

# The Structure and Dynamics of Protein and Nucleoprotein Assemblies Determined with Synchrotron X-ray Radiation

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Reductionism has been remarkably successful in elucidating the biochemistry and function of individual biological molecules. Our interests, however, are to tackle large structures where association of the “parts” leads to behavior that is not predicatable by examining the individual components. The structure determination of large assemblies like viruses, ribosomes, and transcription complexes often requires the marriage of methods such as crystallography, solution x-ray and neutron scattering, and electron microscopy.<sup>1</sup> In addition, the interpretation of these structures requires a well-defined inventory of biological phenomena (e.g.<sup>2,3</sup>). This presentation will address single crystal and solution diffraction studies with synchrotron radiation that have lead to measurement of data that span the range from near atomic resolution to the lowest order resolution diffraction maxima from crystals with unit cells in excess of 500Å.<sup>4</sup> Such complete data sets allow the definition of envelopes defining the accessible volumes of mobile regions of structures and they facilitate the use of models obtained with multiple methods.<sup>5</sup> These data sets have provided insight into RNA organization in viruses and have lead to mechanistic descriptions of large scale virus particle dynamics that result from the assembly of a single type of gene product into a 420 subunit megastructure. Initial ssembly of this particle traps a folding intermediate of the subunits in a prohead. The subunits move to their final folded form when the particle expands by nearly 20% into a mature head.

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<sup>1</sup>Baker T., Johnson J. 1996. Low resolution meets high: towards a resolution continuum from cells to atoms. *Current Opinion in Structural Biology* 6:585-594.

<sup>2</sup>Duda, R. L., Hempel, J., Michel, H., Shabanowitz, J., Hunt, D., Hendrix, R. W. (1995a) Structural transitions during bacteriophage HK97 head assembly. *J. Mol. Biol.* 247:618-635.

<sup>3</sup>Duda, R. L., Martincic, K., Hendrix, R. W. (1995b) Genetic basis of bacteriophage HK97 prohead assembly. *J. Mol. Biol.* 247:636-647.

<sup>4</sup>Wikoff, W., Duda, R., Hendrix, R., Johnson, J. (1998) Crystallization and preliminary x-ray analysis of the dsDNA bacteriophage HK97 mature empty capsid. *Virology* 243:113-118.

<sup>5</sup>Conway, J. F., Duda, R. L., Cheng, N., Hendrix, R. W., Steven, A. C. (1995) Proteolytic and conformational control of virus capsid maturation: The bacteriophage HK97 system. *J. Mol. Biol.* 253:86-99.