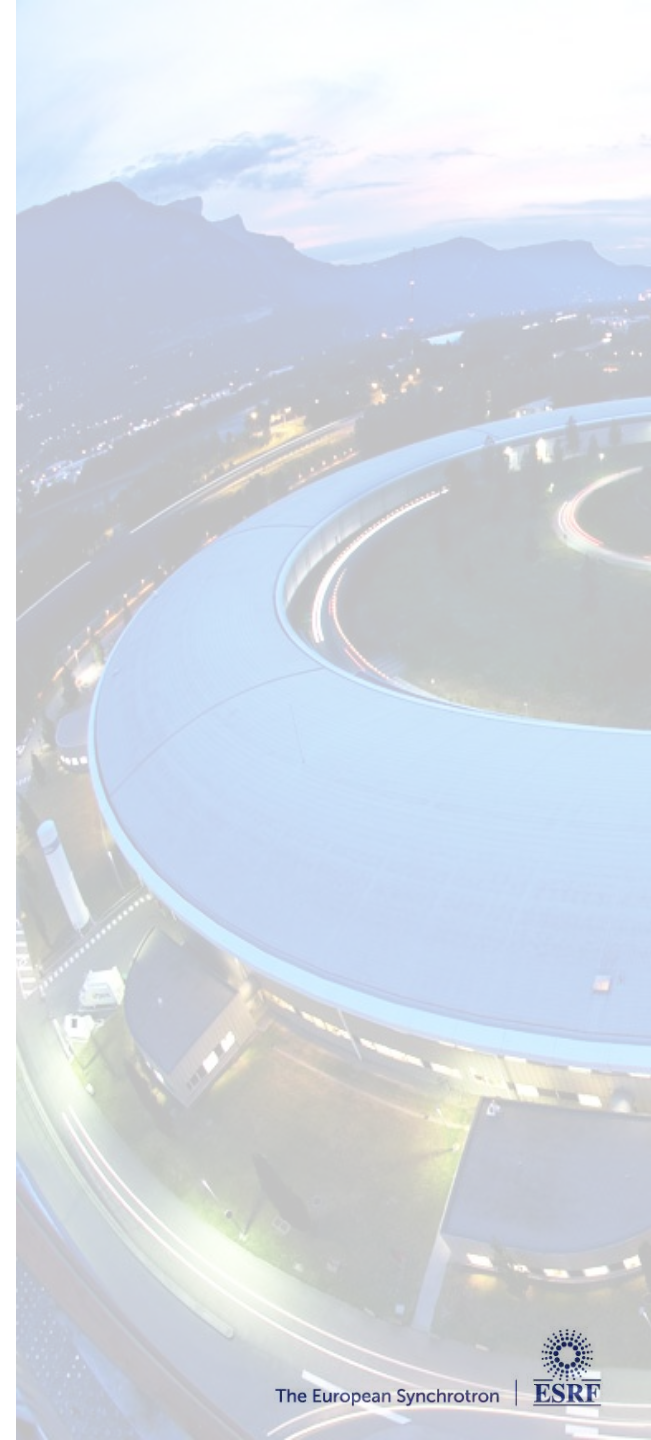




| The European Synchrotron

MXCuBE3 release, and deployment at ESRF

- **Review of main drivers**
- **Improving user experience**
- **MXCuBE on the web**
- **UI Overview**
- **Demo video(s)**



After almost **two and half years** of development and over 2800 commits

Sep 13, 2015 – Jan 19, 2018



Commits per day since 13 sept 2015

- Total of **16411 lines of code**
- With the joint effort of **a lot of people**
- We are finally **ready to deploy MXCuBE 3.0** (3.0.0-beta2) at ESRF

- Commissioning and deployment started on ID29 in December 2017 and MXCuBE3 is to be used for this run
 - *On top of BLISS deployed using Conda (talk by Matias Guijarro)*
- ID23-2 and ID30 A1 (MASSIF 1) will be installed next and the rest of the ESRF MX beamline will follow during the year



