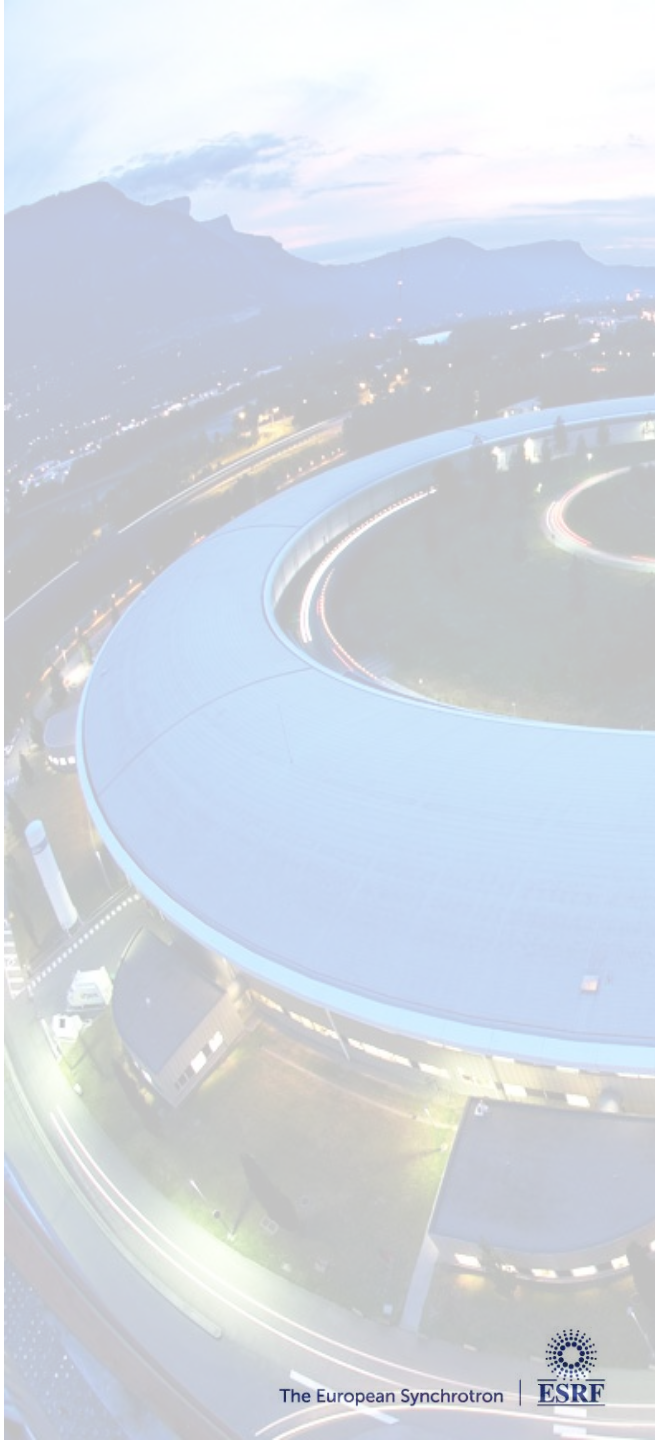
The European Synchrotron

Outline

- News from the developers committee
- Feature review
- MXCUBE at ESRF



Marcus Oskarsson (marcus.oscarsson@esrf.fr)

[DEV]

On behalf of the developers committee

Marcus Oskarsson (marcus.oscarsson@esrf.fr)

News from the developers committee

- **As always monthly meetings - minutes can be found at**
  https://mxcube.github.io/mxcube/doc/developers_meetings/index.html

  From last MXCuBE meeting discussions on: Configuration - XML to YAML conversion, web-security and deployment, new queue features, unattended data collections

- **Code camp on mxcubecore and mxcubeweb development with an introduction to Javascript and React development - October 2023**

  Talks and minutes available on:
  https://mxcube.github.io/mxcube/doc/developers_meetings/index.html

- **Code camp on documentation - March 2024**
  Very nice collaborative effort resulting in:
  https://mxcubeweb.readthedocs.io
  https://mxcubecore.readthedocs.io

  Still in progress and a continuous process !

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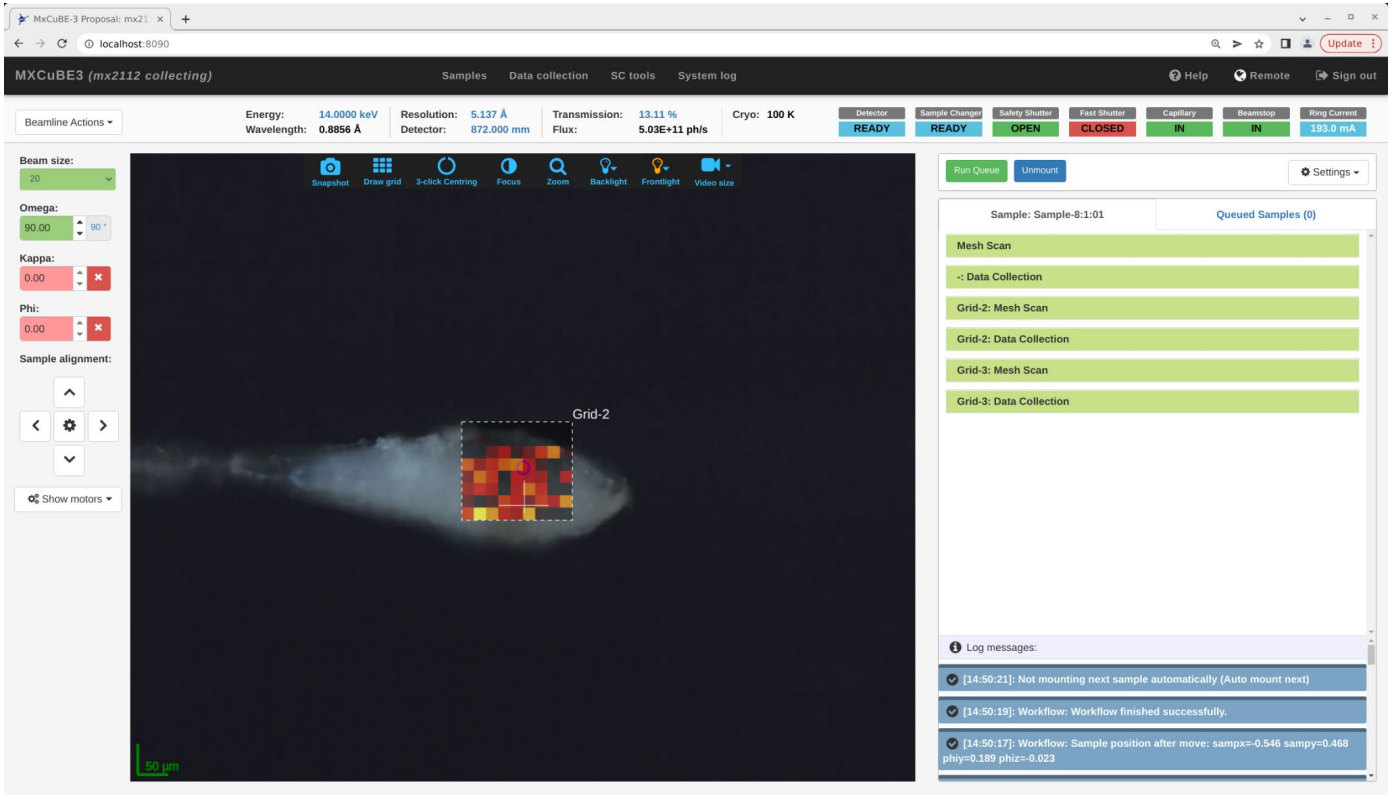
Feature review



