

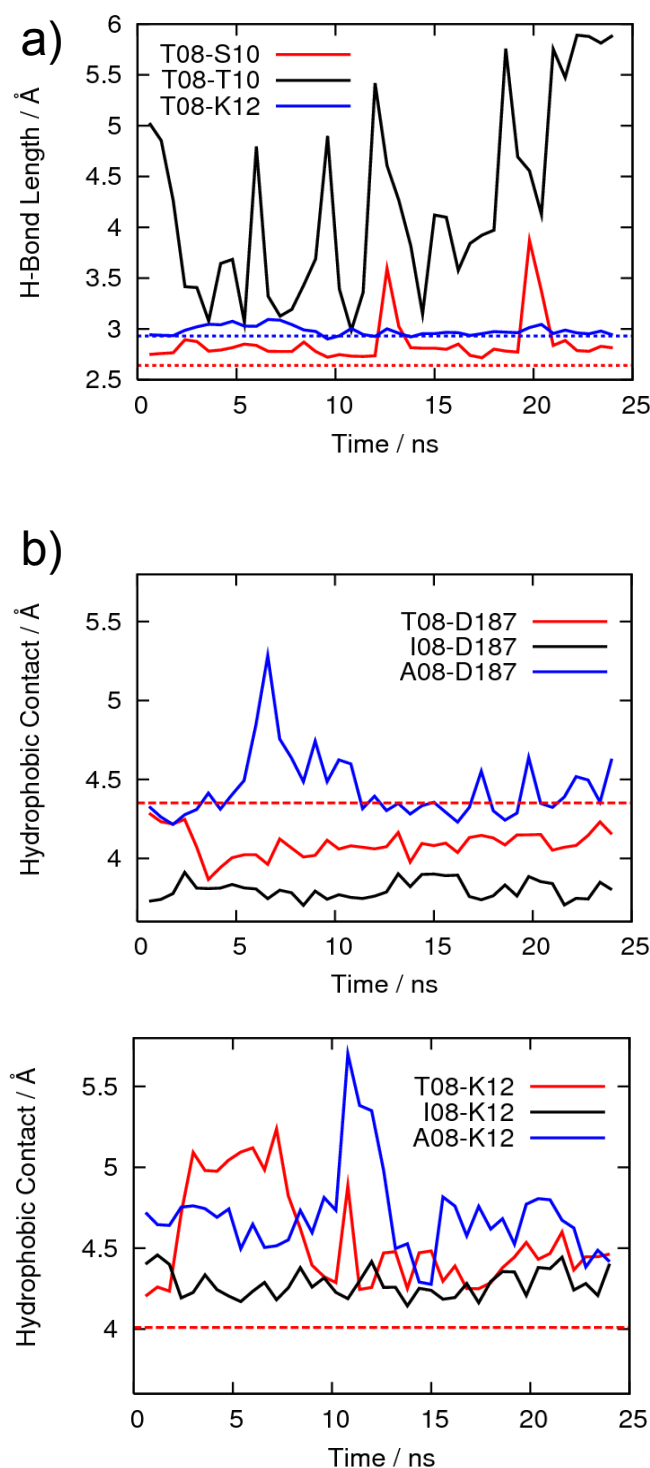


Figure S2. Block averages of non-bonded interactions involving residue 08. a) Residue T08 in BRC4A forms intra-hairpin hydrogen bonds with residues S10 and K12, which are important in maintaining hairpin stability. The corresponding interaction in RAD51 (T08-T10) is less important and fluctuates throughout the simulation. b) T08 also forms hydrophobic contacts with D187 of RAD51 and K12, which may help to stabilise the D187-K12 hydrogen bond. This effect is enhanced following the T08I substitution and reduced in T08A. Dashed lines indicate the corresponding distances in 1NOW.