

Figure S11. Atomic representations of in-phase fluctuating residues in the third and fourth clusters of atomic variables. (A) The third cluster of in-phase fluctuations consists of coupled motions of the backbone of R-loop, side-chains of Asp181, Phe182 on the WPD loop, and Trp96, Tyr124 and Leu160, which make hydrophobic interactions. (B) The fourth cluster of in-phase fluctuations consists of coupled motions of the backbones of β 9, β 10 and β 11 and side-chains of Asn44, Gln61, Trp100 and Leu160. Out of these four residues, the last two make hydrophobic contacts. In both figures, residues with perturbed side-chains are colored with respect their atoms (nitrogen in blue, oxygen in red, carbon in gray), regions of backbones with perturbed dihedral angles are colored in purple, and perturbed H-bonds are shown with black dashed lines.