



	Experiment title: Uppsala (II) BAG, LS-1665 (T. Alwyn Jones BAG) Cellulases; EG3	Experiment number: LS 1935
Beamline: ID 14:EH4	Date of experiment: from: 6 Dec 2001 to: 7 Dec 2001	Date of report: <i>Received at ESRF:</i>
Shifts: 3 (Eg3: 0.5)	Local contact(s): Dr. Gordon Leonard	
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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:EH4

One dataset was collected on a protein crystal of a catalytic inactive mutant of *T. reesei* EG3. The crystal collected on was co-crystallized with one sugar substrate analog:

G2 with a aglycon, umbeferyl, bound at the reducing end of the cellobios. The dataset had high completeness, was of high quality and gave very nice density map. Where a ligand molecule clearly could be found bound in the catalytic active cleft of the protein.

Data statistics for the datasets:

Dataset 1:

Ligand: G2-Umbeferyl 10 mM
Resolution: 100-1.4 Å
Space group: P43212
Cell: a:49.3, b:49.3, c:166.0, $\alpha, \beta, \gamma = 90$
Completeness: 99.1 %