Current UI layout is at its limits

User feedback from interaction with users and usage questionnaire

New requirements on software as new instruments and methods are introduced

Software environment evolves

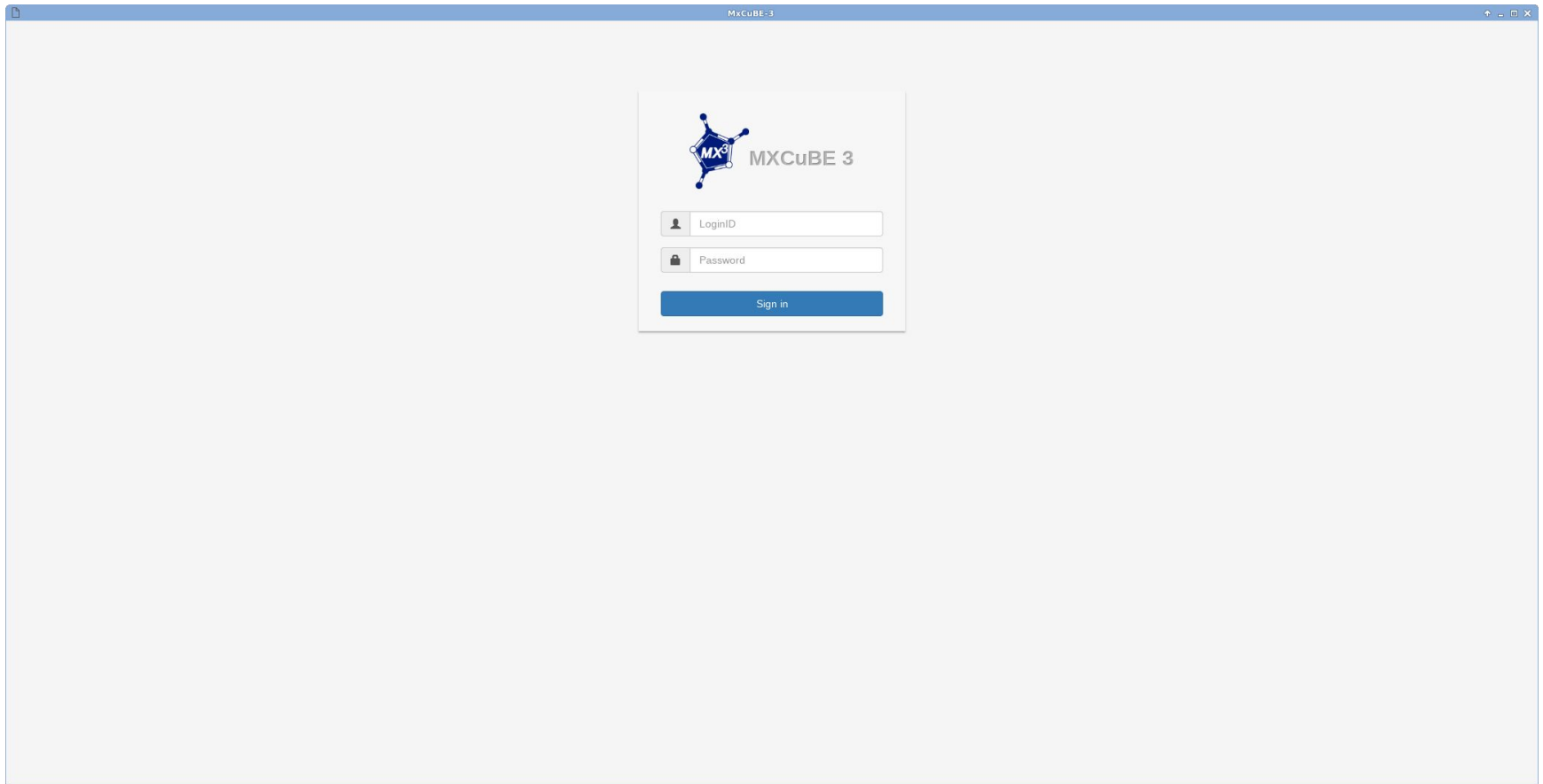
Improving UX

- Context based navigation, functionality / information available when user needs it
 - Guides user
 - Cleans up interface
- Attempt to simplify the main use cases with more intuitive sequence of actions
 - Easier for user to understand what's going on
- Managing information
 - Simplified queue
 - Search / filtering list of available samples
- Over all less clicks
 - Collect without need to actually save position and queue task
 - Keyboard and mouse shortcuts to position the sample
- ... and much more



New platform - MXCuBE as a web application

- Improved remote access feature (remote by design)
- Easier client install (Especially good for remote users)
- Accessibility provided by web technologies,
 - Window scaling, font size, color selection, screen readers
- New **architecture with REST interfaces**, true decoupling of UI and backend **makes it easier to adapt to changes and / or update UI.**
- Easier to achieve **seamless integration** with other web based services, **like ISPyB.**
- Brings MXCuBE into an **dynamic software development environment**, where we can **benefit from a large community of developers.**



- **Login view, perhaps in the future site customizable**
- **Possibility to login directly with proposal or user with one or several proposals**
 - Proposal selection developed by MAX IV (Talk by Fredrik Bolmsten)

