Supplementary Information for

Molecular interaction modes of host-defense peptide cathelicidin LL-37 and its mutants dictate the diverse antimicrobial activities

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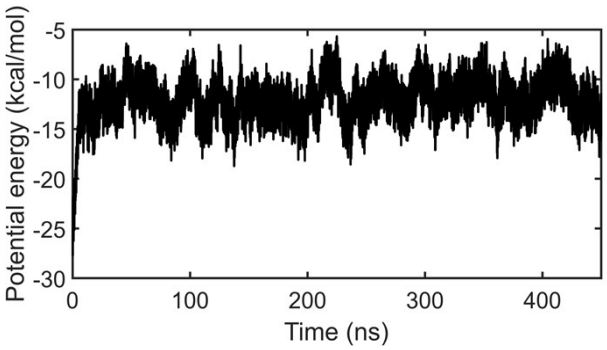

Figure S1. Potential energy of the monomeric LL37(17-29) peptide as a function of simulation time.

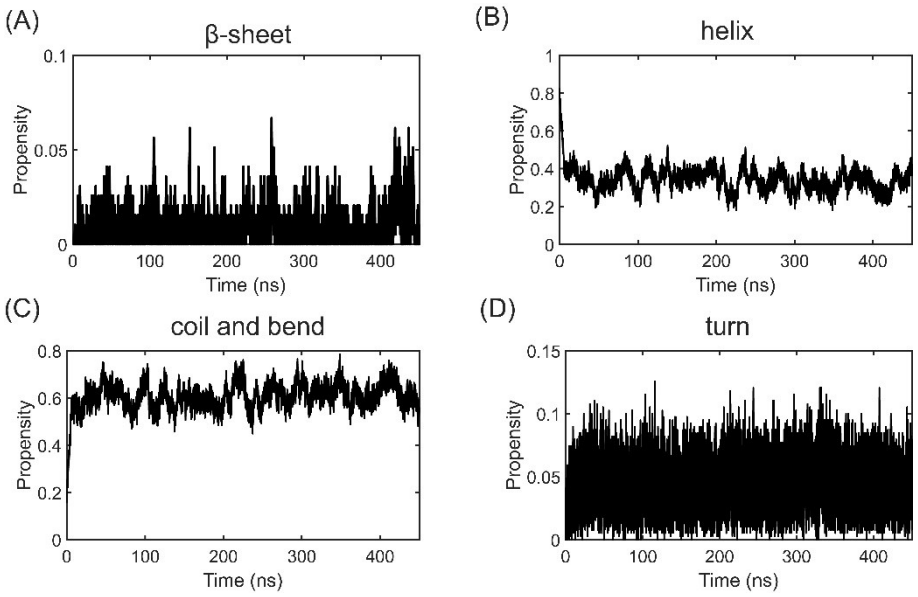

Figure S2. Time-evolution of the secondary structure of the WT LL37(17-29) monomer. (A) Helix, (B) β-sheet, (C) coil and bend, and (D) turn structures.

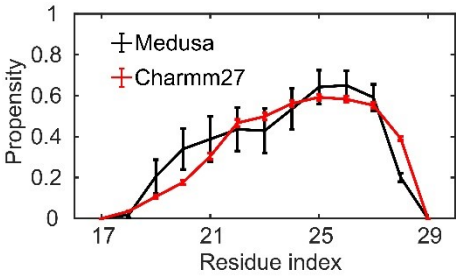

Figure S3 Helical structure propensity of each residue of WT LL37(17-29) peptide obtained by Medusa and Charmm27 force fields.

