Alternate Realities: Searching for the Optimal Supercell Approximate for Incommensurately Modulated Profilin:Actin Crystals

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The Profilin:Actin complex is an important protein complex that plays a critical role in cellular functions such as cytoskeleton organization and cell motility. Examples of this complex existing in an incommensurately modulated crystal have been observed with X-ray crystallography experiments since the mid-1980s. However, the diffraction data obtained could not be successfully processed at that time. Being able to solve and investigate this structure should provide valuable insight into how actin filaments are initiated in cellular systems.

In the mid-2000s incommensurately modulated crystals of the PA complex were successfully reproduced, and the incommensurate state was even cryo trapped and several complete datasets were collected. In the early-2010s software had progressed to the point where this data could be indexed, integrated, and scaled in the $P2_12_12_1(0\gamma0)$ (3+1) D superspace group. We have three processed incommensurate PA datasets with slight differences in unit cell and **q**-Vector values. Currently there is no protein refinement software to deal with this structure in its native 4D space. We are left to work with supercell approximates. Unfortunately, there isn't just a single supercell to evaluate. The 4D data can be processed into multiple theoretically valid 3D supercells.

Our current work is focusing on which of the many possible supercells and space groups evaluated for all three datasets represent the optimal supercell approximate that maximizes symmetry, minimizes the number of subcells needed in the supercell, minimizes R and R_f, and has smooth atomic modulation functions that are expected because only first order satellites have been observed in the data. Additionally, we were curious to see if the variations in **q**-vector and unit cell dimensions effected the modulation functions in our crystals or were they largely the same with the observed differences in the data being caused by variations in **q**-Vector which would change the sampling of common higher dimensional atomic modulation functions shared by all three crystals.