MXCuBE 3 - General Layout and Sample Centring

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

ALBA - MXCuBE meeting - 30 Nov. 2015

Outline

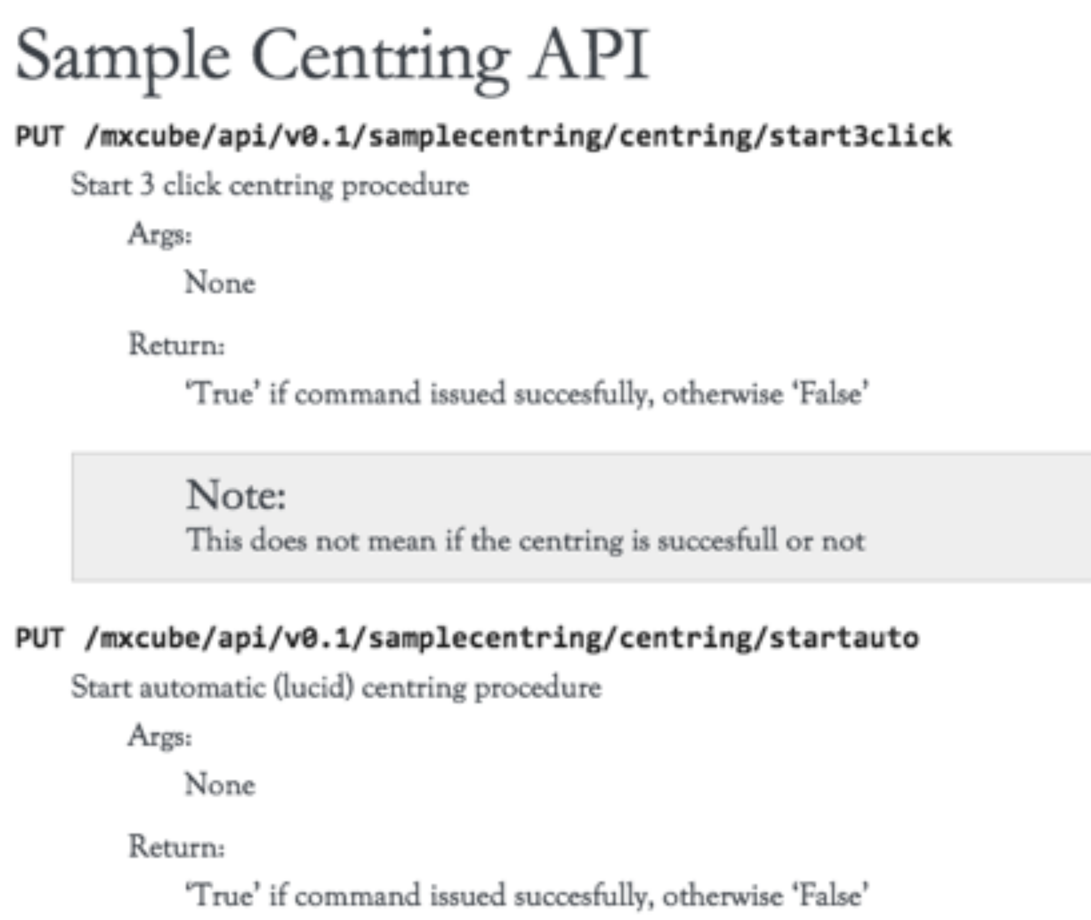
- Review of MXCuBE 3
- Proposed layout for the web interface
- Demo video and current status
- Next steps

Backend

- Python **Flask** microwebframework:
  - web server made simple
  - extensions (database, login, …)
  - easily adaptable to your needs while scalable
  - big community
- http request **API**: rest like (but probably not fully rest)
  - an url for each function
  - Simple to add new features without changing existing ones
- Flask **socketio** for sending HO messages
  - server-client bi-directional communication, websocket based
- Reuse the existing Hardware Repository

Http requests

- API for the calls from client to server (*GET, PUT, POST…*)
- Decoupling the server and the client
- Should be easy to understand by the client
  - ➡ (http://example.com/mybeamline/mymotors/omega/move/45)
- Url routings for sample centring/video: already working



Sample Centring API

PUT /mxcube/api/v0.1/samplecentring/centring/start3click

Start 3 click centring procedure

Args:

None

Return:

'True' if command issued succesfully, otherwise 'False'

