Disorder-to-order transition of an active-site loop mediates the allosteric activation of sortase A

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SUPPORTING MATERIAL

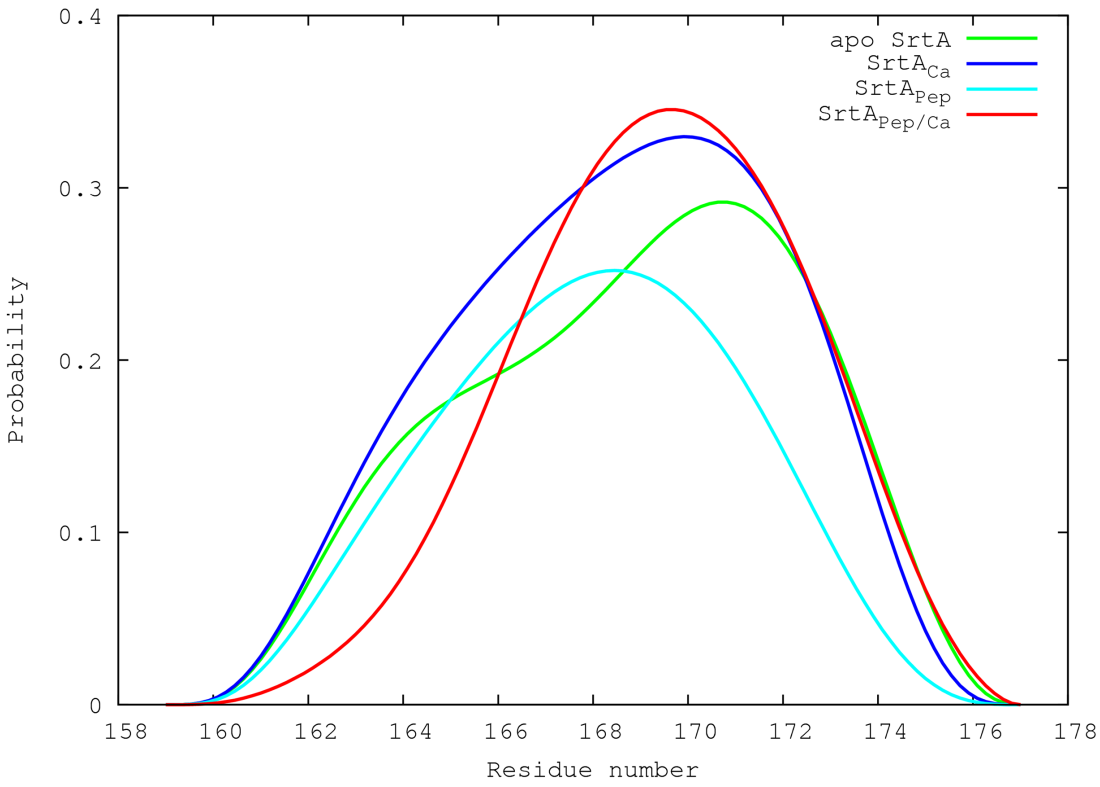

Figure S1 Distributions of the probabilities of residues in the active-site loop for forming 3_{10} helix, obtained from the REST simulations on sortase A in the apo form and in the three liganded forms.