MXCuBE 3 - Sample Video with video controls

MXCuBE 3 Proposal: 291

Sample Overview Data collection Sample Changer System log

Beamline Actions

Energy: 11.5627 keV Resolution: 4.000 Å Transmission: 50.104 % Cryo: 0
Wavelength: 1.0723 Å Detector: 754.569 mm Flux: 0

Beamstop OUT Fast Shutter CLOSED Safety Shutter --- Ring Current

Aperture Control: 30

Omega: 164.34 10°
Kappa: 0.00 0.1°
Phi: 0.00 0.1°
Y: -0.486 0.1 mm
Z: -0.145 0.1 mm
Focus: -0.000 0.05 mm
Samp-X: 0.453 0.1 mm
Samp-Y: 0.287 0.1 mm

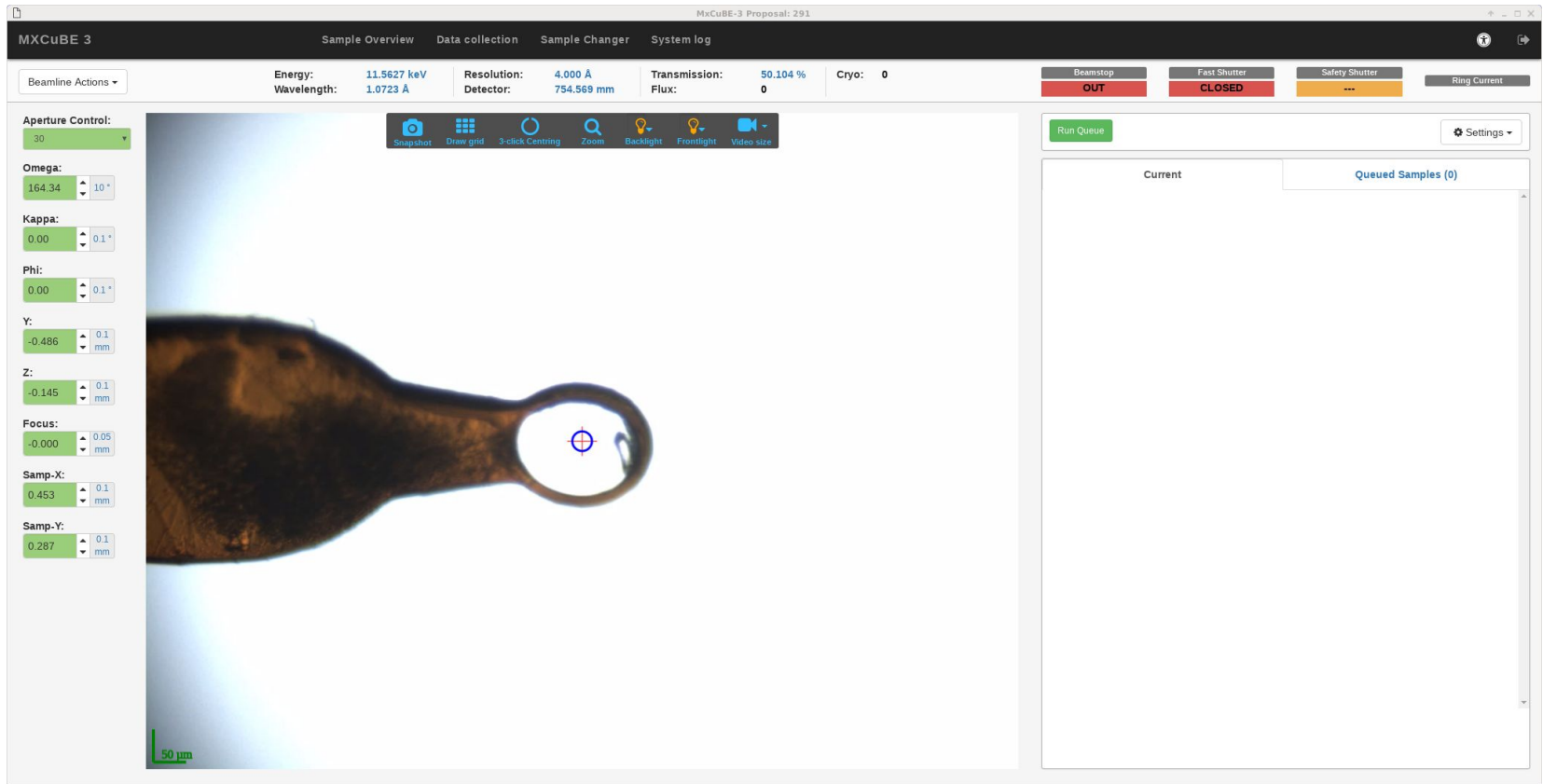
Run Queue

Current Queued Samples (0)

