ESRF	Experiment title: Structural Studies of the Restriction Endonuclease Bgl1 .	Experiment number: LS668
Beamline: D2AM, BM14	Date of experiment: from: 9" June 1997 from: 11 th June 1997 to: 13 th June 1997	Date of report: 13 th August
Shifts:	Local contact(s): Eric Fanchon, Andy Thompson	Received at ESRF: 2 2 AOUT 1997

Names and affiliations of applicants (* indicates experimentalists):

Phillips S.E.V., Newman M.*, Smith L.*, Vinecombe E.*, Wilmot C.M.*

Department of Biochemistry and Molecular Biology,

University of Leeds,

Leeds

LS2 9JT

United Kingdom.

Report:

We collected four complete Bgll/DNA complex data sets during our beam time on D2AM three of which are useful and are being used in ongoing structural determinations:

Native and PCMBS derivative data sets were collected for a Bgll/17mer complex at wavelengths of 1.00911 and 1.00465Å respectively. The derivative data has not been processed but the native data are good to 2.24Å In addition, 2.24Å native and PCMBS derivative data sets were collected for a Bgll/18mer complex at wavelengths of 1.00917 and 1.00465Å respectively.

In total, we collected seven complete Bgll/DNA complex data sets during our beam time on BM14 six of which are useful and are being used in ongoing structural determinations.

Native, PCMBS and hexachloro osmate derivative data sets were collected for the Bgl1/l7mer complex at wavelengths of 0.919, 0.919 and 1.14Å
The 2.2Å native data have an R_{symm} of 0.055 for all data (0.078 in the last resolution shell), the 2.3Å PCMBS data have an R_{symm} of 0.039 for all data (0.107 in the last resolution shell) and the 2.8Å hexachloro osmate data have an R_{symm} of 0.031 for all data (0.054 in the last resolution shell).

2.3Å data sets were also collected for three brominated Bgl1/17mer complexes at a wavelength of 0.919Å These data have R_{symm} 0.034,0.038,0.033 for all data (0.065,0.081, 0.067 in the last resolution shell respectively).

A hexachloro osmate derivative data set was collected for the Bg11/18mer complex at a wavelength of 1.14Å, but these data have not been processed.

The useful data sets have been incorporated into the MIRAS phase calculation using the program SHARP, resulting in a superb electron density map for the Bg11/17rmer complex. A model has been built, including the DNA and all but one residue of the protein and is currntly being refined.

We are pleased with the data collected during this beam time and would like to thank the beam line staff, in particular Eric Fanchon and Andy Thompson, for their assistance.