> Note:
> This does not mean if the centring is succesfull or not

PUT /mxcube/api/v0.1/samplecentring/centring/startauto

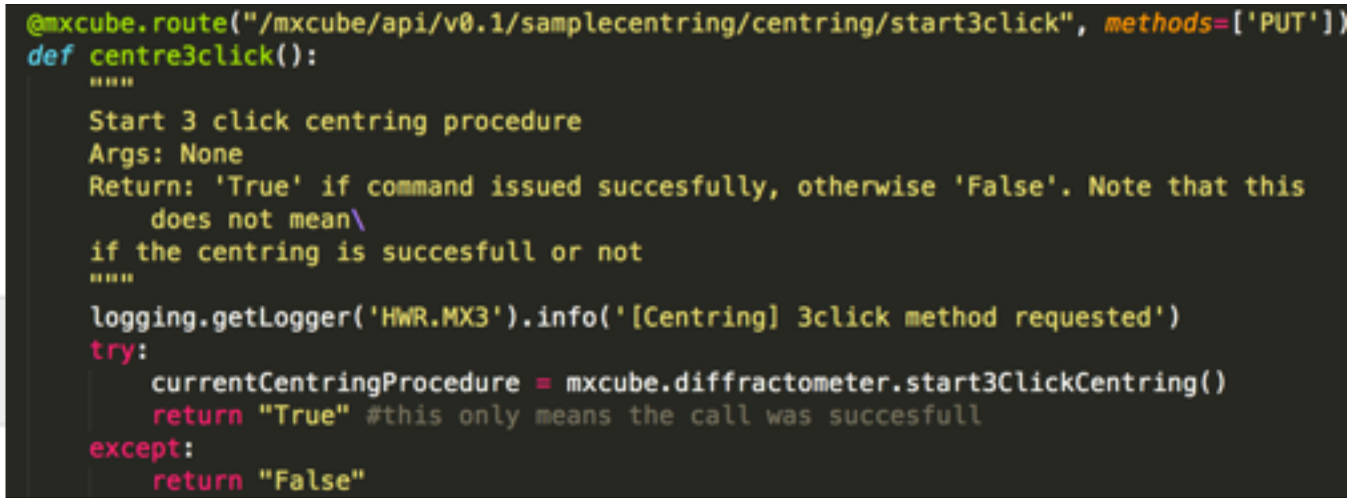
Start automatic (lucid) centring procedure

Args:

None

Return:

'True' if command issued succesfully, otherwise 'False'

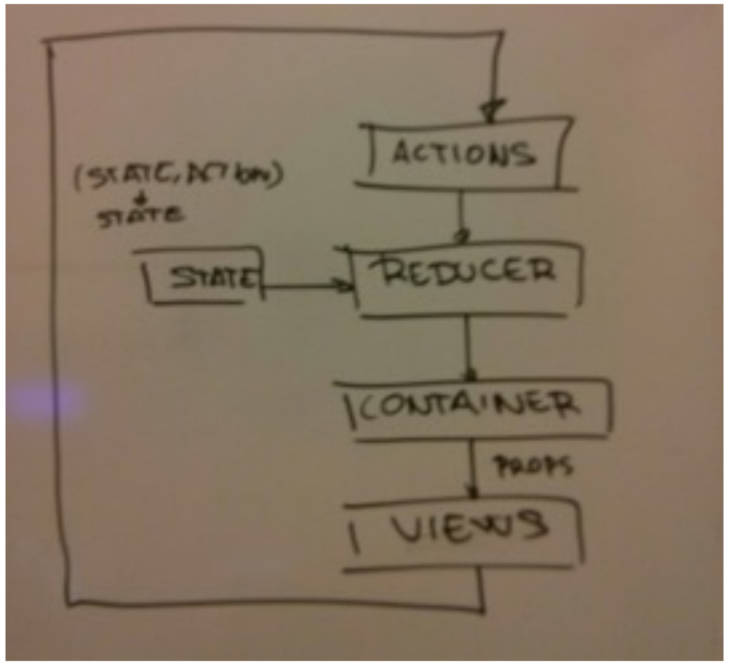


```
@mxcube.route("/mxcube/api/v0.1/samplecentring/centring/start3click", methods=['PUT'])
def centre3click():
    """
    Start 3 click centring procedure
    Args: None
    Return: 'True' if command issued succesfully, otherwise 'False'. Note that this
        does not mean\
    if the centring is succesfull or not
    """
    logging.getLogger('HWR.MX3').info('[Centring] 3click method requested')
    try:
        currentCentringProcedure = mxcube.diffractometer.start3ClickCentring()
        return "True" #this only means the call was succesfull
    except:
        return "False"
```

Frontend

- **Javascript/React** library (Facebook)
- Only for the user interface (the view in MVC)
- Virtual html DOM kept as internal state
  - Different components programmed independently
- Reusing existing code when the layout changes

- **Redux** application architecture/pattern
  - Predictable state container for JavaScript apps …
    - ➡ the way to go if you use React
  - Unidirectional data flow
  - Changes on the internal state in a single place



