

Supplementary information, Figure S4

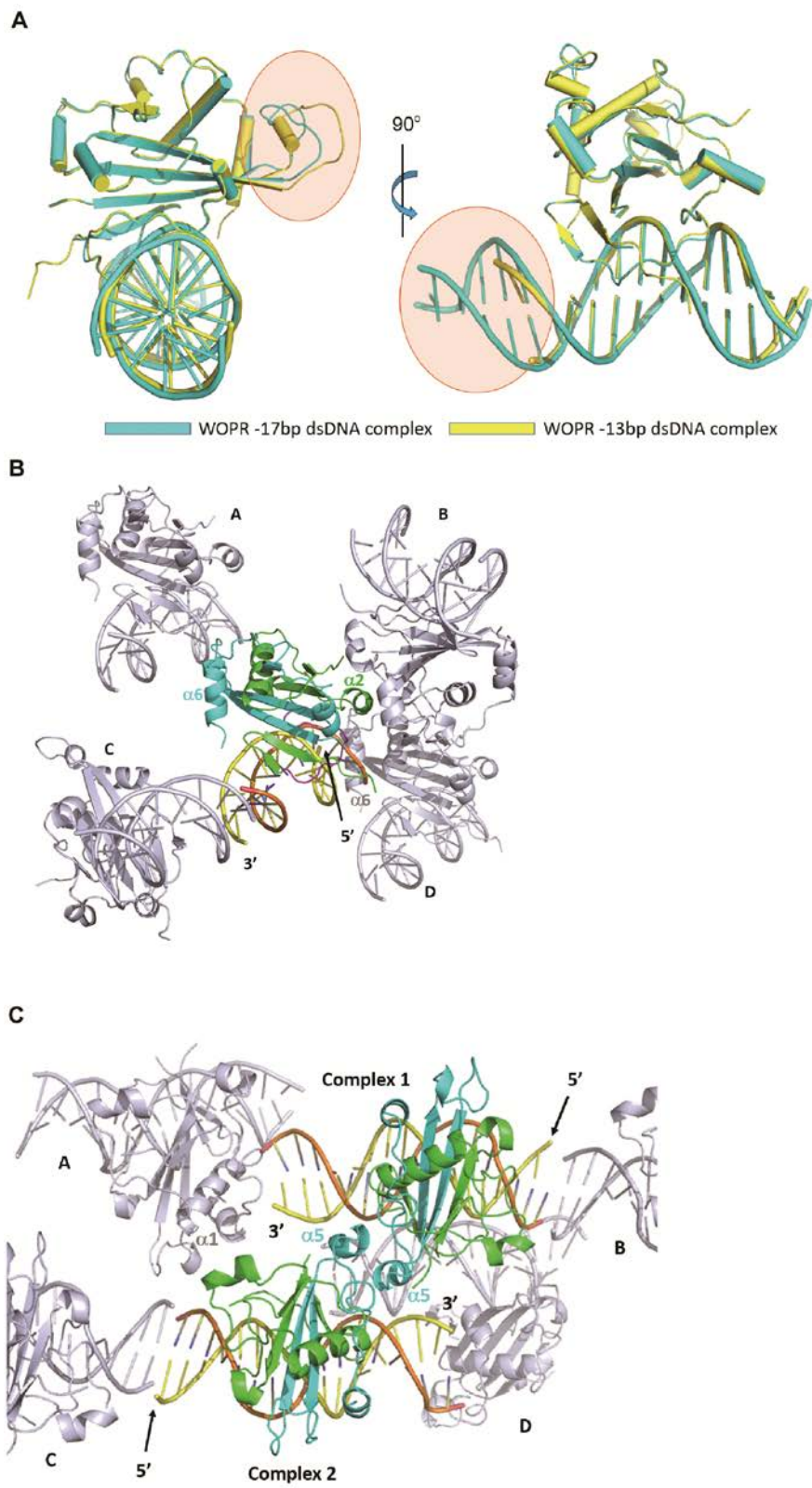


Figure S4 Comparison of the WOPR-13bp dsDNA complex and the WOPR-17bp

dsDNA complex. (A) Superposition of the WOPR-13bp dsDNA complex (in yellow) and the WOPR-17bp dsDNA complex (in cyan). The region with differed conformations is highlighted by an oval. (B) Crystal packing in the WOPR-13bp dsDNA complex. (C) Crystal packing in the WOPR-17bp dsDNA complex. The two complexes have different crystal packing modes. In the WOPR-13bp dsDNA structure, the 3'-end of the dsDNA interacts with the 3'-end of the dsDNA of a symmetry-related complex C and the 5'-end of the dsDNA interacts with $\alpha 6$ of WOPRb of another symmetry-related complex D. In addition, $\eta 1$ and $\alpha 2$ of WOPRa interact with the N-terminus and the $\alpha 1$ - $\eta 1$ loop of WOPRa of a symmetry-related complex B, and the C-terminus of WOPRa interacts with $\alpha 4$ and the $\alpha 4$ - $\beta 6$ loop of WOPRb of another symmetry-related complex A. In the WOPR-17bp dsDNA structure, there are complex molecules in the asymmetric unit. The 5'-end of the dsDNA of complex 1 interacts with the 5'-end of the dsDNA of a symmetry-related complex B and the 3'-end of the dsDNA interacts with $\alpha 1$ of WOPRa of another symmetry-related complex A. In addition, the two complexes in the asymmetric unit interact with each other via $\alpha 5$ and the $\alpha 5$ - $\alpha 6$ loop of WOPRb.