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Crystal structures of two aldo-keto reductase enzymes from *Arabidopsis thaliana*

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There are four *Arabidopsis thaliana* aldo-keto reductase (AKR) enzymes (AtAKR1-4) that share high sequence identity with the human AKR1C subfamily. The human enzymes primarily catalyse the hydride transfer between NADPH and ketosteroids, and the chemistry of this reaction is the same for the AtAKR subfamily. However, the AtAKRs are much more promiscuous turning over steroids, sugars and small aldehydes. Expression analysis suggests that members of the AtAKR subfamily have a role in plant stress responses and development, as well as a house-keeping role. All of the AKRs adopt an $(\alpha/\beta)_8$-barrel fold with three loops (A,B & C) forming a substrate-binding site. In order to understand the function of the AtAKRs and their different substrate profiles we are determining structures of all four members of this subfamily and their complexes with potential ligands. Here we present the NADP-binary complexes of AtAKR1 and AtAKR2 solved to 1.4Å and 1.25Å resolution respectively. Both structures reveal an open and accommodative active sites that explains their ability to bind a broad range of substrates.

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A Glycosyl Hydrolase Family 11 Xylanase With An Extended Thumb Region

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Xylan is one of the major constituents of plant cell walls. It is composed of a linear backbone of β-1,4-linked D-xylopyranosyl units with a variety of substituents depending on its source [1]. The hydrolysis of the xylan backbone is performed by endo β-1,4-xylanases (or xylanases, E.C.3.2.1.8) which release xylooligosaccharides of different lenght [2]. Most xylanases can be found in glycosyl hydrolase families 10 and 11 (GH 10 and 11) [3]. GH 10 xylanases consist of a catalytic domain which is a $(\alpha/\beta)_8$ barrel and one or more carbohydrate binding domains, connected by a flexible linker [4]. The overall structure of GH 11 xylanases has been described as a partially closed right hand. It consists of only one domain that folds into two β-sheets which are packed against each other and one α-helix. The two β-sheets are strongly twisted and form a cleft on one side of the protein in which the active site is situated. This cleft is covered by a long loop region which is called the thumb region [5]. This thumb region is highly conserved throughout the GH 11 xylanases and comparison of several crystal structures has suggested that this region is the most flexible region of the molecule. Several studies have shown that the thumb region opens in a hinge-like fashion by 1.1 Å to accommodate the substrate. During the reaction, the thumb cycles between an open conformation where the ligand can bind and a closed conformation where the reaction can occur [6]. This study describes the structure determination of a *Bacillus subtilis* xylanase mutant of which the thumb region is completely extended. Detailed comparison of this structure and the structures of other GH 11 xylanases reveals that the palm and finger regions have identical conformations. When the thumb is completely extended, the distance between the tip of the thumb (C_α of Ile^{118}) and the finger region (C_α of Gln^{7}) is 28.5 Å in the *Bacillus subtilis* mutant while in *Trichoderma reesei* xylanase II, this distance (from C_α of Ile^{128} to C_α of Ser^{16}) is 11.1 Å in the closed conformation and 12.1 Å in the open conformation. We propose Tyr^{113} and Phe^{125} as the hinge points that accommodate the movement of the thumb region.

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