Crystallographic studies of dsDNA phage HK97 structure and maturation

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HK97 is a double-stranded DNA (dsDNA) λ-like bacteriophage. The process of HK97 assembly and maturation involves large-scale conformational changes in the protein capsid. Intermediates have been identified in the maturation process, the first of which is Prohead I. Prohead I assembles from 420 copies of capsid protein (gp5) into pentamers and hexamers, plus a viral protease (gp4). Maturation to Prohead II occurs when 103 residues of gp5 are cleaved from the N-terminus by gp4. Prohead II matures to Head II *in vivo* when dsDNA is packaged into the empty capsid and *in vitro* under various chemical conditions. The final step of maturation involves covalent peptide bond formation between capsid subunits.

We are using x-ray crystallography to investigate HK97 capsid structure and maturation. Crystals were grown of the HK97 mature capsid, Head II. The space group is $P2_1$, with cell dimensions a = 581.22 Å, b = 628.35 Å, c = 789.45 Å, and β = 89.94°. There is one complete particle in the crystallographic asymmetric unit, allowing for 60-fold noncrystallographic symmetry averaging. Data collection and analysis for a primitive cell of this size is challenging, particularly because cryogenic conditions could not be identified. We found that collecting data from these crystals at the Advanced Photon Source (APS) beamline 14-BM-C allowed the measurement of data to 3.45 Å resolution using a MAR detector. This was a substantial improvement over the 5 Å data set that was collected previously. Data from the APS were collected in two trips (June and August 1998). More than 500 images were collected. The structure determination to 3.5 Å resolution is underway.

Prohead II capsids are a stable intermediate in HK97 maturation. Capsids crystallize in space group $P2_13$ with unit cell a = 707 Å. These crystals diffract x-rays to 6 Å resolution. Data were collected at APS beamline 14-BM-B and 14-BM-D using a Quantum 4 CCD detector. More than 1000 images were collected, and the structure determination is underway.

The structures of both the Head II and Prohead II capsids will elucidate some of the conformational changes that are known to occur during bacteriophage maturation.

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