

*Supplementary Information*

**Proline-Mediated Conformational Rigidity Governs the Ice-Binding  
Behavior of Antifreeze Glycopeptides**

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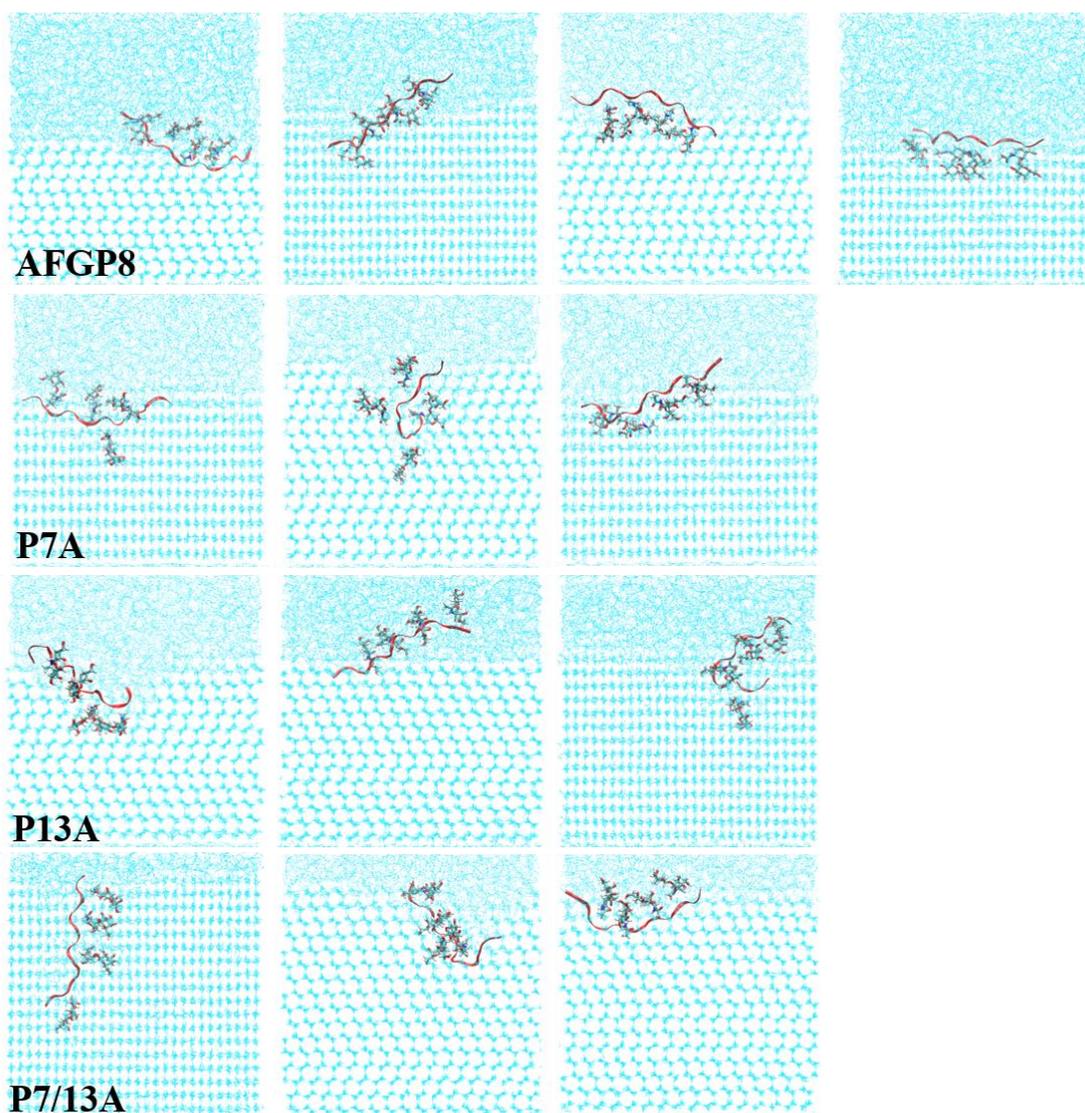