50 μm

- Data collection view

MXCuBE 3 - Sample Video with video controls



Pro tip, use

Shift + **DBL Click**: Move to beam

Z + **Mouse wheel**: microscope zoom

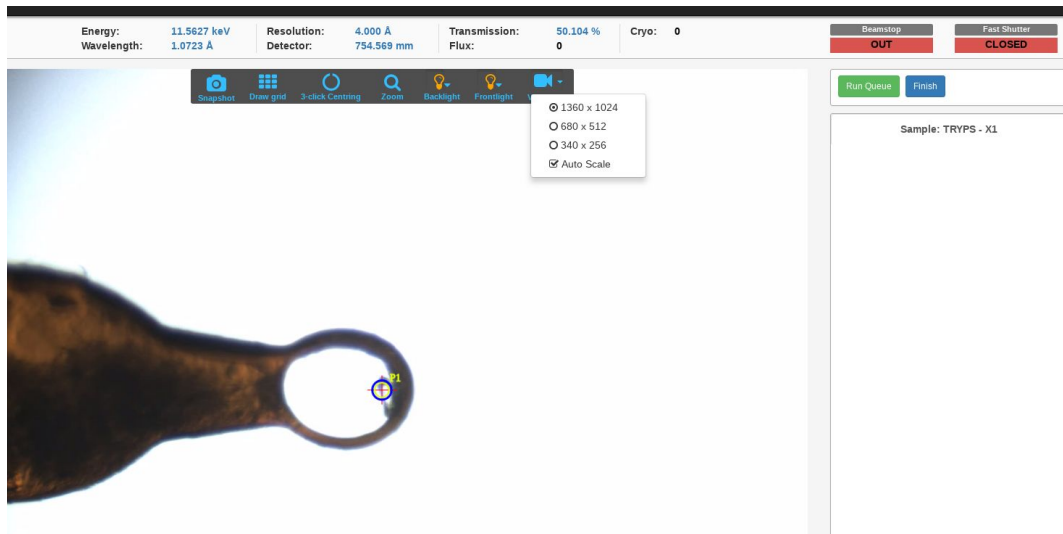
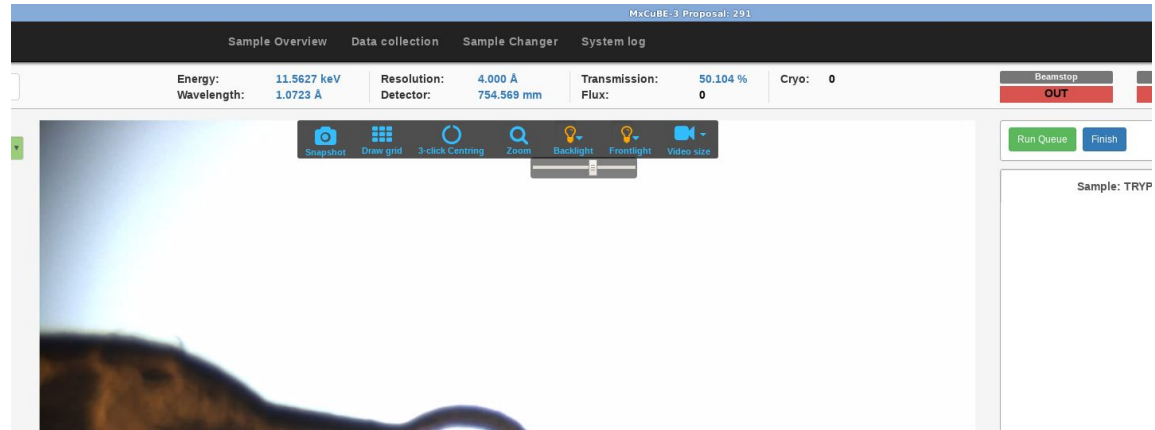
r + **Mouse wheel**: Rotate sample

f + **Mouse wheel**: microscope focus

Or, simply motor controls (located to the left)

