Microsymposium

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Dealing with Aperiodic Protein Crystal Structures

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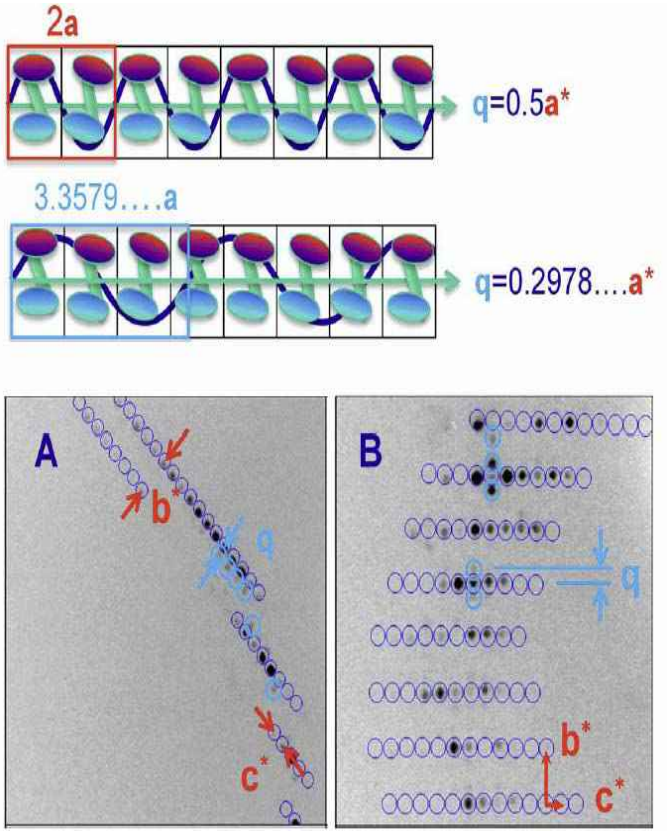
Protein crystals can be aperiodic. They will diffract X-rays, and are therefore a crystal, but their diffraction is not periodic. This means that their diffraction pattern cannot be simply be indexed by a typical three-dimensional unit cell and space group. Aperiodic crystals include "quasi-crystals" as well as "modulated" crystals. In the latter case, the modulation can be positional or occupational and these modulations can be incommensurate with the normal periodic lattice [1]. An overview of aperiodic protein crystal diffraction will be presented with examples. The discussion will then focus on the characteristics of incommensurately modulated crystals followed by a more detailed discussion of how to solve these crystals. The following details of structure solution will be presented: (1) data collection perils; (2) specialized diffraction data processing in (3+1)D space using a q-vector [2]; (3) how to get an approximation of the structure in 3D space; (4) the assignment of the (3+1)D space group; and the ultimate (5) crystallographic refinement in superspace[3]. Future directions and needs will be discussed.

[1] *Lovelace, Murphy, Narayan, Schutt, Lindberg, Svensson, Wynn, Borgstahl "Protein crystals can be incommensurately modulated" J Appl Cryst 41 , 600-605 (2008).,* ***[2]*** *Porta, Lovelace, Schreurs, Kroon-Batenburg, Borgstahl "Processing incommensurately modulated protein diffraction data with EVAL15", Acta Cryst D67, 628-638 (2011).,* ***[3]*** *Lovelace, Simone, Petricek, Borgstahl, "Simulation of modulated protein crystal structure and diffraction data in a supercell and in superspace" Acta Cryst D69, 1062-1072 (2013).ace, Murphy, Narayan, Schutt, Lindberg, Svensson, Wynn, Borgstahl "Protein cr*



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