

Supporting information (SI)

**Molecular Insight into the Adsorption of Spruce Budworm Antifreeze
Protein to an Ice Surface: A Clathrate-Mediated Recognition Mechanism**

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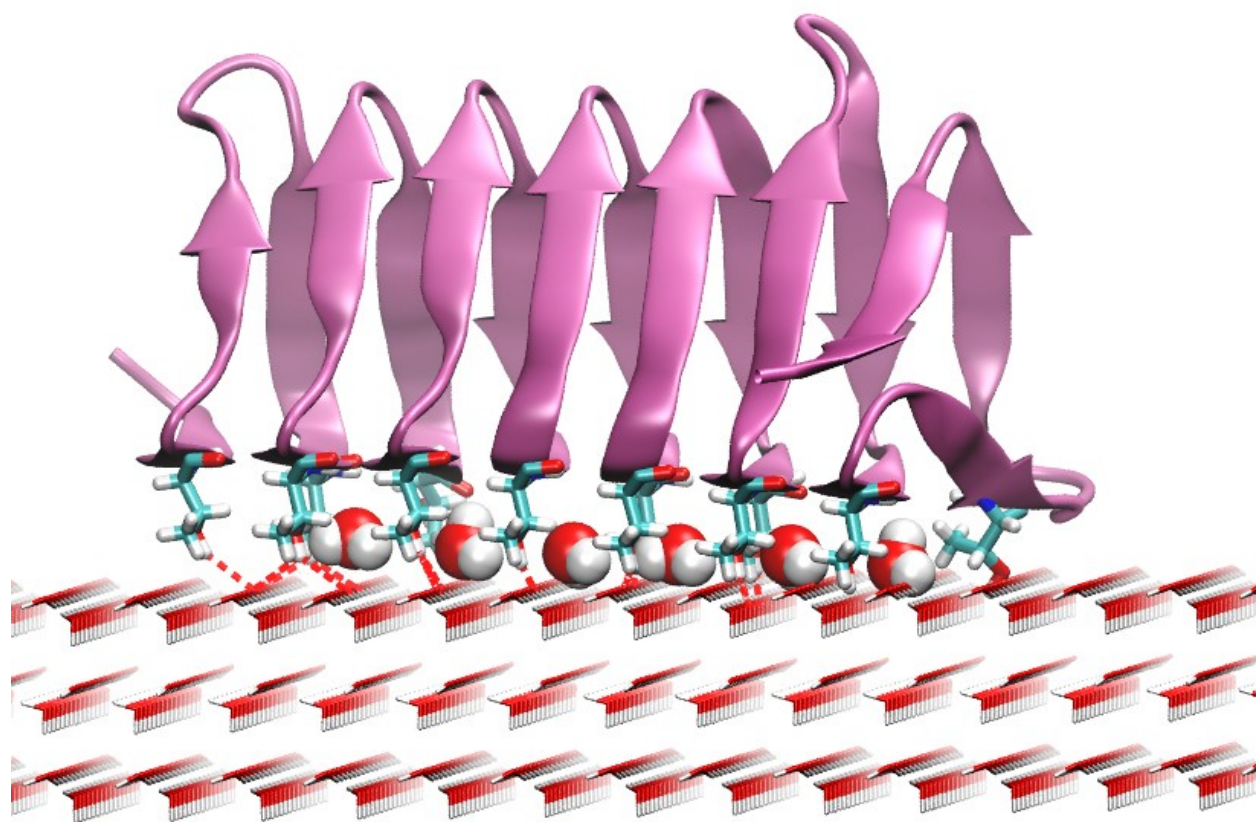


Figure S1: Initial structure of AFP-ice complex obtained from molecular docking. Protein is shown in cartoon representations and the THRs ladder is shown in stick. Ice plane is represented in line mode. Ordered waters are shown in sphere representation and hydrogen bonding interactions are shown as red dots.