Redux architecture

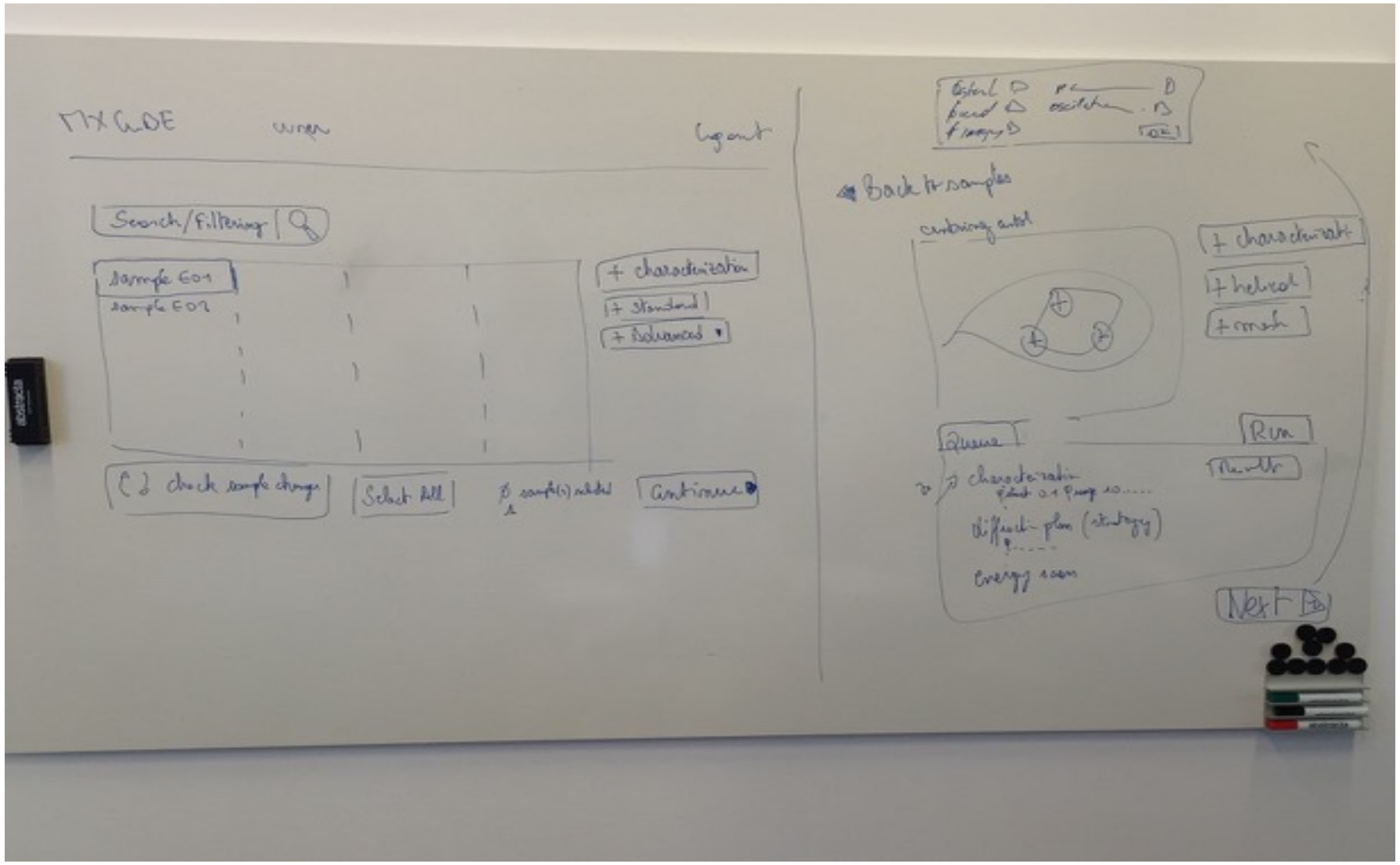
Layout

- Before going to *react* a main objetive was identified
  - Improve the user experience !!!

- And for that it is useful to
  - Have a clean interface
  - Use modern web technologies
  - Learn current usage and feedback

- And finally… a big question arises:
  - Is this really possible?

