

Figure S1. Deviation of C^α positions in models. The deviation is calculated from the corresponding X-ray structures, with models and the X-ray structures superimposed by minimizing RMSD. (A) Histidines in 6 Å models. (B) Comparison of homology and NEB models.

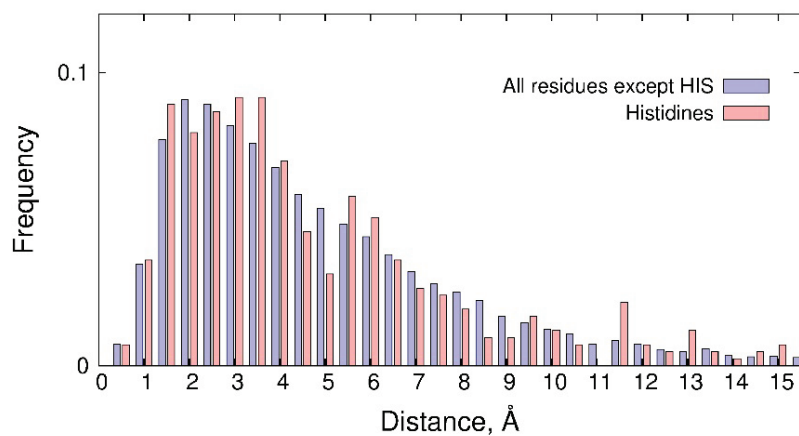


Figure S2. Deviation of C^α positions in histidines and all other residues in 6 Å NEB models.