

Supplementary Figures

Figure S1

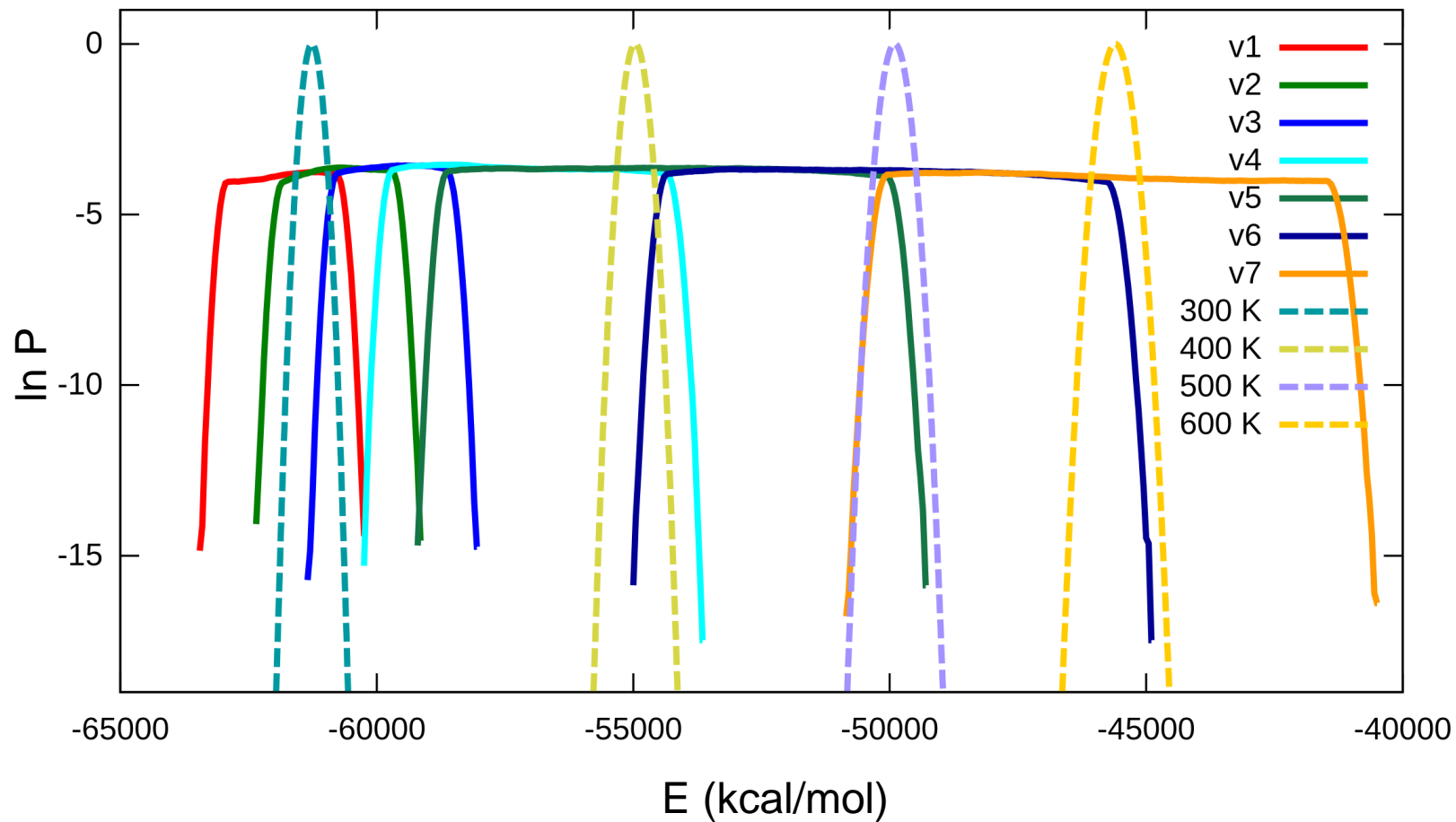


Figure S2

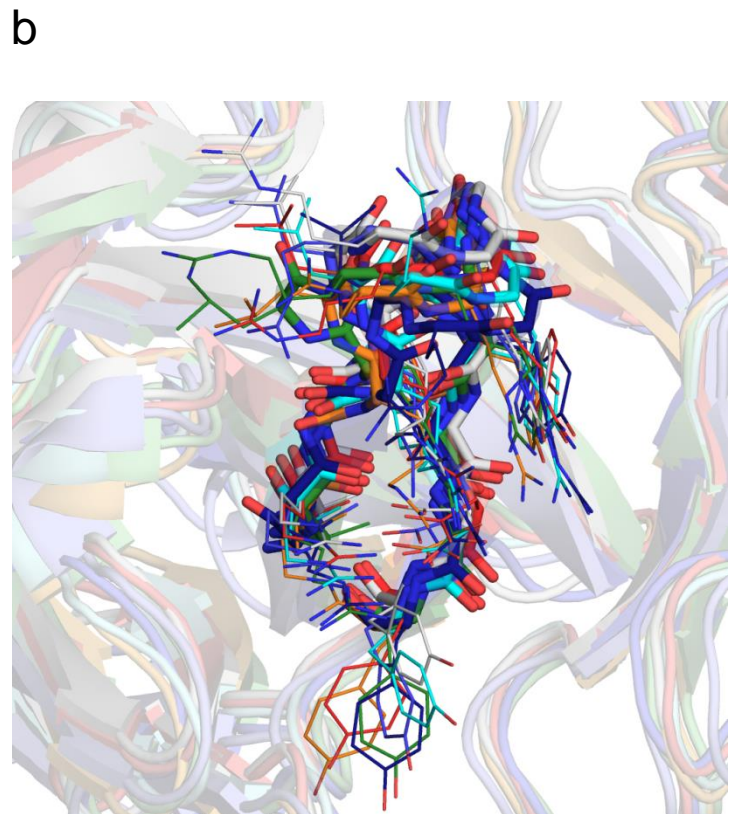
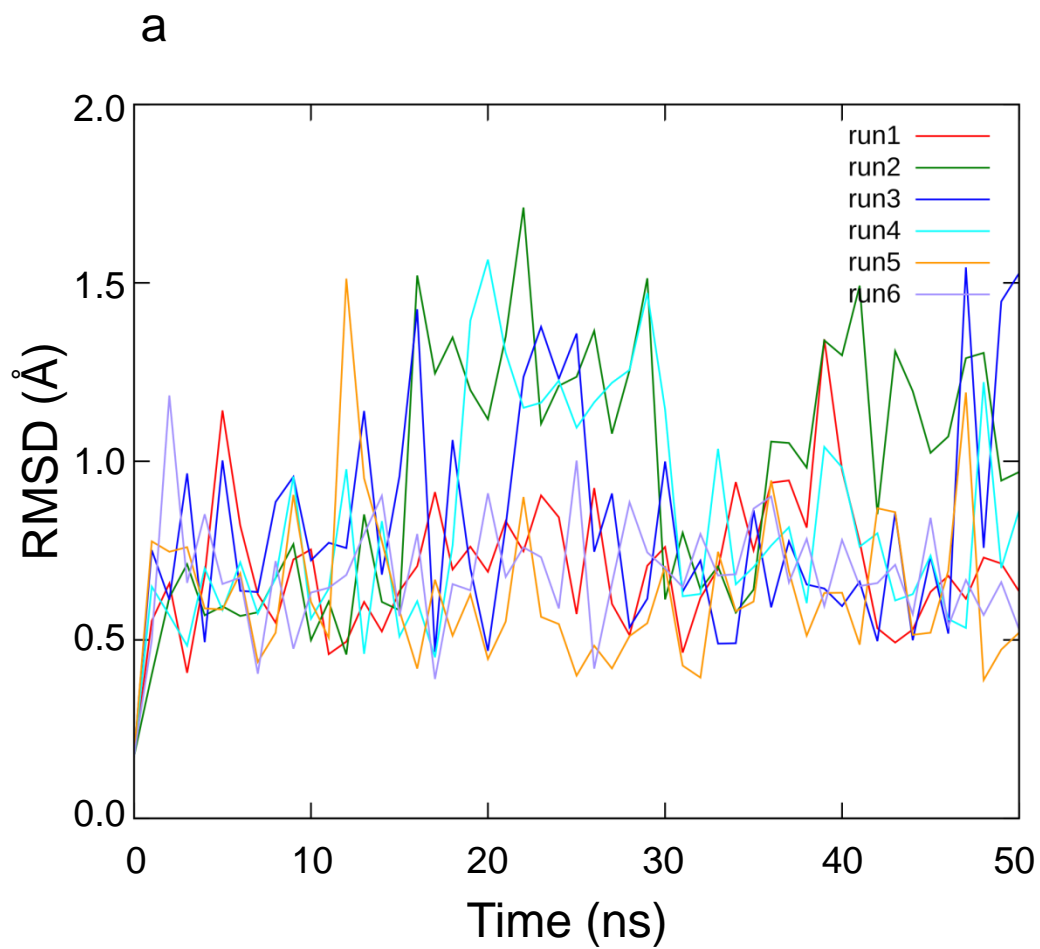
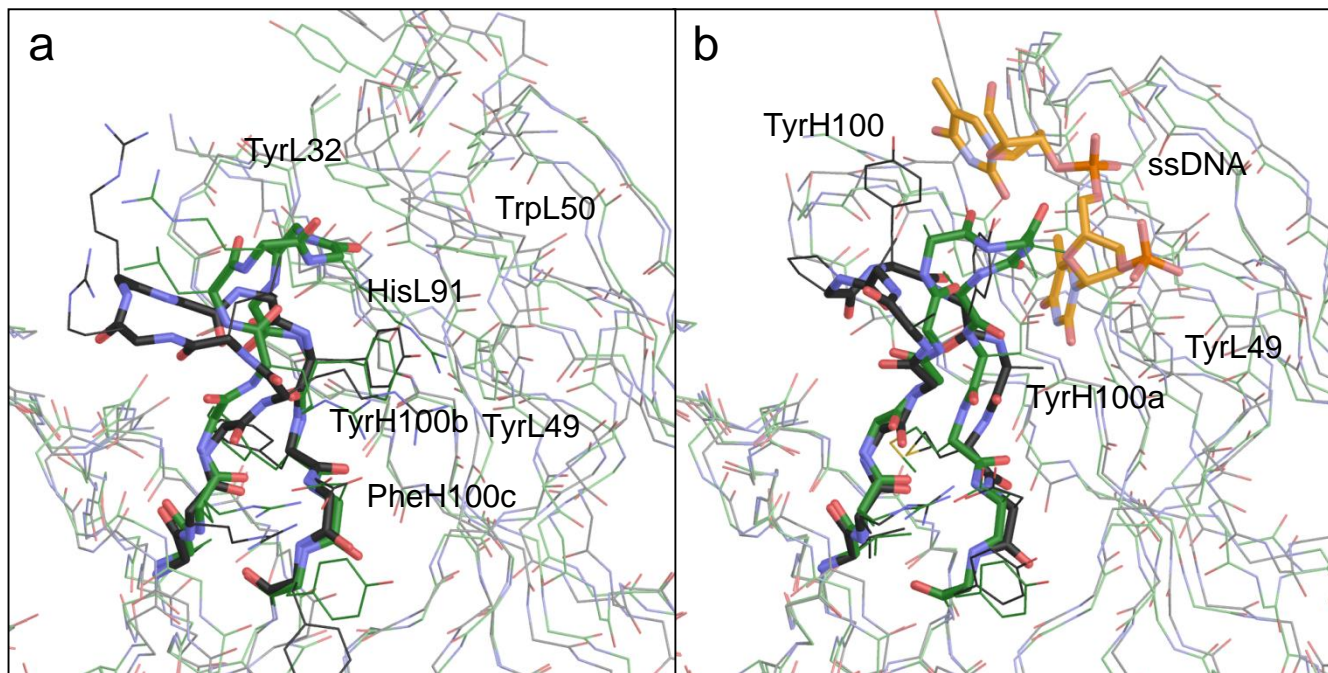


Figure S3



Supplementary Figure Legends

Fig. S1: Probability distributions of the potential energy obtained from the TTP-V-McMD simulation ($v1-v7$) and the reweighted canonical distributions at 300, 400, 500, and 600 K. Each curve corresponds to each distribution, according to the figure legend.

Fig. S2: (a) The RMSDs of the CDR-H3 loop along the canonical MD simulations. Each simulation from run1 to run6 is colored according to the legend in the figure. (b) Final structures of each canonical MD with the X-ray structure. The colors of the structures correspond to the trajectories in the legend of (a). The X-ray structure is colored gray.

Fig. S3: (a) The X-ray structure and our model a of the A52 antibody. The X-ray structure (PDBID 4m61, chains A and B) and our model a are colored green and black, respectively. (b) The X-ray structures of the apo- and holo-antibodies of the DNA-1 antibody. The apo-antibody (PDBID 1xf3, chains L and H) and the holo-antibody (PDBID 1xf2) with the bound antigen single-stranded DNA (ssDNA) are shown in green, black, and orange, respectively. The backbone atoms of the CDR-H3 loops and the ligand atoms are shown by thick stick models, and the others are depicted by thin wire models.