Layout - first sketch



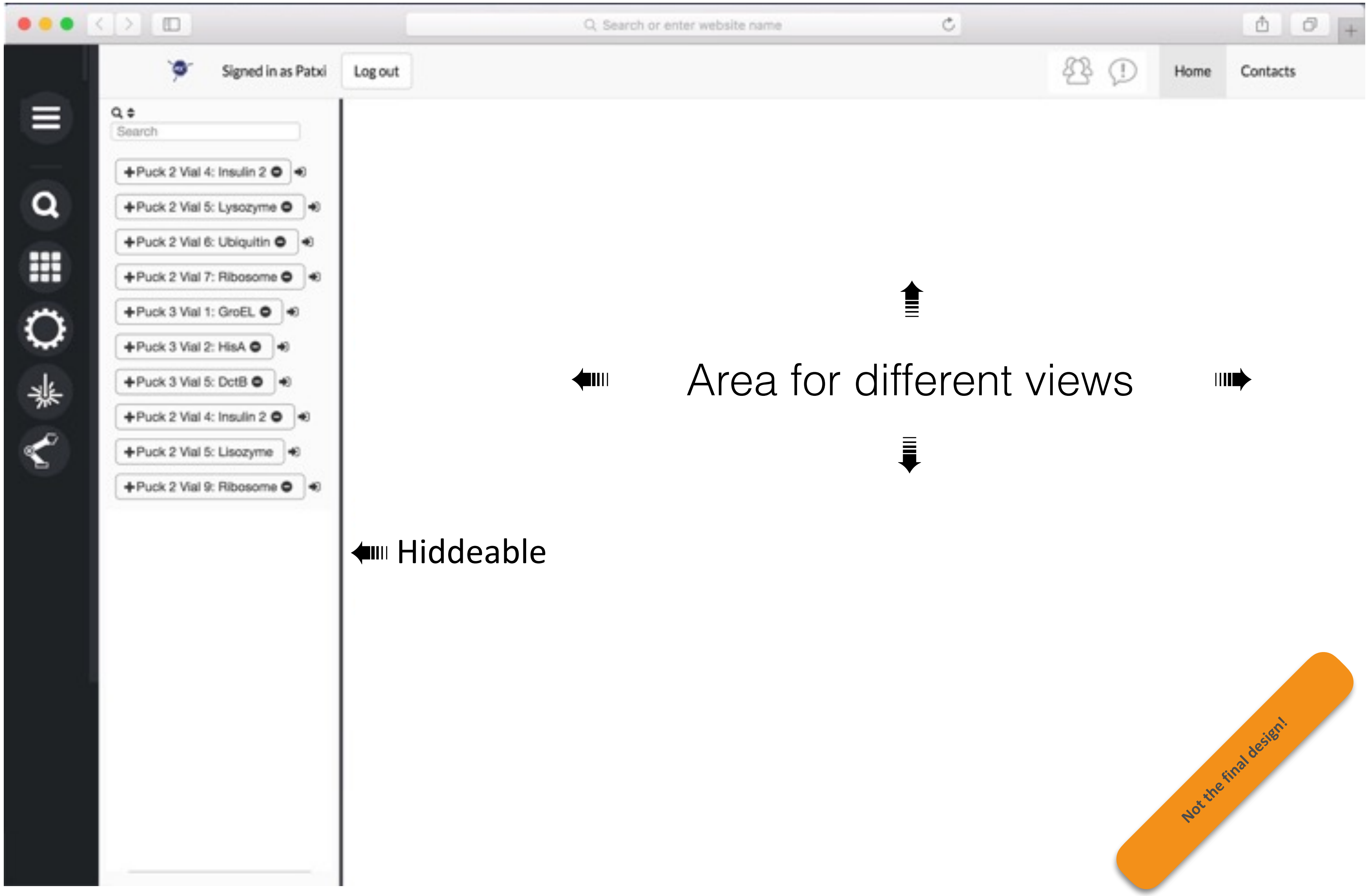
MAXIV-ESRF Sep. 2015

- Experiment configuration in a batch like mode
  - All available samples
- Experiment management for each sample
  - centring mechanism
  - should also be automatic and transparent for the user

Transitions between views to be defined

Layout - first real design

- Common parts



- +Puck 2 Vial 4: Insulin 2
- +Puck 2 Vial 5: Lysozyme
- +Puck 2 Vial 6: Ubiquitin
- +Puck 2 Vial 7: Ribosome
- +Puck 3 Vial 1: GroEL
- +Puck 3 Vial 2: HisA
- +Puck 3 Vial 5: DctB
- +Puck 2 Vial 4: Insulin 2
- +Puck 2 Vial 5: Lisozyme
- +Puck 2 Vial 9: Ribosome