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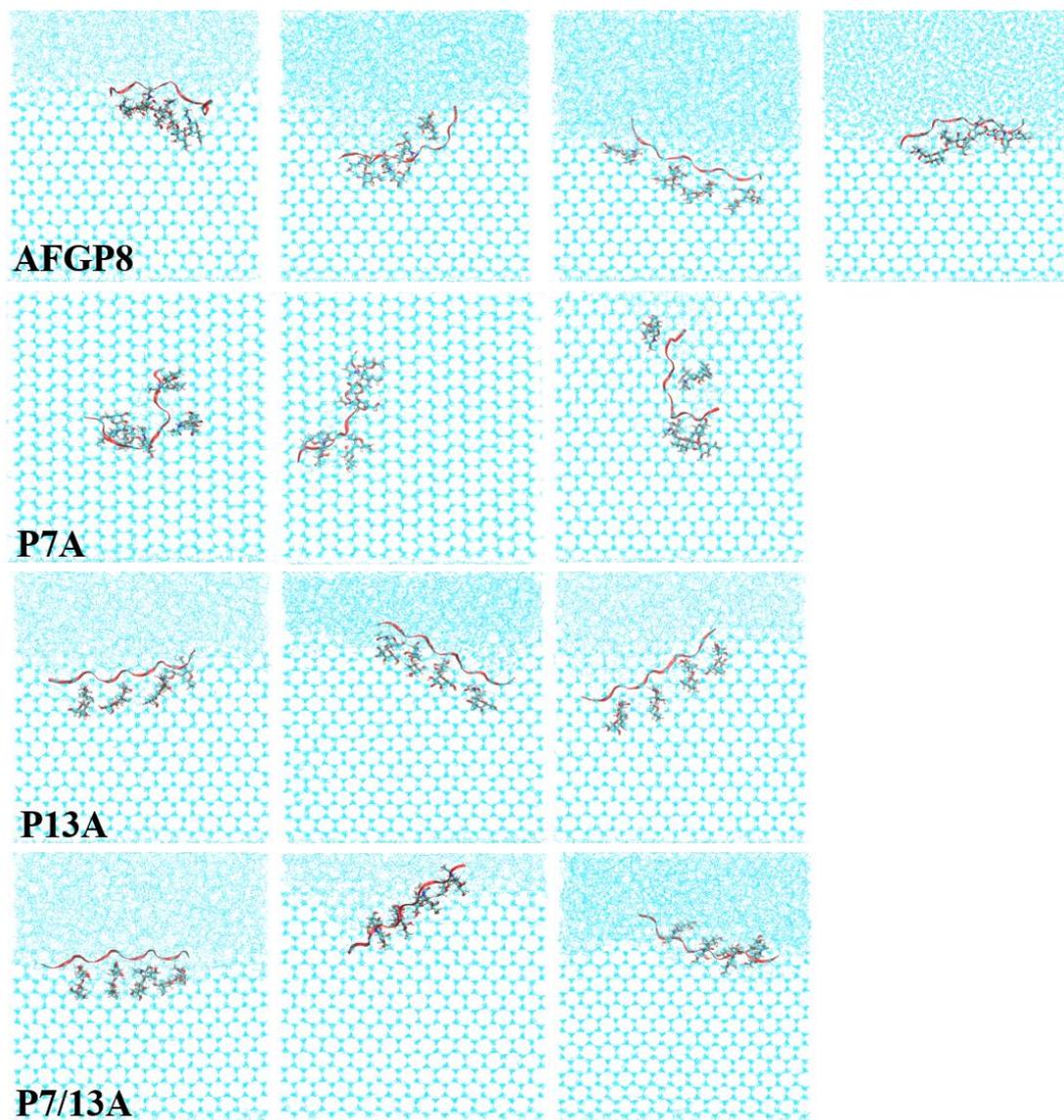
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**Table S1** Parameters used in DIKI.

