

## Experimental report, MX-425 25.4-27.6 2005

### 1. Structure of an urasil DNA glycosylase

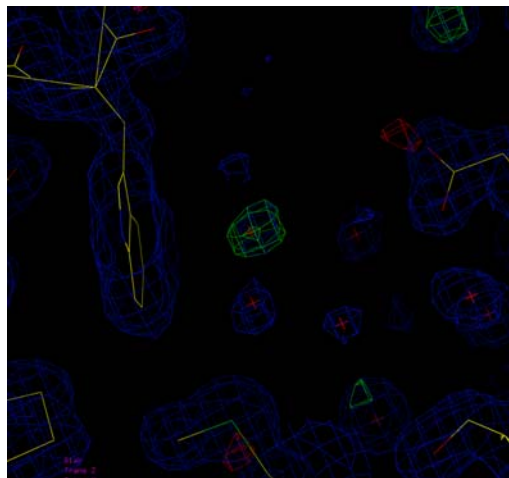
We tried to collect data for series of crystals, however, only one sample gave diffraction to a resolution of about 3.25Å. Since we have no in-house diffractometer, assessment of crystal quality prior to visits to ESRF is currently not possible. The crystal turns out to have a unit cell of about 85 x 85 x 505 Å in space group P422. Even with the high Laue symmetry, calculation of the Matthews coefficient gives 6 molecules per asymmetric unit. Attempts to solve the structure by MR have not succeeded.

	Best Xtal
Resolution	3.25Å
I/sI	10.1
R(sym)	15.8%
Completeness	100%

### 2. Structure of a protein:nucleotide complex

We collected in total 12 datasets of the protein Mag2 from *S. pombe* of crystals treated with 3mA or urasil in order to capture the protein\_nucleotide complex. We have tried both co-crystallization (3mA) and soaking (3mA and urasil). Analysis of the difference electron density maps after refinement shows no sign of a bound substrate (see figure below for a representative case). Crystal data 71.3Å, 84.5Å, 124.5Å, 90, 90, 90. Space group P2<sub>1</sub>2<sub>1</sub>2. Statistics for best data sets:

	3mA co-crystal	3mA soak	Urasil
Resolution	1.75Å	1.9Å	2.0Å
I/sI	17.3	12.5	11.8
R(sym)	7.4%	9.8%	10.1%
Completeness	99.9%	100%	100%



Difference map in the putative binding pocket in Mag2.