

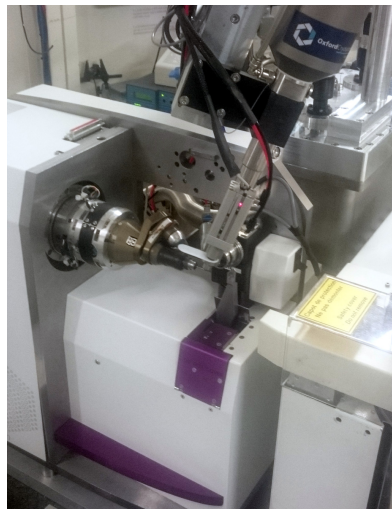
MASSIF-3 News

David von Stetten
February 6th, 2017

MASSIF-3 (ID30A-3)

Beamline characteristics:

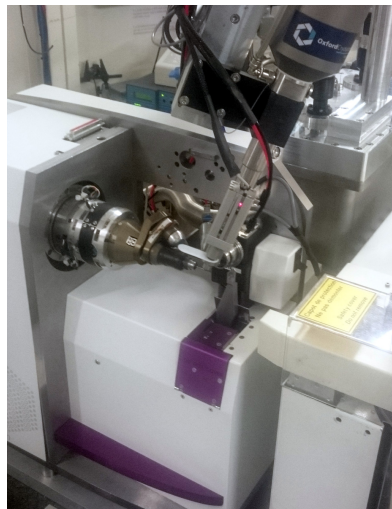
- fixed energy: 12.8 keV
- beam diameter: 15 μm
- 1.5×10^{13} ph/s
- Eiger 4M: up to 750 img/s
- SC3 sample changer
(soon replaced by FlexHCD)



MASSIF-3 (ID30A-3)

MD2 diffractometer:

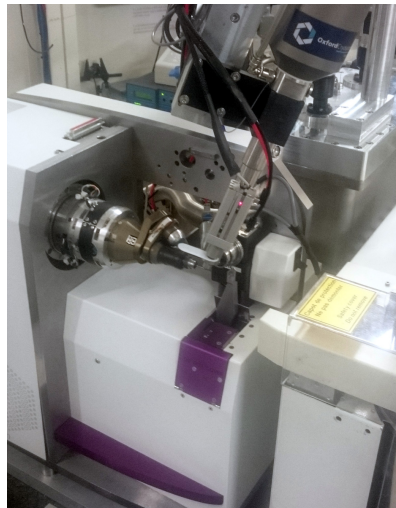
- installed in January 2017
- built-in scintillator
- mini-kappa



MASSIF-3 (ID30A-3)

MD2 diffractometer:

- installed in January 2017
- built-in scintillator
- mini-kappa
- option for fast mesh scans
- option for apertures $< 15 \mu\text{m}$
- option for in-plate screening
- option for faster omega rotation
- new microspec in development



Computing infrastructure news

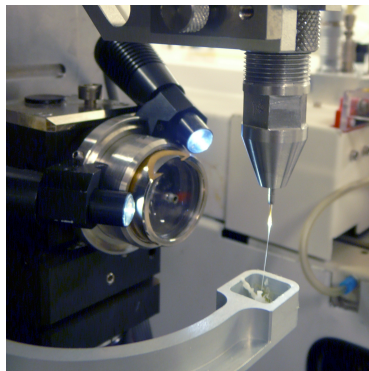
For all MX beamlines:

- new ESRF data storage system (GPFS)
- upgrade of MX computing cluster for autoprocesing
- upgrade of NX soft- and hardware for remote access

SSX on MASSIF-3: High Viscosity Extruder (HVE)

High Viscosity Extruder (HVE):

- injector filled with 30 μl synthetic grease
- mixed with 10% v/v protein crystal suspension ($\approx 0.3\text{mg}$ protein)



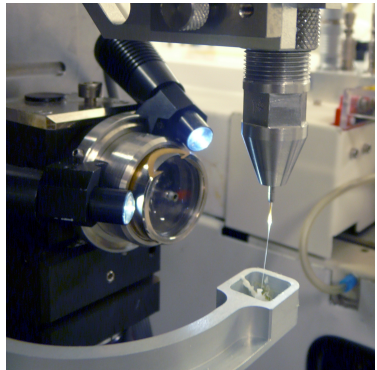
[Botha *et al.*, Acta Cryst. D71, 387 (2015)]

SSX on MASSIF-3: High Viscosity Extruder (HVE)