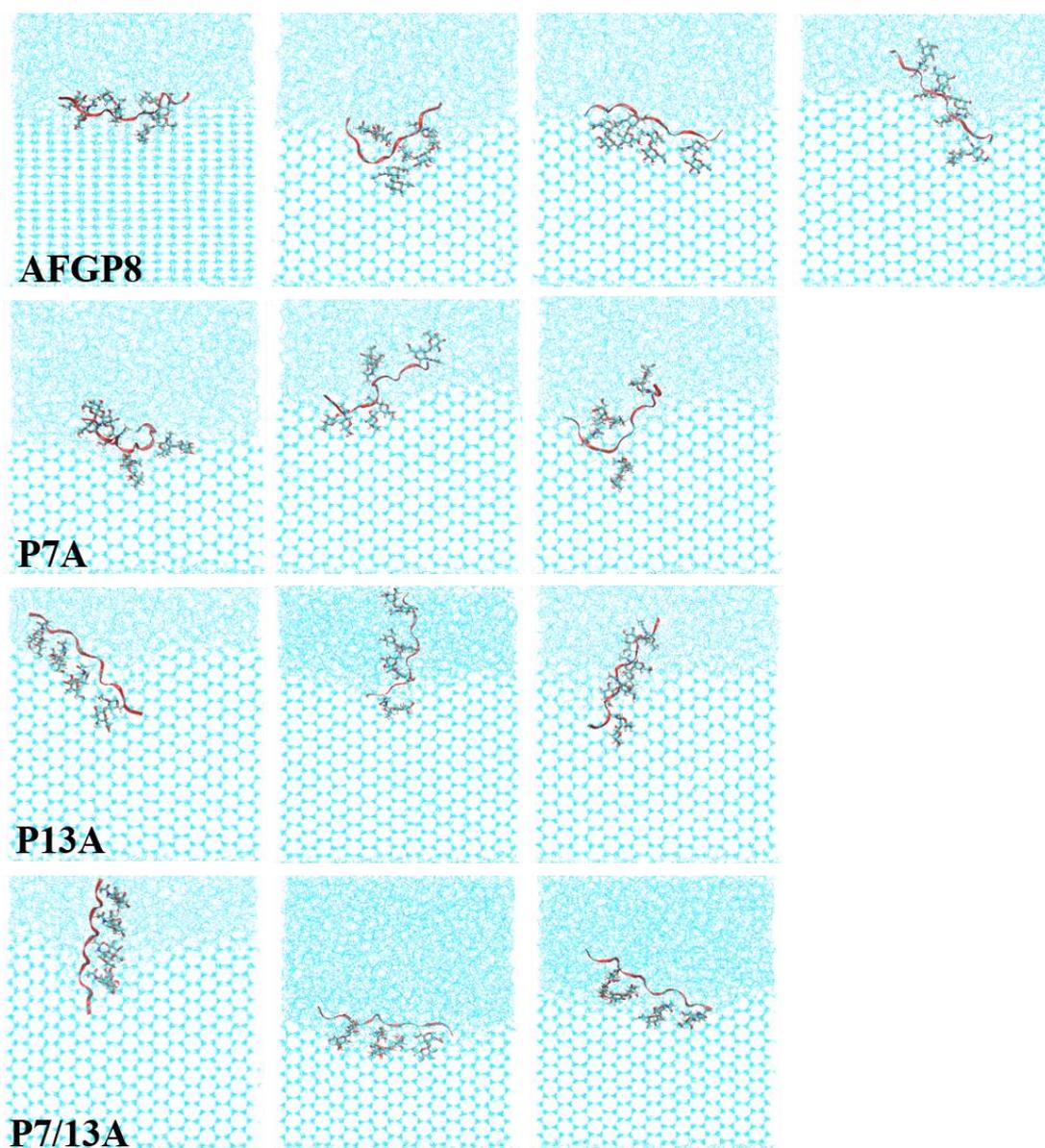
	BP	PP	SP
$\sigma$ (CFK)	10	10	10
$s$ (FFK)	3000	6000	1000