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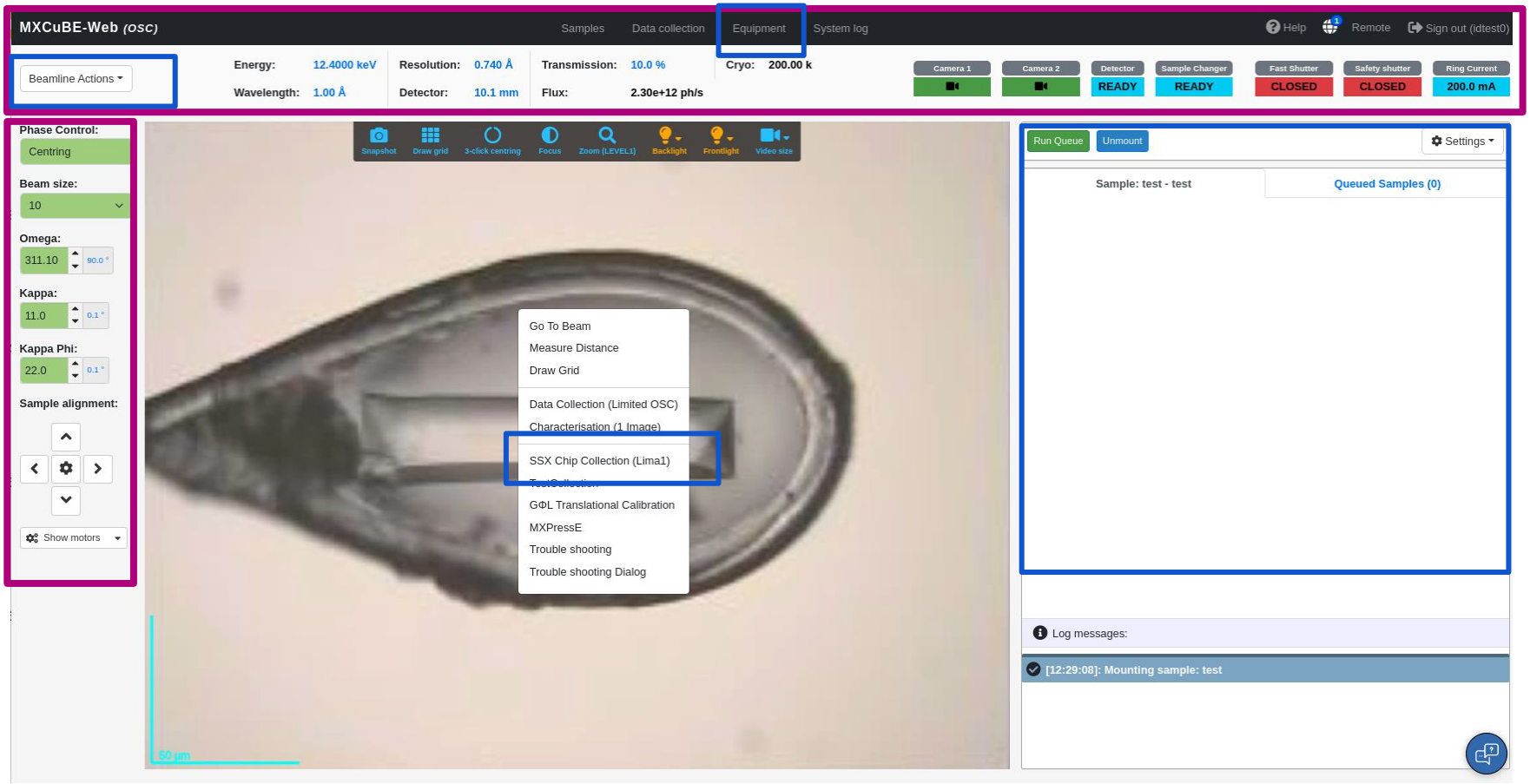
Feature review

Same principle interface on all sites

To a certain extent configurable instrumentation control, procedures / methods



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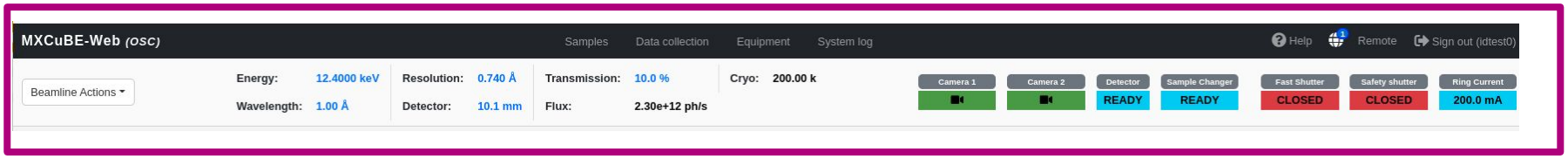
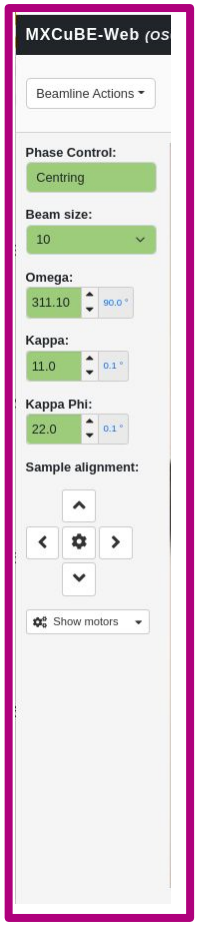
Feature review





