

Figure S1 E_{HB} of H-bond in *abc* and after Gly of chain b and c 17th site was mutated. Index 1-30 is the position of each H-bond in the collagen.

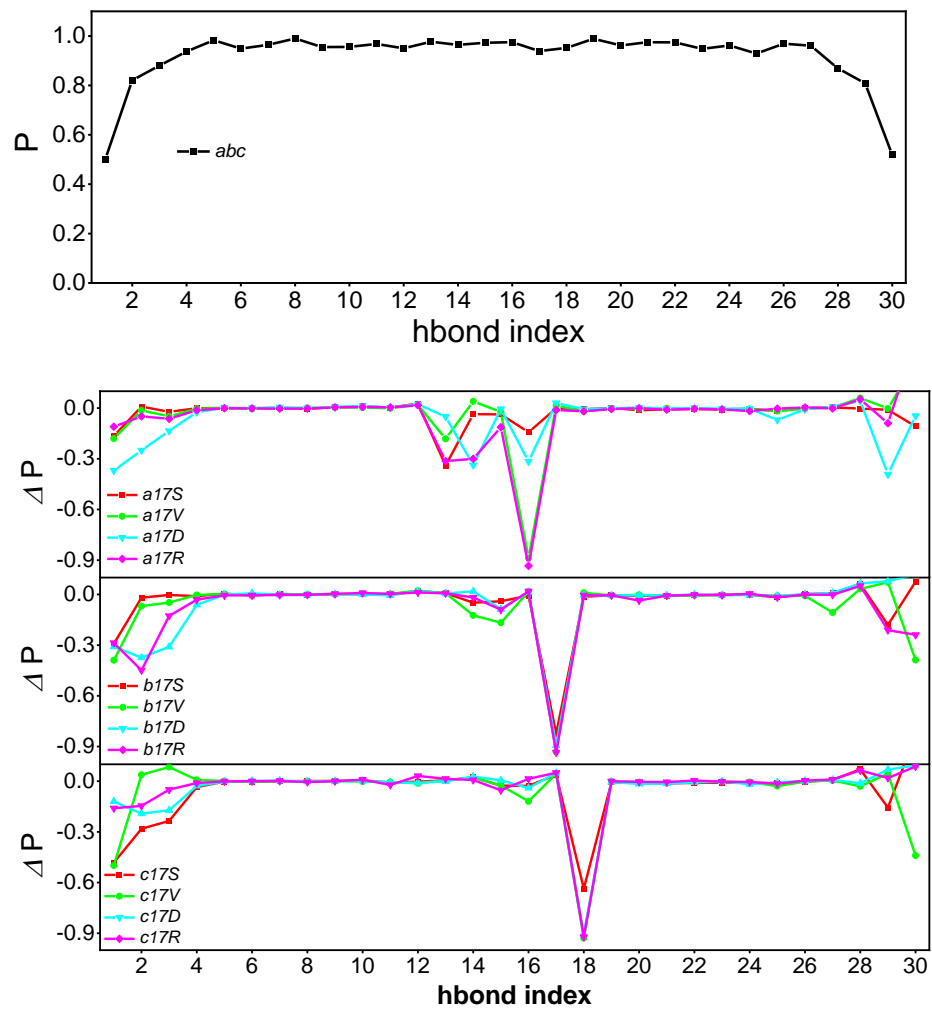


Figure S2 Probability of H-bond binding of abc and change after Gly of chain b and c 17th site was mutated. Index 1-30 is the position of each H-bond in the collagen.