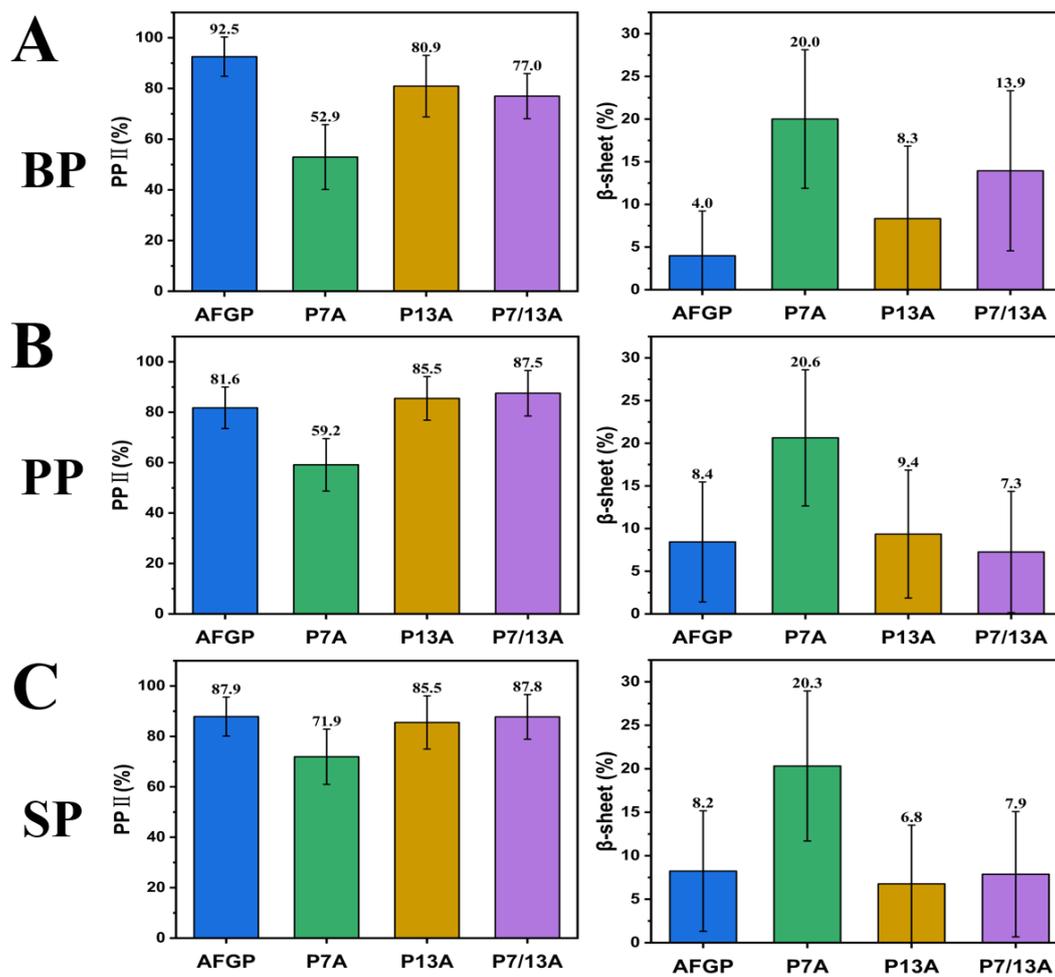
**Fig. S1** Snapshot of AFGP8 and its three mutants on the basal plane from 1000 ns parallel simulations.