The display of available instrumentation is configurable in ui.yaml

To the left motor control and on the top “beamline setup”

```yaml
sample_view:
  id: sample_view
  components:
    -
      label: Omega
      attribute: diffractometer.phi
      role: omega
      step: 90
      precision: 2
      suffix: °
    -
      label: Kappa
      attribute: diffractometer.kappa
      role: kappa
      step: 0.1
      precision: 1
      suffix: "°"
```

```yaml
beamline_setup:
  id: beamline_setup
  components:
    -
      label: Beamstop
      attribute: beamstop
    -
      label: Capillary
      attribute: capillary
    -
      label: Fast Shutter
      attribute: fast_shutter
    -
      label: Safety shutter
      attribute: safety_shutter
    -
      label: Detector
      attribute: detector
    -
      label: Energy
      attribute: energy
      step: 0.001
      precision: 4
      suffix: keV
```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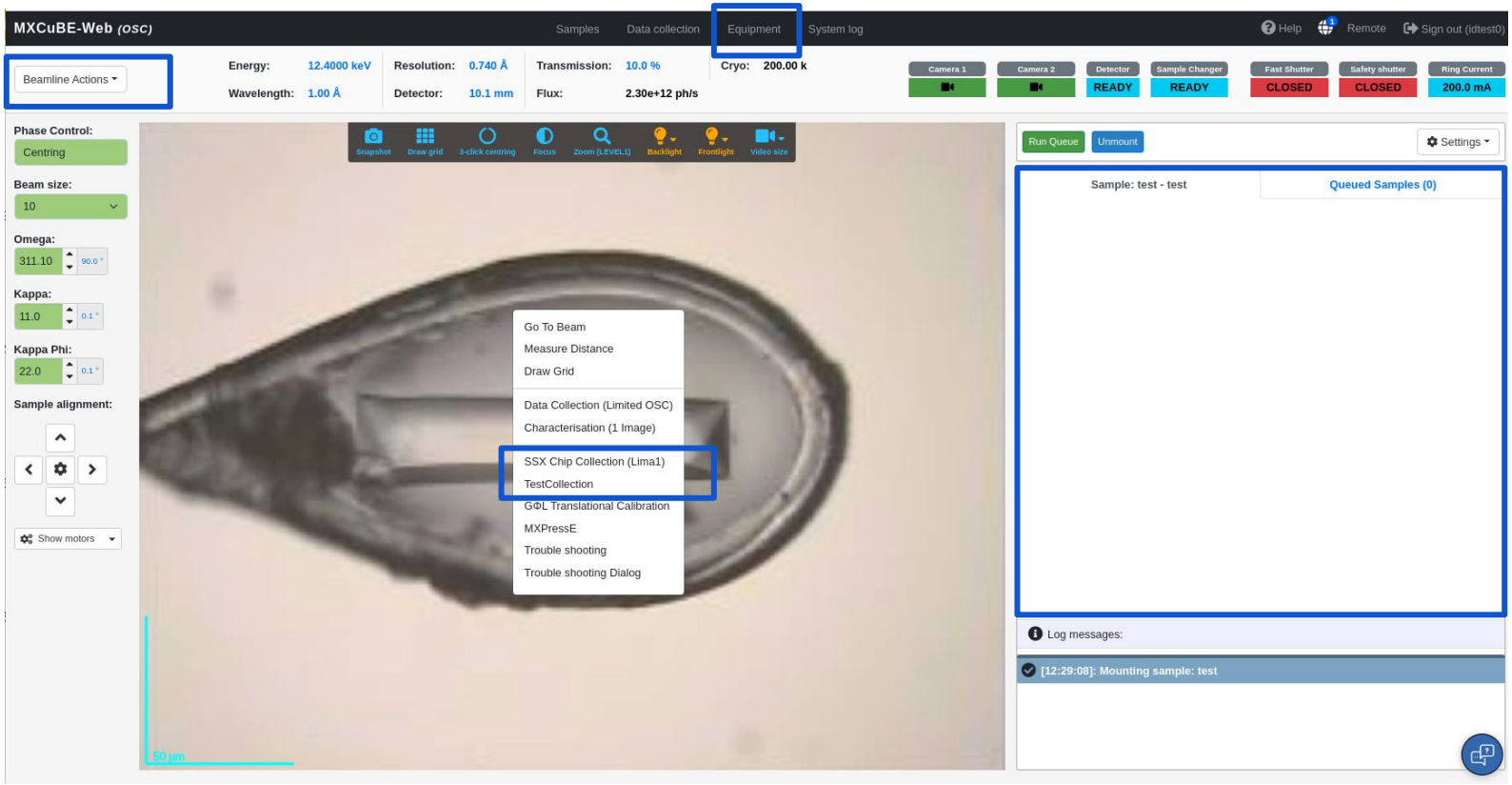
Feature review



- Equipment view - For not so often used or temporary instrumentation commands
- Beamline action - For procedures that are frequently used and involves more than a simple command
- Queue entry / task - For collecting data

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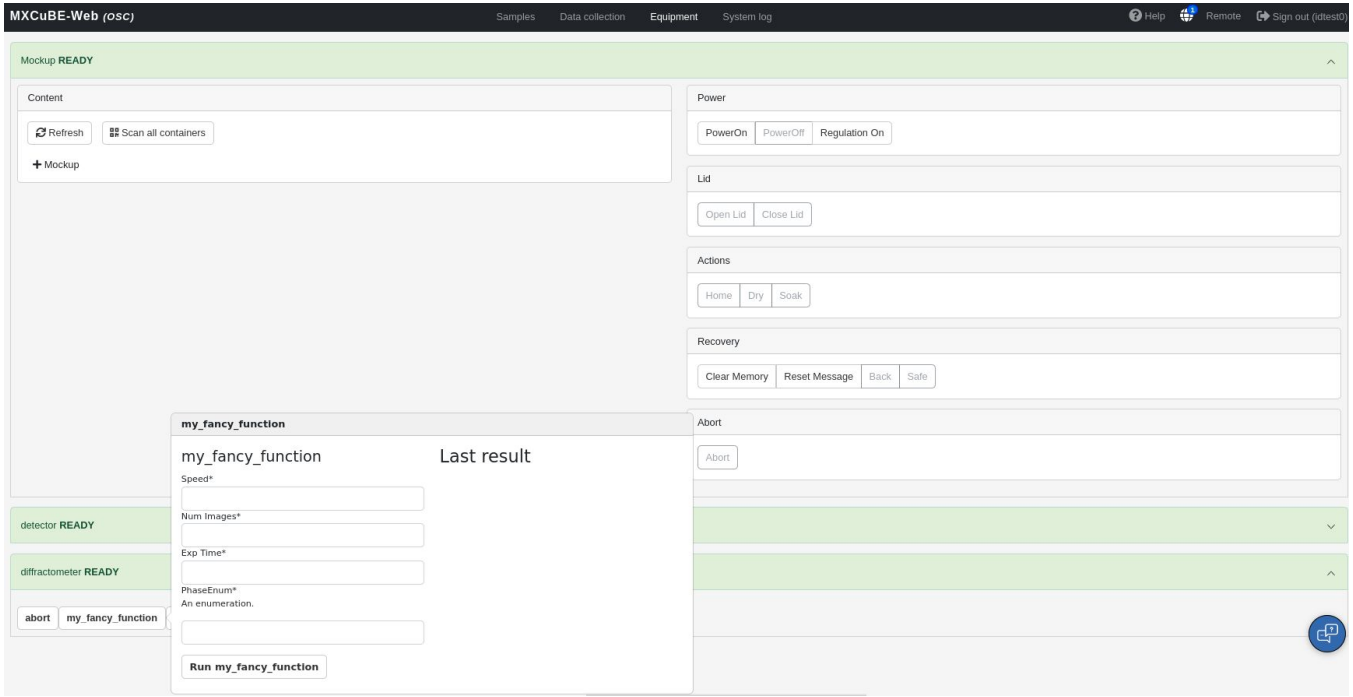
Feature review

