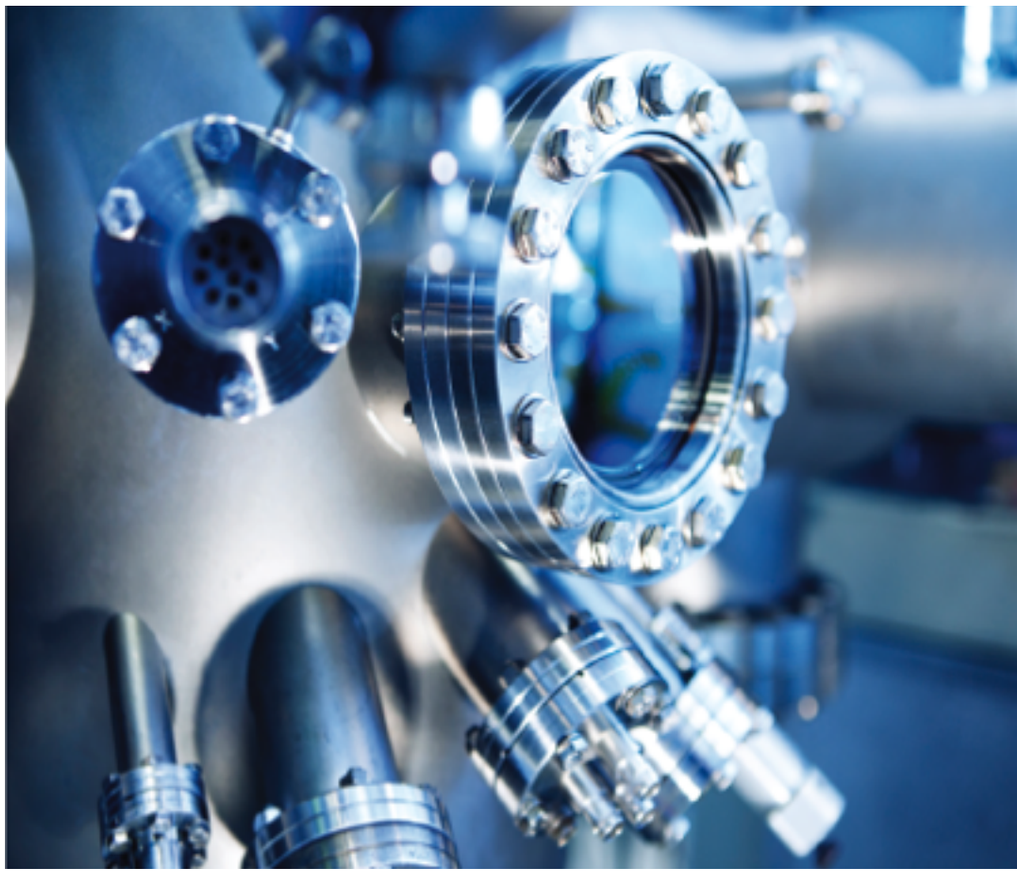
MXCuBE 3: status, ongoing developments and milestones