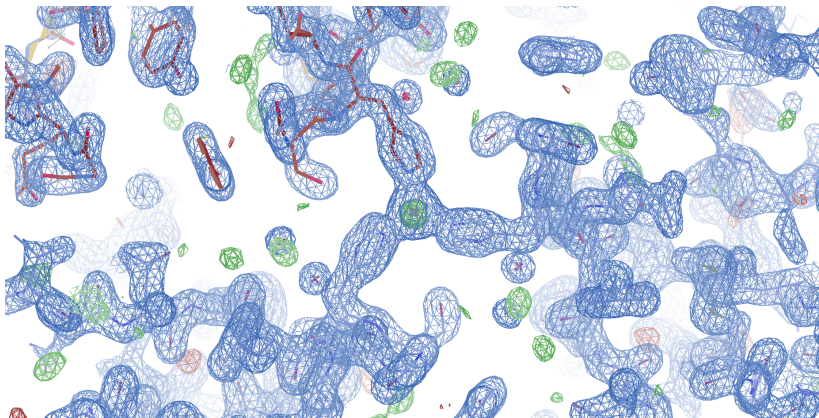
High Viscosity Extruder (HVE):

- injector filled with 30 μl synthetic grease
- mixed with 10% v/v protein crystal suspension ($\approx 0.3\text{mg}$ protein)
- runs for 30–120 min at 200–500 img/s
- 100% transmission
- about 7 kGy per crystal

[Botha *et al.*, Acta Cryst. D71, 387 (2015)]



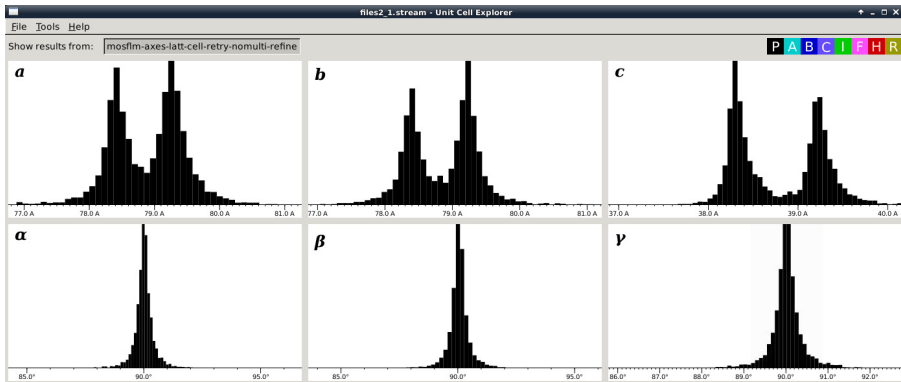
SSX example: insulin



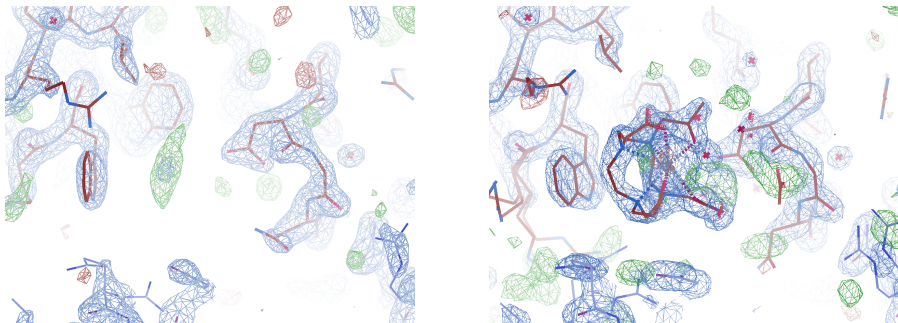
(crystal size: 4–8 μm)

SSX example: lysozyme soaked with gadolinium

Two crystal populations that could be separated into two datasets:



SSX example: lysozyme soaked with gadolinium



(crystal size: 20–25 μm)

SSX examples: data processing statistics

Processing with NanoPeakCell and CrystFEL:

	insulin	lysozyme	lysozyme+Gd
space group	<i>H3</i>	<i>P4₃2₁2</i>	<i>P4₃2₁2</i>
images/second	500	200	200
number of images	1 000 000	539 000	539 000
indexed patterns	37 462	20 683	47 482
resolution range [Å]	41.3– 1.6	56.0– 1.8	55.4– 1.8
completeness [%]	100.0 (100.0)	100.0 (100.0)	100.0 (100.0)
redundancy (low / high)	404 / 117	613 / 101	1093 / 175
R_{split} [%]	12.5 (41.6)	11.9 (62.9)	9.3 (52.2)
CC* [%]	99.4 (89.9)	99.1 (49.5)	99.5 (65.1)
SNR	6.2 (2.4)	7.2 (2.0)	8.2 (2.2)
R_{work} / R_{free}	14.9 / 19.9	17.5 / 19.8	14.7 / 19.3

SSX examples: data processing statistics

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If you have a suitable project with microcrystals and are interested in trying this HVE device, please let us know.

Acknowledgements

MPI Heidelberg:

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