Equipment view - For less often or temporary instrumentation commands

- For convenience, maintenance and workarounds
- Automatic simple test/maintenance UI for type hinted and “exported” (in .xml file)
- Possible via typehints



Methods are automatically added if they are “exported” with the export tag and the method is type hinted (at least with a return type)

```
<exports>["abort", "status", "my_fancy_function", "my_other_funny_function"]</exports>
```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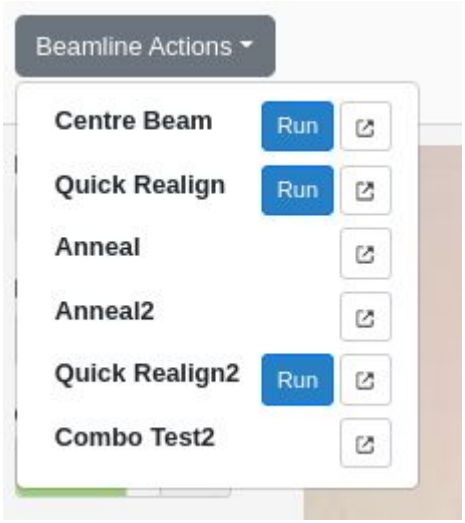
Feature review

Beamline action - For procedures that are frequently used and involves more than a simple command

Configured as the beamline_actions of the Beamline hardware object




```
<object class="BeamlineActionsMock
    <commands>[
      {"type": "controller", "name": "Centre Beam", "command": "HardwareObjects.m
      {"type": "controller", "name": "Quick Realign", "command": "HardwareObjects
      {"type": "controller", "name": "Anneal", "command": "HardwareObjects.mockup
      {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMoc
      {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMoc
      {"type": "annotated", "command": "HardwareObjects.mockup.BeamlineActionsMoc
    ]
    </commands>
</object>
```

The controller commands define the command arguments programmatically via the CommandObject.add_argument method

The annotated command uses the method typehints and Pydantic models to define the arguments

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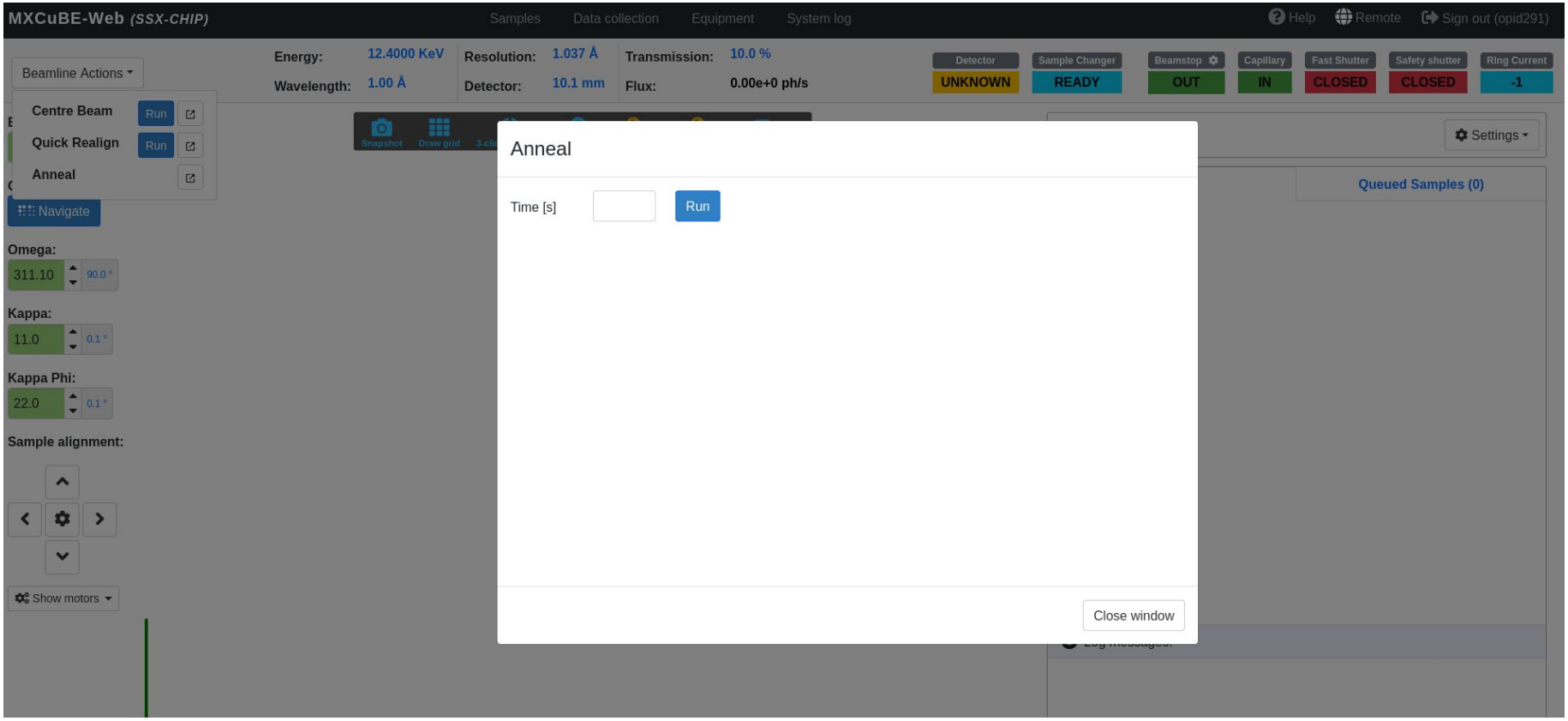
Beamline actions

