

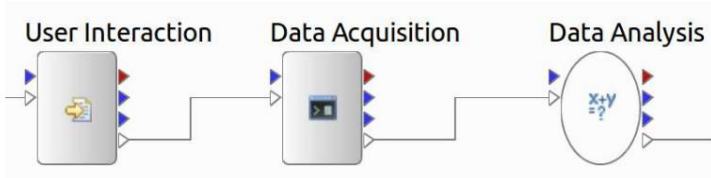
# Workflows and ISPyB/EXI

**Olof Svensson**  
**Data Analysis Unit**  
**ISDD / ESRF**

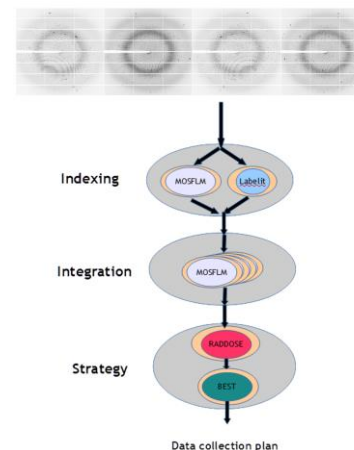
# EXAMPLES OF COMPLEX DATA COLLECTION

## • Combination of:

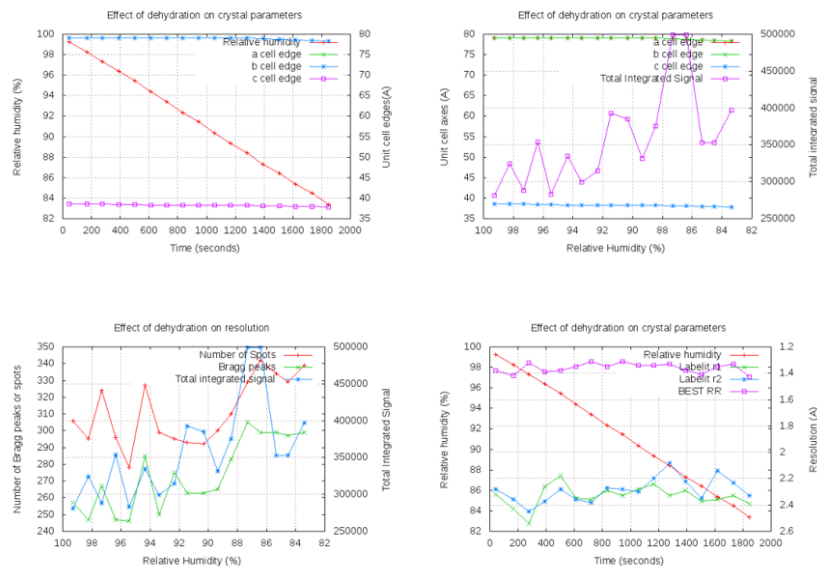
- Data collection
- Data processing
- [User interaction]



