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## Crystallographic studies of 1,3-β glucanase from potato

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1,3-β Glucanases from plants are polysaccharide endohydrolases possessing the ability to hydrolize 1,3-β glucosyl linkages, but only when several contiguous 1,3-β -linked glucosyl residues are present. They are classified as PR-2 (phatogenesis-related class 2) proteins because they are expressed in the plant tissue when the organism is subjected to attack by pathogenic microorganisms, and also because 1,3- β glucans are commonly found in fungal cell walls. Potato 1,3-β glucanase with molecular mass of 35.5 kDa has been crystallized by the hanging drop vapor diffusion method and diffraction data extending to 1.5 Å resolution were collected at 100 K using synchrotron radiation. The crystals are monoclinic, space group $P2_1$, with $a$ = 75.5, $b$ = 49.3, $c$ = 83.0 Å, β = 103.5°, and contain two protein molecules in the asymmetric unit, corresponding to a Matthews volume of 2.0 $Å^3$/Da and 37.2% solvent content. The crystal structure was solved by molecular replacement using barley 1,3-β glucanase as the search model. The protein possesses an eight-stranded α/β-barrel fold. The main feature of this structure is a deep groove, approximately 35 Å long, lying between α-helices α2 and α3 at the N-terminus of the polypeptide chain and α5 and α6 at the C-terminus of the chain (Fig.1 α-helices - light grey). The electronegatively charged catalytic cleft harbors glutamate residues Glu93 and Glu234, which act as hydrogen donor and the nucleophile, respectively. They are located at the C-terminal end of strand β4 (Glu93) and the C-terminal end of strand β7 (Glu234) (Fig. 1, β-strands - dark grey). The length of the groove suggests that it can accommodate seven or eight glucan residues from a polysaccharide chain.

*Fig. 1. Ribbon diagram of 1,3-β glucanase from potato showing the extended catalytic groove.*

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## Cost, space, time: what are the limits for publishable structures?

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Access to modern single-crystal diffraction experiments continues to be limited to those with the significant funding, laboratory facilities, training and time (or personnel) required for the techniques. Most of us would also hope to produce publishable material from such experiments. So what are the lower limits for cost, space, time and training that might enable access to to the technique to a larger pool of scientists?
The accepted paradigm for single-crystal experiments might need to be suspended to reach some of these goals. In terms of cost and space, what can we do without and still produce acceptable results? In terms of time and training, how much automation can be implemented?
A side benefit of an affordable, minimal system for single-crystal diffraction is the ability to include the technique in undergraduate teaching situations. The new Rigaku SCXmini benchtop crystallography system will be described as a possible answer to these problems. Several examples of published or publishable structures from such a system are included as examples.