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Direct Probing of Solvent Accessibility and Mobility at the Binding Interface of Polymerase (Dpo4)-DNA Complex YANGZHONG QIN, DONGPING ZHONG, Ohio State Univ - Columbus — Water plays essential structural and dynamical roles in protein-DNA recognition through contributing to enthalpic or entropic stabilization of binding complex and by mediating intermolecular interactions and fluctuations for biological function. These interfacial water molecules are confined in nanospace but mostly highly mobile. Here, we report our studies of interfacial water dynamics in the binary and ternary complexes of a polymerase (Dpo4) with DNA and an incoming nucleotide using a site-specific tryptophan probe with femtosecond resolution. By systematic comparison of the interfacial water motions and local sidechain fluctuations in the apo, binary and ternary states of Dpo4, we observed that the DNA binding interface and active site is dynamically solvent accessible and the interfacial water dynamics are slightly slow but similar to the surface hydration water fluctuations on picosecond time scales. Our MD simulations also show the binding interface full of water molecules and nonspecific weak interactions with protein and DNA. Such a fluid binding interface facilitates the polymerase sliding on DNA for fast translocation while the spacious and mobile hydrated active site contributes to the low fidelity of the lesion-bypass Y-family DNA polymerase.

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