



<b>Experiment title:</b> X-Ray Crystal Structure determination of Cyclophilin-40: A chaperone and intracellular messenger protein	<b>Experiment number:</b> LS-1356	
<b>Beamline:</b> BM30	<b>Date of experiment:</b> from: 02-Jul-99 to: 03-Jul-99	<b>Date of report:</b> 31-Aug-99
<b>Shifts:</b> 1	<b>Local contact(s):</b> Fanchon Eric (PLUO A)	<i>Received at ESRF:</i>

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**Report:**

The original experiment was to collect high quality data on cyclophilin-40 and use this data in the solution of the cyclophilin 40 (Cyp40) structure. Two crystal forms of Cyp40 have now been obtained and since the original application (1-Sep-98) the crystal structure of the monoclinic form has been solved and refined. Our primary aim for this data beamtime was the collection of high quality/high resolution data from the tetragonal form ( $a=94.58$ ,  $c=118.32$ , Space Group  $P4_2 2 2$ ) of the protein. A complete data set (33 frames at  $1.5^\circ$  per frame) was collected out to a resolution of  $1.8 \text{ \AA}$ . The structure determination of this form indicates that the TPR-domain (tetratricopeptide repeat) consisting of residues 180 to 370 adopts a significantly different conformation in which two helix-turn-helix motifs are changed into long helical rods. This structure is currently being refined.

We were able to make significant use of the remaining beam time to collect data on another protein crystal; the SeMet derivative of *ocr*, the gene product of bacteriophage T7

which binds and inhibits bacterial endonucleases. With the help of the station personnel we were able to collect X-ray fluorescence spectra from a selenomethionine form of this protein (this crystal is monoclinic Space group  $C2$   $a=78.80$   $b=37.69$   $c=35.47$   $\beta=98.39$ ) and subsequently collect two datasets, one each at the maximum  $f$  and  $f'$  anomalous effects at wavelengths  $0.980895$  and  $0.981171$  Å. These datasets are currently being used in attempts to solve this structure in combination with datasets collected from this crystal at other wavelengths. A third dataset was to be attempted however the latter third of the shift was lost to equipment failures in the optics of the beamline.