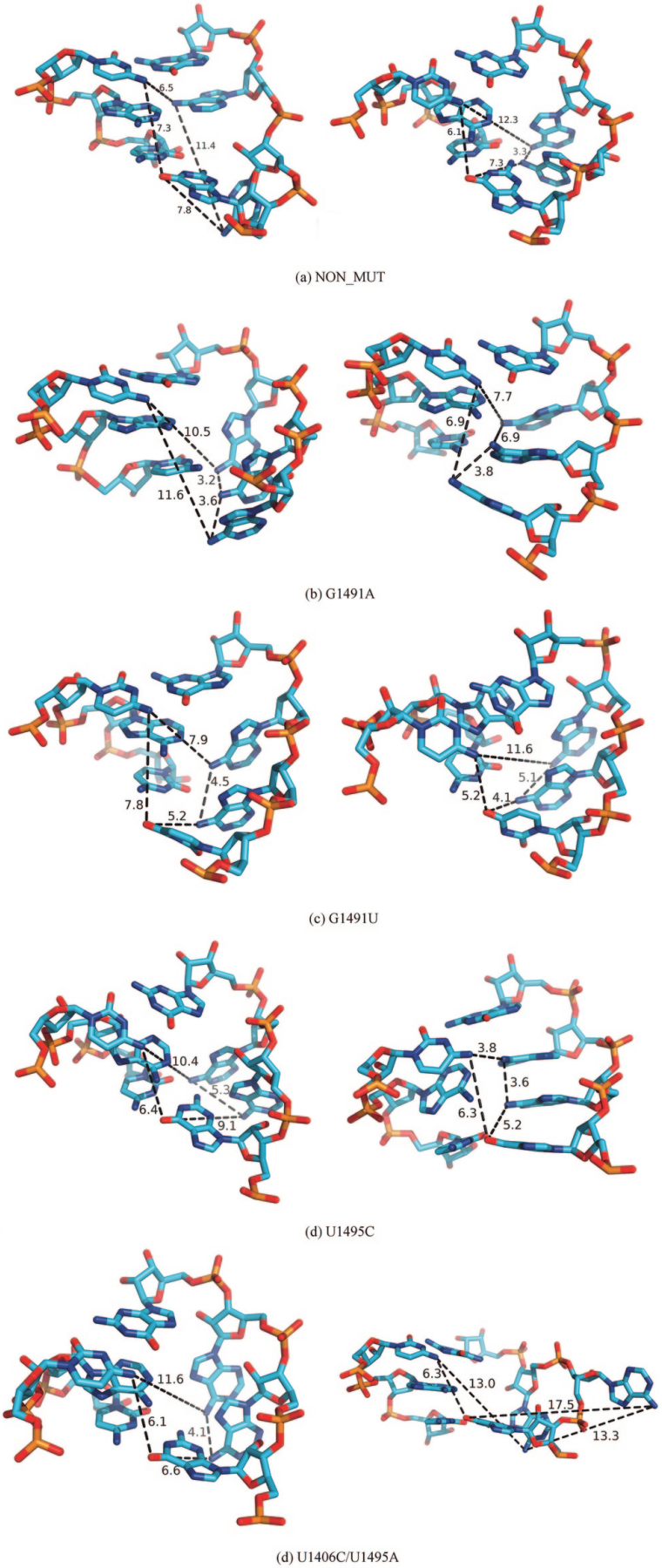

Figure S4: **Conformations of bases forming the A-site in the most populated clusters in different MD simulations**. The distances (in Å) between chosen atoms are shown as black dotted lines; two snapshots per simulation correspond to two A-sites in the crystal structure; for base numbering see the inset in the Figure S5 and Figure 1a.