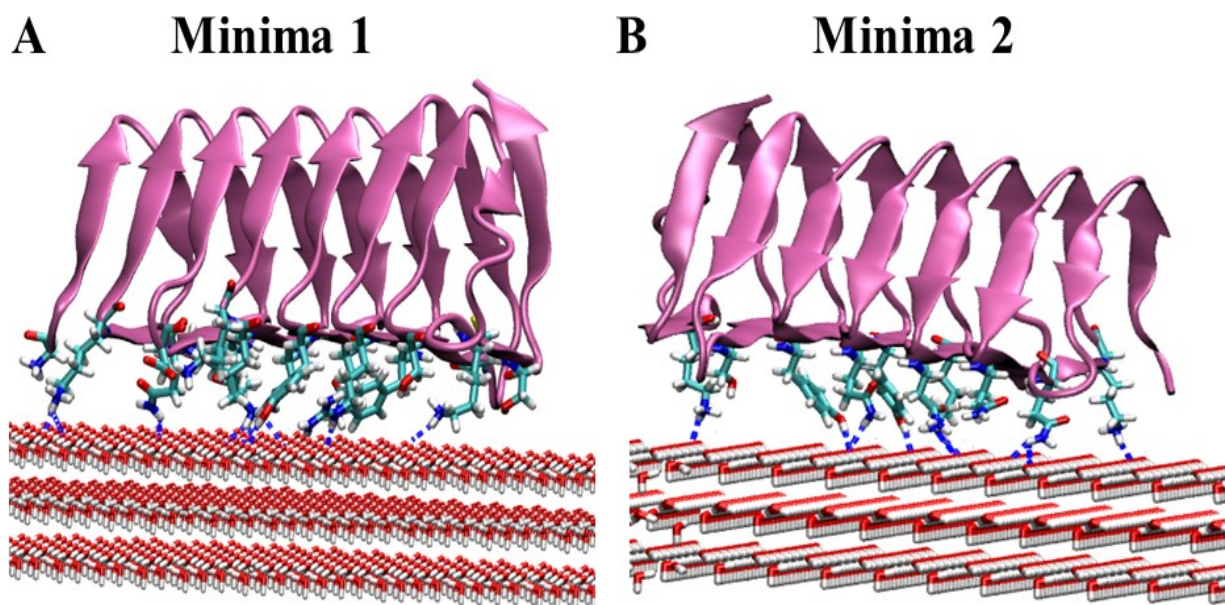


Figure S2: Two different bound structures of the *sbw*AFP-ice complex corresponding to two minima of the PMF profile where the AFP interacts with the ice plane through the non-IBS plane. Structures of the *sbw*AFP-ice complex corresponding to the first (A) and second (B) minima of the PMF profile are shown. The protein is shown in cartoon representations and THR ladder is shown as cyan sticks. Ice plane is represented in red stick representation and hydrogen bonding interactions are shown in blue dotted line.