Area for different views

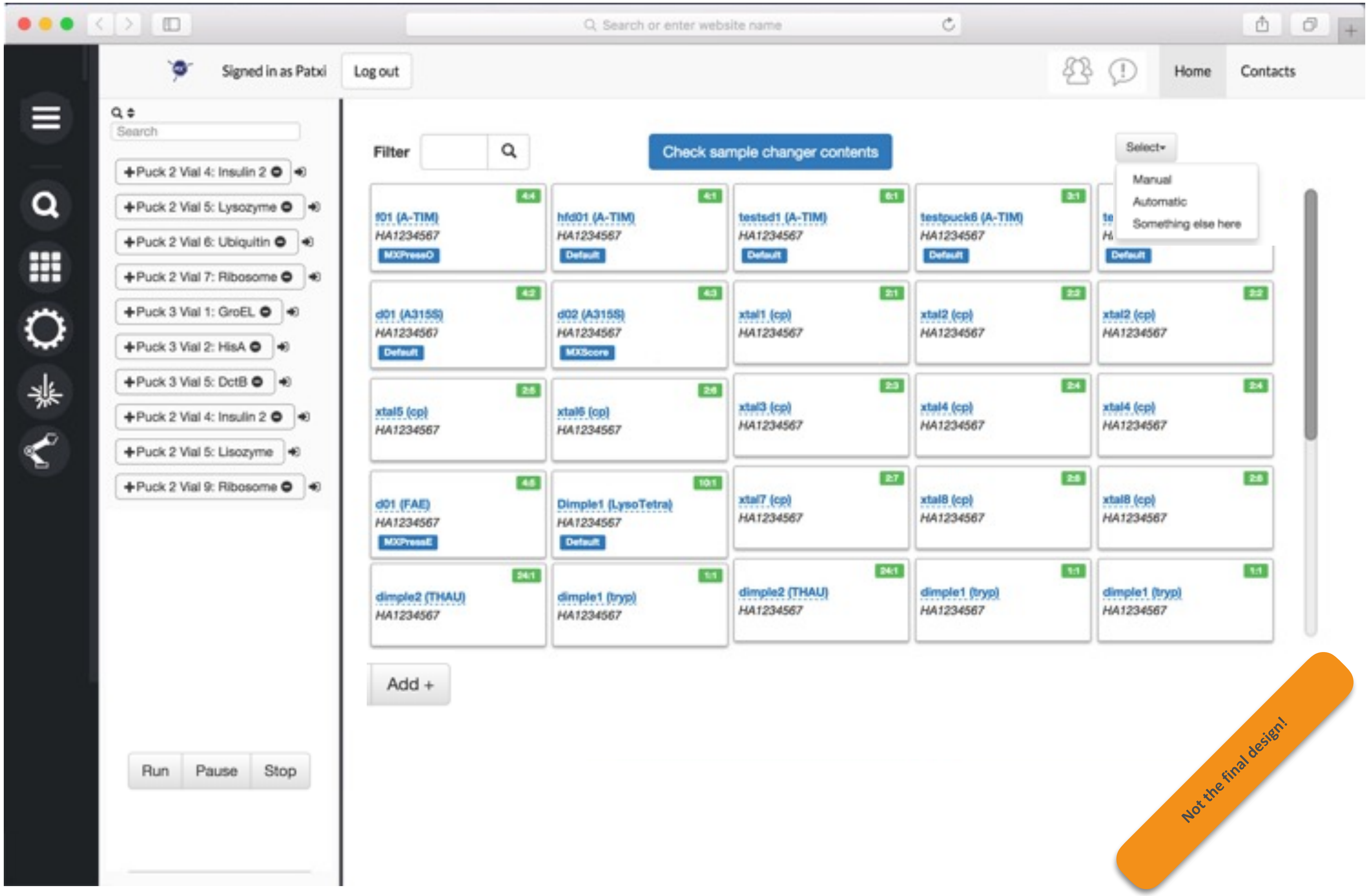
Hiddeable

Not the final design!

View selector

Layout - first real design

- Sample Grid



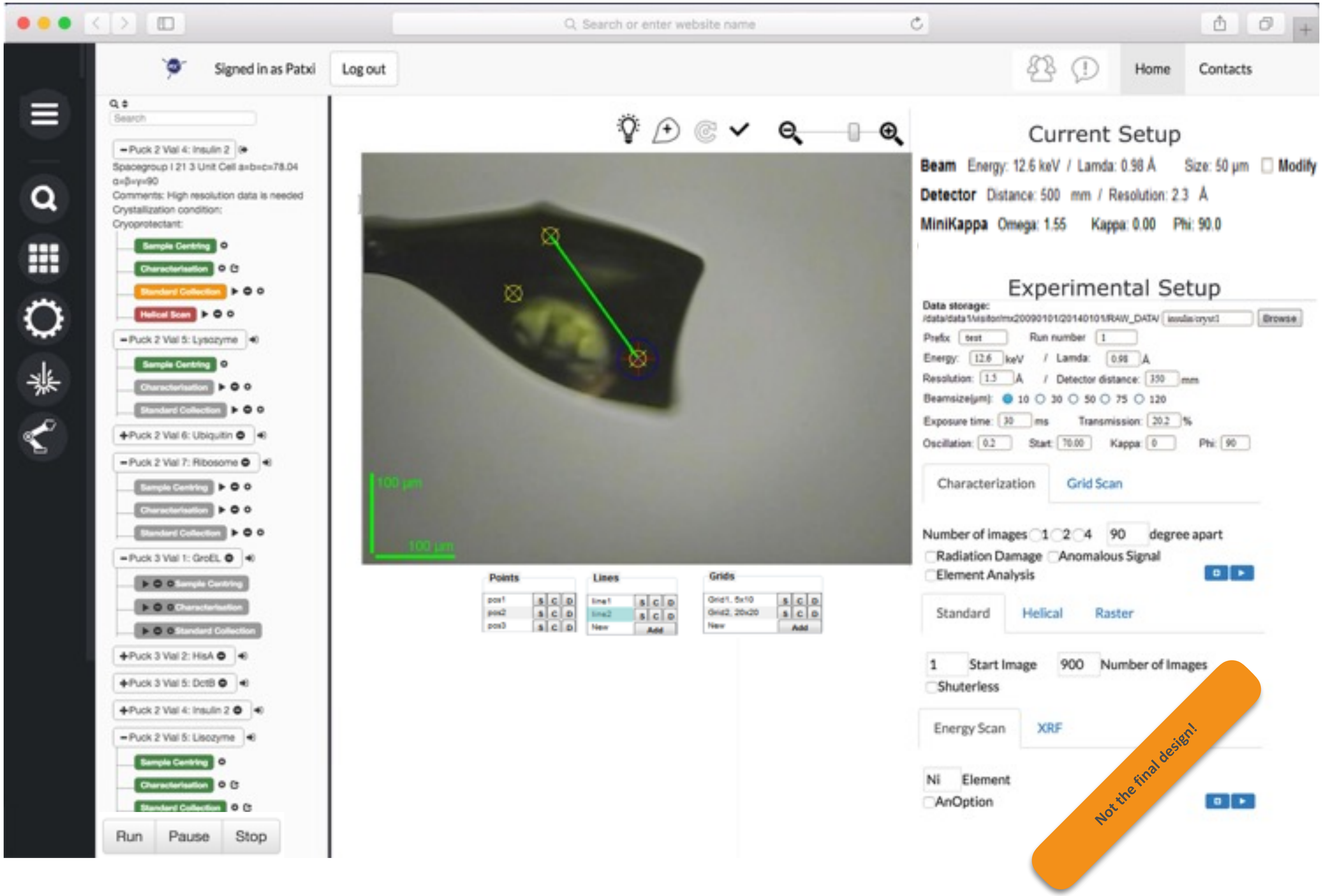
- Puck 2 Vial 4: Insulin 2
- Puck 2 Vial 5: Lysozyme
- Puck 2 Vial 6: Ubiquitin
- Puck 2 Vial 7: Ribosome
- Puck 3 Vial 1: GroEL
- Puck 3 Vial 2: HisA
- Puck 3 Vial 5: DctB
- Puck 2 Vial 4: Insulin 2
- Puck 2 Vial 5: Lisozyme
- Puck 2 Vial 9: Ribosome

