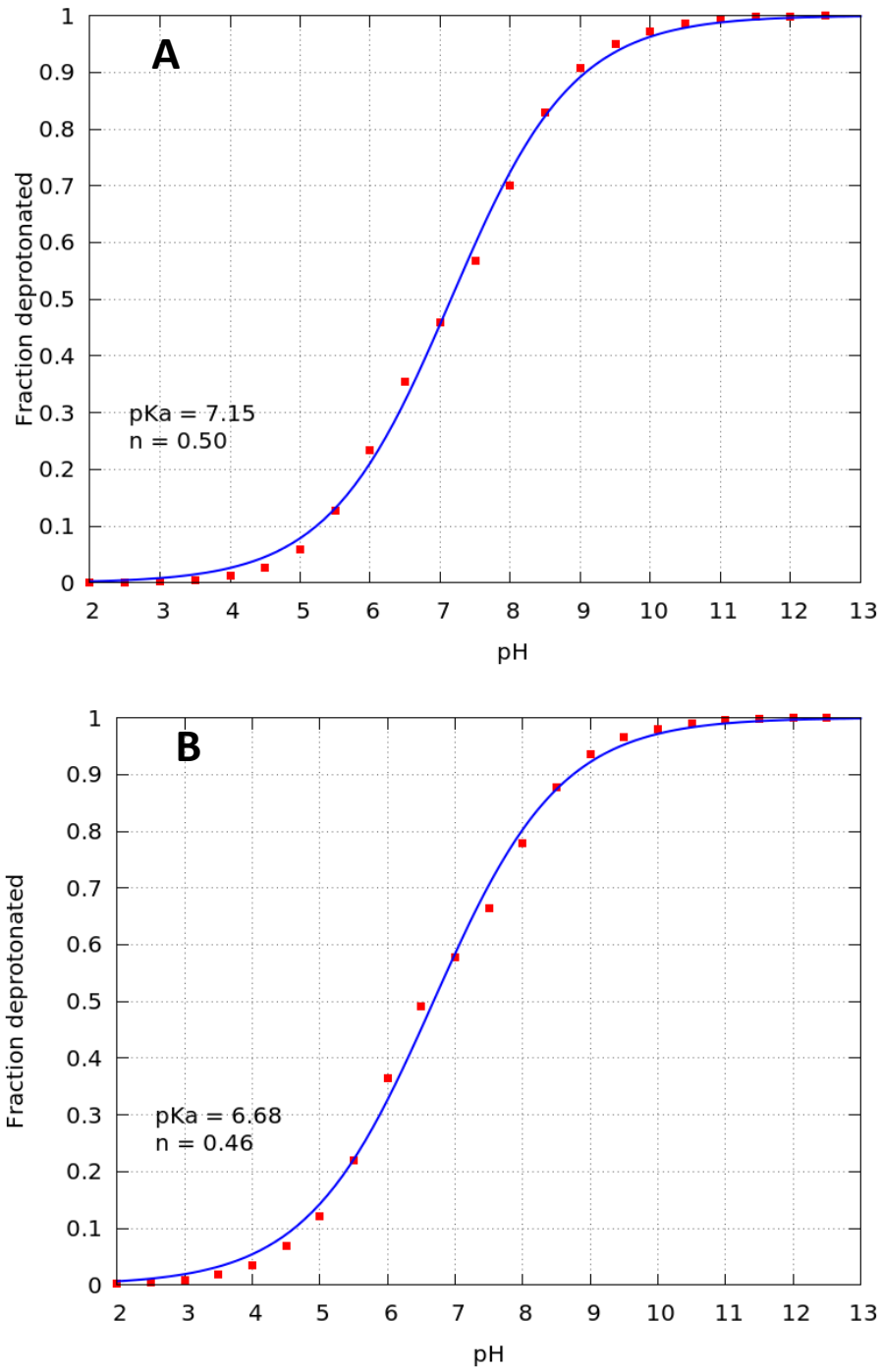

Figure S3. Titration curve of (A) Lys125 and (B) His121 obtained from one independent pH-REMD simulation, when all the titratable residues are allowed to change their protonation states. Data from the simulations (red dots) have been fitted to Eq 1. In this particular calculation, Lys125 titrates with a pK_a of 7.15 and has a Hill coefficient of 0.50. His121 titrates with a pK_a of 6.68 and has a Hill coefficient of 0.46.

