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Crystallization and X-ray diffraction data for a new form of concanavalin A

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A new crystal form of concanavalin A, a well studied lectin from the jack bean (*Canavalia ensiformis*) is reported. These crystals, with the symmetry of orthorhombic space group $C222_1$, grow as large roughly equi-dimensional blocks. Unit-cell parameters at 120 K are a = 118.67 (12), b = 101.36 (13), c = 111.94 (9) Å. On density considerations for two molecules per asymmetric unit, the water content is ∼60%. Data to a nominal resolution of 1.5 Å were collected.

1. Introduction

The structure of concanavalin A (conA) was first reported over 30 years ago (Reeke *et al.*, 1971; Hardman *et al.*, 1971; Edelman *et al.*, 1972; Hardman & Ainsworth, 1972) using orthorhombic (*I*222) crystals. The molecule consists of two large antiparallel β-sheets joined by numerous loops and turns. There are two native metal-binding sites, a Ca^{2+} site and a transition-metal site (predominantly Mn^{2+}), and there is evidence of a third (Naismith *et al.*, 1993). Selective repopulation of the transition-metal site markedly improves the diffraction limit of the *I*222 crystal form (Kalb *et al.*, 1988), allowing higher-resolution refinements to reveal ever greater detail (Emmerich *et al.*, 1994). True atomic resolution is attainable from native *I*222 conA crystals cooled to cryogenic temperatures, with concomitant increases in refinable detail (Parkin *et al.*, 1996; Deacon *et al.*, 1997). In spite of such high resolution, model accuracy and precision are difficult to assess in molecules as large and flexible as proteins (Kleywegt & Jones, 1997). Comparison of different crystal forms of the same species, however, can yield important information even at lower resolution. This provided the impetus to search for new crystal forms of this well studied protein.

2. Materials and methods

2.1. Crystallization

Crystals of conA (type 5V, C7275, Sigma–Aldrich, St Louis, MO, USA) grew in hanging drops containing 10 µl of a 30 mg ml^{-1} protein solution and 10 µl precipitant [100 m*M* Tris–HCl pH 8.0 and 25%(*v*/*v*) ethanol] in water equilibrated against a 1 ml precipitant reservoir. Large block-shaped crystals formed over a few weeks.

2.2. Data collection

Data extending to 1.5 Å resolution were collected at 120 K on Xuong–Hamlin dual-multiwire area detectors attached to a Huber four-circle goniometer and Rigaku RU-200 Cu $K\alpha$ X-ray source. A crystal 0.4 mm on each side was washed briefly in antifreeze (∼30% 2-methyl-2,4-pentanediol in the reservoir buffer), plunged into liquid nitrogen and mounted into the cold-stream path of a modified Siemens LT-2 low-temperature apparatus using specially designed tongs (Parkin & Hope, 1998).

3. Results

The crystals are orthorhombic, space group $C222_1$, with unit-cell parameters a = 118.67 (12), b = 101.36 (13), c = 111.94 (9) Å at 120 K. Given two molecules of conA per asymmetric unit, the solvent content is ∼60%. Further details, including intensity statistics, appear in a separate paper (Kantardjieff *et al.*, 2002), where these crystals and data are used in a comparison with the two atomic resolution models from *I*222 form crystals (Parkin *et al.*, 1996; Deacon *et al.*, 1997).

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