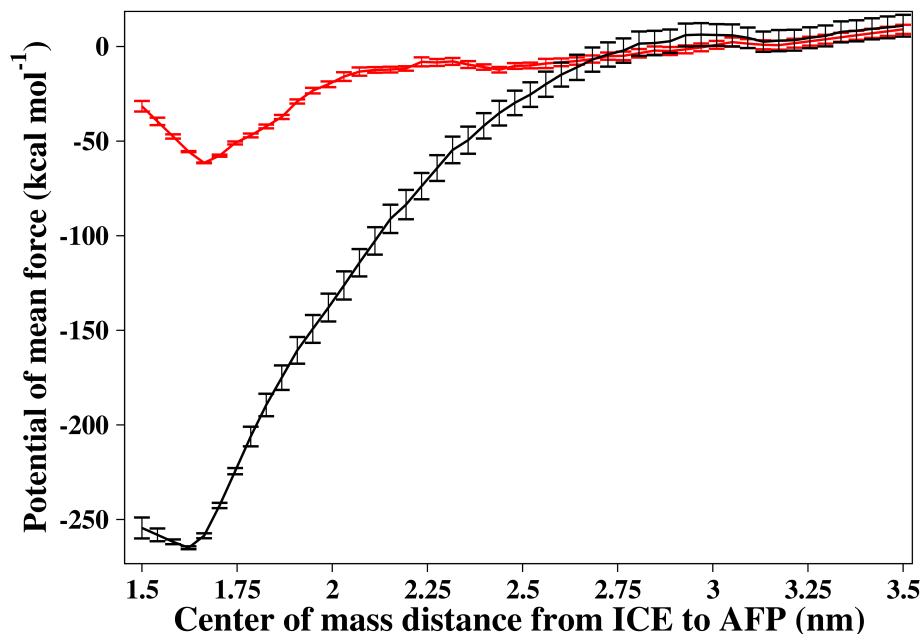


Figure S3: Comparison of the PMF profiles for the binding of *sbw*AFP to the basal plane of ice through the ice binding surface in presence of anchored clathrate water using two different water models, SPC/E (black) and TIP4P (red). Error estimation was obtained from the bootstrap analysis. We have performed free energy simulations at 225 K and 240 K using SPC/E and TIP4P water model, respectively. Due to high simulation temperature, the binding affinity of AFP adsorption reduces in TIP4P model. However, the position of the minima remains invariant in both the water models which indicate that AFP adsorbs at the ice/water interface rather than forming direct hydrogen bonds with the ice surface. A point to mention is that in case of TIP4P we have observed that the ice/water interface changes during the simulation timescale. During the free energy calculation, there is a growth of solid phase on top of ice surface which can interfere with the PMF profile. Growth of such ordered layer upon minor undercooling has been reported earlier also. Therefore, we have presented the binding free energy calculation data using SPC/E water model in the manuscript.

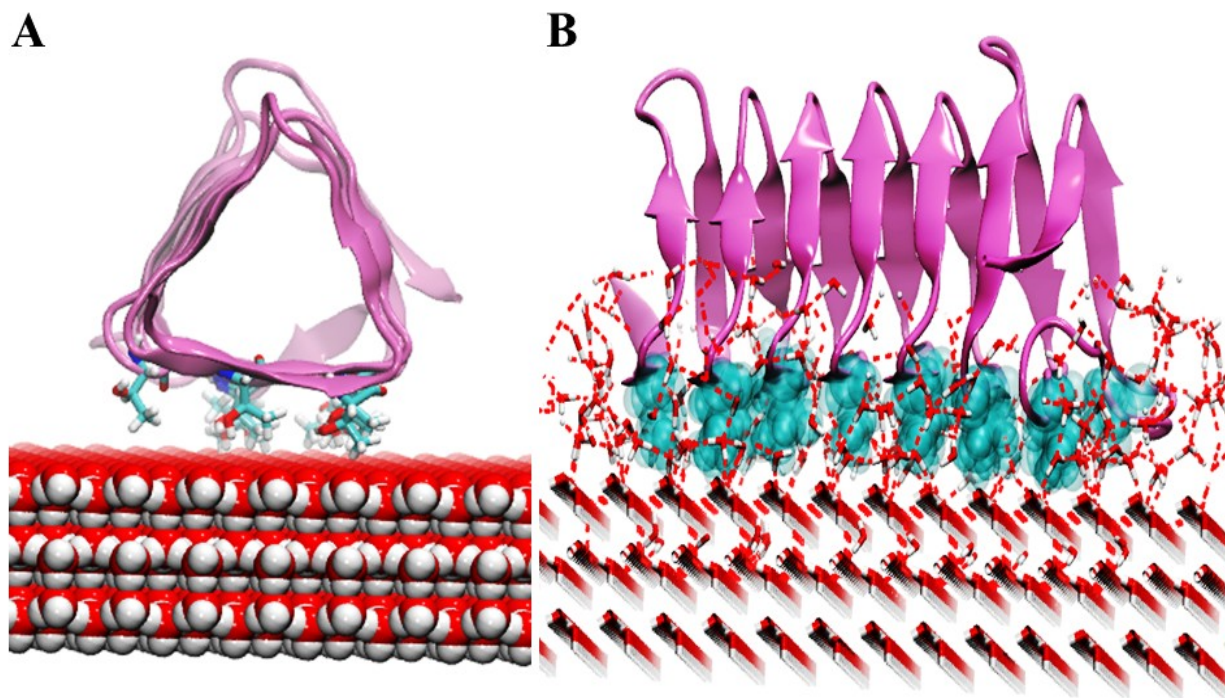


Figure S4: Structures of the *sbw*AFP-ice complex corresponds to the PMF minima where the AFP binds to the ice plane through the IBS in absence of anchored clathrate water. (A) Front view of the bound state of the complex is shown where the protein is shown in cartoon representations and THR ladder is shown as cyan sticks. Ice plane is represented in vdW representation. (B) Side view of the bound state of the *sbw*AFP-ice complex is shown where the protein is shown in cartoon representations and THR ladder is modeled as cyan vdW mode. Ice and ice/water interfacial water surrounding the THR ladder is shown in stick representation and hydrogen bonding interactions are shown as red dotted lines.