Example beamline action - anneal dialog



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Feature review

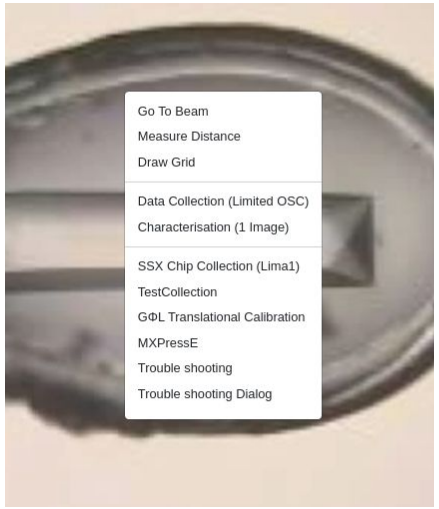
Queue entry / task - For collecting data

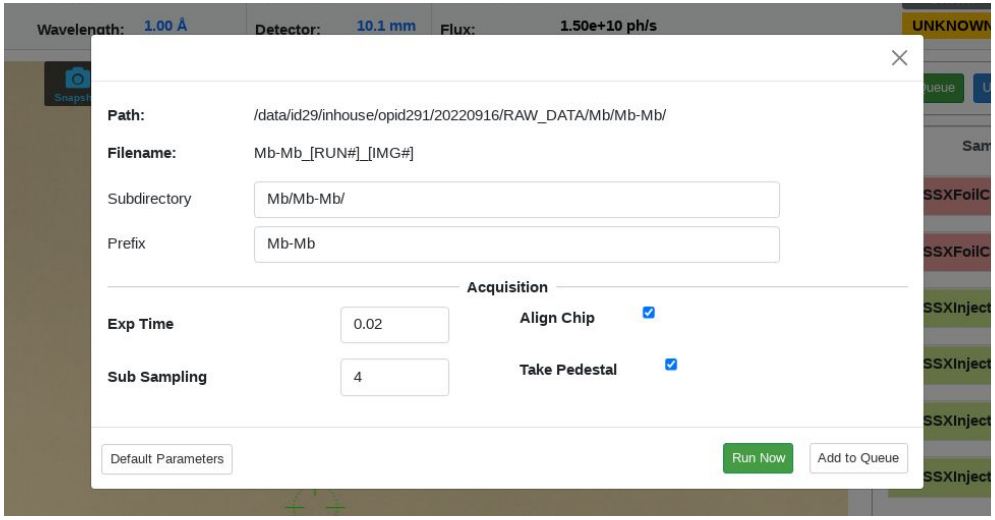
Write a task that takes a PyDantic model and add it to available_methods of Beamline object

```
82      legacy_parameters: LegacyParameters
83
84
85  class SsxChipCollectionQueueEntry(BaseQueueEntry):
86      """
87      Defines the behaviour of a data collection.
88      """
89      DATA_MODEL = SsxChipColletionTaskParameters
90      NAME = "SSXChipCollection"
91      REQUIRES = ["point", "line", "no_shape", "chip", "mesh"]
92
93      # New style queue entry does not take view argument,
94      # adding kwargs for compatability, but they are unsued
95      def __init__(self, data: SsxChipColletionTaskParameters, view=None,
96          super().__init__(view=view, data_model=TaskNode(data))
97
98
99      def execute(self):
100         super().execute()
```

```
available_methods:
    datacollection: True
    characterisation: True
    helical: True
    xrf_spectrum: True
    energy_scan: True
    mesh: True
    ssx_chip_collection: True
    gphlworkflow: True
    test_collection: True
```

Model parsed JSONSchema generated and a dialog can be created





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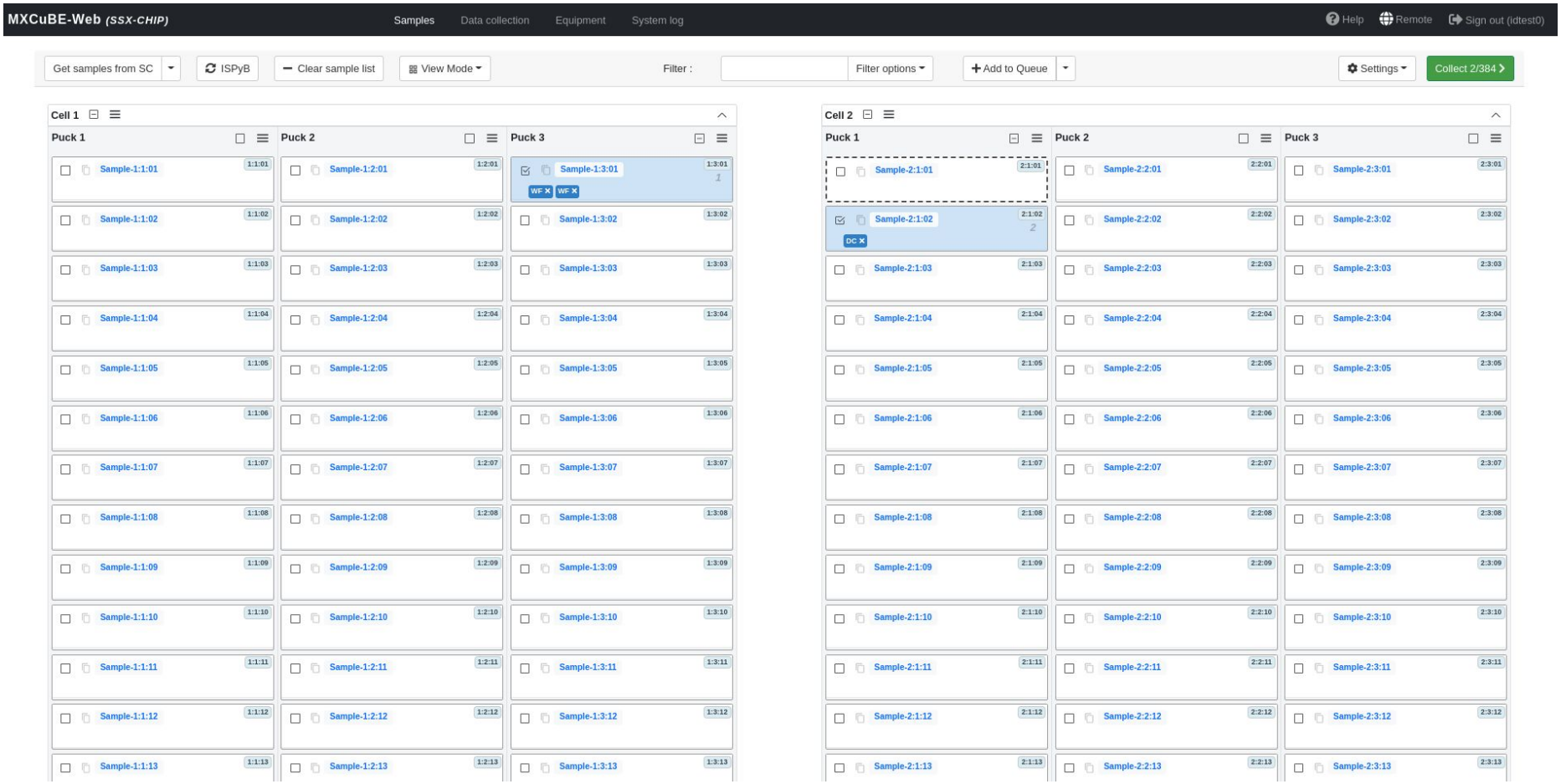
New sample list



