



Experiment title: Block Allocation Group: Portugal		Experiment number: LS-1384/5
Beamline: ID14-4	Date of experiment: from: 6-May-99 to: 7-May-99	Date of report: 10-Aug-1999
Shifts: 3	Local contact(s): Sean McSweeney	<i>Received at ESRF:</i> 16 AOUT 1999

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Report:

A wavelength of 0.932 Å and a working temperature of 100 K were used throughout.

1. ATP sulfurylase from *Desulfovibrio desulfuricans* ATCC 27774

Native data collected. Crystal size was 0.2 x 0.3 x 0.05mm. The intensity of the beam oscillated very much during the data collection. The spacegroup given by the autoindexing routine in Denzo was dependent on the initial image used. When using Scalepack it was observed that the scale factors and the chi-squared values varied a lot from one image to the next. The completeness is low. The best statistics correspond to the following: Space group C222, a=120.9, b=129.0 c=160.4 Å; Resolution limits: 3.23 - 30 Å; Nr. observed reflections: 22,845; Nr. unique reflections: 11,063; R-factor (I) 0.142; I/σ(I): 5.78; Completeness: 63.2%. The structure wasn't solved nor are there other attempts of processing the data currently being made due to the poor quality of the data.

2. Multi-haem Nitrite Reductase from *Desulfovibrio desulfuricans* ATCC 27774

Native data collected from a crystal 0.4 x 0.15 x 0.1mm in size. The crystals belong to space group $P2_12_12_1$ with cell constants: $a=78.9$, $b=104.6$, $c=143.2$ Å. Resolution limits: 2.3 - 30.0 Å; Nr. observed reflections: 96,142; Nr. unique reflections: 53,714; R-factor (I): 0.084; $I/\sigma(I)$: 11.7; Completeness 94.0%. This data set will be used for extending the resolution of the maps obtained from the BM-14 MAD experiment (see report) or to try a molecular replacement solution of the model from the MAD data.

3. Cinnamomin from *Phytophthora cinnamomi*

Native data were collected. The crystals belong to space group P1 with cell dimensions $a=31.47$, $b=36.82$, $c=43.94$ Å, $\alpha=76.9$, $\beta=86.2$, $\gamma=80.4^\circ$. Resolution limits: 30.0-1.45 Å; Nr. observed reflections: 83,599; Nr. unique reflections: 32,402; R-factor(I): 0.088; $I/\sigma(I)$: 8.8; Completeness: 95.1%. The protein structure was determined by molecular replacement, and refinement is in its early stages.

4. [NiFe] Hydrogenase from *Desulfovibrio desulfuricans* ATCC 27774

Native data were collected. The crystals belong to space group $P2_1$ with cell dimensions $a=64.09$, $b=169.98$, $c=72.62$ Å, $\beta=92.8^\circ$. Resolution limits: 32.0-1.80 Å; Nr. observed reflections: 337,524; Nr. unique reflections: 135,264; R-factor(I): 0.072; $I/\sigma(I)$: 4.5; Completeness: 95.4%. The protein structure was determined by molecular replacement, and refinement converged to $R=0.175$, $R\text{-free}=0.231$. A manuscript is currently in preparation.