ESRF	**Experiment title:** Structure determination of the infectivity protein, g3p, of filamentous phage fd	**Experiment number:** LS-927
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The two N-terminal domains (Dl-D2) of the infectivity protein g3p of Ff filamentous phages (M13, fd, fl) contain the binding sites for the two receptors of phage infection: the F'-pilus primary receptor as well as the TolA coreceptor. Recently, we have shown that during phage infection, the two receptors are contacted in a sequential manner, with binding site for TolA on the Dl domain blocked by the D2 domain in the absence of F'-pilus. In order to better understand this process we have solved the crystal structure of the two N-terminal domains Dl-D2 of the infectivity protein g3p of filamentous phage fd by a combination of MIR and molecular replacement phasing using data collected at ESRF's ID14-3 beamline.

We collected data for a native crystal of a deletion variant of g3p consisting of the Dl and D2 domains, a crystal of a selenomethionine-substituted DlD2, and a native crystal for a deletion variant consisting of Dl

only. The crystals had unit cell a=125 Å, b=78 Å, c=63 Å with symmetry P212121. The data were collected to 1.8 Å, 2.5 Å and 1.6 Å for the DlD2, Se-Met DlD2 and Dl crystals, respectively. The structure of DlD2 was refined to 2.0 Å with a free R-factor of 0.29. A schematic diagram of the DlD2 structure is illustrated in Fig. 1.

While individual domains Dl and D2 superimpose well with the respective Dl and D2 domains in the g3p Dl-D2 structure from the related Ff phage M13, the two overall structures superimpose poorly. This is due to a 5 Å movement of D2 with respect to Dl around a hinge located in a strand of a short anti-parallel beta-sheet that connects Dl to D2. The movement results in an opening up of a hydrophobic groove running between the two domains, postulated to contain the binding site for the F'-pilus. We propose a mechanism for the early steps of phage infection, whereby interaction with the pilus tip causes a conformational change that opens this groove and frees Dl for coreceptor binding.

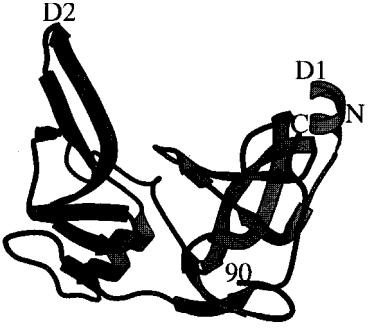

Fig. 1. A schematic of the DlD2 structure of g3p.