$\overline{\mathrm{ESRF}}$	Experiment title: Dundee-St. Andrews BAG	Experiment number: LS-1683
Beamline: BM14	<b>Date of experiment:</b> from: 28-04-2000 to: 29-04-2000	Date of report: 30-08-2000
Shifts:	Local contact(s): Gordon Leonard	Received at ESRF:

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## Report:

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FadR is an *E. coli* fatty acyl responsive transcription factor, representative of the large GntR family of bacterial regulators. Using the time on BM14, a suitable derivative was identified, and a full 3-wavelength MAD dataset (C2221, 1.85 Å, Rsym=0.074) and a native (2.0 Å, Rsym=0.070) were collected. The MAD dataset yielded readily interpretable anomalous and dispersive Pattersons. Together with a dataset of another derivative at 1.65 Å, this resulted in excellent phases to 1.65 Å, from which the structure was built with warpNtrace. The structure reveals a DNA binding domain and a novel C-terminal acyl-CoA binding fold, and gives insight in how acyl-CoA would bind and how that might result in a conformational change.

## **Publication**

D.M.F. van Aalten, C. C. DiRusso, J. Knudsen and R.K. Wierenga Crystal structure of FadR, a fatty acid responsive transcription factor with a novel acyl-coenzyme A binding fold. EMBO J. (2000) in press.