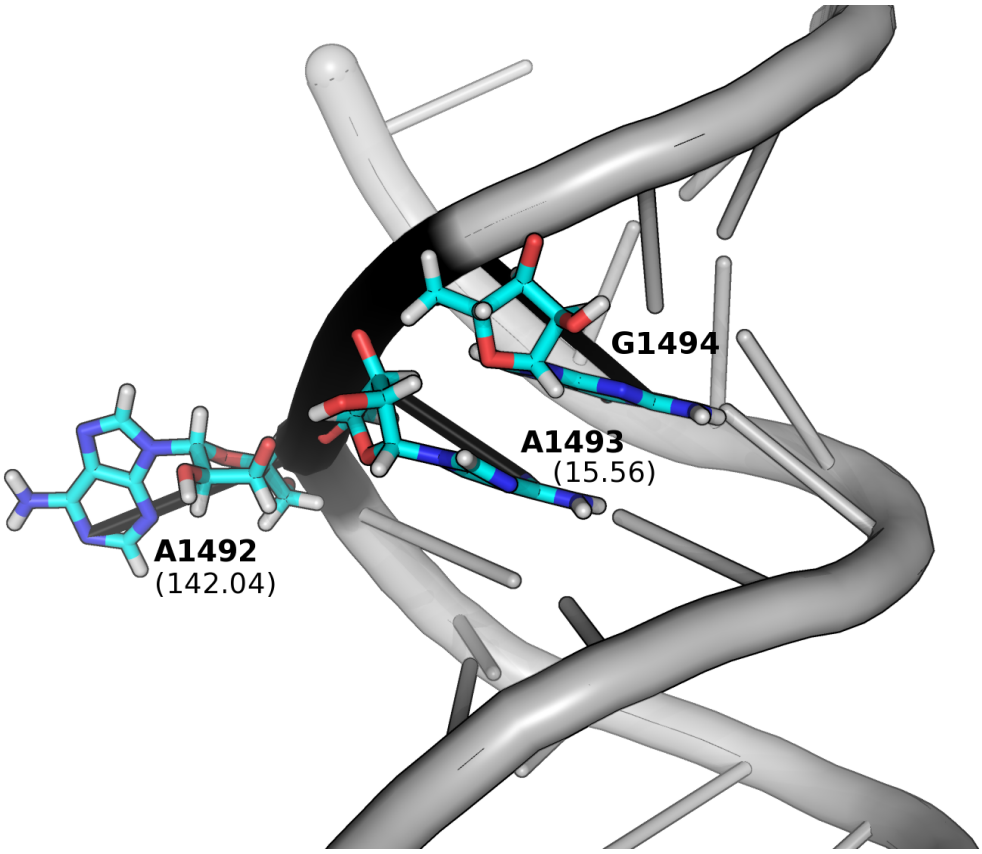

Figure S3: **Pseudo-dihedral angles describing the variation in the conformations of A1492 and A1493**. The angle θ_{A1493} is calculated as a torsion angle between the four atoms: G1494(N1) – G1494(P) – A1493(P) – A1493(N1), as depicted by black sticks (analogously for θ_{A1492}: G1494(N1) – G1494(P) – A1492(P) – A1492(N1)). The exemplary snapshot is taken from the NON_MUT simulation, with the values of the pseudo-dihedral angles (in degrees) shown in brackets.