4:4 f01 (A-TIM) HA1234567 MXPressO	4:1 hfd01 (A-TIM) HA1234567 Default	6:1 testsd1 (A-TIM) HA1234567 Default	3:1 testpuck6 (A-TIM) HA1234567 Default	te H Default
4:2 d01 (A315S) HA1234567 Default	4:3 d02 (A315S) HA1234567 MXScore	2:1 xtal1 (cp) HA1234567	2:2 xtal2 (cp) HA1234567	2:2 xtal2 (cp) HA1234567
2:5 xtal5 (cp) HA1234567	2:6 xtal6 (cp) HA1234567	2:3 xtal3 (cp) HA1234567	2:4 xtal4 (cp) HA1234567	2:4 xtal4 (cp) HA1234567
4:5 d01 (FAE) HA1234567 MXPressE	10:1 Dimple1 (LysoTetra) HA1234567 Default	2:7 xtal7 (cp) HA1234567	2:8 xtal8 (cp) HA1234567	2:8 xtal8 (cp) HA1234567
24:1 dimple2 (THAU) HA1234567	1:1 dimple1 (tryp) HA1234567	24:1 dimple2 (THAU) HA1234567	1:1 dimple1 (tryp) HA1234567	1:1 dimple1 (tryp) HA1234567

Not the final design!

Layout - first real design

- Sample Video



−Puck 2 Vial 4: Insulin 2
Spacegroup I 21 3 Unit Cell a=b=c=78.04
α=β=γ=90
Comments: High resolution data is needed
Crystallization condition:
Cryoprotectant:

- Sample Centring
- Characterisation
- Standard Collection
- Helical Scan

−Puck 2 Vial 5: Lysozyme

- Sample Centring
- Characterisation
- Standard Collection

+Puck 2 Vial 6: Ubiquitin

−Puck 2 Vial 7: Ribosome

- Sample Centring
- Characterisation
- Standard Collection

−Puck 3 Vial 1: GroEL

- Sample Centring
- Characterisation
- Standard Collection

+Puck 3 Vial 2: HisA

+Puck 3 Vial 5: DctB

+Puck 2 Vial 4: Insulin 2

−Puck 2 Vial 5: Lisozyme

- Sample Centring
- Characterisation
- Standard Collection

Points			
pos1	S	C	D
pos2	S	C	D
pos3	S	C	D

Lines			
line1	S	C	D
line2	S	C	D
New	Add		

Grids			
Grid1, 5x10	S	C	D
Grid2, 20x20	S	C	D
New	Add		

Current Setup

Beam Energy: 12.6 keV / Lamda: 0.98 Å Size: 50 µm □ **Modify**

Detector Distance: 500 mm / Resolution: 2.3 Å

MiniKappa Omega: 1.55 Kappa: 0.00 Phi: 90.0

Experimental Setup

Data storage:
/data/data1/visitor/mx20090101/20140101/RAW_DATA/ insulin/cryst1 Browse

Prefix: test Run number: 1

Energy: 12.6 keV / Lamda: 0.98 Å

Resolution: 1.5 Å / Detector distance: 350 mm

Beamsize(µm): ● 10 ○ 30 ○ 50 ○ 75 ○ 120

Exposure time: 30 ms Transmission: 20.2 %

Oscillation: 0.2 Start: 70.00 Kappa: 0 Phi: 90

Characterization | Grid Scan

Number of images ○1 ○2 ○4 90 degree apart
□ Radiation Damage □ Anomalous Signal
□ Element Analysis

Standard | Helical | Raster

1 Start Image 900 Number of Images
□ Shutterless

Energy Scan | XRF

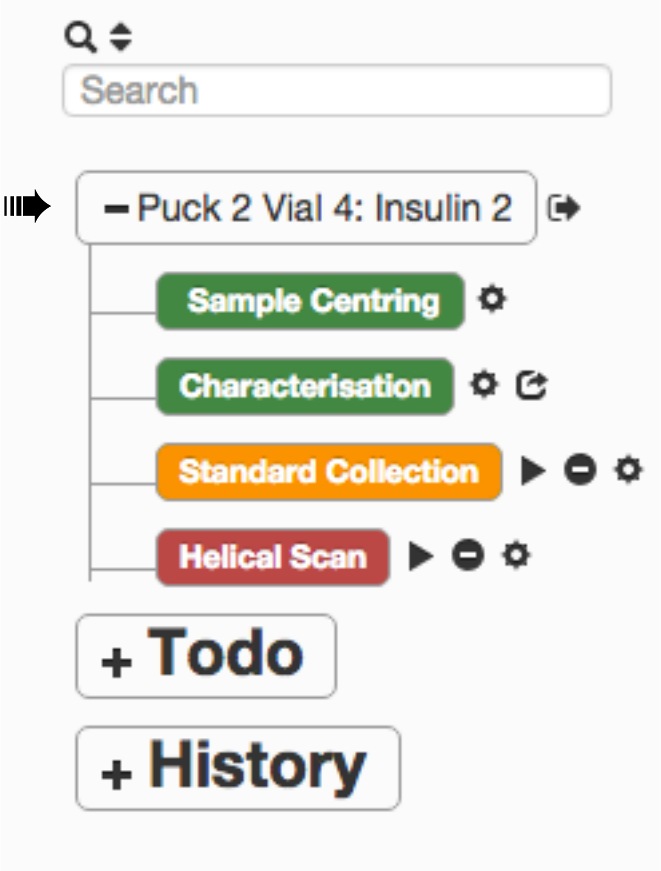
Ni Element
□ AnOption

Not the final design!