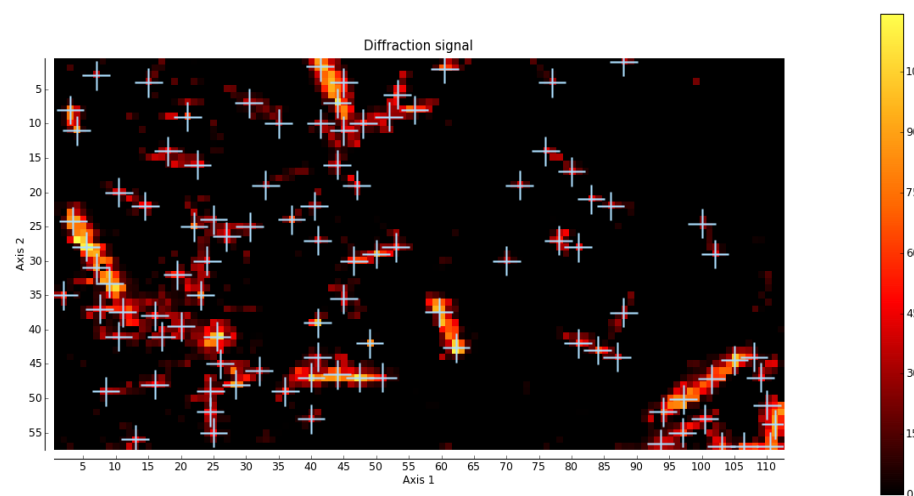
## Example: Characterisation



## Example: Dehydration

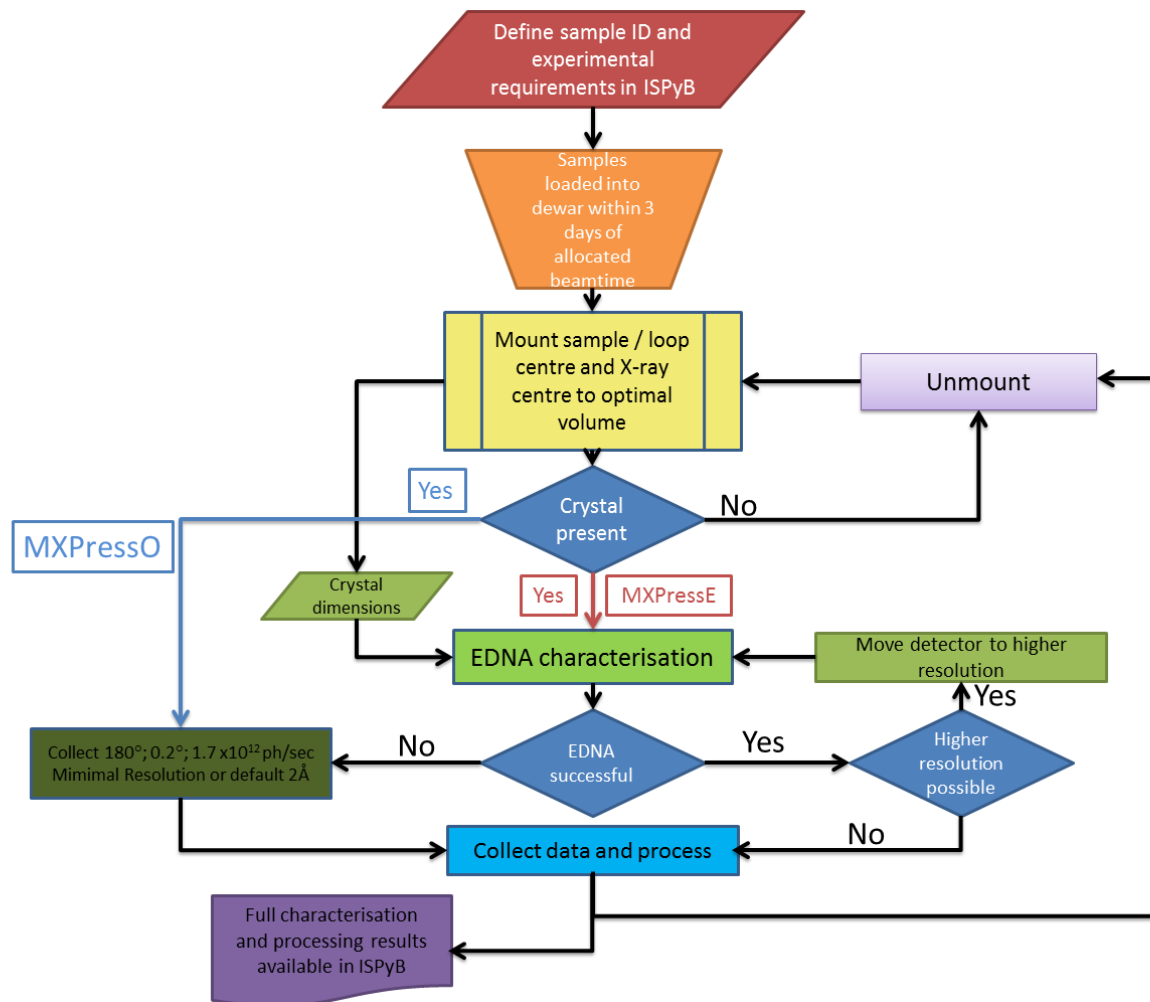


## Example: Mesh and collect



# THE MOST COMPLEX DATA COLLECTION: MXPRESSA

## MXPressA (~10000)



- **The BES (Beamline Expert System)**
  - A customized version of Passerelle EDM for the ESRF
  - Similar to the SES (Soleil Expert System)
- **Passerelle EDM:**
  - Based on the open-source passerelle workflow engine, which is based on the Ptolemy II workflow engine (written in Java)
  - Combines the passerelle workflow engine with a workflow design tool
  - Both the engine and the design tool are connected to a data base
  - Accessed via a web GUI (Jboss Application Server 7)
- **Passerelle EDM is a commercial product:**
  - Initial one-off purchase followed by one-year maintenance contracts
  - ESRF license costs shared between the ESRF and EMBL Grenoble
  - Contact person: Erwin de Ley (erwin.de.ley@isencia.be)

