Supplementary Information

Long-ranged Protein-glycan Interactions Stabilize von Willebrand Factor A2 Domain from Mechanical Unfolding

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Figure S1. (A): SASA profile as a function of D_{EE} for system $S_{C(repeat)}^{+G}$ and those in **Figure 2A**. (B): Energy profile as a function of D_{EE} for systems $S_{C(repeat)}^{+G}$ and S_{C}^{+G} . (C): Snapshot of structures in state E for systems $S_{C(repeat)}^{+G}$ and S_{C}^{+G} . Only the unfolded structures are labeled. (D): Force profile as a function of D_{EE} for systems $S_{C(repeat)}^{+G}$ and S_{C}^{+G} . Solid lines are the averages over every 1000-step of the raw data (shaded lines of the same color).

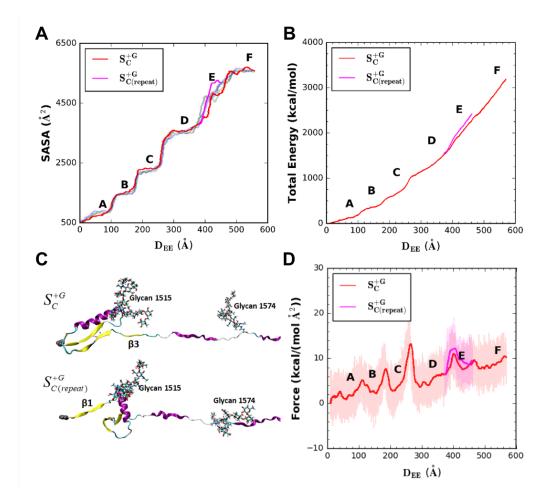


Figure S2. (A): SASA profile as a function of D_{EE} for independent simulations and those in Figure 2A. (B): Energy profile as a function of D_{EE} for independent simulations and those in Figure 6. (C,D): Force profiles as a function of D_{EE} for independent simulations and those in Figure 5. Solid lines are the averages over every 1000-step of the raw data (shaded lines of the same color).

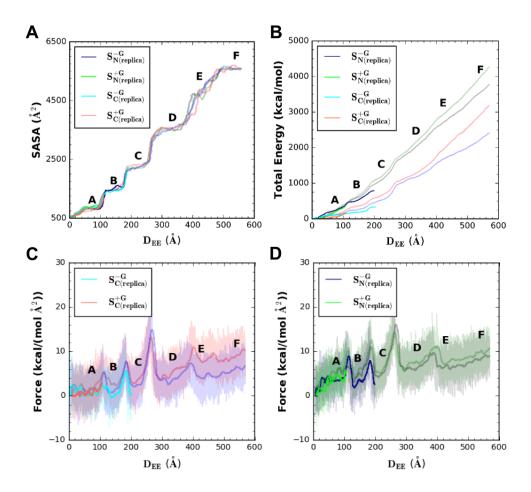
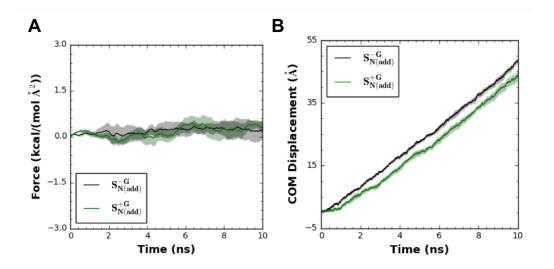


Figure S3. (A) Force profiles for different systems: $S_{N(add)}^{+G}$ (green) and $S_{N(add)}^{-G}$ (back). (B) The corresponding COM profiles. Each solid line represents the averaged value of four independent simulations, and the error bars with the same color indicate the standard errors among them.



Movie S1. Interaction pattern changes as a function of time.