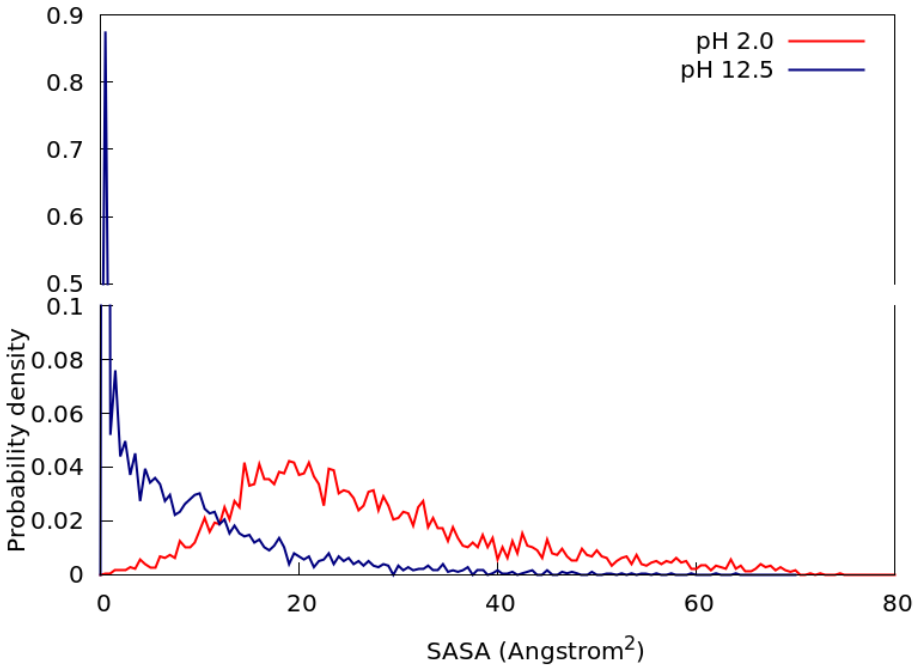

Figure S4. Normalized histogram of the solvent exposed surface area (SASA) of Lys125 at low and high pH.

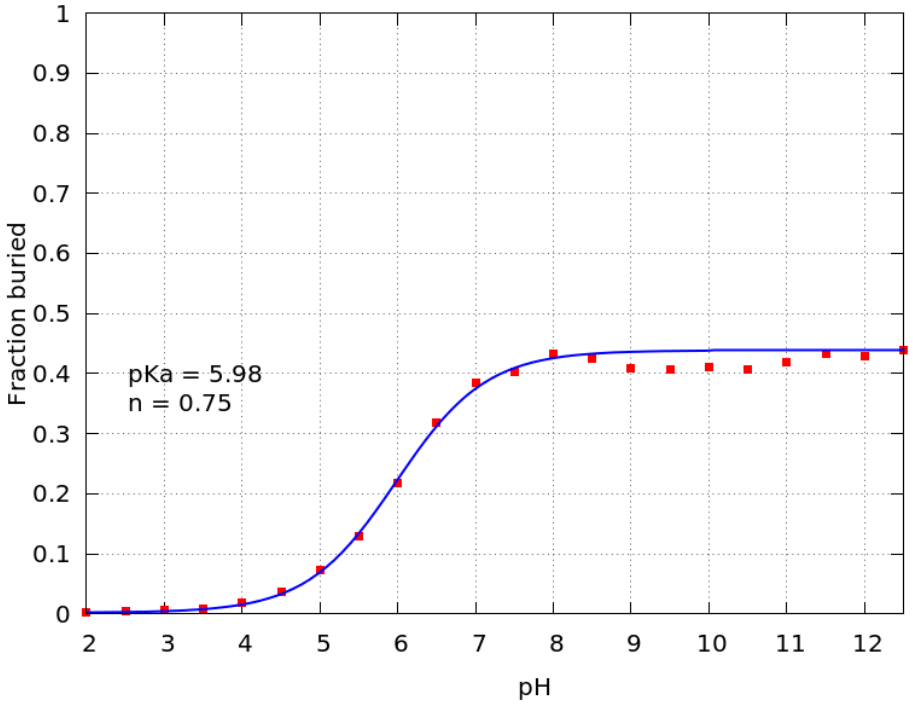

Figure S5. Fraction of buried conformation at each pH for L125K, based on the SASA criteria of both Lys125 and His121.