

The role of flexibility of capsid proteins in the symmetry of viral shells

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1. Abstract

Several self-assembly experiments conducted with model icosahedral plant viruses have shown that, under physiological conditions, capsid proteins initially interact with the viral genome, forming nucleoprotein complexes in a disordered state, which raises the question of how these virions ultimately assemble into highly ordered structures in the host cell. Here, we present a model that enables us to explore the viral assembly pathways while taking into account the elastic energy involved in the growth process. We show that as a capsid grows, the structures of disordered intermediates in which the distribution of pentamers does not belong to the icosahedral subgroups become energetically so unfavorable that the malformed shells can dissociate and reassemble, overcoming the energy barriers for the formation of perfect icosahedral shells. We find that the key for the disorder–order transition lies in the strength of flexibility of capsid proteins compared to the other forces in the system including protein–protein interactions and the entropy of free subunits.