ESRF	**Experiment title:** PROTEIN CRYSTALLOGRAPHY AT AFMB-CNRS, MARSEILLE	**Experiment number:** LS1657
Beamline: ID14-2	**Date of experiment:** from: 03.03.2000 to: 04.03.2000	**Date of report:** Aug00
Shifts: 1	**Local contact(s):** Steffi Artzt	*Received at ESRF:*

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Report:

Many glycoside hydrolases are modular proteins. Modules are defined as structural and functional independent subunits of a polypeptide chain. The modules, the most often associated with glycoside hydrolase catalytic domains are the so-called "Carbohydrate Binding Modules" (CBM's). They display high affinities for the oligosaccharridic substrate of the corresponding catalytic domain.

The xylanase U (xylU) from *Clostridium thermocellum* consists of four modules, one of which is a CBM (family 6). No structure is available for this type of CBM to date. The xylanases play a major role in the synergetic degradation of cell walls, consisting of cellulose imbedded in xylane, in that it makes the cellulose chains accessible to the cellulosomes of the bacterium. The structures of several "Cellulose Binding Domains" (CBD) have been determined, but no xylane binding domain is known to date. In order to get more information on how variation of substrate specificity is performed by these proteins it is of great importance to be able to compare the different types of CBM's. We have recently crystallized the CBM6 of xylU and have obtained needle-formed crystals with space group $P6_122$ or $P6_522$ and unit cell parameters a=b=60 Å and c=158 Å. We intend to determine the 3D structure, using the MAD method, on a mutant protein of CBM6 of xylU in which a seleno-methionine has been introduced. A native data set has been collected on beamline ID14-EH2. The data collection and processing statistics are given below.

	CBM6 of xylU
Resolution (Å)	39-2.0 (2.15-2.0)
Oscillation range (°)	30
Number of unique reflections	11947 (1131)
Redundancy	4.3 (4.4)
Completeness (%)	99.9 (99.9)
R_{sym}	11.6 (18.5)
$\langle I \rangle / \sigma(I)$	4.3 (3.2)