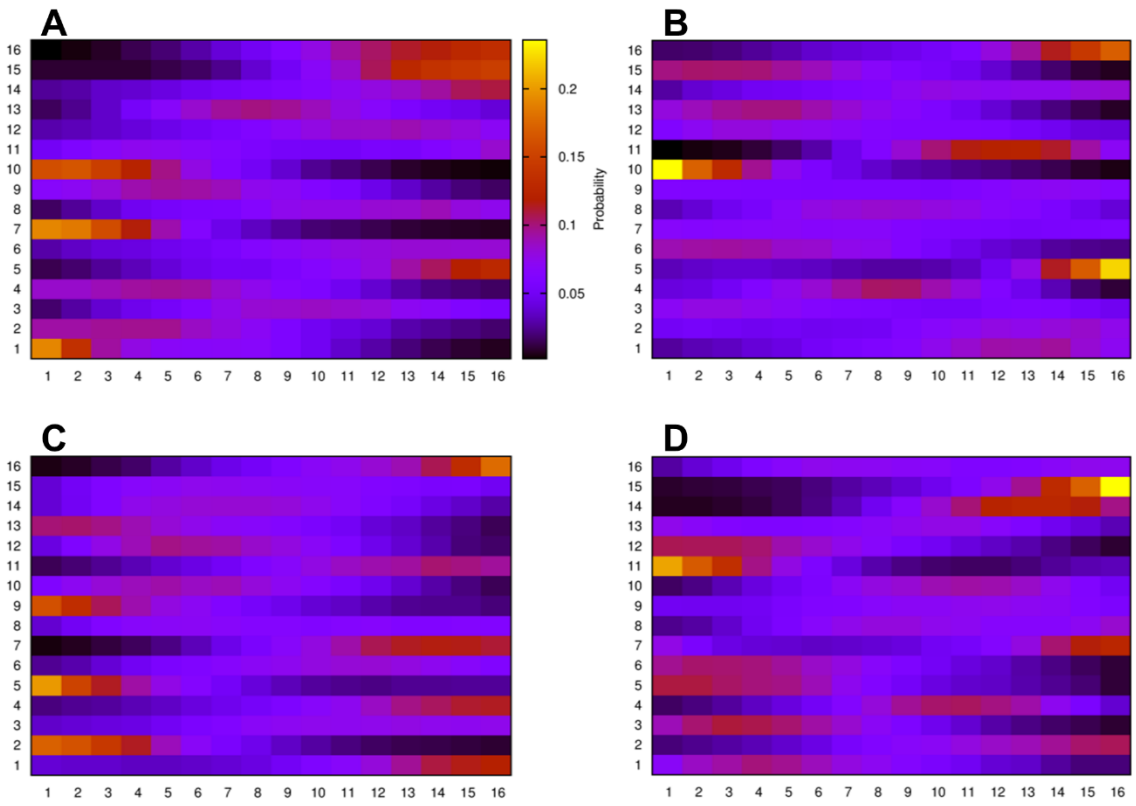

Figure S2 Probabilities of each replica, started from a particular position along the temperature ladder, to be at all the 16 positions in the ladder during the 100-ns simulations. The vertical axis indicates the starting position. (A) Apo SrtA. (B) $SrtA_{Ca}$. (C) $StrA_{Pep}$. (D) $StrA_{Pep/Ca}$.

