

Small crystal analysis

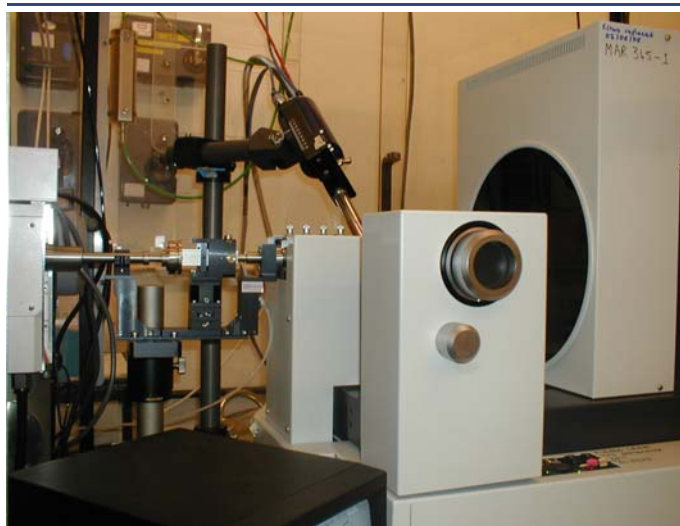
A full dataset using the Xenocs FOX2D CU 25_25P mirrors was collected from a small cryo-cooled crystal of IP3-3 kinase, supplied by Dr Beatriz Gonzalez-Perez. These mirrors were then exchanged for Osmic blue mirrors and a second dataset was collected from the same crystal under identical experimental conditions.

The generator was an MSC/Rigaku RuH3R running at 50kV, 100mA (300 micron focus) and the data were collected on a Mar345 image plate detector. The crystal was a thin plate with approximate dimensions 200x75x50 microns. In both cases the image plate was operated in 300mm scan mode with a crystal to detector distance of 200mm, giving a maximum resolution of 2.43Å. When collecting the data with the Xenocs mirrors, the Mar collimation slits were set to 0.5mm (upstream slits) and 0.25mm (downstream slits). The corresponding values were 0.5mm/0.4mm when using the Osmic blue mirrors. The Mar second ion chamber readings were 53 for the Xenocs mirrors and 41 for the Osmic mirrors.

The crystal belongs to space group C222 with cell dimensions a=72.1Å, b=97.4Å, c=191.0Å. Images were collected with an oscillation angle of 0.4° and an exposure time of 4 minutes.

All data were processed with MOSFLM and scaled with SCALA (both programs are part of the CCP4 package). The effective mosaic spread (which includes the beam

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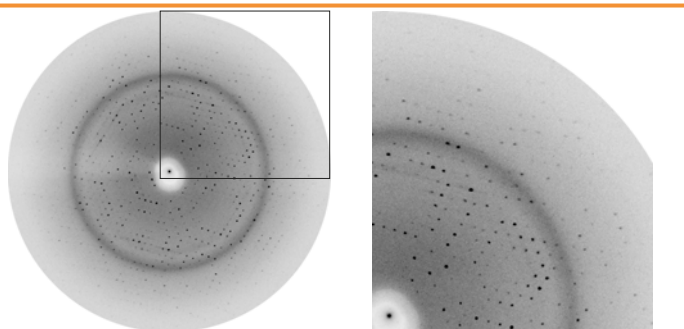


divergence) refined to 0.51° for the Xenocs data and 0.47° for the Osmic data, suggesting that the beam divergence is only slightly higher for the Xenocs optics.

Spot sizes were 9x9 pixels (1.35mmx1.35mm) in both cases (in the centre of the detector).

The merging statistics for the two datasets are listed below:

	Osmic Blue	Xenocs FOX2D CU 25_25P
Exposure time per frame	4 min	4 min
R _{merge} (22.7.-2.43A)	8.8%	6.4%
R _{merge} (2.57-2.43A)	44.1%	26.2%
$\langle I \rangle / \langle \text{sig} \rangle$ (22.7.-2.43A)	12.1	15
$\langle I \rangle / \langle \text{sig} \rangle$ (2.57-2.43A)	2.5	4.1
Mean multiplicity	3.3	3.3



One of the diffraction patterns taken from crystal dataset

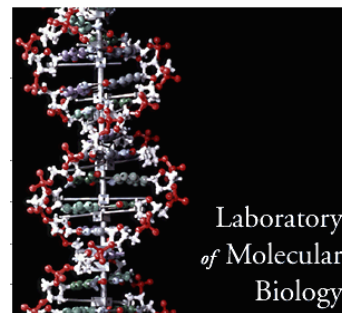
Conclusion

In both cases the standard deviation estimates from MOSFLM were adjusted in SCALA to reflect the true discrepancies between symmetry related reflections.

The results for the highest resolution shell show an improvement in signal to noise by a factor of 1.64. This is consistent with the average scale factor of 2.43 between the two datasets, which provides a good estimate of the relative X-ray flux hitting the crystal. If the data quality is determined solely by counting statistics, an increase in flux by a factor of 2.43 would give a factor of $\sqrt{2.43} = 1.56$ in the signal to noise.

Use of the Xenocs mirrors provides a clear improvement in data quality for this relatively small crystal.

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