Mikel Eguiraun - mikel.eguiraun@maxiv.lu.se

Outline

- Project status update
- User interface updates
- Demo video
- Next steps



MXCuBE 3: looking back

- Kickoff in October 2015

January 2016
Core packages

March 2016
MD3

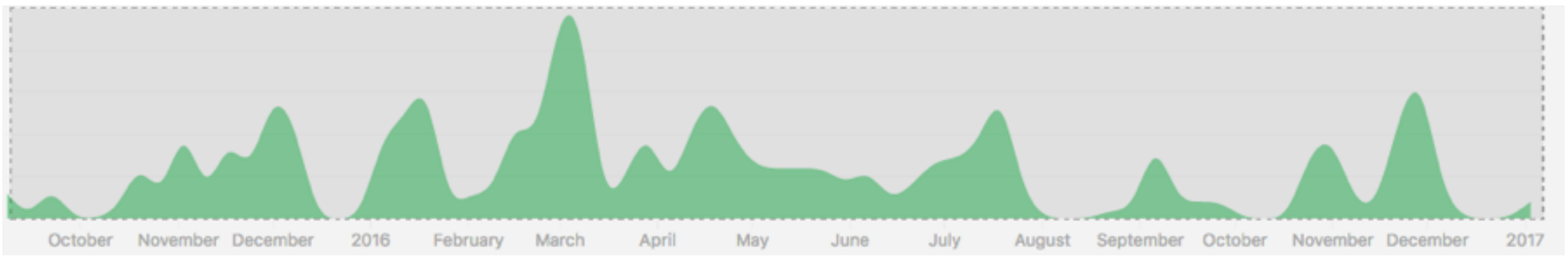
June 2016
First Data Collection

October 2016
MAD experiment
Sample Changer
Characterisation
ISPYB

December 2016
Energy Scan
XRF Scan

MXCuBE 3: Current status

- Under development but first data collection during Biomax commissioning (June 2016, MAX IV)
- MAXIV in production usage (real users … watching over our shoulders)
- ESRF testing routinely in several beamlines
- 297 PRs accepted
- 38 open issues | 104 closed
- Active development and less bugs than ever!
- bi-weekly Skype meetings + face2face meetings ~3 months

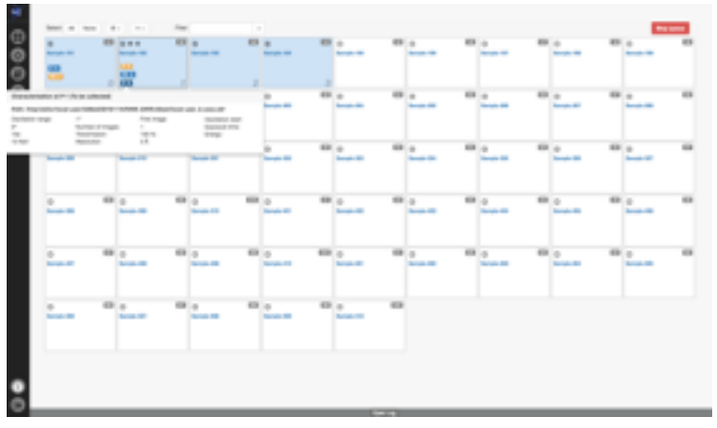


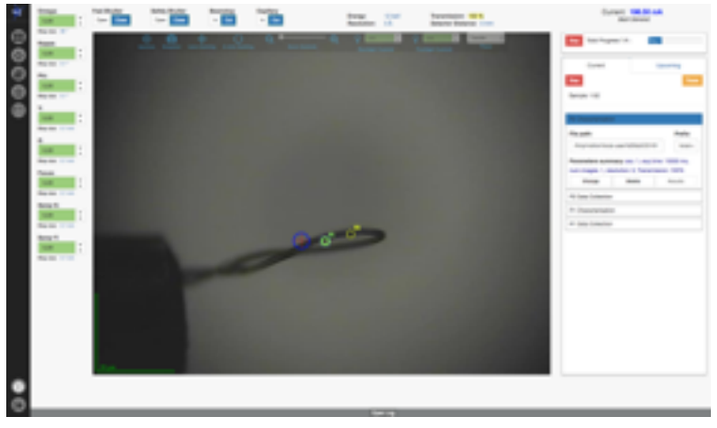
MXCuBE 3: Current status

- Sample imaging and operation
- Experiment queue configuration and execution
- Basic data collection strategies
  - standard dc, characterisation, helical
- Master-slave remote operation (hype for Marcus)
- LIMS integration
- Basic sample changer integration
- But also:
  - application architecture refined
  - usability improvements everywhere
  - debugging, performance improvements, compatibility, testing, refactoring, robustness, etc.