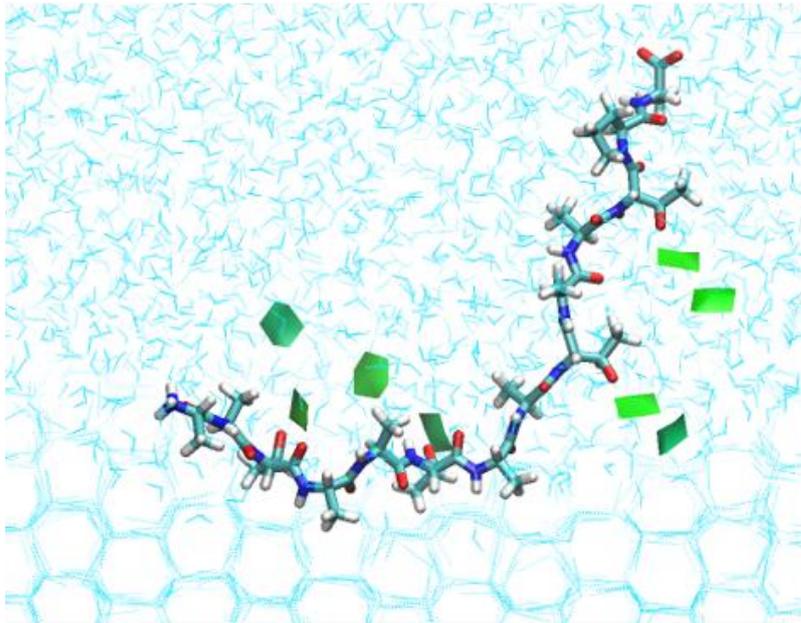
**Fig. S2** Snapshot of AFGP8 and its three mutants on the primary prism plane from 1000 ns parallel simulations.



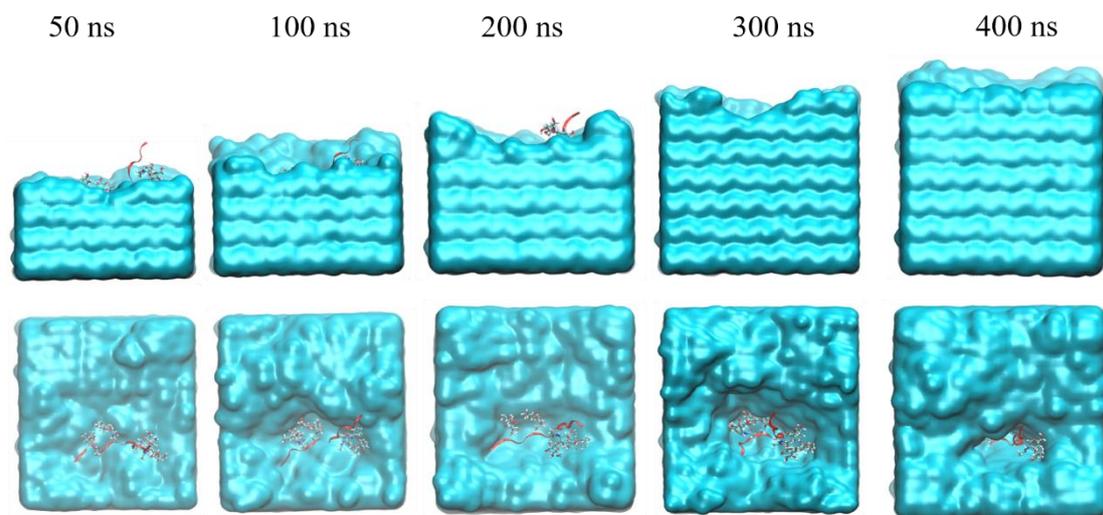
**Fig. S3** Snapshot of AFGP8 and its three mutants on the secondary prism plane from 1000 ns parallel simulations.



