| ESRF | **Experiment title:** Structural studies on HSV- 1 thymidine kinase, UvrA and a drug-DNA complex. | **Experiment number:** LS965 |
|---|---|---|
| **Beamline:** BM14 | **Date of experiment:** from: March 30" 1998 to: March 31st 1998 | **Date of report:** 3 1st August 1998 |
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**Report:** Solution of a crystal structure of DNA complexed with porphyrin by multi-wavelength anomalous dispersion phasing

**Crystal preparation:** Prior to the experiment at the ESRF, crystals of the DNA complexed with porphyrin were grown. These crystals were flash frozen at 100K in house and tested for diffraction quality, then transferred, using a new cryo-torch device which we have developed for the mounting of flash frozen crystals at synchroton stations, to a nitrogen-vapour storage device. At the ESRF, a crystal was removed from storage and mounted using the cryo-torch device.

**Data Collection:** Crystal diffraction data was collected at three wavelengths $\lambda_1$=0.919Å, $\lambda_2$=0.920Å and $\lambda_3$= 0.7747Å. Data was processed in the space group P41 with crystal unit cell dimensions a = b = 32.161 and c = 61.190 using crystallographic software from the **HKL** suite and CCP4 suite. For data of resolution 1.59Å, the Rmerge statistics for $\lambda_1$, $\lambda_2$ and $\lambda_3$ were 1.82%, 1.84% and 1.91% respectively, and the $R_{anom}$ statistics were 10.12%, 5.56% and 6.12% respectively.

**MAD phasing:** The positions of four bromines in the asymmetric unit cell were found using anomalous difference, dispersive difference and isomorphous difference Patterson maps.

Phases were calculated for the data, giving a high mean figure-of-merit of 0.84, the resulting maps revealed a clear solvent boundary and crudely revealed two A-DNA helices in the unit cell.

**Model building:** Although the connectivity in the initial electron-density map was very poor, it has been possible to model DNA and porphyrin to the map, shown in *fig1*. This model is now in the process of refinement and this high-resolution (1.2Å) A-DNA structure will be published.

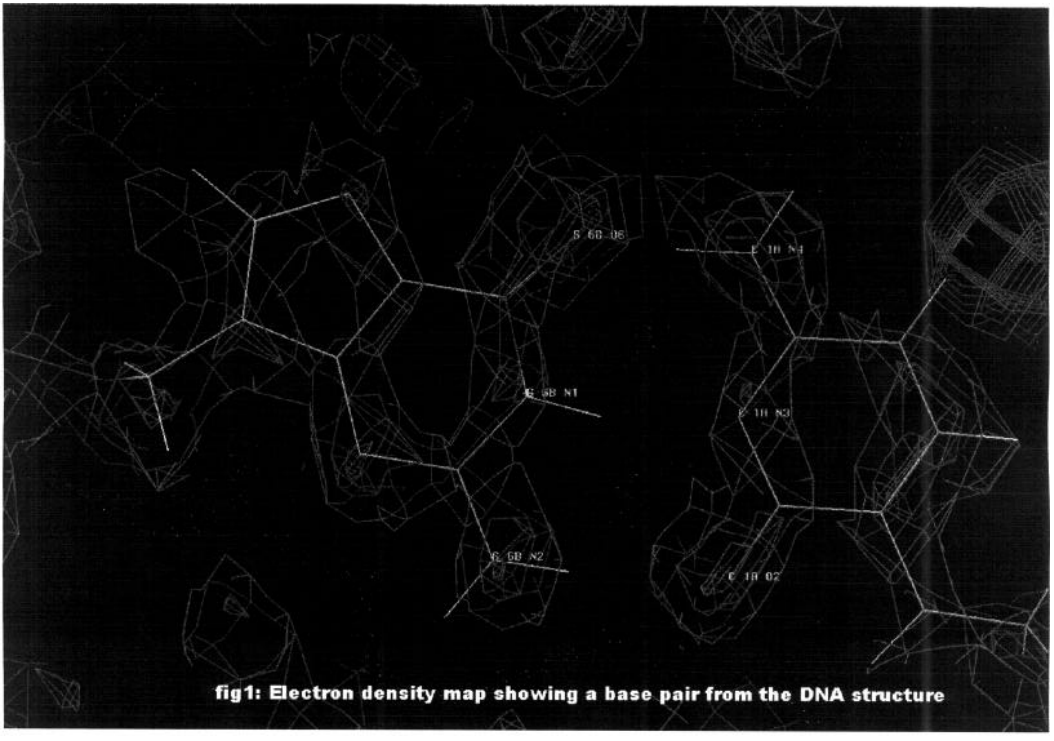

**fig1: Electron density map showing a base pair from the DNA structure**