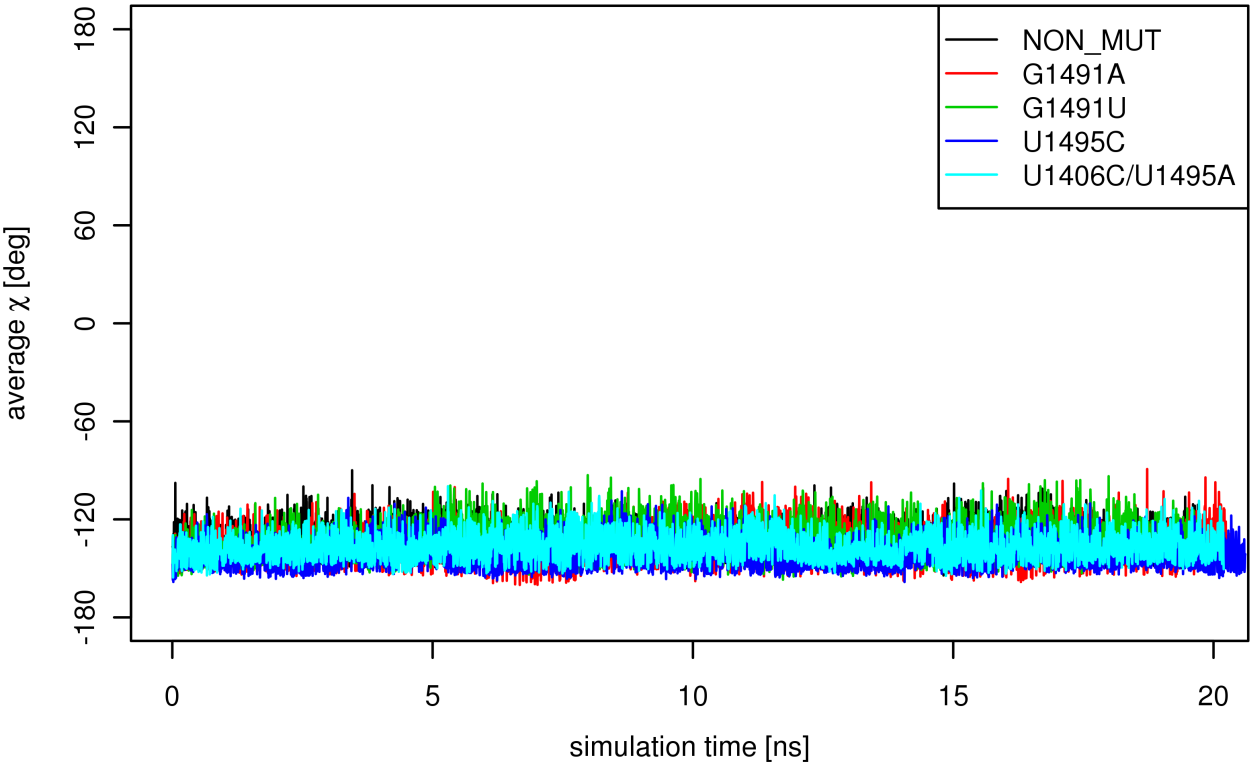

Figure S12: **Average glycosidic torsion angle** χ, calculated for all the residues in each simulation per each frame. The scale on y axes spans the possible range of χ (-180, +180); compare with Figure 6 in [Banáš, P. *et al.*, Journal of Chemical Theory and Computation. **2010**, 6, 3836-3849].