



	Experiment title: Uppsala (II) BAG, LS-1665 (T. Alwyn Jones BAG) Cellulases; EG3	Experiment number: LS 1665
Beamline: ID 14:EH2	Date of experiment: from: 21 Feb 2002 to: 22 Feb 2002	Date of report: <i>Received at ESRF:</i>
Shifts: 3 (Eg3: 1)	Local contact(s): Dr. Cecile Jamin	
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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 Å) and which could hopefully yield structures at atomic resolution.

Datasets collected on ID14:EH1

Two datasets were collected on protein crystals of a catalytic inactive mutant of *T. reesei* EG3. The crystals were co-crystallized with two different sugar substrate analogs:

G4, and G2SG2. The two datasets had high completeness, were of high quality and gave very nice density maps. There was a ligand bound in the catalytic active cleft of the protein, in both datasets.

Data statistics for the datasets:

Dataset 1:

Ligand: G4 20 mM
Resolution: 50-1.7 Å
Space group: P43212
Cell: a:49.5, b:49.5, c:167.6, $\alpha, \beta, \gamma = 90$
Completeness: 98.9 %

Dataset 2:

Ligand: G2SG2 20 mM
Resolution: 50-1.5 Å
Space group: P43212
Cell: a:49.3, b:49.3, c:166.0, $\alpha, \beta, \gamma = 90$
Completeness: 99.3 %