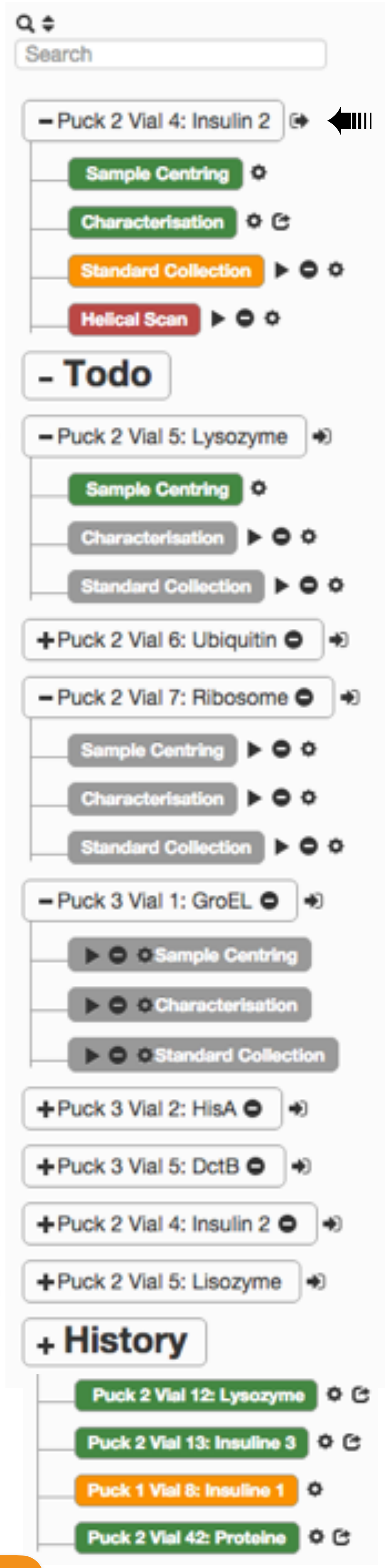
Layout - Queue

- Queue:
  - Current sample always on top
  - Todo and History (collapsable)
  - Drag&Drop, search, reorder, skip …

