ESRF	**Experiment title:** Dundee-St. Andrews BAG	**Experiment number:** LS-1683
Beamline: ID14-1	**Date of experiment:** from: 27-03-2000 to: 28-03-2000	**Date of report:** 30-08-2000
Shifts: 2	**Local contact(s):** Hassan Berlhani	*Received at ESRF:*

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Report:

We previously solved the structure of chitinase B from Serratia Marcescens. Although this structure has aided us in interpretation of biochemical data, we had no complexes with substrates/inhibitors and thus no insight in the catalytic mechanism. Using ESRF time on ID14-1, we have collected data on an inactive mutant (P212121, 1.7 Å, Rsym=0.063), the inactive mutant soaked with a chitin pentamer (2.25 Å, Rsym=0.046), wild type soaked with partially de-acetylated chitin (pentamer: 1.83 Å, Rsym=0.057 and hexamer: 1.90 Å, Rsym=0.051) and a novel natural inhibitor isolated from sea-spunges near the Fiji islands (1.85 Å, Rsym=0.055). The structures of the inactive mutant have been completely refined and are currently being written up. The map of WT with natural inhibitor shows density for the soaked molecule, but is not readily interpretable. The complexes with partially de-acetylated chitin show one or two disordered NAGs in the active site, but have not been properly refined yet.