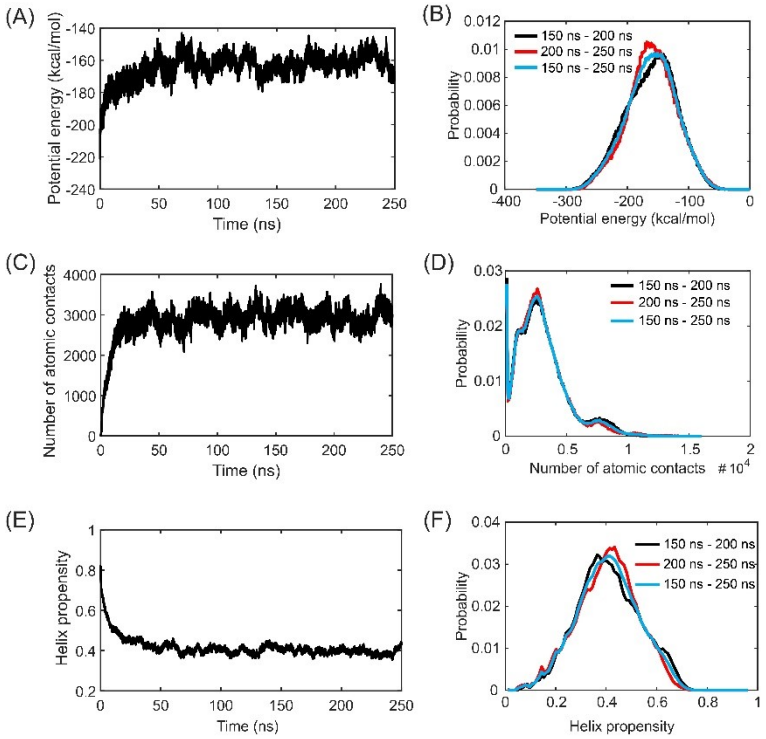

Figure S4 Convergences of the aggregation simulations. Evolutions of potential energy (A), the number of atomic contacts (C), and the helical property (E) of the WT LL37(17-29) peptides as a function of the simulation. Histograms of potential energy (B), the number of atomic contacts (D), and the helical property (F) during 150-200 ns, 200-250 ns, and 150-250 ns

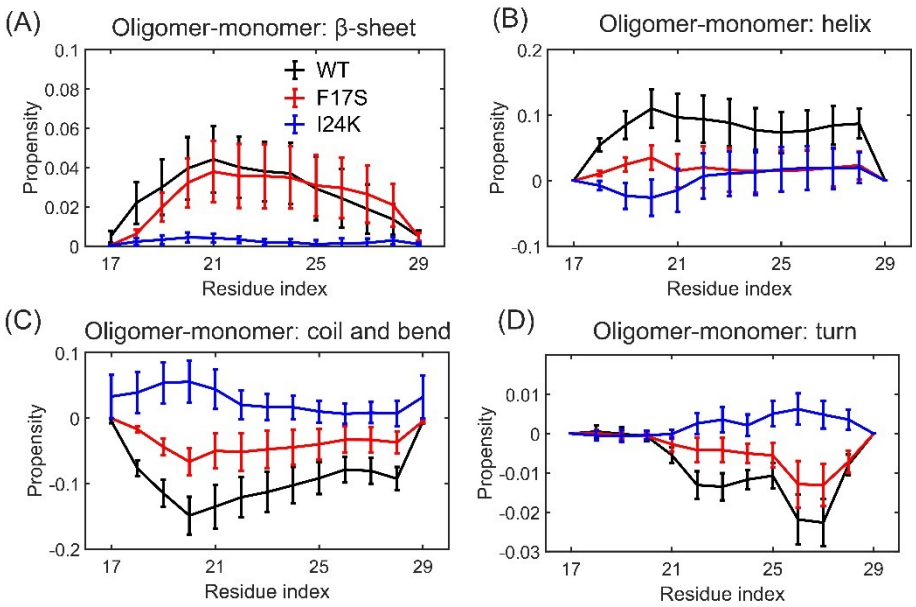

Figure S5. **Variations of the secondary structures during the aggregation of LL37(17-29) peptides and mutants.** (A) β-sheet, (B) helix, (C) coil and bend, and (D) turn structures.