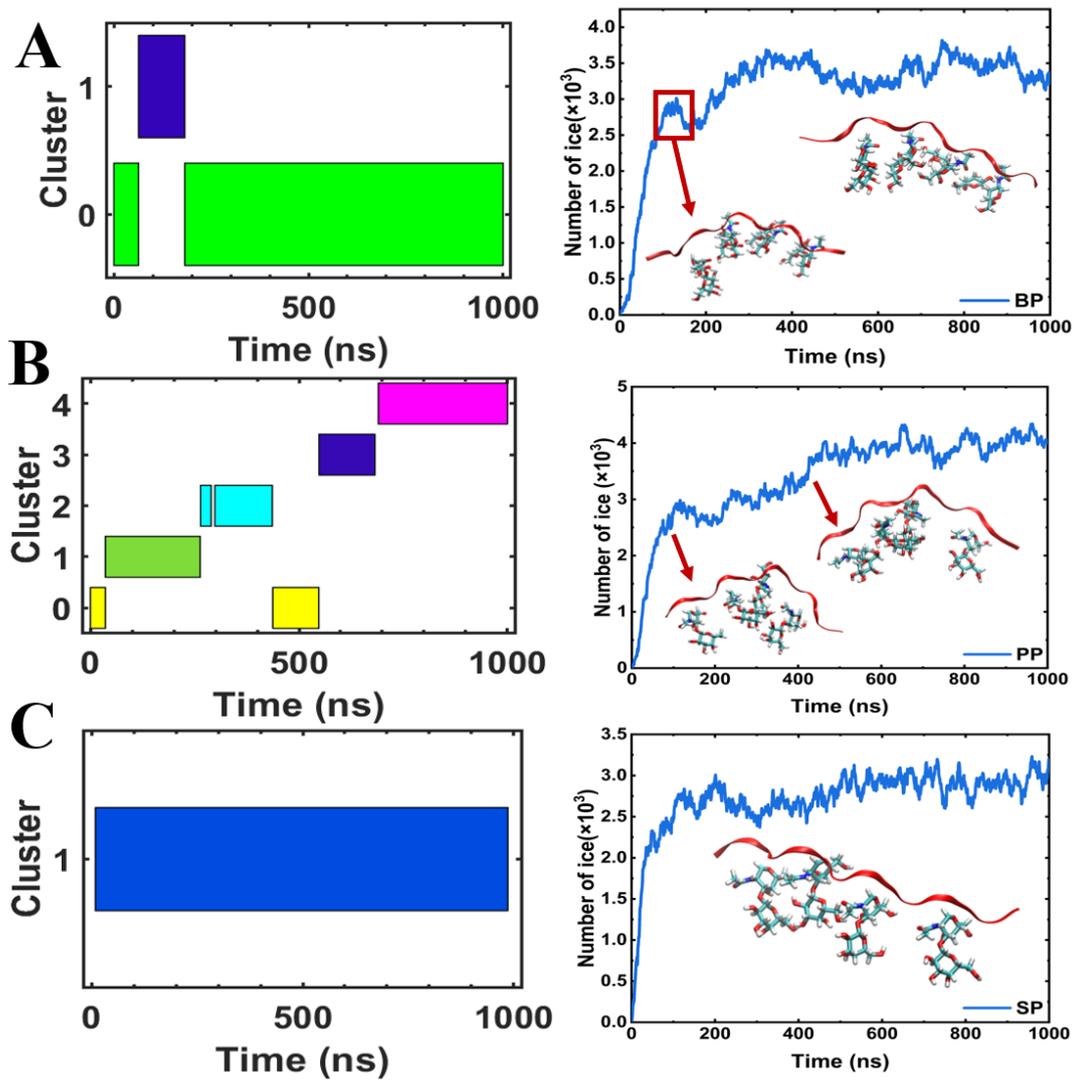
**Fig. S4** The average content of PPII helices and  $\beta$ -sheets of the four glycopeptides. (A) BP. (B) PP. (C) SP.