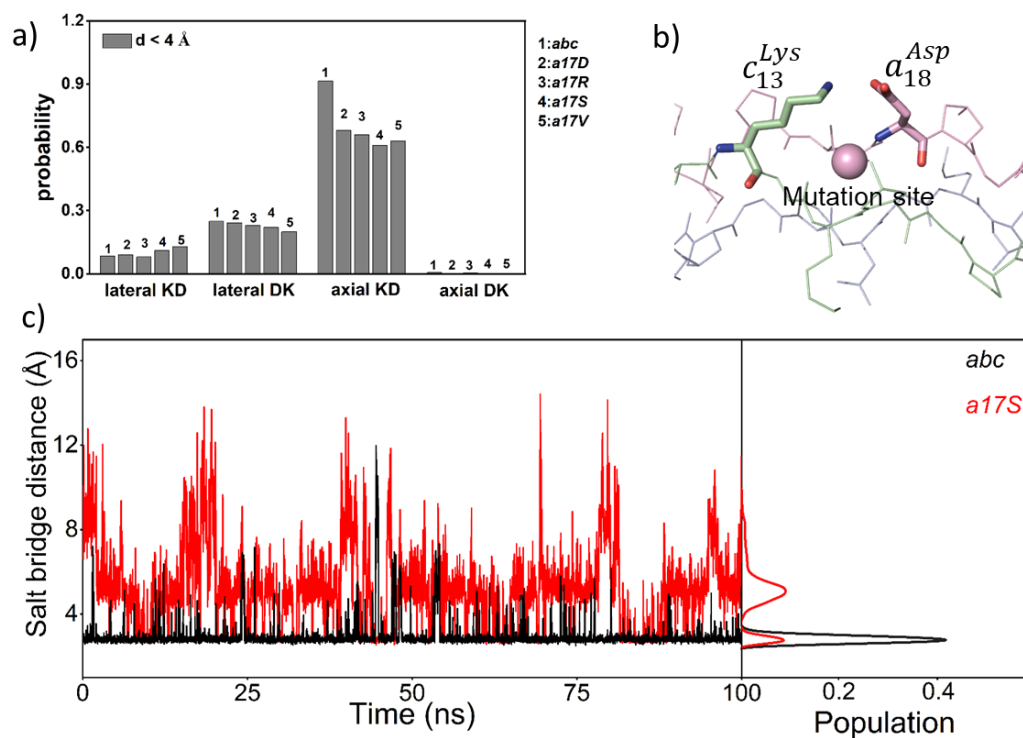


Figure S3 Salt-bridge changes. a) probability of salt-bridge distance change under 4 Å; b) mutation site around a broken salt-bridge formed by Lys and Asp; c) change in salt bridge distance over simulated time.

Since the substitution site is in the middle of the salt bridge, when the side chain is changed to a longer amino acid, NO distance of the salt bridge changed from one peak near 4 Å to two peaks in 4 Å and 6 Å, steric hindrance blocks the charge effect and the salt bridge is destroyed.