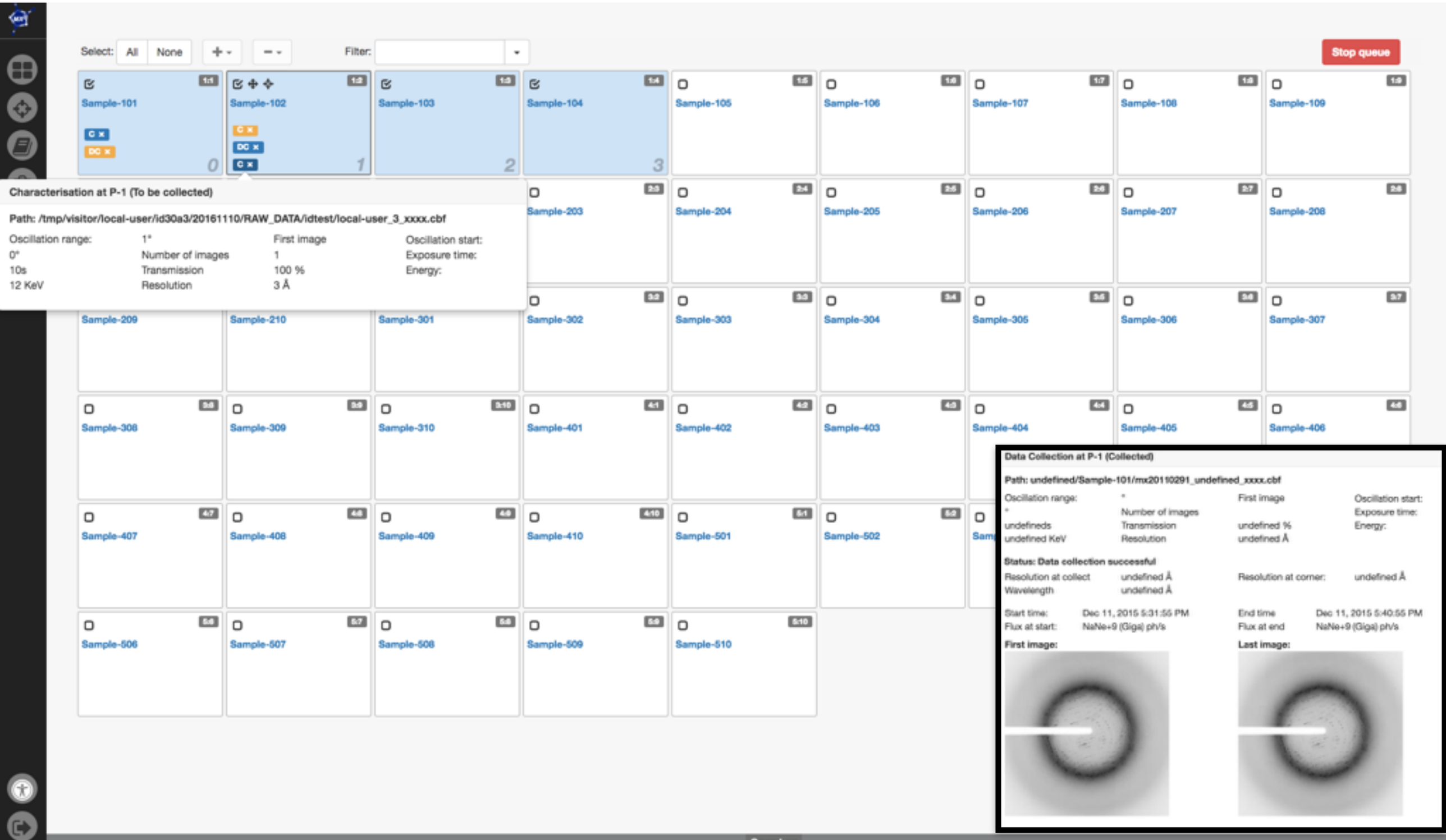
User Interface

- Two main operation modes:
  - Automatic:
    - multiple sample selection and configuration
    - Workflows
  - Manual:
    - sample by sample
    - manual operation and configuration