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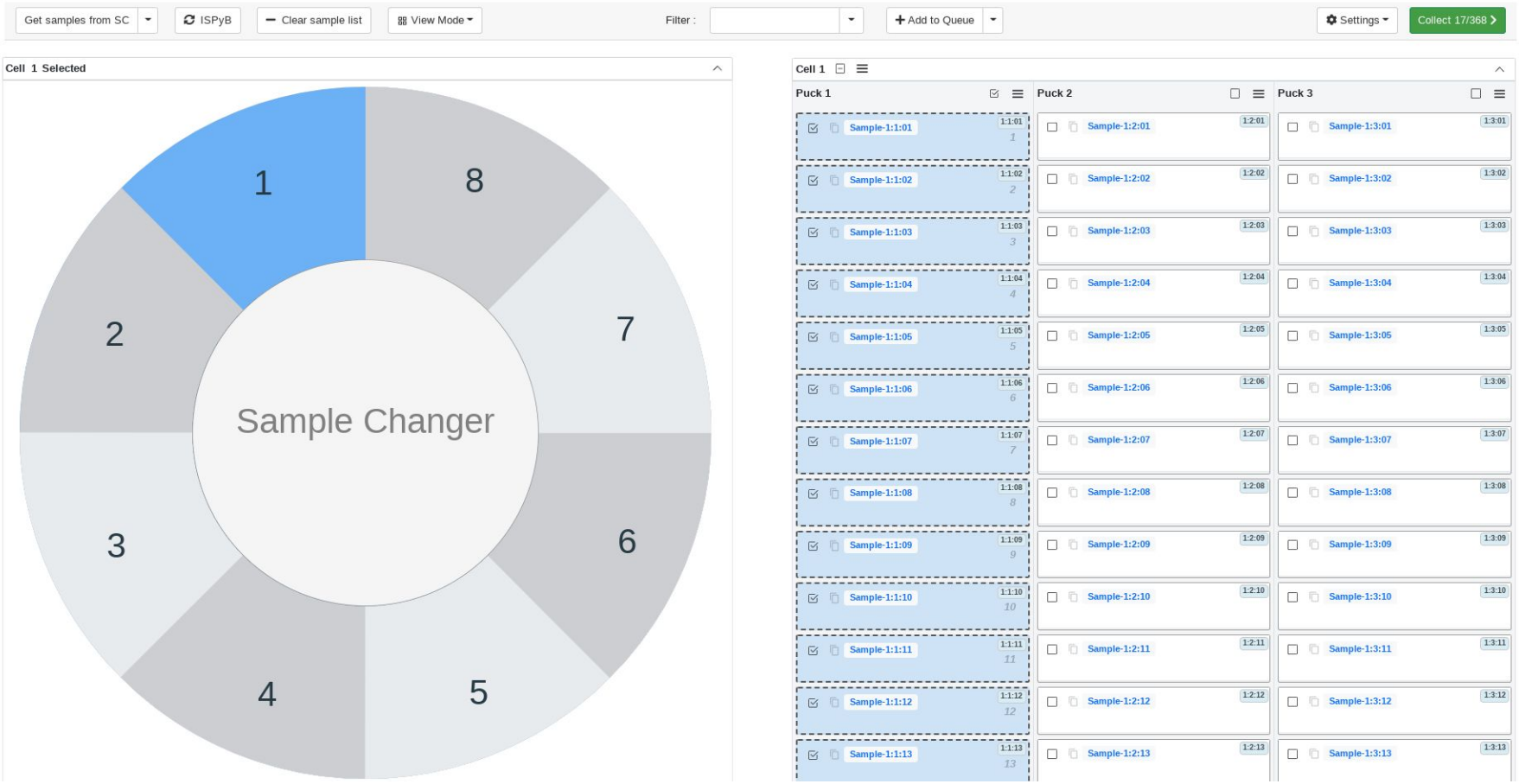
New sample list



Thanks JB

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MXCUBE at ESRF

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MXCUBE at ESRF

- ID23-1. ID23-2, ID30B and ID29 on mxcubeweb-4.72.0+esrf.0516 and mxcubecore-1.104.0+esrf.0516 (ID30A1 and ID30A3 are being updated)
- We try to rebase on upstream and deploy roughly every two weeks - this would be helped by better test coverage :)
- SSO with two factor authentication
- ICAT integration ongoing

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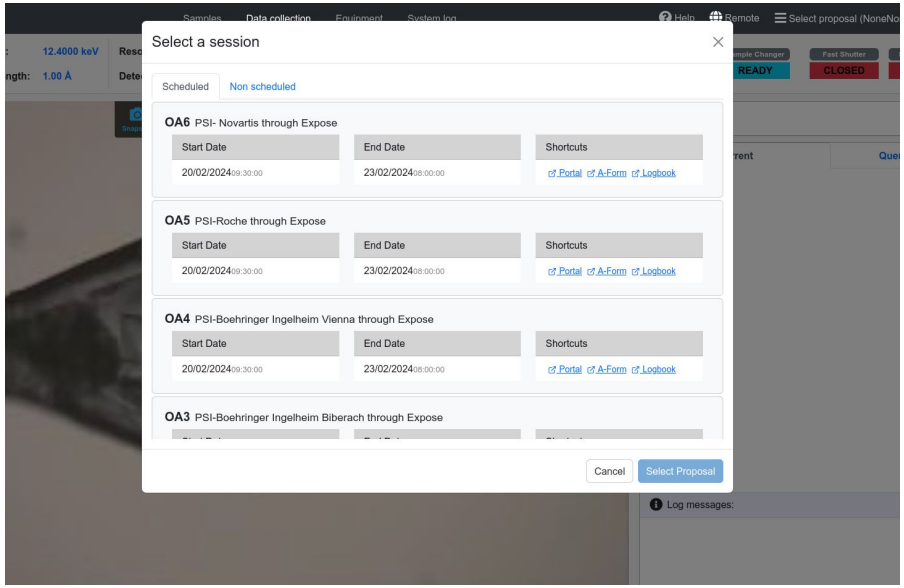
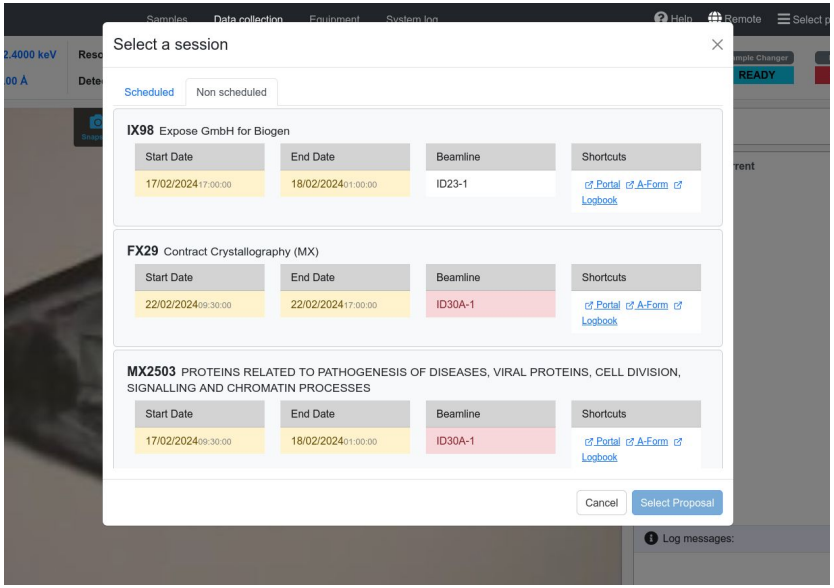
Single sign on with new proposal selection interface