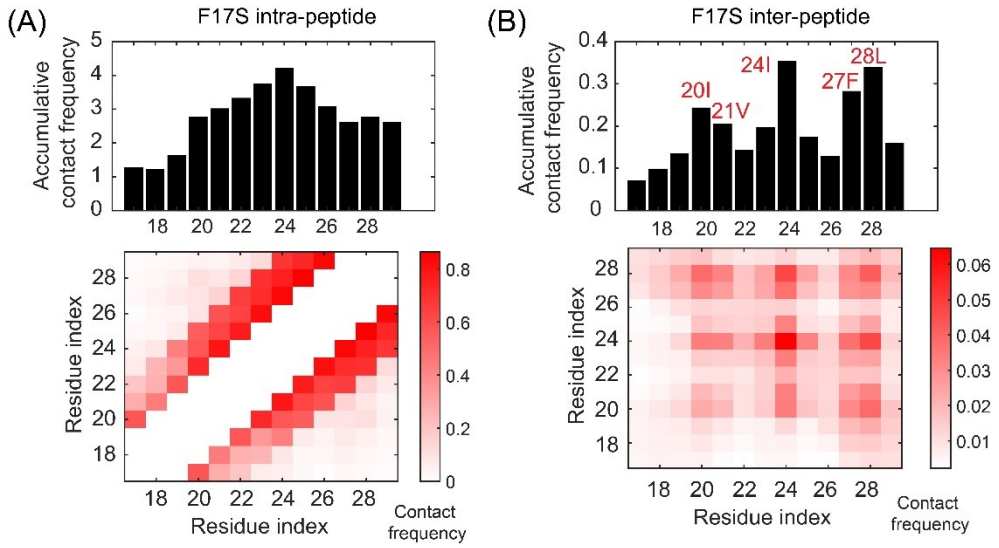

Figure S6. Residue-wise contact frequency maps of F17S mutation. (A) Intrapeptide contact frequency map, and (B) interpeptide contact frequency map. The accumulative contact frequency of each residue with the rest residues are shown in the top panels.

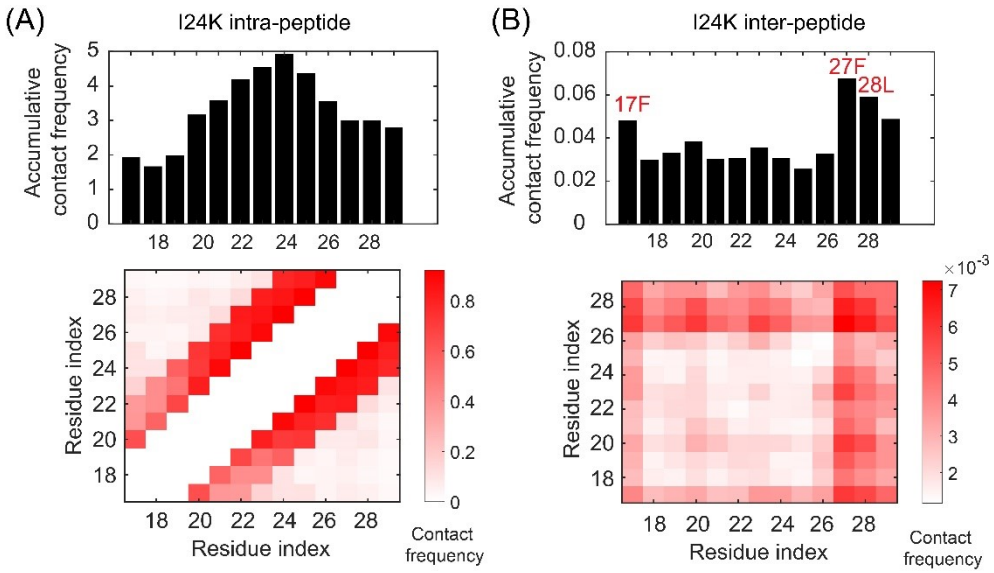

Figure S7. Residue-wise contact frequency maps of I24K mutation. (A) Intrapeptide contact frequency map, and (B) interpeptide contact frequency map. The accumulative contact frequency of each residue with the rest residues are shown in the top panels.

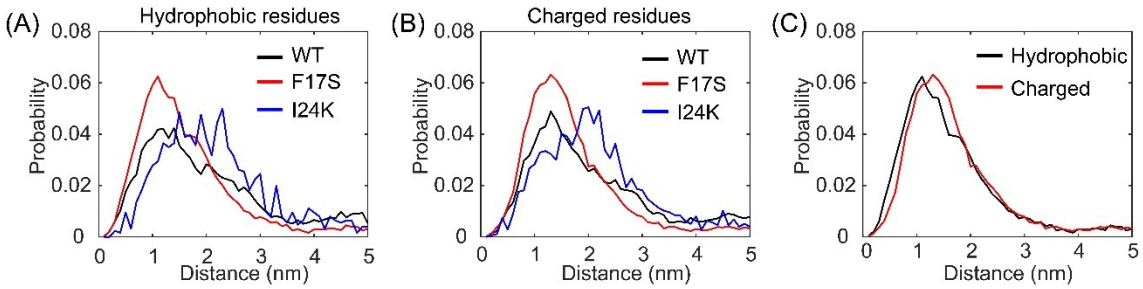

Figure S8. Structures of oligomers formed by LL37(17-29) peptides. Distributions of (A) hydrophobic and (B) charged residues in the oligomers formed by the WT and mutants of LL37(17-29).