

Water Follows Polar and Nonpolar Protein Surface Domains

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All-atom molecular dynamics simulations revealed that protein surface domains distinctly affect the orientation of neighboring water molecules.

The hydration of molecules affects their physical and chemical properties. In particular, the functions and interactions of various proteins are determined by the conformation of water molecules around polar and nonpolar protein surface domains. Therefore, understanding the local interactions between water molecules and the polar and nonpolar protein surface domains, such as water molecule conformations in protein hydration layers, benefits targeted protein engineering, and recognition of molecules including proteins, DNA/RNA, cell membranes, and drugs.

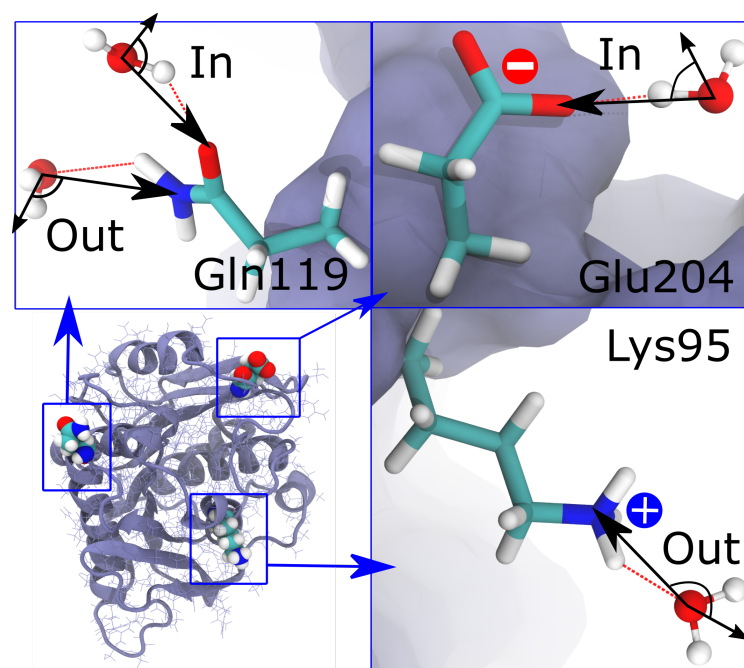


Figure 1: Surface amino acids distinctly orient water neighbors, leading to water In-orientation and Out-orientation.