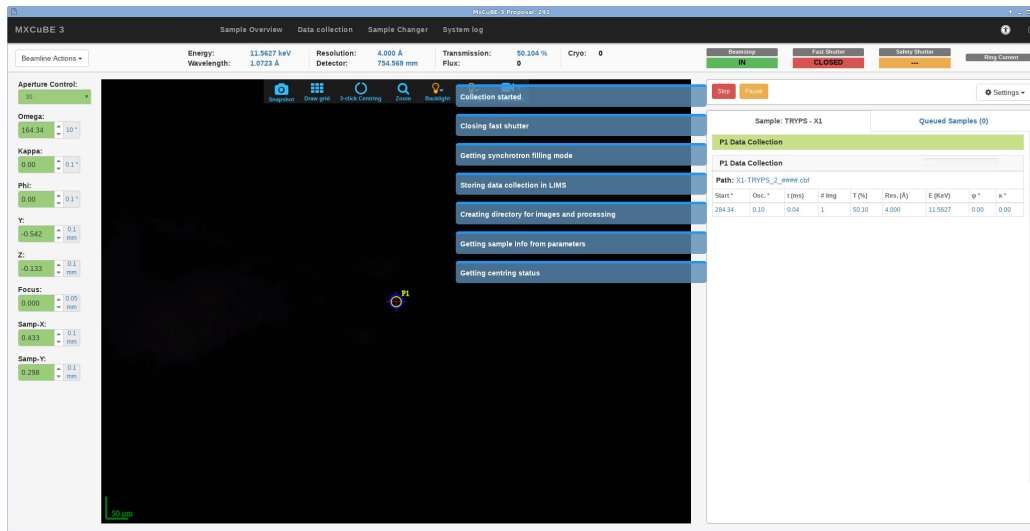
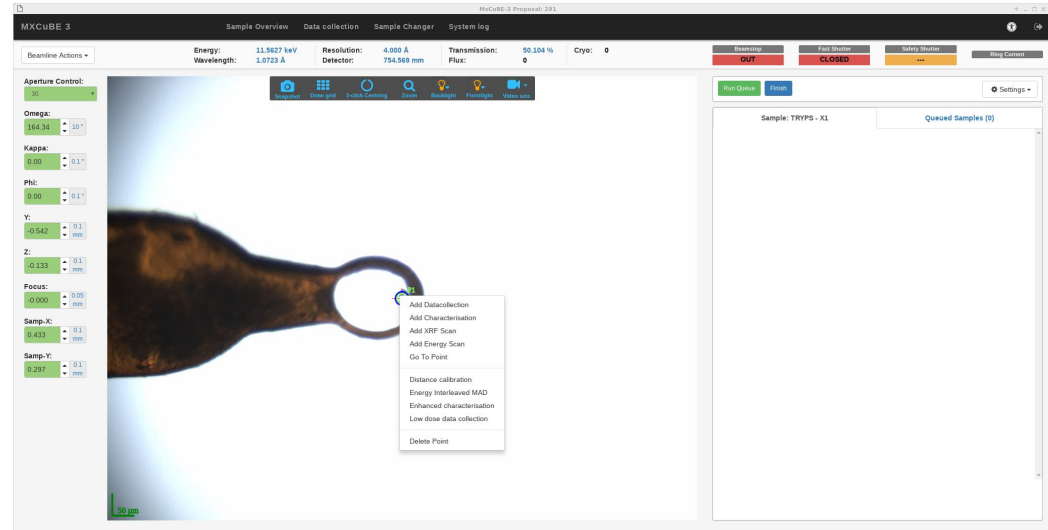
Microscope / video controls:

