Structural Basis for the Influence of A1, 5A, and W51W57 Mutations on the Conductivity of the *Geobacter sulfurreducens* Pili

Supplementary Information

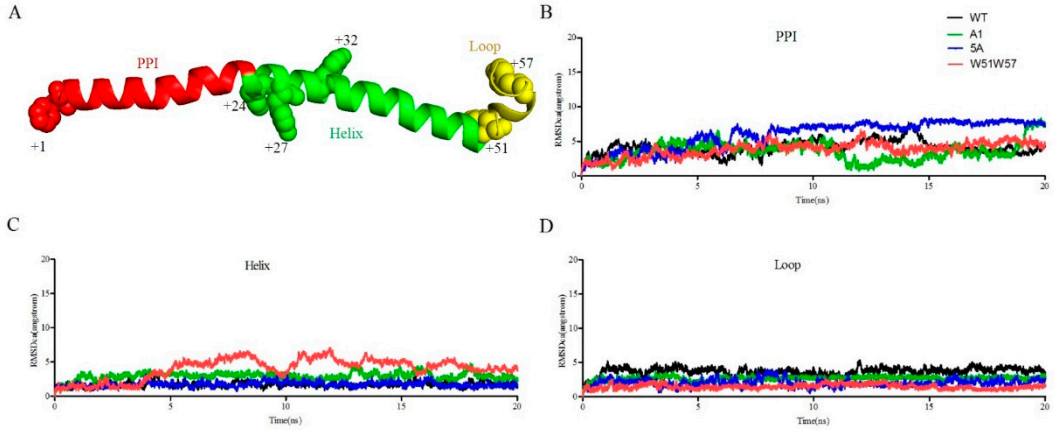

Figure S1. RMSD landscapes of four types of pilins for the PPI, Helix, and Loop domain. (**A**) The three-dimensional structure of PilA. Three domains, i.e., PPI, Helix, and Loop, are highlighted with red, blue, and yellow, respectively. The aromatic amino acid sites are shown using location and sphere. Time series of RMSDs of backbone Cα atoms to the initial structures for the (**B**) PPI, (**C**) Helix, and (**D**) Loop domain of the wild type and its mutants are computed and plotted.

Table S1. The shortest aromatic pathway for GC pili.

	Pathway	Distance(Å)
GC	($F24_p$, $Y27_p$, $F24_{p+1}$, $Y27_{p+1}$, $F24_{p+2}$, $Y27_{p+2}$, $F24_{p+3}$ $Y27_{p+3}$	(7.0,10.6,7.0,10.6,7.0,10.6,7.0,10.6)

GC represent the pili of *N. gonorrhea*.