Beamline Expert System x

mxhpc2-1705:8090/BES/bridge/app/

ESRF | EMBL | BES 3.2.0

Design Configuration Testing Support Admin

Olof Svensson

Commit Save Lock General Validate Flow Run Customize

Editor Debug

Shared Submodel MXPressDataCollection (2.1)  
Original layout

Palette


- Throttling Delay
- Error Observer
- Error Catcher
- Router
- Transform
- I/O
- Expert
- Cluster
- Events
- Monitoring
- Continuation
- ESRF actors
  - Error Handler by Causing actor
  - Error Handler by ErrorCode raised
  - Error Handler by Severity
  - Python Actor
- Shared Submodels
  - AnalyseKappa
  - CenterRotationAxis
  - CollectAndProcessBurningStrategy
  - CollectReferenceImages
  - CollectWithoutStrategy
  - CommonDataCollection

MXPressDataCollection

# BES – WORKFLOW EXECUTION LOG

Beamline Expert System

mxhpc2-1705:8090/BES/bridge/app/



**BES**  
3.2.0

Design Configuration Testing Support Admin

Olof Svensson

← Refresh ↑ Export ↻ Flow

Reference: 9070  
Id: 4734179  
Type: MXPressA  
Creation Date: 2016-12-09 16:02:31  
Status: Finished  
External Reference: fx57  
Correlation Id:  
Initiator: id30a1  
Executor:

Request details

Request ( id= 4734179, type = MXPressA )

7 rows 10

Name	Value	Data Type	+
collection_software	mxCuBE_-2.0	STRING	
directory	/data/visitor/fx57/id30a1/20161209/RAW_DATA/BIPDE1/BIPDE1-CD014403_H04-3_DI01318464	STRING	
modelpath	MXPressA	STRING	
prefix	BIPDE1-CD014403_H04-3_DI01318464	STRING	
run_number	1	STRING	
sample_lims_id	575403	STRING	
sample_node_id	119	STRING	

Task Result Item Event

Enter search string here

Id: Status: ☐ Created ☐ Error ☐ Finished ☐ Cancelled ☐ Started ☐ Timeout


Type: Discriminator: Initiator:

View

101 rows 400

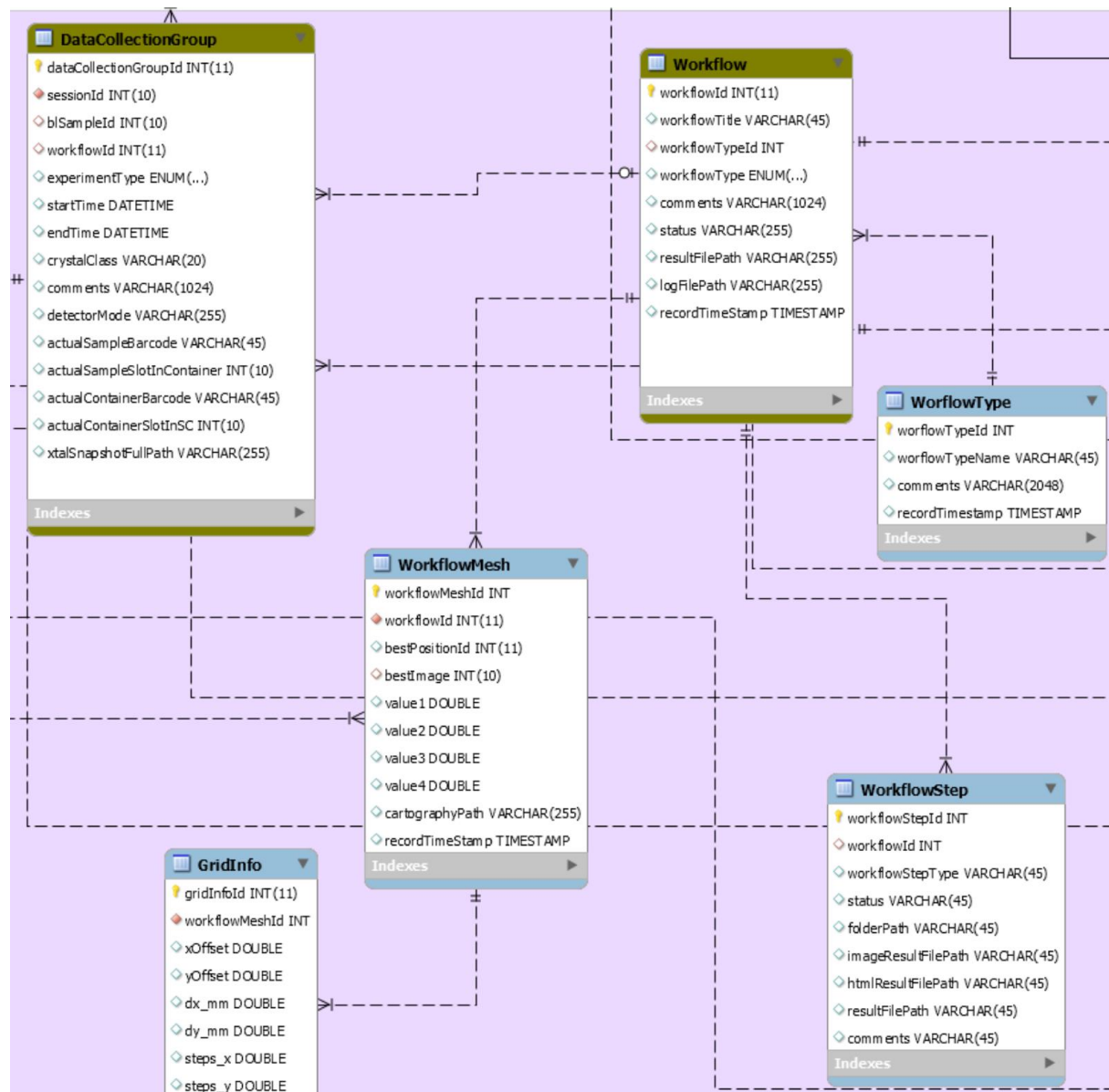
		Id	Creation Date	Duration(ms)	Status	Type	Initiator
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734180</a>	2016-12-09 16:02:31	8	Finished	Start	actor:/MXPressA.Start
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734291</a>	2016-12-09 16:02:31	632	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.Beamline%20setup
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734292</a>	2016-12-09 16:02:32	576	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.Prepare%20MXPressA
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734293</a>	2016-12-09 16:02:32	1850	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.CommonPrepareExperiment.Init%20workflow
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734294</a>	2016-12-09 16:02:34	768	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.CommonPrepareExperiment.Read%20motor%20positions
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734295</a>	2016-12-09 16:02:35	299	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.CommonPrepareExperiment.Default%20parameters
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734296</a>	2016-12-09 16:02:35	2295	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.MXPressMultiCrystal.Interpretation%20of%20diffraction%20p
<input type="checkbox"/>	<input type="checkbox"/>	<a href="#">4734297</a>	2016-12-09 16:02:37	315	Finished	eu.esrf.services.python.v2.6	actor:/MXPressA.MXPressMultiCrystal.Contact%20user%20if%20first%20acroi

Page 6 | Workflows and ISPyB / EXI | 2017-01-17 | Olof Svensson

The European Synchrotron | 



# ISPYB DATA BASE AND WORKFLOWS





- The results of the workflows are accessed from the summary page

ISPyB Information System for Protein crystallography Beamlines

TEST SERVER on Validation db

Home Lab-contacts Shipment Samples Prepare experiment Data collection Feedback References Help

View last sessions View all sessions Search data collections

**Selected Session**

Proposal: mx415  
Start Date: 16-01-2017  
BeamLine: ID30A-2  
[Back to this session](#)  
[Back to sessions](#)