- Light and zoom intensity changed by slider

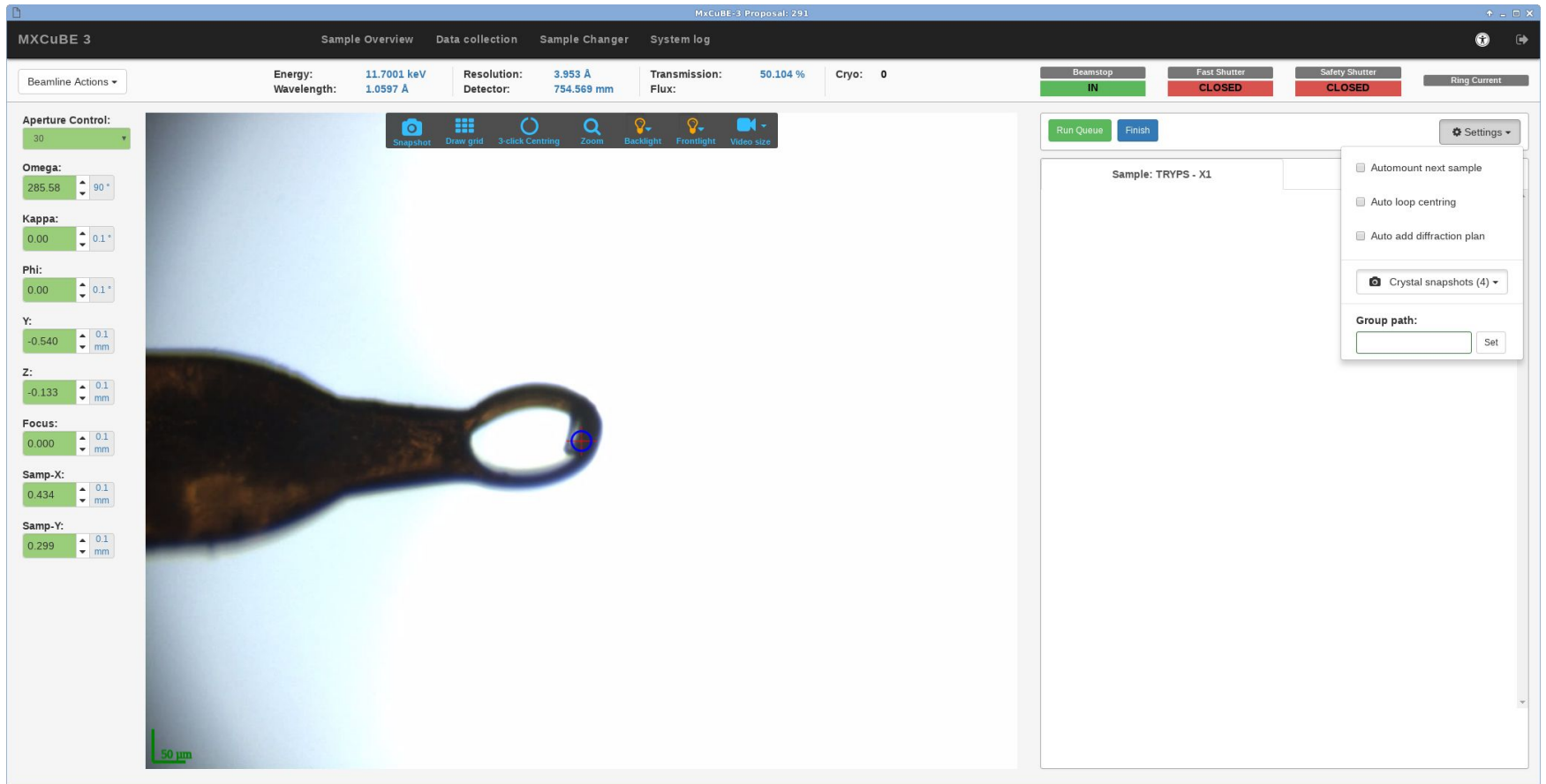


- Video is streamed as MPEG-1, perhaps adaptive MPEG-4 in the future
- Possibility to select video stream size (particularly useful for remote users)
- With auto scale option
- Perhaps possibility so select compression ratio

- Right click context menu to add tasks



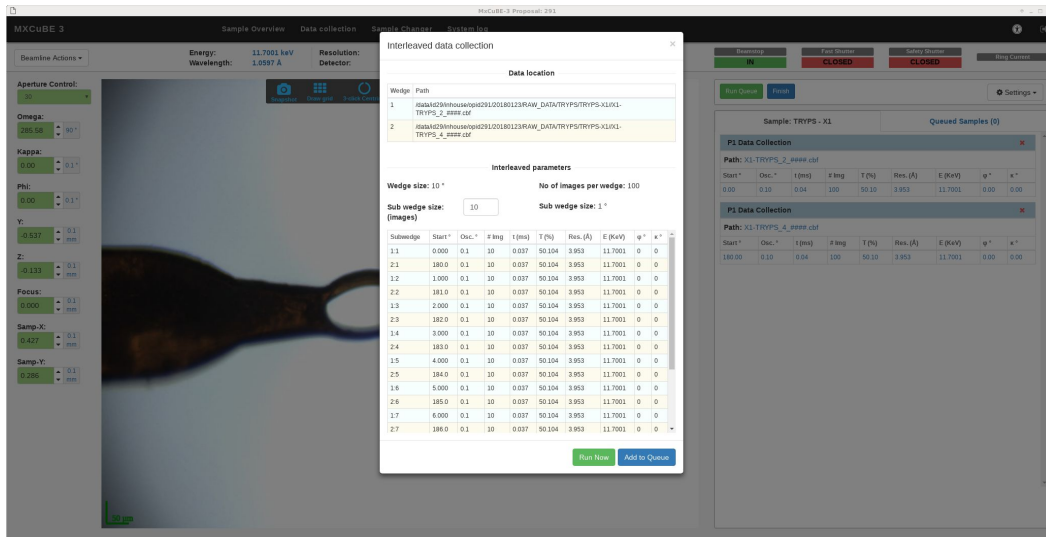
- Messages shown next to the queue during execution