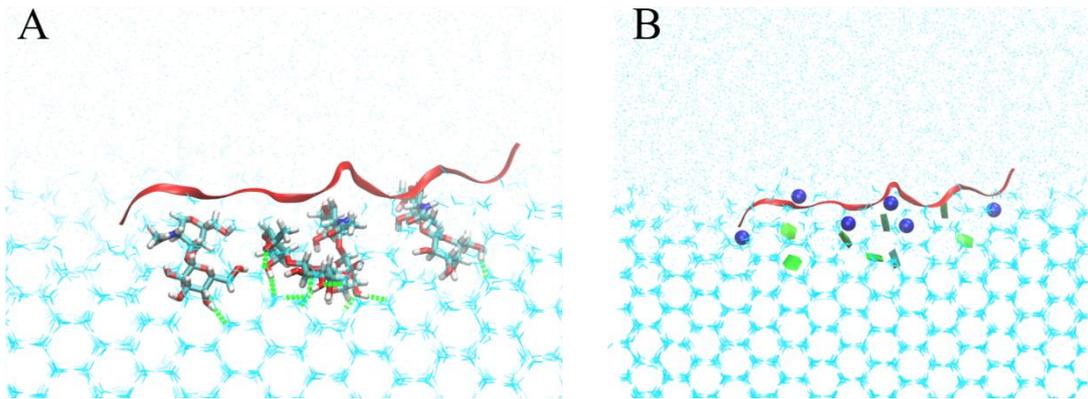
**Fig. S5** Cluster 0 conformation of P7A on the primary prism plane, showing two saccharides above the peptide chain and two saccharides below. Sugar are represented by Paperchains



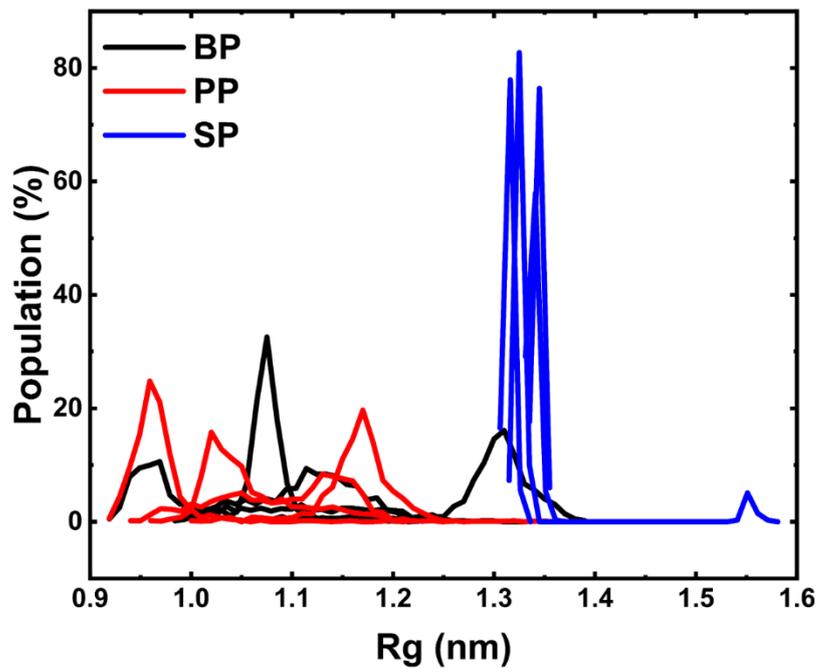
**Fig. S6** Snapshots of P7A being progressively engulfed on the primary prism plane.



**Fig. S7** Temporal evolution of AFGP8 on the three ice planes and the time-dependent change in ice content. (A) BP. (B) PP. (C) SP.



**Fig. S8** Interaction of P7A/P13A with the ice lattice at 1000 ns. (A) Hydrophilic interactions, with hydrogen bonds shown as green dashed lines. (B) Hydrophobic interactions, with methyl groups represented as blue spheres.



**Fig. S9** The Rg distribution of the three ice planes.