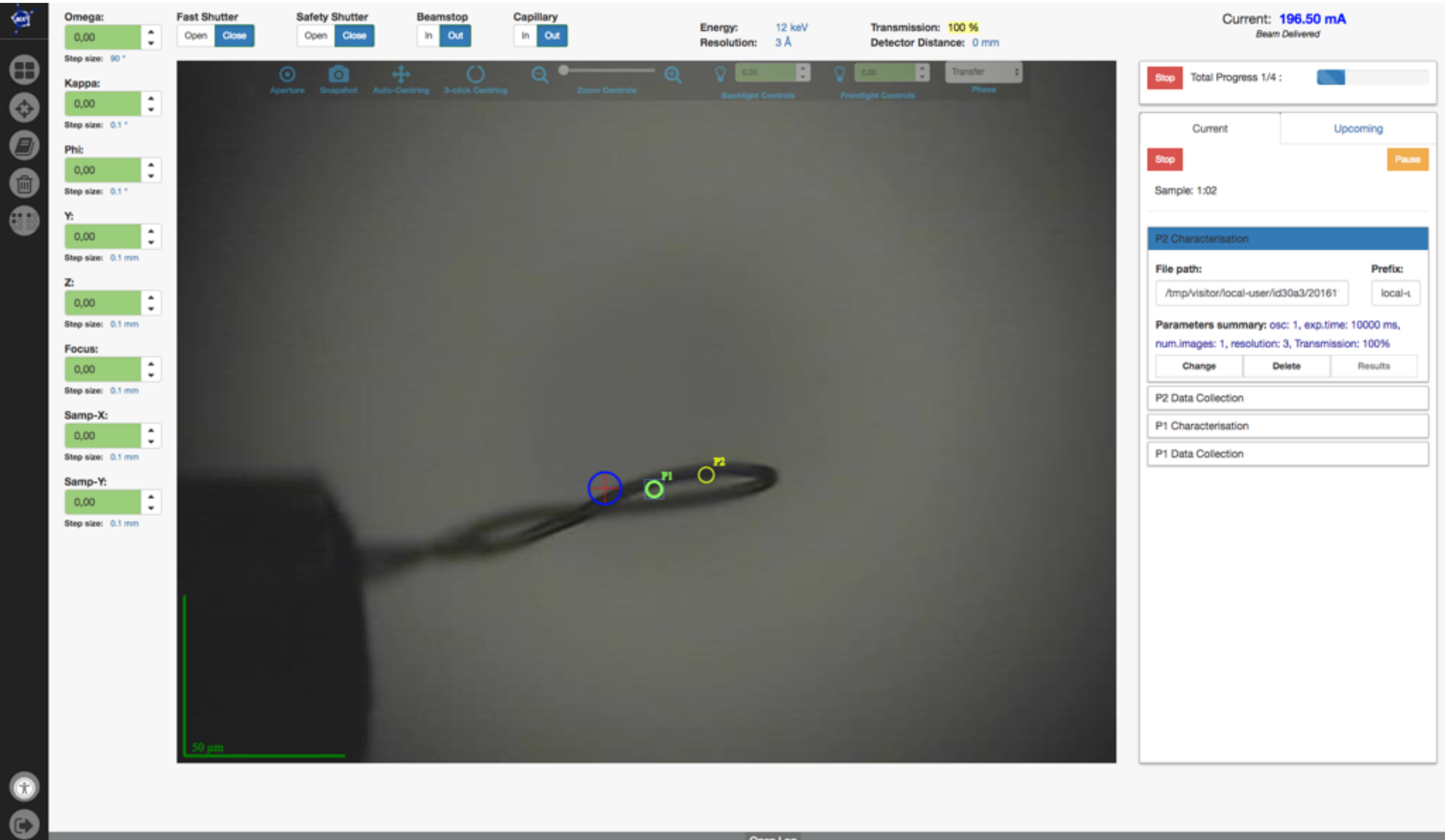




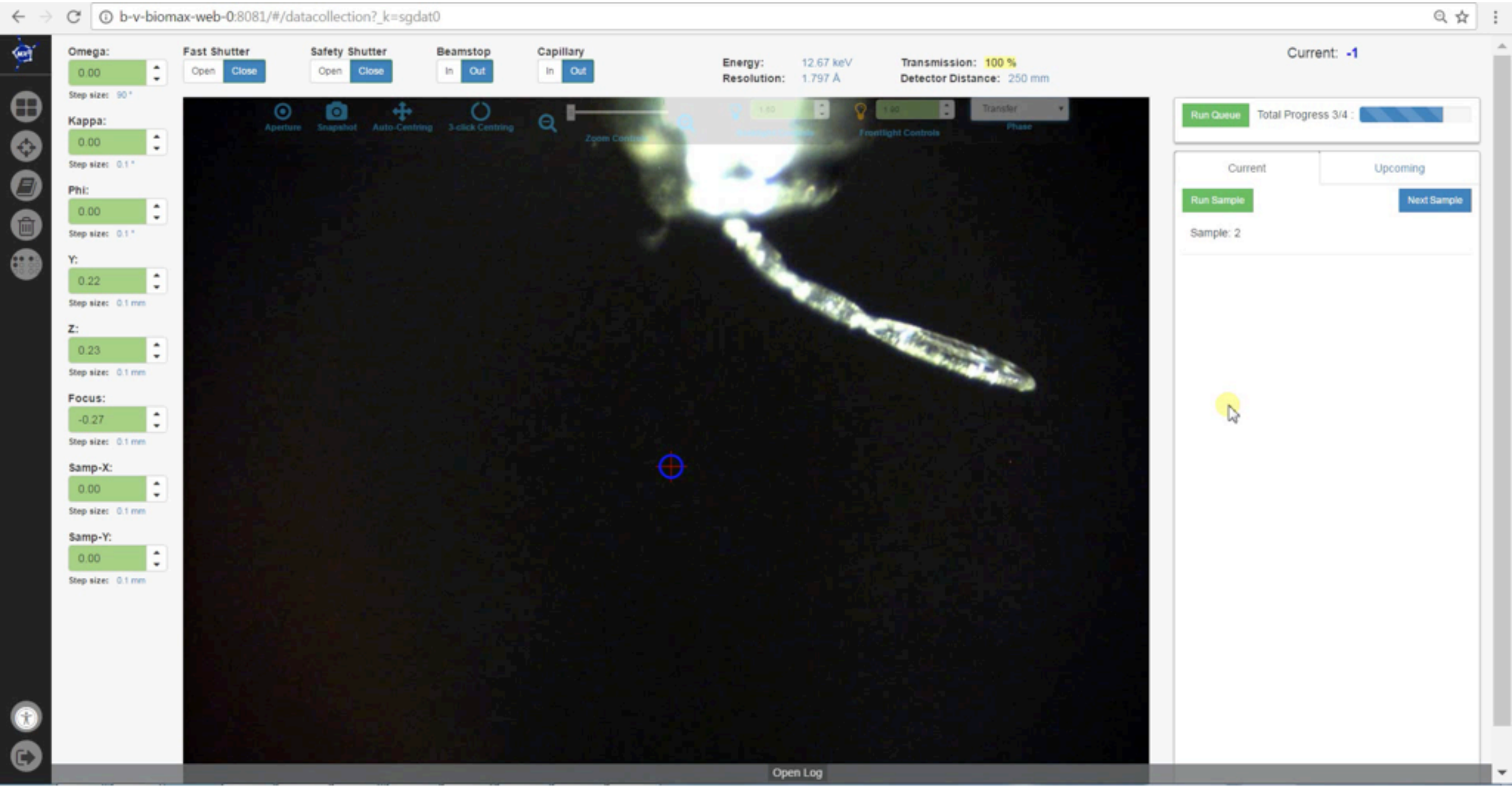
Samples


Select: All None
Filter:
Stop queue
Sample-101
Sample-102
Sample-103
Sample-104
Sample-105
Sample-106
Sample-107
Sample-108
Sample-109
Characterisation at P-1 (To be collected)
Path: /tmp/visitor/local-user/id30a3/20161110/RAW_DATA/idtest/local-user_3_xxxx.cbf
Oscillation range: 1°
First image
Oscillation start: 0°
Number of images 1
Exposure time: 10s
Transmission 100 %
Energy: 12 KeV
Resolution 3 Å
Sample-203
Sample-204
Sample-205
Sample-206
Sample-207
Sample-208
Sample-209
Sample-210
Sample-301
Sample-302
Sample-303
Sample-304
Sample-305
Sample-306
Sample-307
Sample-308
Sample-309
Sample-310
Sample-401
Sample-402
Sample-403
Sample-404
Sample-405
Sample-406
Sample-407
Sample-408
Sample-409
Sample-410
Sample-501
Sample-502
Sample-506
Sample-507
Sample-508
Sample-509
Sample-510
Data Collection at P-1 (Collected)
Path: undefined/Sample-101/mx20110291_undefined_xxxx.cbf
