ESRF	**Experiment title:** Block Allocation Group: Portugal	**Experiment number:** LS-1384/5
Beamline: BM14	**Date of experiment:** from: 7-May-99 to: 9-May-99	**Date of report:** 10-Aug-99
Shifts: 6	**Local contact(s):** Andrew Thompson	*Received at ESRF:*

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Report:

Data collection:

Data were collected using a Mar345 Image Plate at three wavelengths : 1.7403 Å (inflexion point), 1.7390 Å (peak), 0.9919 Å (remote) from a crystal 0.3 x 0.1 x 0.1mm in size, at T=100K. The crystals belong to space group $P2_12_12_1$ with cell constants: a=78.88Å b=104.49Å c=143.06Å at 100K.

Data processing:

Data were processed with DENZO/SCALEPACK/CCP4. During data scaling with Scalepack, it was observed that the chi squared values of the fitting increased from about 0.48, 0.56 and 0.62 in the first images to about 2.49, 2.25 and 2.05 in the last images for the point of inflexion, peak and remote datasets, respectively. Since this behaviour was observed during data collection for the 3 working wavelengths using the same crystal, it cannot be explained by radiation damage.

The output statistics from Scalepack are the following:

Wavelength:	1.7403 Å (inflex. point)	1.7390 Å (peak)	0.9919 Å (remote)
Resolution limits:	2.7 - 35 Å	2.7 - 35 Å	2.5 - 35 Å
No. of observed reflections:	33843	33686	42079
No. of unique reflections:	60779	60354	76770
R factor(I):	0.092	0.092	0.042
I/sigma(I):	6.9	7.3	14.6
%Completeness:	95.1	94.9	96.2

Structure solution:

Using program Solve, a solution for the heavy atoms was found with an overall Z-score of 44.8. Ten iron sites were located in the asymmetric unit. Since both the self-rotation function and Matthews volume calculations indicate the existence of 2 molecules (of the large sub-unit) per asymmetric unit, the sites found would correspond to 5 heme groups per molecule. After the final refinement, the Solve figure of merit for this solution was 0.62 which is an indication that the solution is good.

The solution obtained by Solve was further refined using the program SHARP. After refinement, a figure of merit (FOM) of 0.49 for the acentric reflections and 0.45 for the centric reflections were obtained, before solvent flattening. After solvent flattening with the program Solomon, the overall FOM improved to 0.92 indicating at least statistically that the phases are of good quality.

The structural model is presently being built.