	Experiment title: Cellobiohydrolase CelS from *Clostridium thermocellum*	Experiment number: LS-1685
Beamline ID-14.3	**Date of experiment:** April 7th, 2000	**Date of report:** August 28th
Shifts:	**Local contact(s):**	*Received at ESRF:*

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Report:

Cellobiohydrolase CelS is the major enzymatic component of the *C. thermocellum* cellulosome, a bacterial multi-protein complex which is very efficient in degrading crystalline cellulose. Orthorhombic crystals of the catalytic domain of CelS (Mw=60 kDa) have a large unit cell with six molecules in the asymmetric unit, but they diffract X-rays beyond 2.5 Å resolution using a synchrotron source. Our objective is to carry out structural studies of CelS in complex with different substrates/inhibitors to gain further insight into the mode of action of this processing enzyme in cellulose degradation.

The 3D structure of CelS has been determined by molecular replacement techniques and is currently being refined against a previous data set (collected at EMBL-DESY, Hamburg) of the enzyme-cellobiose complex at 2.3 Å resolution. During this period, we have collected a single data set from another CelS-cellobiose complex, but the crystals diffracted X-rays to lower resolution (probably due to freezing problems). Data collection statistics is summarized in the table below.

Crystal form	Beam-line	λ (Å)	No. of images	Space group	a (Å)	b (Å)	c (Å)	Data resolution (Å)	Data complet. (%)	R_{merge} (%)	Multipli-city
CelS - cellobiose	ID-14.3	0.931	100	$P2_12_12_1$	146.5	206.3	212.7	2.5	82.5	12.5	3.2

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