Structure of a Biological Cell Wall Penetrating Device

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Abstract:
Bacteriophages infect bacterial cells by injecting their genome through the cell wall, a \textasciitilde150Å thick barrier formed by two lipid bilayers and peptidoglycan. We have determined the crystal structure of phage P22 tail-needle gp26, a specialized protein fiber used by the virus to penetrate the \textit{Salmonella} enterica cell wall. The 2.0Å crystal structure of the tail needle gp26 reveals a 240Å elongated protein fiber formed by two trimeric \textalpha-helical coil-coiled domains interrupted by a triple-\textbeta helix. The first coil-coiled domain of gp26 spans 165Å and is held together by four trimerization \textit{octads}, which confer a slender and stiff conformation to the fiber. This helical core relates gp26 to class I membrane fusion proteins, while the C-terminal helical domain exposes \textbeta-hairpins with hydrophobic tips, homologous to those seen in class II fusion peptides. The extended topology of the trimer minimizes the surface exposed to solvent that is largely hydrophobic. This is consistent with the knowledge that gp26 is ejected through the bacterial cell wall during infection.

The crystal structure of tail needle gp26 was determined using Xenon gas as derivatization agent. Remarkably, eight well-occupied Xenon sites were found inside the protein fiber at the trimeric helical interface. To accurately measure the anomalous signal of Xenon, low energy X-ray data were recorded from Xenon-derivatized crystals at \textasciitilde7000 eV. This was found to dramatically improve the quality of the initial set of phases used in the subsequent steps of structure determination.