**Session Information**

Local Contact:   
Comments: Session created by the BCM

**Session Statistics**

Nb Collect: 5  
Nb Test: 0  
Nb Energy Scan: 0  
Nb XRF Spectra: 0

**Reports**

**General report:**  
[Word](#) [PDF](#)

**Screening report:**  
[Word](#) [PDF](#)

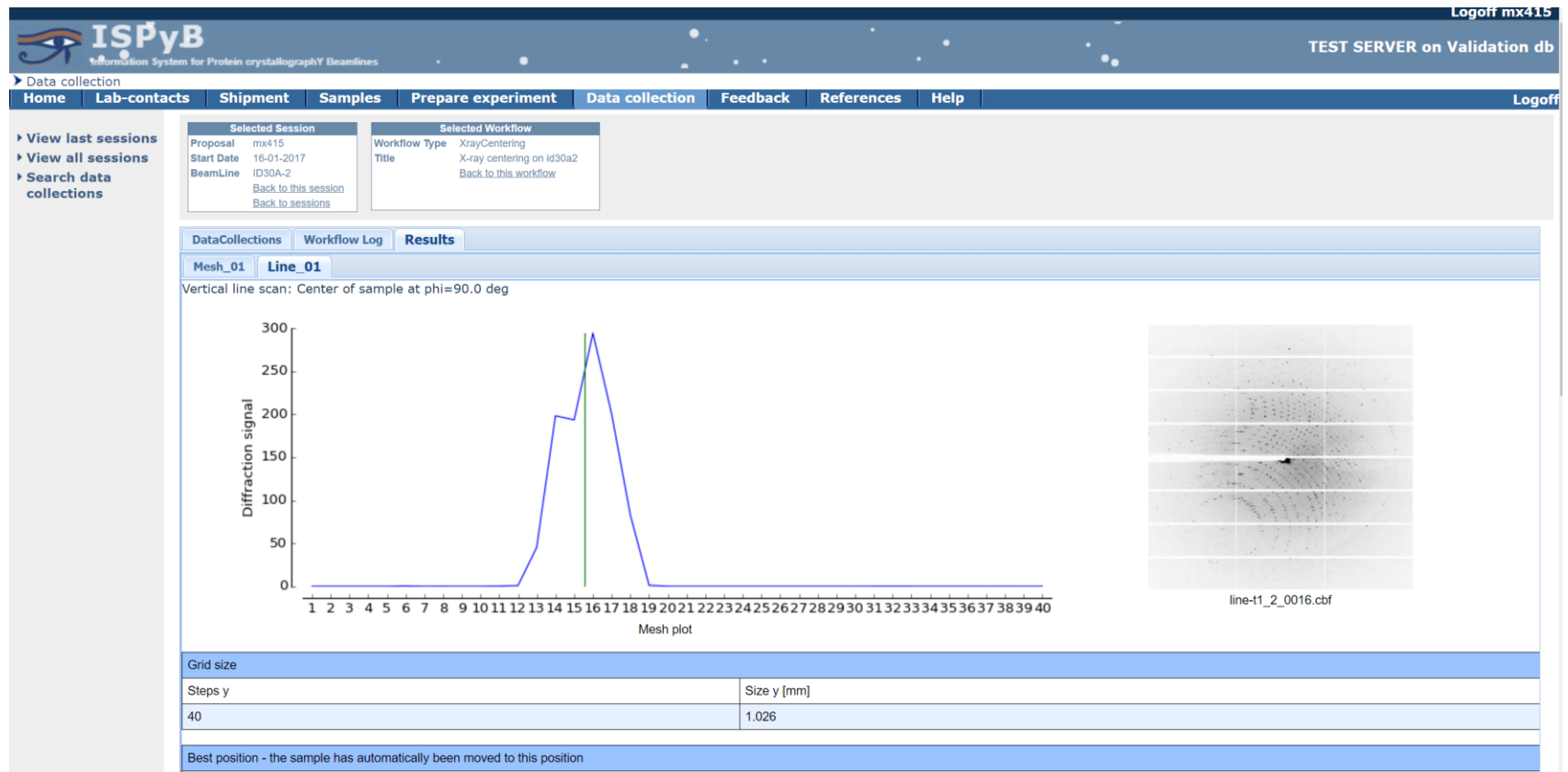
**Session**

[Save Comments](#) [View All Summary info](#) [View All DataCollection](#) [Expand All](#) [Collapse All](#) [Clear Grouping](#)

