ESRF	**Experiment title:** HUMAN GELSOLIN	**Experiment number:** LS 163
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Names and affiliations of applicants (* indicates experimentalists):

Paul McLaughlin*, Department of Biochemistry, University of Edinburgh, Scotland
Robert Robinson*, Laboratory of Molecular Biophysics, University of Oxford, England
Les Burtnick*, Laboratory of Molecular Biophysics, University of Oxford, England

Report:

Having solved the structure of whole gelsolin in a calcium free (un-activated state), we attempted in these experiments to locate the Ca^{2+} site and the active conformation. Crystals soaked in Ca^{2+}, Cd^{2+} and Tb^{2+} did not survive the freezing protocol. Therefore we had to revert to collecting at room temperature. Crystals proved radiation sensitive and many were required to complete a data set. In the end, this was 94% complete to 4.0Å (Rmerge=0.097) and 81 .6% to 3.0Å (Rmerge 0.163). This data set was isomorphous to the Ca^{2+} free form and no calcium ion or changes in the protein structure were observed.

We must conclude that Ca^{2+} cannot bind in the crystal because the high ammonium sulphate concentration in which the crystals are grown reduces the volubility of the ion and/or the lattice contacts in the crystal make the binding site unavailable to the ion.

The second experiment was to locate an ATP binding site. Crystals were soaked in ATP and a 90% complete data set to 3.0 Å was collected (Rmerge 0.100). These data were also isomorphous to the native and the binding site could not be identified. It is not unlikely that because of the high concentration of the precipitant, sulphate ions compete with the binding sites for the nucleotide phosphate groups.

On the home source, it is impossible to collect data at sufficient resolution with these crystals due to the weak diffraction from the 164kD contents of the asymetric unit. Our time at ESRF was valuable because we quickly found out that we need to stabilise the crystals in salts other than Ammonium Sulphate and we have now shown that we can do this successfully in Ammonium Acetate.