Automatic execution is achieved by:

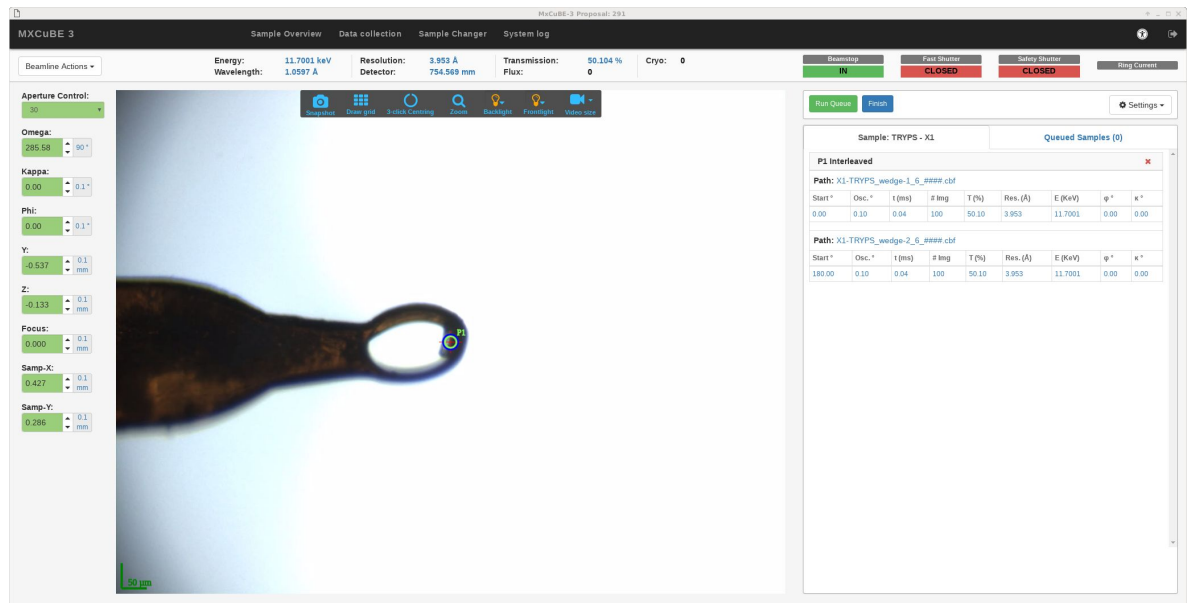
- “Automount next”, “Autoloop centring” and “Auto add diffraction plan”.
- The user no longer select Full/Semi automatic mode for the queue

Interleaved data collection



- Now possible to **interleave n data collections**.
- Also possible to **interleave any parameter** like energy, kappa omega, resolution ...
- In the future **pie chart like display**, potentially with the possibility to **change subwedge order**

- The two principal wedges to be collected are shown in the task



Energy scan

MXCuBE 3

Sample Overview Data collection Sample Changer System log

Beamline Actions

Energy: 11.7001 keV Resolution: 3.953 Å Transmission: 50.104 % Cryo: 0
Wavelength: 1.0597 Å Detector: 754.569 mm Flux: 0

Beamstop IN Fast Shutter CLOSED Safety Shutter CLOSED Ring Current

Aperture Control: 75

Omega: 285.58 90°
Kappa: 0.00 0.1°
Phi: 0.00 0.1°
Y: -0.537 0.1 mm
Z: -0.133 0.1 mm
Focus: 0.000 0.1 mm
Samp-X: 0.427 0.1 mm
Samp-Y: 0.286 0.1 mm

Vertical Spacing: 0 Horizontal Spacing: 0 Overlay: [slider]