Exp. Type	Image Prefix	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Second Graph	Comments
<b>Start</b> time: 09:41:14 16-01-2017 (1 Item)									
XrayCentering	line-t1	2	<i>Nb tot images:</i> 112 <i>Exp. time:</i> 2.500 s <i>Phi range:</i> 0.25 ° <i>Flux:</i> 1.0E12 ph/sec <i>Detector resolution:</i> 2.00 Å <i>Transmission:</i> 100.00 <i>Wavelength:</i> 1.000 Å <i>Total expo time:</i> 100.00 s	XrayCentering V1: 1.49 V2: 4.58 N:					

ESRF | EMBL | BM14 | SPINE | MSD | MAX IV | SOLEIL

- The results of web pages are presented as HTML pages
  - The directory location of the web pages is stored in Workflow.resultFilePath. Every directory inside this directory that contains a “index.html” page is rendered as a tab, the name of the tab is the name of the directory



- Results of workflows are accessed from the summary page

ExiMX Extended ISPyB for MX<sub>BETA</sub>

Version: 0.9.8  
Released: 2016/12/22

Home Shipment Proteins and Crystals Prepare Experiment Data Explorer Offline Data Analysis Help

search by protein acronym

Log out MX415@svensson

New Tab

1 Data Collections Energy Scans Fluorescence Spectra

View

enter search prefix, sample or protein

Run #2 Helical Jan 16, 2017 9:41:14 AM  
/data/vsutor/mx415/d30a2/20170116/RAW\_DATA/1/XrayCentering\_01

Summary Beamline Parameters Data Collections (5) Sample Results Workflow (2)

Workflow	Type	Helical
Protein	Res. (corner)	2 Å (1.6 Å)
Sample	Wavelength	1 Å
Prefix	Phi range	0.25 °
Images	Phi start (total)	95° (10°)
Transmission	Exposure Time	2.5 s
Flux start	Flux end	1e+12 ph/sec

Workflow XrayCentering

Image of a crystal

Plot of data collections

ExiMX Extended ISPyB for MX<sub>BETA</sub>

Version: 0.9.8  
Released: 2016/12/22

Home Shipment Proteins and Crystals Prepare Experiment Data Explorer Offline Data Analysis Help

search by protein acronym

Log out MX415@svensson

New Tab

1 Data Collections Energy Scans Fluorescence Spectra

View

enter search prefix, sample or protein

Run #2 Helical Jan 16, 2017 9:41:14 AM  
/data/vsutor/mx415/d30a2/20170116/RAW\_DATA/1/XrayCentering\_01

Summary Beamline Parameters Data Collections (5) Sample Results Workflow (2)

