Report of experiment MX386 at ID14.3 (14/07/2005)

The 3 shifts at ID14.3 were particularly productive for many of our projects.
In general we had no problems using the beamline devices, although we would like to bring to the attention one minor detail which, once fixed, would definitely improve the beamline quality. Despite the fact that the refill is very fast, there is no electronic link to ProDC to hold on the data collection, therefore we had to stop and go back to the appropriate Phi, after having looked for the last collected frame.

Project Schistosoma haematobium GST mutants: R21L and R21Q
We collected two data sets of R21L: the first data set at 1.7 Å, number of frames 360. The second data set was collected at 1.9 Å, number of frames 484, the oscillation was 0.5 degree. It was possible to scale the data processed with Denzo. The statistics parameters were good for both data sets. No data set was collected for R21Q due to poor crystal quality.

Project Cytochromes c551
We are interested in the structural basis of the thermal stability in cytochrome c family. The structures of the cytochromes c552 from the thermophilic bacterium *H. thermophilus* has already been solved in our lab; we are now trying to determine the crystal structure of a point mutant (F7A) of the cytochrome c551 from *P. aeruginosa* whose folding mechanism is currently being investigated. F7A is almost as stable as the thermophilic protein. Our aim is to establish the structural requirements of the surprisingly enhanced stability of this mutant. In order to obtain a high resolution dataset we tested several crystals, finally we were able to collect data at 1.86 Å resolution. Data collection parameters are summarised in the table below.

F7A (resolution 30.0-1.86 Å)	
Space group	P65
Unit cell dimensions	a= 66.766, b=66.766, c= 62.462
Completeness (last shell) %	100 (100)
Mosaicity	0.28
Rsym (last shell)	0.057 (0.520)

Project CcmH
We are working on the structure of CcmH protein. At present the structure (solved by MAD on ID29) is going to be refined and we are now trying to solve the structure of the reduced form of the protein. In fact CcmH contains one disulphide bridge with a putative functional role in the maturation of c-type cytochrome in vivo. Our aim is to establish if

the protein undergoes structural rearrangement during the oxidation-reduction cycle. We tested several crystals soaked with DTT and TCEP as reducing agent at different concentration and collected two data sets on hopefully reduced crystals with both agents. Data collection parameters are reported in the following table.

CcmH DTT 2mM (resolution 30.0-2.3 Å)	
Space group	P212121
Unit cell dimensions	a=31.273, b= 65.283, c=81.429
Completeness (last shell) %	99.6 (95)
Mosaicity	1.4
Rsym (last shell)	0.124 (0.528)
CcmH TCEP 3mM (resolution 30.0-2.3 Å)	
Space group	P212121
Unit cell dimensions	a=32.155, b=41.358, c=65.582
Completeness (last shell) %	98.9 (95.0)
Mosaicity	0.95
Rsym (last shell)	0.07 (0.45)