

Set-up

| | | |
|---------------------------------|----------------------------|--|
| Source | Type: | Rotating anode, Cu |
| | Model: | Siemens M18XH-SRA |
| | Filament: | 300 μm |
| Optics | Model: | Xenocs focusing optics FOX2D CU 12_38P |
| | | |
| X-Ray Diffraction system | Model: | MAR345 |
| | Detector Type: | Image Plate |
| | Detector Mode: | 345/100 |
| | Mar Slits: | S1 = 0.5 x 0.5 mm ² S2 = 0.3 x 0.3 mm ² |
| | Distance Crystal-detector: | 150 mm |



Fig. 1 : Crystallographic setup at the EMBL, Grenoble

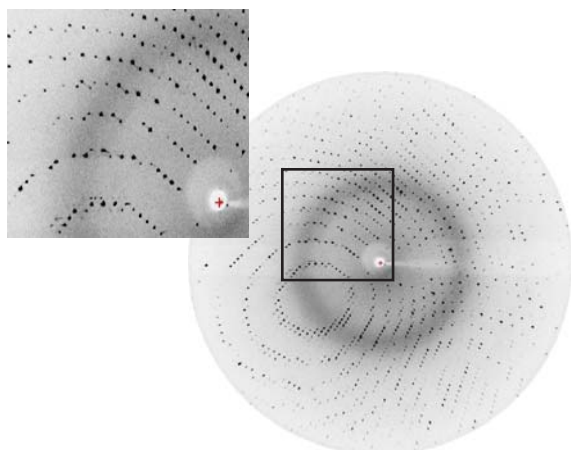


Fig. 2 : One of the diffraction patterns taken from the Elastase crystal dataset. No visible contamination from the Cu K- β ray could be detected. The individual diffraction spots are intense and nicely shaped.

Protein Crystallography application

Data courtesy of Dr. Hassan Belrhali, European Molecular Biology Laboratory (EMBL), Grenoble, France.

Introduction

This application note presents the improved results from an in-house protein crystallography application using the focusing FOX2D CU 12_38P optics from Xenocs. All experiments were performed at the European Molecular Biology Laboratory (EMBL) in Grenoble, France. Dr. Hassan Belrhali, responsible for crystallography applications at EMBL, Grenoble, conducted the experiments and carried out the data treatment.

The related results were generated using a rotating anode and a MAR 345 diffractometer, equipped with an image plate detector. Elastase and Thaumatin crystals, known as reference systems for protein crystallography, served as test samples. The resulting data was processed with a rectangular integration mask (MOSFLM).

Experiment

Experiment 1

Source power

50 mA x 40 kV

Crystal parameters

Type: Elastase (P2₁2₁2₁)

Size: 300 x 300 x 300 μm^3

Frozen at 100 K

$\Delta\phi$ / image 1°: 220 images

Exposure time: 600 s

Experimental details

Overall R_{sym} : 2.4 %

R_{sym} at 1.9 Å: 3.7%

I/σ : 16.7

Refined mosaicity: 0.47°

Completeness: 97.5%

Redundancy: 8.6

Experiment 2

Source power

100 mA x 40 kV

Crystal parameters

Type: Thaumatin (P4₁2₁2)

Size: 250 x 250 x 250 μm^3

Frozen at 100 K

$\Delta\phi$ / image 1°: 120 images

Exposure time: 60 s

Experimental details

Overall R_{sym} : 6.0 %

R_{sym} at 1.9 Å: 19.7%

I/σ : 10.9

Refined mosaicity: 0.19°

Completeness: 99.9%

Redundancy: 7.9

Conclusion

Comparing the crystallographic results for the two samples, one must take into account the difference in source power and exposure time.

The instrumental configuration (source, optics, diffractometer slits) typically delivers a flux of approximately 3.2×10^8 counts/sec at the sample position. The good crystallographic results are achieved due to the high flux coming from the focusing optics. The crystal sizes are rather large but the crystal diameter can be reduced down to 50 μm .