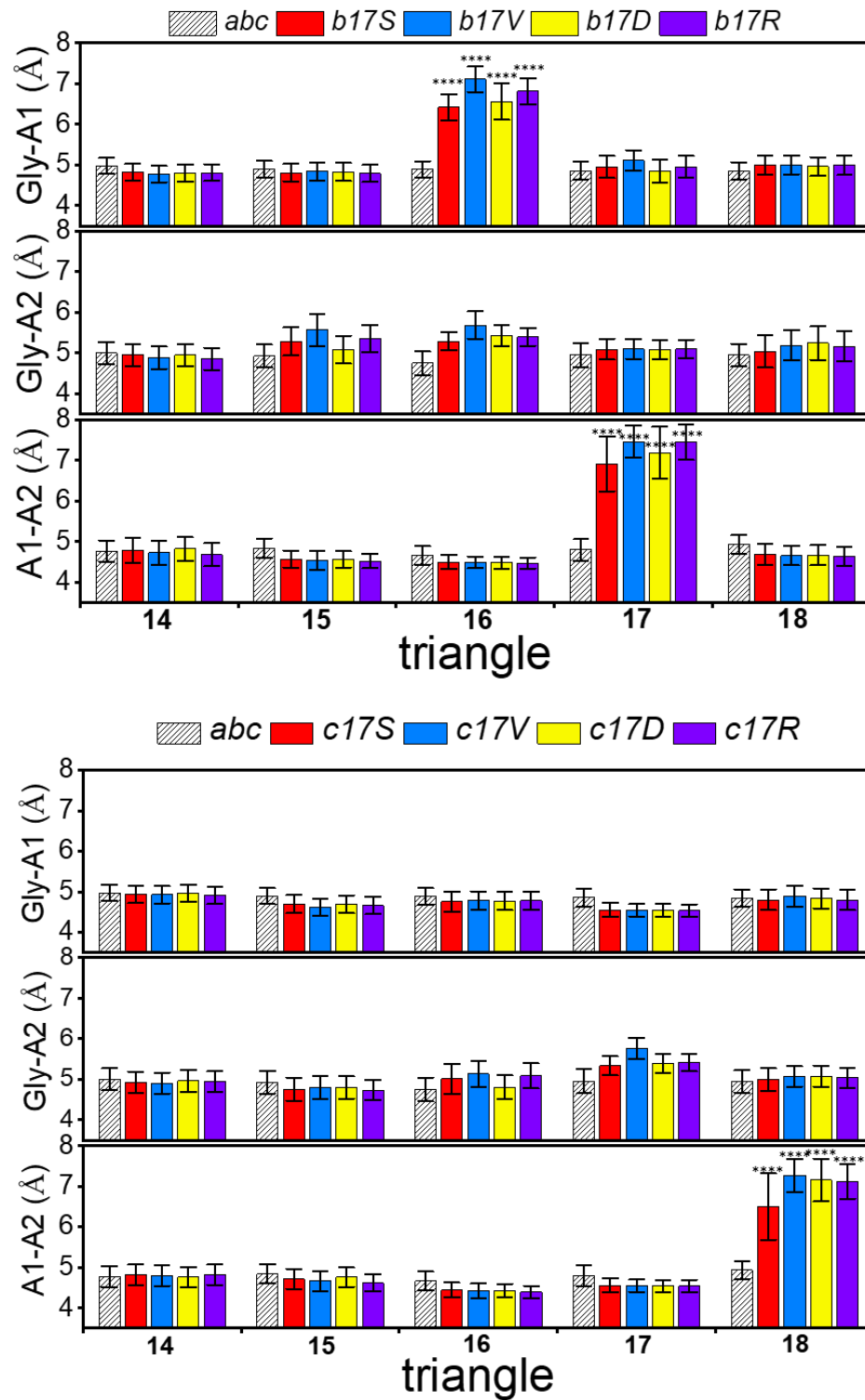


Figure S4 The side length after chain *b* and *c* mutation in *Ca* triangle. Collagen have a stable state is triple helix, each distance of *Ca*-*Ca* in same plane is between 4.5 to 5 Å. All kind of mutant have similar tendency in broken these length of *Ca*. Indicate a strong decrease of collagen stability in consistent with loss of H-bond.

Statistical significance was calculated using one-way ANOVA. Values are mean±SD.

**** $P < 0.0001$, versus abc alone

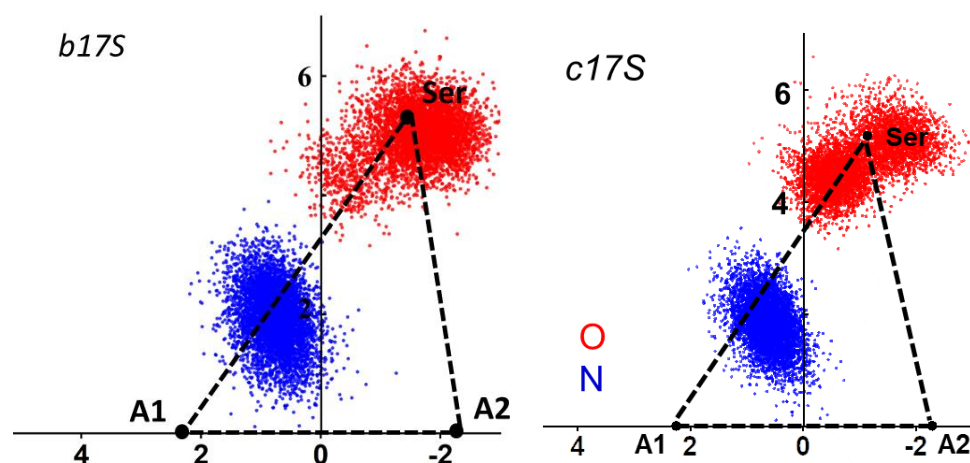


Figure S5 The distribution of nitrogen and oxygen atoms in a broken H-bond in *b17S* and *c17S*. Nitrogen atoms are shown in blue, and oxygen atoms are shown in red.

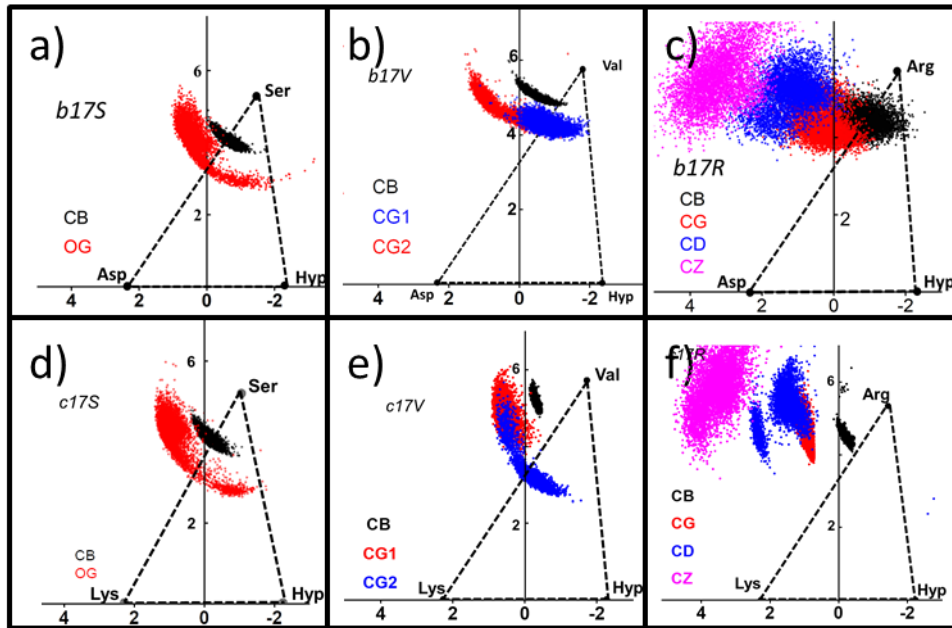


Figure S6 The distribution of mutant amino acid side-chains in chain b and c mutants. a-c) The side-chain distribution of b17S, b17V and b17R; d-f) The side-chain distribution of c17S, c17V and c17R