ESRF	Experiment title: **Cellulases.** *BAG: Uppsala (II)*	**Experiment number:** LS-1520 d
Beamline: ID14-EH4	**Date of experiment:** from: 22 Sept 1999 to: 25 Sept 1999	**Date of report:** 29 Aug 2000
Shifts: 3	**Local contact(s):** Sean McSweeney	*Received at ESRF:*

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Report:

During this visit to ID14-4 more than 40 crystals were tested and 9 datasets were collected. The time was mainly devoted to two projects: Epoxide hydrolases (Experiment report LS-1520 c) and Cellulases, reported here.

Three datasets were collected of ligand complexes with Cellobiohydrolase 1 (CBH1, Cel7A) from *Trichoderma reesei*: One of the datasets (exo-loop mutant, 2.0 A) were later found too disordered to be useful.

One complex of CBH 1 E212Q mutant (crippled nucleophile, catalytically deficient) with insoluble oligosaccharides was solved at 1.8 A. We have previously solved the structure of this ligand in complex with the acid/base-crippled mutant CBH1 E217Q and may now compare the effect of the active site residue mutations upon carbohydrate substrate distortion.

Another dataset (1.3 A) was collected of CBH1 E212Q in complex with a synthetic penta-saccharide derivative, a methylumbelliferyl-tetraoside with an alpha-1,4-linked glucose residue attached to the non-reducing end. The alpha-1,4-linked glucosyl unit is binding in the expected subsite of the active site tunnel of CBH1, but it is rotated around 180 degrees, i.e. turned upside-down, compared to the usual binding configuration observed. All glc-binding subsites in the cellulose binding tunnel of CBH1 should be able to accomodate the glucosyl unit in the "upside-down" configuration if the cellulose chain is sliding through the tunnel during processive hydrolysis. The new structure is a starting point for modelling of the cellulose sliding process.

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