Currently being validated - to be deployed within shortly

Thanks Alejandro !

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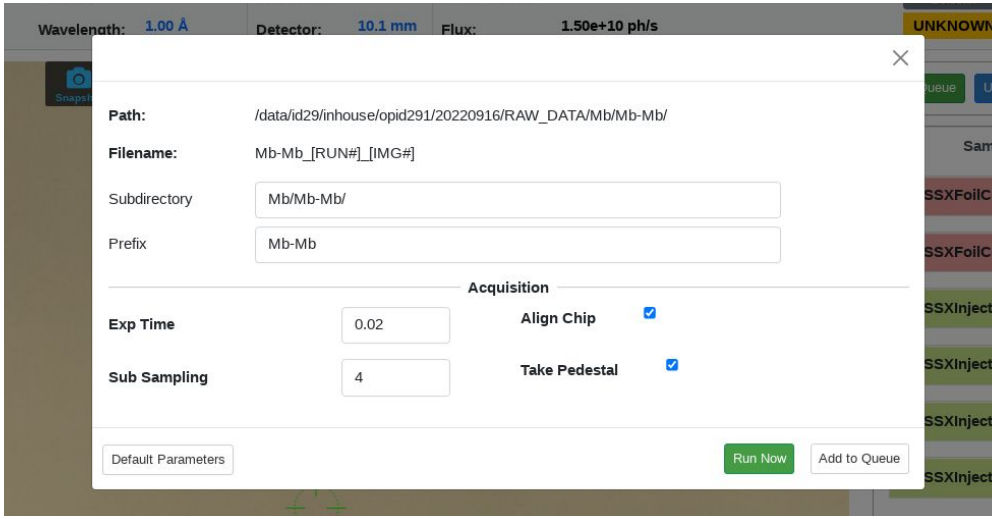
MXCUBE at ESRF

- Automation features developed on MASSIF1 now available everywhere
- Automation speed up - we are now up to 16 samples per hour (depending on workflow)
- Continued SSX development
  - Chip
  - Foil
  - Injector
  - *Laser triggered*



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Future perspectives

- Continue SSX development
- Continue development on new queue functionality
- Continue development of automation
- Continue ICAT integration
- Continue work on AbstractProcessing - been on hold for sometime
- Migrating from XML to YAML
- Deploy video stream solution for hutch videos
- Move to TypeScript ?
- Increase testing both backend and e2e
- Cleanup REST API and possibly exchange spectree for FlaskOpenAPI3 ?

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Questions

Thank you for your attention

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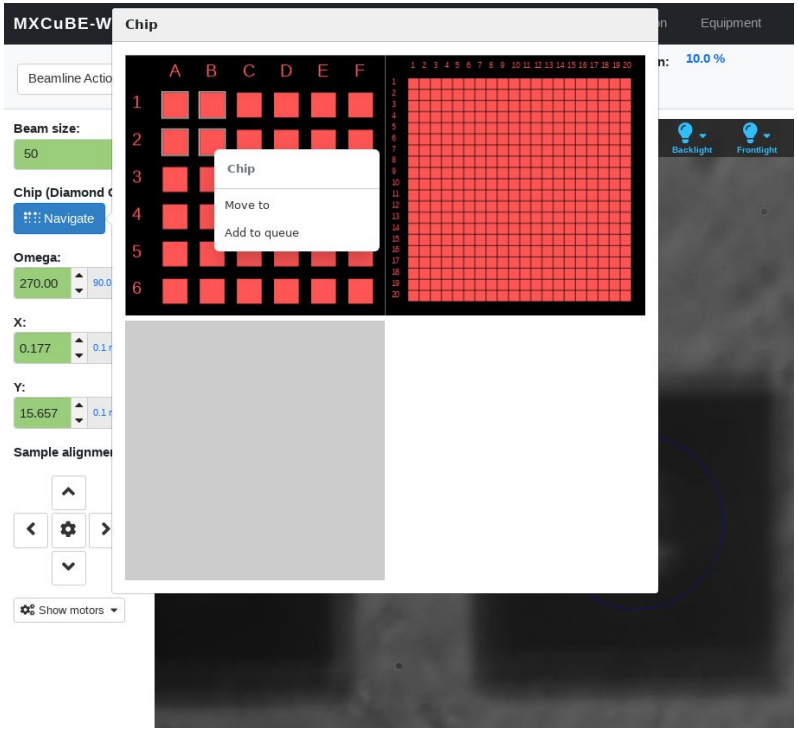
MXCUBE at ESRF



