

Experimental report, MX-298 29.4-30.4 2005

1. Structure of an urasil DNA glycosylase

We tried to collect data for a large number of crystals, however, only one sample gave diffraction to a resolution of about 4.5Å. 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.

2. MAD collection of an Xth crystal

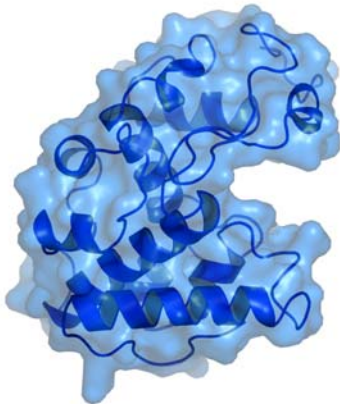
We collected four full MAD datasets of a crystal we believe is a Xth enzyme, however, we have not been able to solve the structure by SAD/MAD phasing using solve. Crystal data 108.8Å, 108.8Å, 163.9Å, 90, 90, 90. Space group P4_{1/3}22. Listing of statistics for peak datasets:

	Set 1	Set 2	Set 3
Resolution	2.5Å	2.25Å	2.0Å
I/sI	7.3	8.9	4.4
R(sym)	19.4%	12.2	12.9%
R(anomal)	22.7%	17.8	18.3%
Completeness	80%	94.6%	51.7%

3. ChiG

As a backup project, we collected two datasets of ChiG, the structure of which have been solved. The structure will be published in due course. Crystal data : 48.31Å, 74.0Å, 63.3Å, 90, 108, 90. Space group P2₁ with 2 molecules in the asymmetric unit.

Dataset	Completeness	R(sym)	Resolution	I/sI
ChiG1	97.4 %	9.6%	1.6 Å	12.5
ChiG2	98.5 %	7.6%	1.5 Å	13.2



3D-structure of ChiG