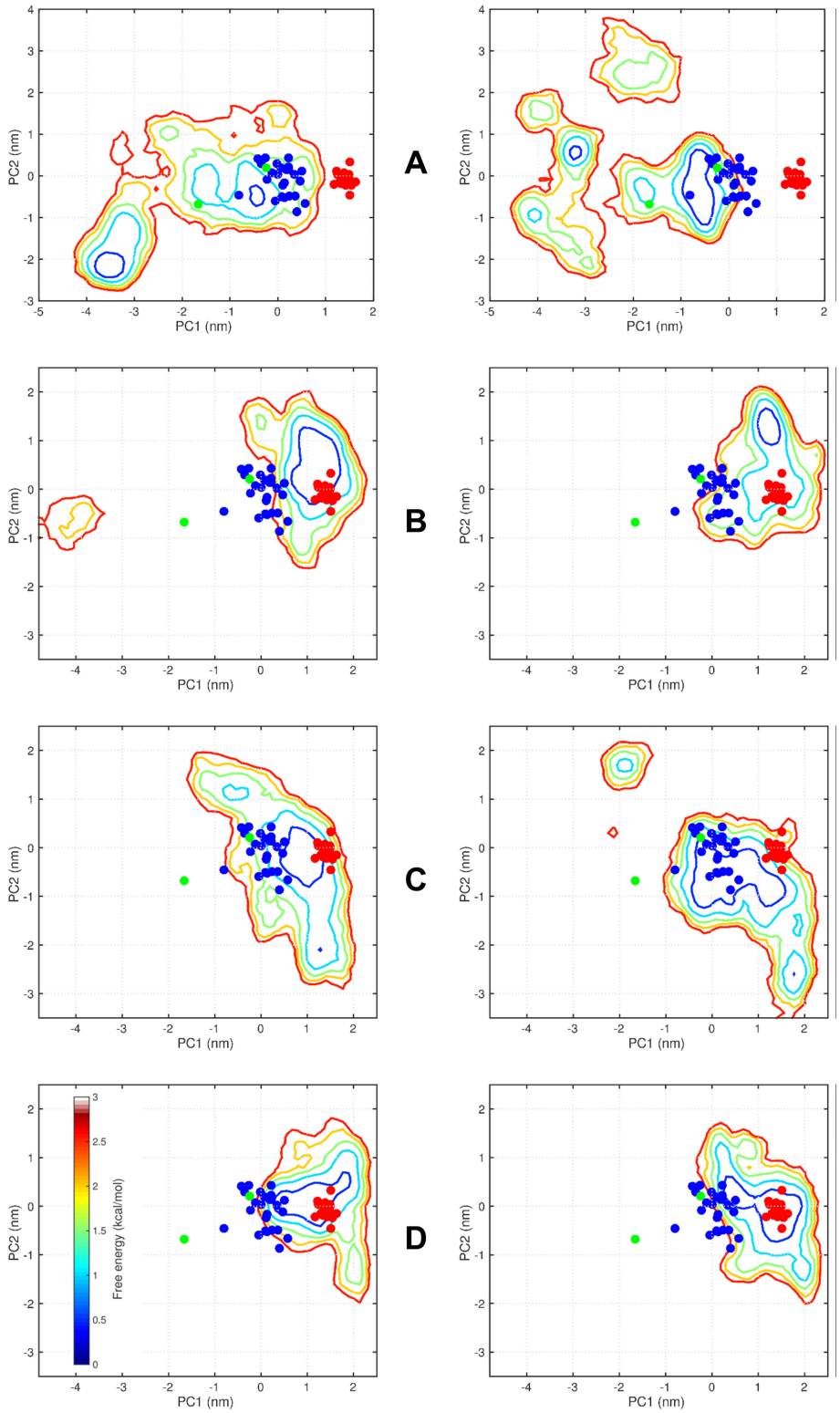

Figure S3 Conformational ensembles of the four forms of SrtA. (A) Apo. (B) $SrtA_{Ca}$. (C) $StrA_{Pep}$. (D) $StrA_{Pep/Ca}$. Left and right panels display results calculated from 0-50 ns and 50-100 ns of the simulations.

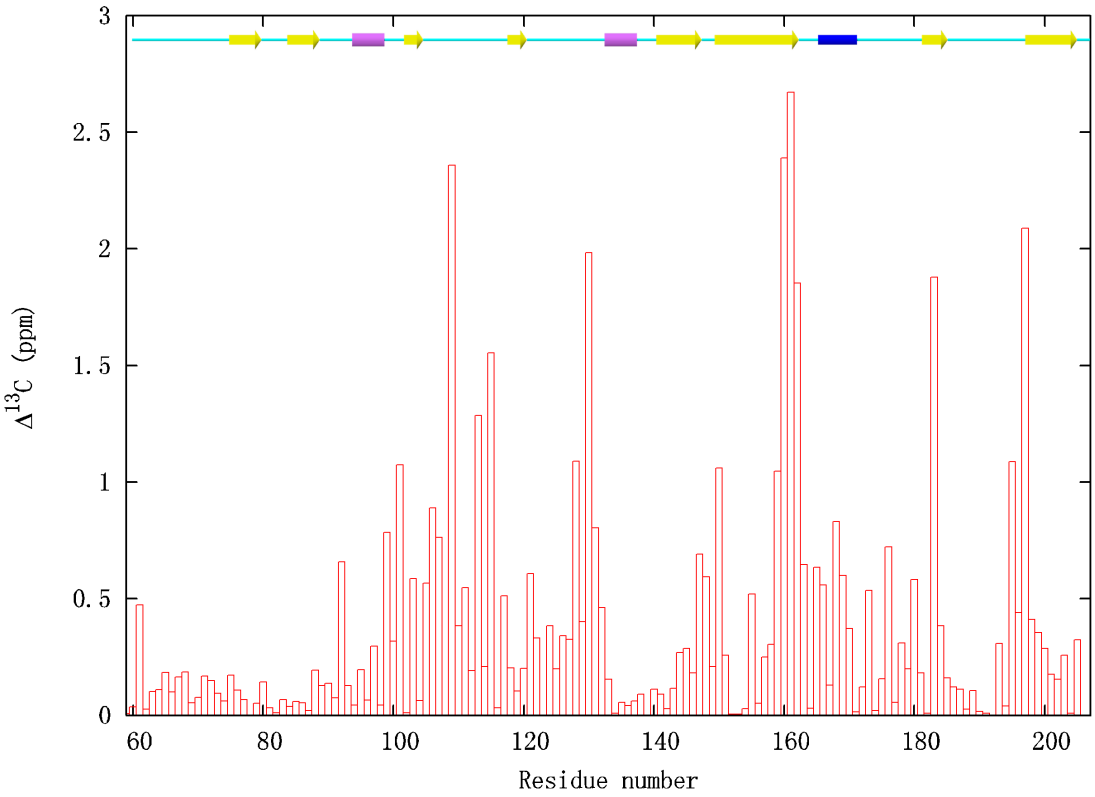

Figure S4 Predicted changes in Cα chemical shifts of sortase A upon Ca^{2+} binding. The secondary structure of the protein is shown at the top.