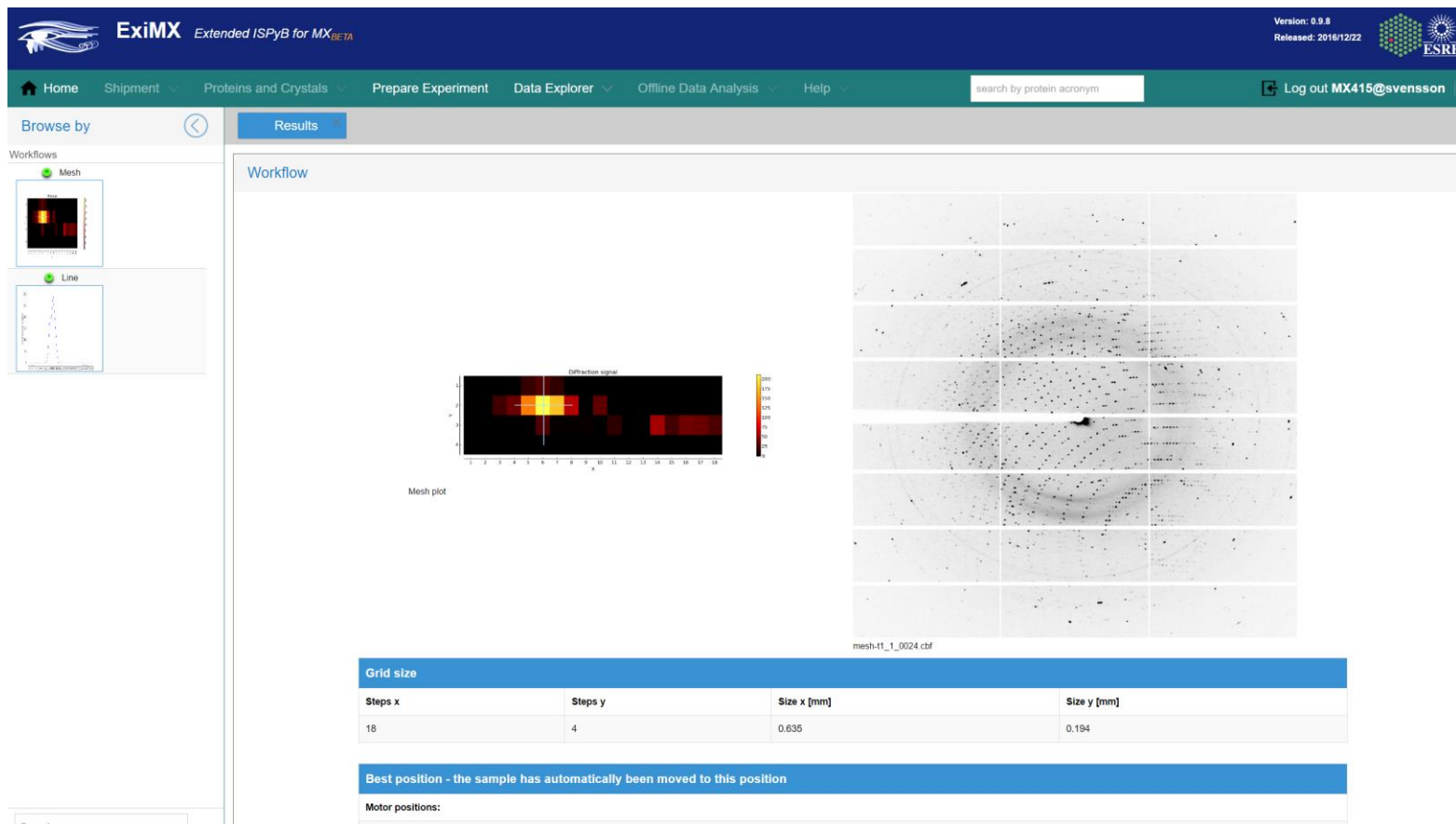
Mesh Line

Success Success

# DIFFERENCE BETWEEN ISPYB GUI AND EXI

- **EXI:**

- The results are stored as json files.
- The json file contains all data (text, tables and encoded images)
- The location of the json file is stored in WorkflowStep.resultFilePath



- David von Stetten, Max Nanao, Sasha Popov, Daniele de Sanctis, Stéphanie Monaco, Didier Nurizzo, Matias Guijarro, Solange Delagenière, Alejandro de Maria, Marcus Oskarsson (ESRF)
- Matthew Bowler (EMBL Grenoble)
- Erwin de Ley and Koen Heunick (Isencia, Belgium)
- The ESRF Data Analysis Unit, Beamline Control Unit and Structural Biology group

### Further reading:

- **Fully automatic characterization and data collection from crystals of biological macromolecules**, Svensson, O., Malbet-Monaco, S., Popov, A., Nurizzo, D., & Bowler, M. W. (2015). Acta Crystallographica Section D: Biological Crystallography, 71(Pt 8), 1757–1767. <http://doi.org/10.1107/S1399004715011918>
- **MeshAndCollect: an automated multi-crystal data-collection workflow for synchrotron macromolecular crystallography beamlines**, Ulrich Zander · Gleb Bourenkov · Alexander N Popov · Daniele De Sanctis · Olof Svensson · Andrew A McCarthy · Ekaterina Round · Valentin Gordeliy · Christoph Mueller-Dieckmann · Gordon A Leonard, ACTA CRYSTALLOGRAPHICA SECTION D BIOLOGICAL CRYSTALLOGRAPHY 71(11):2328-2343 · NOVEMBER 2015
- **Facilitating best practices in collecting anomalous scattering data for de novo structure solution at the ESRF Structural Biology Beamlines**, Daniele de Sanctis · Marcus Oscarsson · Alexander Popov · Olof Svensson · Gordon Leonard, Acta Cryst. (2016). D72, 413-420
- **The use of workflows in the design and implementation of complex experiments in macromolecular crystallography**, S. Brockhauser, O. Svensson, M. W. Bowler, M. Nanao, E. Gordon, R. M. F. Leal, A. Popov, M. Gerring, A. A. McCarthy and A. Gotz., Acta Cryst. (2012). D68, 975-984