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Structural Studies on the Receptor-Recognition Protein P2 of Bacteriophage PRD1

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Beamline(s): X12C

PRD1 and adenovirus have striking similarities in capsid architecture and in their major coat proteins, P3 from PRD1 and hexon from adenovirus. Although PRD1 has an internal membrane, and infects its *E. coli* host by a mechanism that differs from that used by adenovirus, both viruses attach to their hosts through vertex complexes. In PRD1, the vertex complex has three proteins (P2, P5 and P31) while the adenovirus penton has two (penton base and fiber). P2 is the functional counterpart of adenovirus fiber, or at least its knob region. With 590 residues (63.9 kDa), P2 is almost exactly the same size as ad2 fiber (582 residues, 62.0 kDa), but P2 is monomeric rather than trimeric. A structure determination, enabled by its crystallization [1], is resolving this puzzle.

Orthorhombic P2 crystals have space group $P222_1$ ($a = 137.8 \text{ \AA}$, $b = 46.5 \text{ \AA}$, $c = 136.4 \text{ \AA}$). The P2 structure was solved using an oxidized selenomethionine (Se-Met) derivative for a multiwavelength anomalous dispersion experiment conducted at beamline X12C. Since P2 only has six methionines, additional phases obtained from four heavy atom derivatives were necessary to obtain an interpretable electron density map. The current P2 model has been refined to 2.4 \AA , with an R-factor of 23.2% and an R_{free} of 25.2%. The crystal structure of P2 (Figure 1) reveals an elongated seahorse-shaped molecule, with dimensions of $146.0 \text{ \AA} \times 46.5 \text{ \AA} \times 33.5 \text{ \AA}$, composed mostly of β -strands. Despite P2's elongated shape, its fold is quite different from adenovirus fiber. The "head" of the molecule has similar architecture to the β -propeller family of proteins, which includes haemopexin, neuraminidase, and G protein. These proteins have four to eight repeated blades composed of a four-stranded antiparallel β -sheet "W" motif. A thorough investigation into the properties of this family of related proteins is being conducted to obtain further insights into the structural and functional properties of P2.

References:

1 L. Xu, S.J. Butcher, S.D. Benson, D.H. Bamford and R.M. Burnett, "Crystallization and preliminary X-ray analysis of receptor-binding protein P2 of bacteriophage PRD1," *J. Struct. Biol.*, **131**, 159-163 (2000).

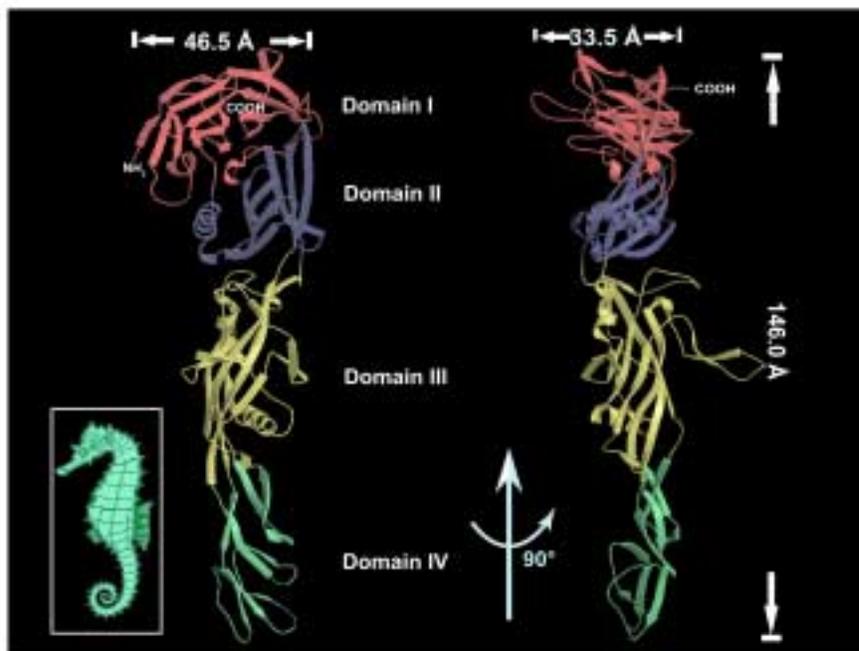


Figure 1. Ribbon diagram of the P2 molecule with its domains colored in red, blue, yellow and green. The front view (left) shows that P2 has a shape like a seahorse (inset) and that domains I and II form a β -propeller "head" with five "W" motif blades. The molecule is rotated 90° in the side view (right) to show that the head is shaped like a shallow cup.