Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information:

Membrane pore formation and ion selectivity of the Ebola virus delta peptide

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Structural modeling of the delta-peptide:

The structure modeled by Phyre2 was based on the crystal structure of S. Cerevisiae (pdb id 2J6A), which was the top template identified by Phyre2. Despite having only 18% sequence identity, it predicted most of the amphipathic helix described in literature. Fig. S1 shows the sequence comparison information provided by Phyre2.

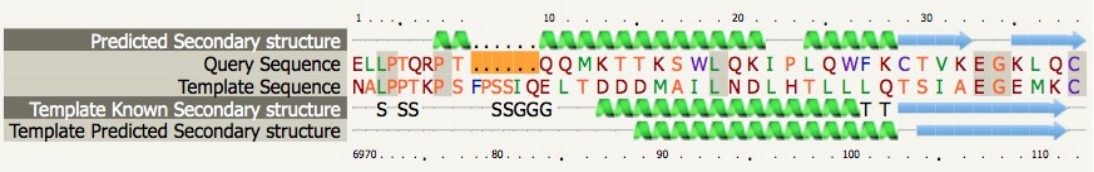


Figure S1. Secondary structure comparison between the template (pdb id 2J6A) and delta-peptide.

Simulations performed:

Table S1: List of different systems and the length of the simulations used in this work.

Membrane Systems	Number of Atoms	Simulation Time (ns)
Single Peptide for Umbrella sampling	22472	10 ns x 20 windows
Tetramer with disulfide	69824	750
Pentamer with disulfide	72697	1100
Hexamer with disulfide	75380	500
Pentamer without disulfide	88906	500
Hexamer without disulfide	92944	500

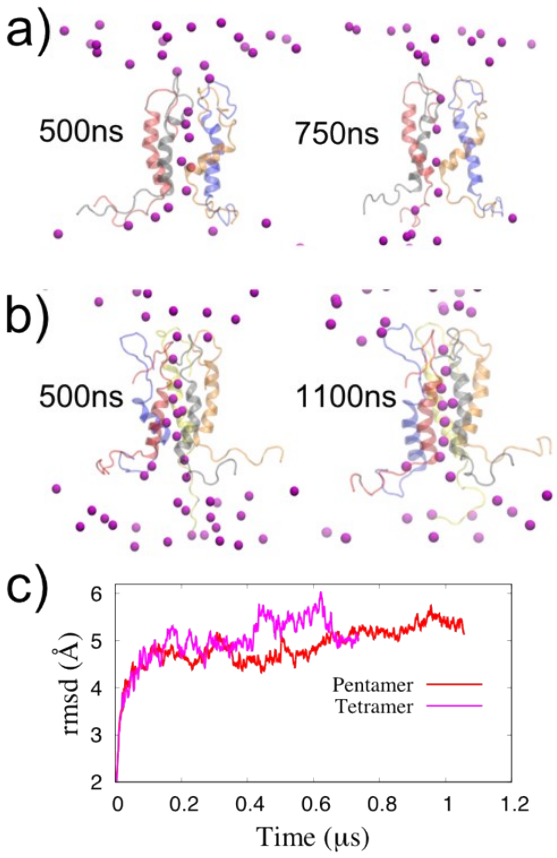


Figure S2. Snapshots of the a) tetramer and b) pentamer structures at different timescales. The Cl^- ions are shown as purple spheres which can also be seen in the pore. c) Evolution of RMSD as a function of time for the tetramer and pentamer models for extended simulation times.

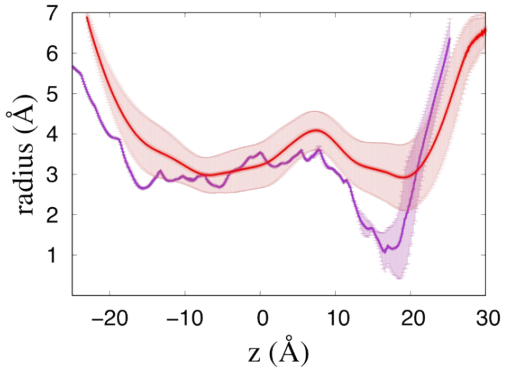
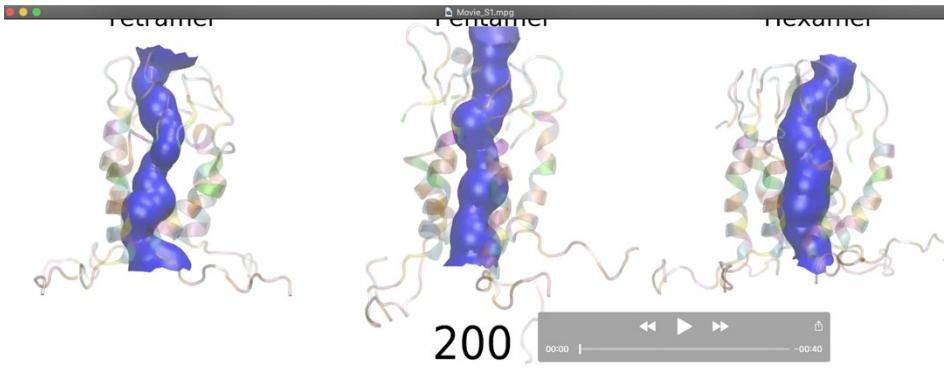
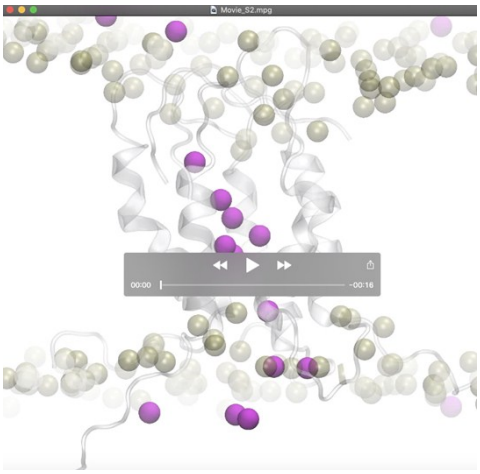


Figure S3. Pore radius for the pentamer model calculated for different times: red curve for 300 to 500 ns purple curve for 900 to 1100 ns. With time, pore structure becomes more stable as shown by significantly small error-bars (shaded region), indicating reduced fluctuations in the pore radius for 900-1100 ns. The pore is still able to pass Cl- ions but the narrowing at one end may help in ion selectivity.



Movie S1. Pores formed by four, five, and six delta-peptide assemblies, calculated by HOLE, showing the changes in pore radius as a function of time (200-500 ns). The sections that are too narrow to pass any water molecules are colored red, green if they allow one water molecule to pass, and blue if they are wide enough to pass two or more water molecules.



Movie S2. Chloride ion permeation through pentameric pore.