Multidisciplinary structural characterization of helical plant viruses by small angle X-ray scattering and tritium planigraphy data.

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A virion of flexible Potato virus X (PVX) was studied using combination of tritium planigraphy (TP) and small angle X-ray scattering (SAXS). Homological modeling of coat protein (CP) structure in PVX virion was based on the available high-resolution structure of CP from the other member of the Potexvirus - Papaya Mosaic virus. We propose an algorithm for determining the orientation of the CPs and refinement the coordinates of amino acids atoms in PVX virion by TP data. The search of optimal correlation between the maximum inclusion of tritium labels and the side of molecule forming the terminal face of the helical assembly permits to restore a detailed image of the quaternary structure of the virus, and to determine the interfaces between the CPs. Additionally, low resolution *ab initio* shapes were reconstructed using bead modelling approach against solution scattering data. Given the structural parameters of the solute, which pointed to the extended architecture of the viruses and their CPs, the initial round of the shape determination was performed without symmetry restrictions using elongated cylinders as the search volumes. As the resulting shapes possessed quazi-helical symmetry, corresponding solid helical models were generated yielding the best agreement with the typical P1 reconstructions and a refinement cycle was launched within such search volume. The reconstructed models were still able to neatly fit the experimental SAXS data confirming the helical arrangement of the particles and revealed sparse bead occupancies in the core region of the helix in a full agreement with the expected virus architecture. Both structural reconstructions, on the base of TP and SAXS, complement each other giving the detailed spatial PVX virion organization. This work was supported in part by Russian Foundation for Basic Researches (projects 15-54-74002 EMBL, 16-03-00375, 15-04-01406).