

You Would Think 1.2 Angstrom Resolution Would be Enough for Structure Solution...

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Self-assembling protein nanotubes (PNTs) are an intriguing alternative to carbon nanotubes for applications in bionanotechnology, in part due to greater inherent biocompatibility. The type IV pilus of the gram-negative bacteria *Pseudomonas aeruginosa* is a protein-based fibre composed of a single monomeric subunit, the type IV pilin. Engineered pilin monomers from *P. aeruginosa* strain K122-4 (K122) have been shown to oligomerize into PNTs both in solution and at surfaces. In order to fully exploit PNTs in application settings, an in-depth understanding of their assembly, physical characteristics, robustness etc., both in solution and when constrained to surfaces, is required. Characterization of the oligomerization process in solution suggests that protein is in a monomer-dimer equilibrium in solution, and that oligomerization is a fibril-mediated process. In addition to the K122-4 pilin, pilins from other strains of *P. aeruginosa* also appear to oligomerize into PNTs; therefore, a comparison of their structures should provide insights into the protein determinants that drive PNT oligomerization. We have crystallized and collected X-ray diffraction data for the pilin from *P. aeruginosa* strain P1 (space group P21, $a = 22.40 \text{ \AA}$, $b = 54.90 \text{ \AA}$, $c = 37.85 \text{ \AA}$; $\beta = 96.08^\circ$) at 1.2 \AA resolution. You would think that structure solution at this resolution would be straightforward, however it has proven recalcitrant. We will discuss the data and challenges in dealing with the problem of a protein that crystallized and diffracted well, which should have led to a straightforward solution, but remains frustratingly out of just out of reach.