

## Report of experiment MX386 at ID14.4 (15/07/2005)

The 24h shift at ID14-4 was not as successful as expected due both to the bad quality of the crystals (too small to be even tested with home source) and to some failure at the front end, which forced the beamline scientists to eliminate the attenuator thereby causing enormous radiation damage to the well diffracting crystals even with 0.5 sec exposure. In any case we managed to collect two data sets of CcmH co-crystallized in the presence of 2.0 mM of TCEP.

CcmH co-crystallized with TCEP in three different conditions. All the three crystal forms were tested. CcmH crystals belonging to the C form did not diffract well and we did not collect them. The crystals form A and B diffracted very well, in particular one crystal diffracted at 1.7Å.

Data collection parameters are reported in the following table.

CcmH FORM A (resolution 30.0-1.7 Å)	
Space group	P212121
Unit cell dimensions	a= 40.073Å, b=45.414Å, c=48.127Å
Completeness (last shell) %	97.7 (96.5)
Mosaicity	0.5
Rsym (last shell)	0.044 (0.458)
CcmH FORM B(resolution 30.0-2.0 Å)	
Space group	P4
Unit cell dimensions	a=45.008 b=45.008 c=40.159
Completeness (last shell) %	97.7 (96.5)
Mosaicity	1.332
Rsym (last shell)	0.125 (0.627)

The other project which worked partially well was a MAD experiment on a DNR protein C-terminal domain deletion mutant (N152stop). At present we are trying to solve the phases.

We tested several crystals, some did not diffract well while others suffered severe radiation damage during data collection.

DNR N152stop (resolution 30.0-3.1 Å)	
Space group	P21
Unit cell dimensions	a= 57.04, b=167.82, c= 59.08, β=116.97
Mosaicity	0.75
peak (12.6574eV)	
Rsym (last shell, 3,1 Å )	0.086 (0.369)
Completeness (last shell) %	99.4 (98.9)
remote (12.7500eV)	
Rsym (last shell, 3,4 Å )	0.093 (0.386)
Completeness (last shell) %	99.2 (98.4)
Inflection point (12.6549eV)	
Rsym (last shell, 4,0 Å )	0.097 (0.375)
Completeness (last shell) %	98.7 (97.3)

We then passed into the project of XendoU for which we wanted to collect a native data set at high resolution. After having tested many crystals, we started collecting 1 data set, whose spot went up to 2.3Å at the beginning (wavelength 0.977744 and 0.8 mosaicity), but we had to cut the resolution to 2.7 at the end for severe radiation damage. Therefore we shall try to improve crystals for the next beamtime shift.

In the table there is the result from scala:

	Low resolution limits 63.50-2.42	High resolution limits 2.42- 2.3
Rmerge	0.175	0.579
Rmeas (within I+/I-)	0.191	0.630
Total no. of observations	259412	34888
Total number unique	42808	5786
Mean(I)/sd(I)	11.4	2.1
Completeness	95.0	88.3
Multiplicity	6.1	6.0