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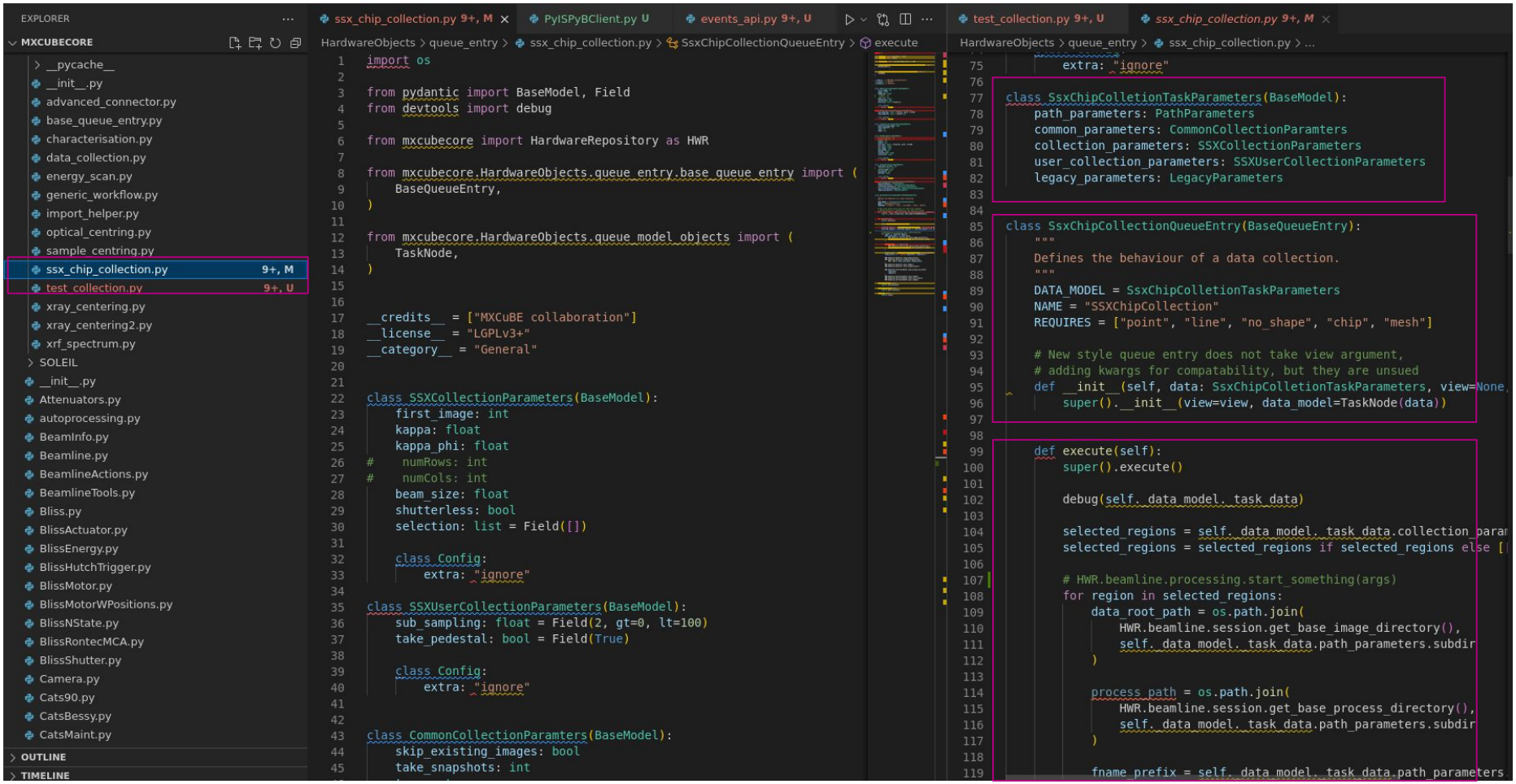
New Queue Proposal

Example - New style queue entry



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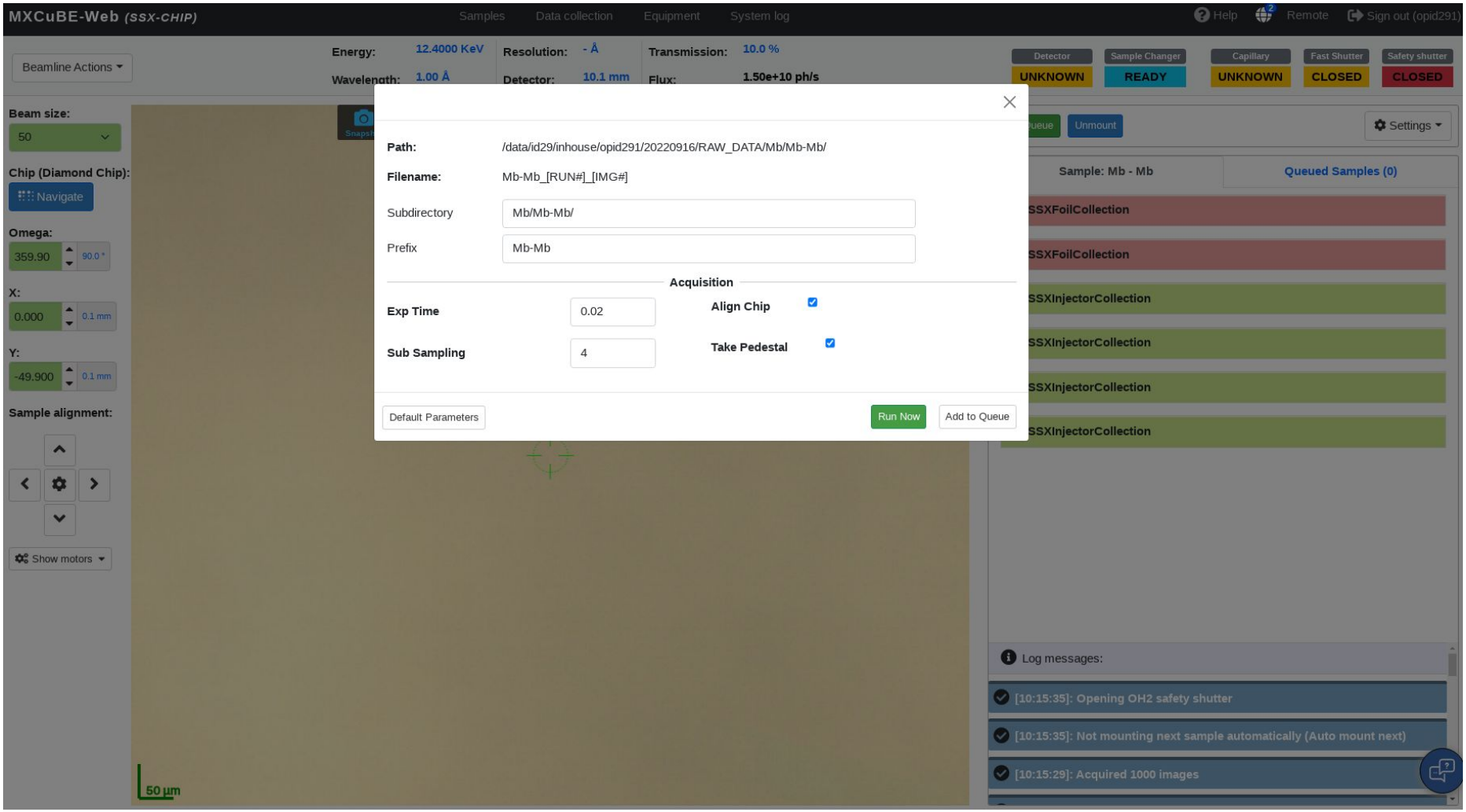
Example UI



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