Current sample



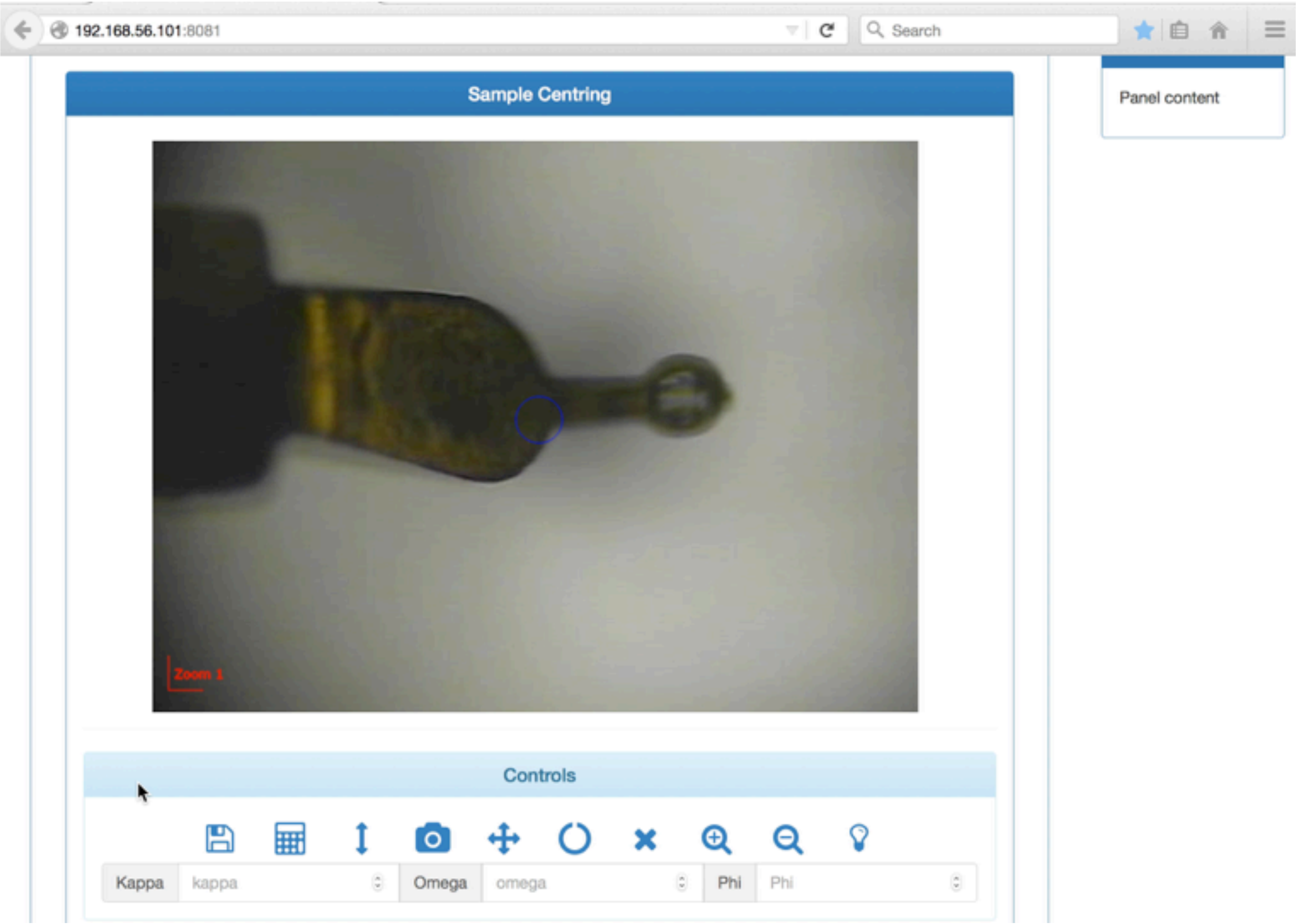
Current sample



Not the final design!

MXCuBE 3 - demo

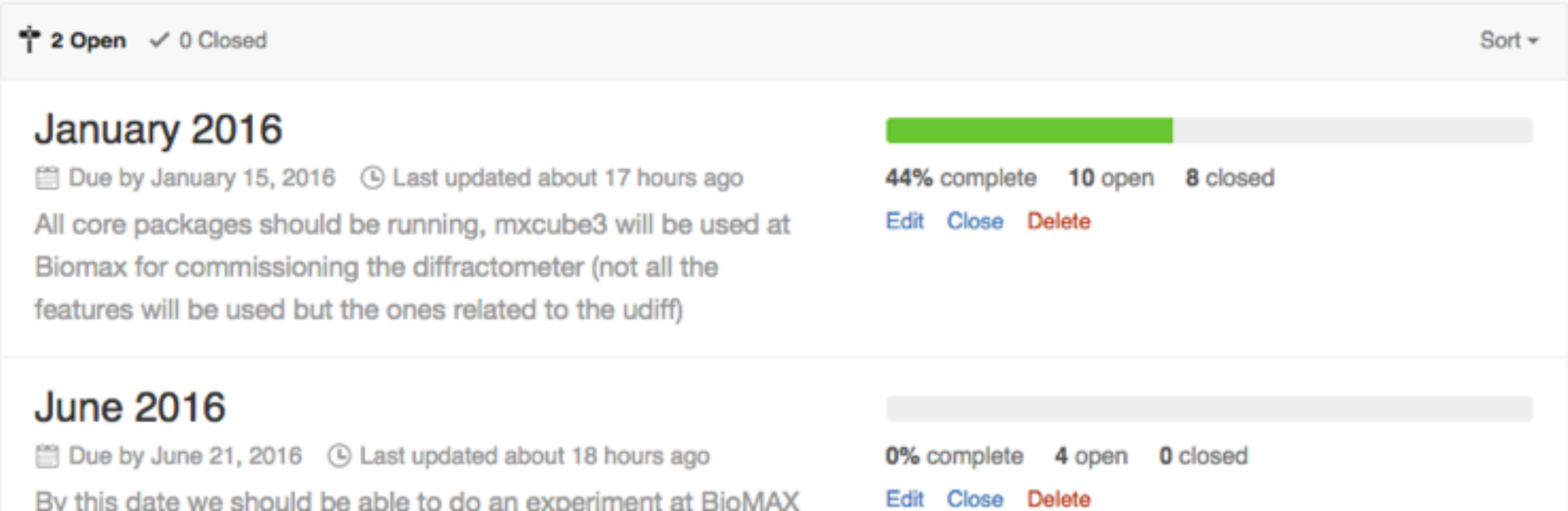
- Sample Centring and video



Current Status

- Working on core packages - Jan16 milestone (*Antonio's talk*)
  - Diffractometer controlled: code reused in *any* layout
  - Setting up development environment/workflow (*Matias' talk*)
  - Web interface layout designed (at least until further discussion)
  - Mockups + real environment
  - Github => 138 commits | 25 pull requests | 38 issues

https://github.com/mxcube/mxcube3



2 Open ✓ 0 Closed

January 2016

Due by January 15, 2016 Last updated about 17 hours ago

All core packages should be running, mxcube3 will be used at Biomax for commissioning the diffractometer (not all the features will be used but the ones related to the udiff)

44% complete **10** open **8** closed

June 2016

Due by June 21, 2016 Last updated about 18 hours ago

By this date we should be able to do an experiment at BioMAX

0% complete **4** open **0** closed

Next steps

- Real testing
  - Maxlab 911 mx beamline to be closed…
  - MaxIV laboraty setup: MD2? + virtual beamline
  - ESRF beamlines (Matias)

- Work towards Jan16 milestone
  - HO integration in the server (http requests)
  - Frozen design: gimp => web
  - Implementation of the queue
  - Sample Grid

MXCuBE3 People

Main developers:

MAX IV: M. Eguiraun, A. Milan-Otero, J. Nan, F. Bolmsten

ESRF: M. Guijarro

Supported by:

MXCuBE collaboration

MAX IV MX and KITS teams

ESRF BCU team

Thanks for your attention!