ESRF	**Experiment title:** Uppsala (II) BAG, LS-1665 (T. Alwyn Jones BAG) Cellulases; EG3	Experiment number: LS 1935
Beamline: ID 14:EH1	**Date of experiment:** from: 4 Oct 2001 to: 5 Oct 2001	**Date of report:**
Shifts: 3 (Eg3: 1.5)	**Local contact(s):** Dr. Edward Mitchell	*Received at ESRF:*

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Report:
Protein Name EG3: Endoglucanase 3 from *T. reesei*

Brief background and outline of project

(Cel12A, GH family 12). EG3 is a minor component in the cellulase system, but may nevertheless play an important role. It differs from the other cellulases in that it does not contain the additional cellulose binding module and linker typical for many cellulases. It is also smaller than other fungal cellolytic enzymes and subsequently appears to have a larger ability to penetrate the cellulose substrate. We have recently solved the structure and now aim at obtaining ligand complexes with wild-type and mutated enzymes for understanding catalytic mechanism, substrate binding and specificity. Very large crystals have been obtained that diffract to very high resolution (0.9-1.0 A) and which could hopefully yield structures at atomic resolution.

Datasets collected on ID14:EH1

Four datasets were collected on protein crystals of a catalytic inactive mutant of T. reesei EG3. The crystals were co-crystallized with four different sugar substrate analogs:
G2, G3, G5 and G6. All four datasets had high completeness, were of high quality and gave very nice density maps. In two of the four datasets a ligand could clearly be found bound in the catalytic active cleft of the protein.

Data statistics for the datasets:

Dataset 1:

Ligand:	G2 20 mM
Resolution:	50-1.5 Å
Space group:	P43212
Cell:	a:49.3, b:49.3, c:166.2, $\alpha, \beta, \gamma = 90$
Completeness:	99.3 %

Dataset 2:

Ligand:	G3 20 mM
Resolution:	50-1.6 Å
Space group:	P43212
Cell:	a:49.4, b:49.4, c:166.3, $\alpha, \beta, \gamma = 90$
Completeness:	99.6 %

Dataset 3:

Ligand:	G5 20 mM
Resolution:	50-1.4 Å
Space group:	P43212
Cell:	a:49.3, b:49.3, c:166.1, $\alpha, \beta, \gamma = 90$
Completeness:	99.7 %

Dataset 4:

Ligand:	G6 20 mM
Resolution:	50-1.5 Å
Space group:	P43212
Cell:	a:49.4, b:49.4, c:166.2, $\alpha, \beta, \gamma = 90$
Completeness:	100 %