Oscillation range: °
First image
Oscillation start: °
Number of images
Exposure time: undefineds
Transmission undefined %
Energy: undefined KeV
Resolution undefined Å
Status: Data collection successful
Resolution at collect undefined Å
Resolution at corner: undefined Å
Wavelength undefined Å
Start time: Dec 11, 2015 5:31:55 PM
End time Dec 11, 2015 5:40:55 PM
Flux at start: NaNe+9 (Giga) ph/s
Flux at end NaNe+9 (Giga) ph/s
First image:
Last image:

Data Collection



Demo video


b-v-biomax-web-0:8081/#/datacollection?_k=sgdat0
Omega:
0.00
Step size: 90 °
Kappa:
0.00
Step size: 0.1 °
Phi:
0.00
Step size: 0.1 °
Y:
0.22
Step size: 0.1 mm
Z:
0.23
Step size: 0.1 mm
Focus:
-0.27
Step size: 0.1 mm
Samp-X:
0.00
Step size: 0.1 mm
Samp-Y:
0.00
Step size: 0.1 mm
Fast Shutter
Open
Close
Safety Shutter
Open
Close
Beamstop
In
Out
Capillary
In
Out
Energy: 12.67 keV
Resolution: 1.797 Å
Transmission: 100 %
Detector Distance: 250 mm
Current: -1
Aperture
Snapshot
Auto-Centring
3-click Centring
Zoom Control
Frontlight Controls
Transfer
Phase
Run Queue
Total Progress 3/4 :
Current
Upcoming
Run Sample
Next Sample
Sample: 2
Open Log

Looking ahead

- Next milestone: March 2017

March 2017

Manual data collection ready for users

Beamline specifics

Synchrotron specifics

Sample changer page for advanced controls

Update Samples View

Mesh scan

Energy Scan and XRF

Looking ahead

- Next milestone: March 2017
  - Workflow
  - Display characterisation results
  - Polish the interface (icons, buttons, minimal layout changes, joystick)
  - Clarify the relationship and data sharing between Samples and DataCollection view (simplify usage)
  - Debugging

MXCuBE3 People

MAX IV: M. Eguiraun, A. Milan-Otero, J. Nan, F. Bolmsten, M. Thunnissen
ESRF: M. Guijarro, M. Oskarsson, A. Beteva, D. de Sanctis

Supported by:

MXCuBE collaboration
MAX IV MX and KITS teams
ESRF BCU and SB teams

Thanks for your attention!