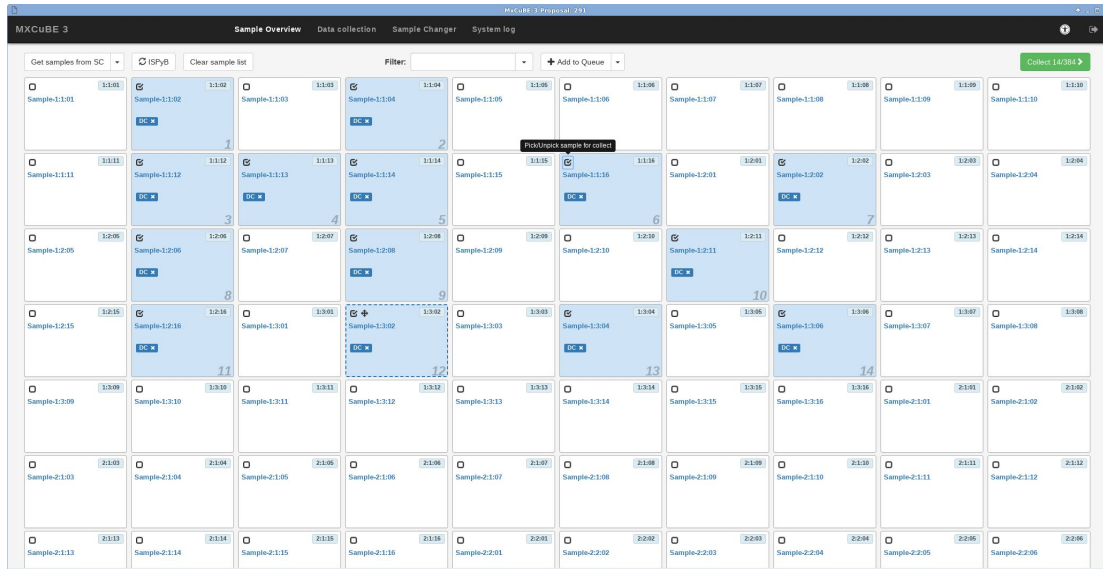
Grid cells: 1-81 (8x9 grid)

Context menu options:
Centring Point on cell
Mesh and collect
Mesh and collect from file
WF Mesh Scan
X-ray Centring
Delete

Sample: TRYP5 - X1 Queued Samples (0)

- Mesh interface similar to MXCuBE 2
- Possibility to change transparency of grid
- Also possible to add centring point to cell

Sample Grid

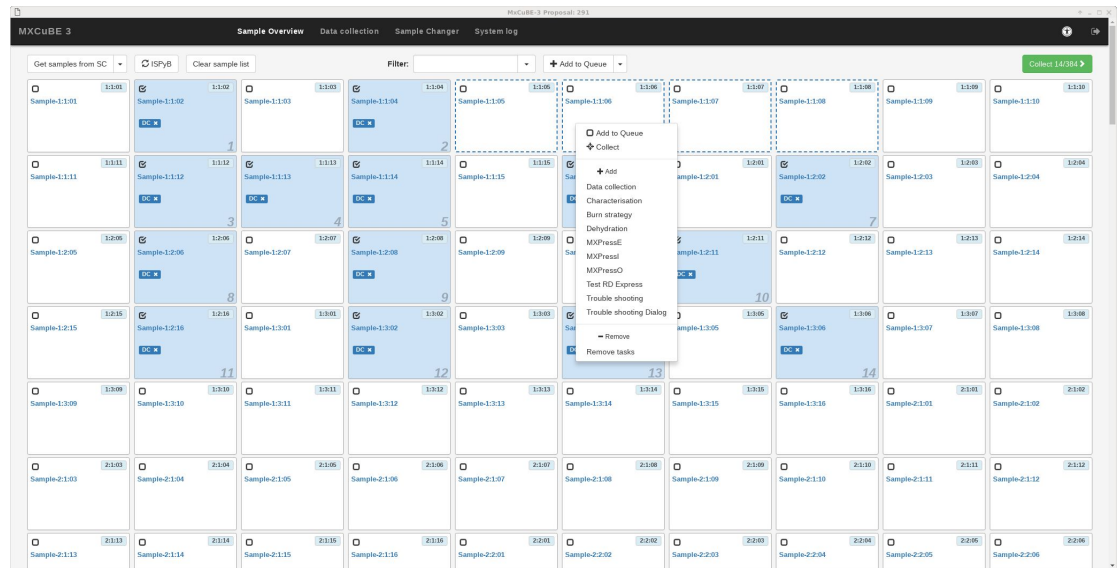


Sample grid contains available samples

- Synch with lims
- Filtering
- Results view
- Tasks to be executed

Sample grid context menu

- Preparing for automated execution by selecting multiple samples
- Use context menu to add tasks



Remaining features for 3.0:

- Remote access chat
- Remote access give away control

Project page: <https://github.com/mxcube/mxcube3>

Docker images: <https://hub.docker.com/u/oscarsson/>

Questions ?



Thanks to everybody involved in the project, especially staff from MAX IV and ESRF
(Picture from last MXCuBE ISPyB meeting at Soleil)