



| The European Synchrotron

Latest advances on EXI-MX

# Development aim

- Faster display of summary page especially with complex workflows (WF)
- no going back and force to other pages to visualize more details
- Intuitive accesses to avoid manual reading
- Simplification of the processes (vs. an interface evolving over 10 years with multiple add-ons)

# Enrichment of the session summary page

ExiMX Extended ISPyB for MX BETA

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 MX1862@smonaco

New Tab

Very weak diffraction

Run #1 OSC Dec 15, 2016 8:51:38 AM  
/data/visitor/mx1862/nc29/20161215/RAW\_DATA

Summary Beamline Parameters Data Collections 1 Sample Results 15 Workflow

Workflow	Type	OSC
Protein	Res. (corner)	1.3 Å (1.07 Å)
Sample	Wavelength	0.977 Å
Prefix	Pil range	0.1 °
Images	Pil start (total)	200° (83°)
Transmission	Exposure Time	0.037 s
Flux start	Flux end	2.02e+11 ph/sec

P 42 212	Completeness	Res.	Rmerge
Inner	92%	3.7	3.7
Outer	98%	1.3	82.6
Overall	97%	1.3	9.0

cell A	cell B	cell C
67.2964	67.2964	100.883
Alpha	Beta	Gamma
90	90	90

Workflow Characterisation

Type	Characterization
Res. (corner)	1.3 Å (1.07 Å)
Wavelength	0.977 Å
Pil range	1 °
Pil start (total)	540° (180°)
Exposure Time	0.037 s
Flux end	2.5e+12 ph/sec

Isotropy	Mosaicity	0.45
Space Group	P4	
Rank Res.	1.33 Å	Eip. Time
Images	830	Total rotation
Transmission	7.3324	

cell A	cell B	cell C
67.25	67.25	100.66
Alpha	Beta	Gamma
90	90	90

Run #2 Characterization Dec 15, 2016 8:45:46 AM  
/data/visitor/mx1862/nc29/20161215/RAW\_DATA

Summary Beamline Parameters Data Collections 1 Sample Results Workflow

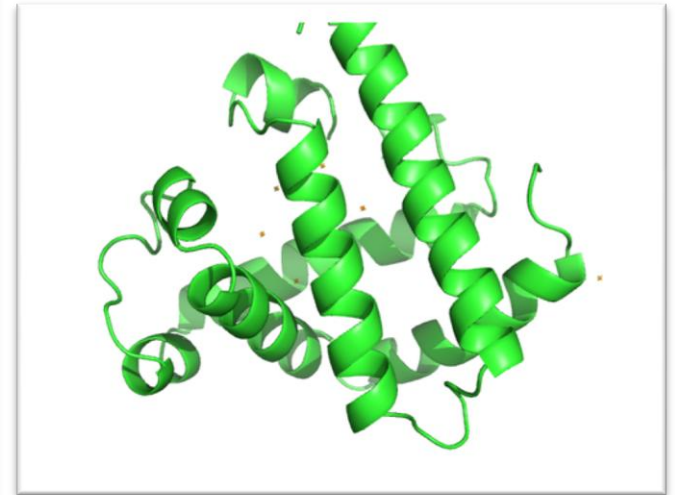
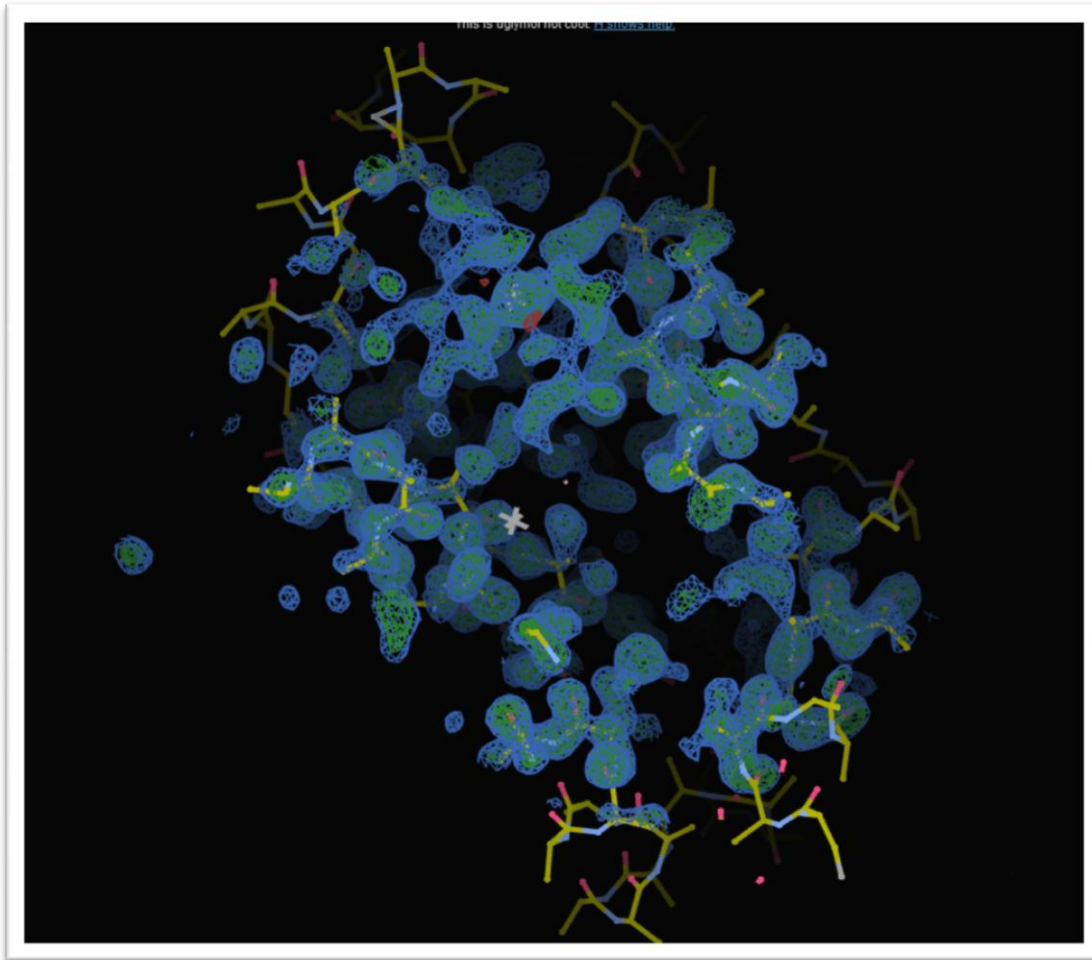
Workflow

Type

Characterization


# Structure solution results


## AutoSAD phasing pipeline




# Shipments - 1

- Description of more generic shipment to fulfill all BL needs – *to be validated*


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

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 **ESRF**

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 **ESRF**

[Home](#) [Shipments](#) [Proteins and Crystals](#) [Prepare Experiment](#) [Data Explorer](#) [Offline Data Analysis](#) [Help](#)

search by protein acronym

[Log out mx415@mx415](#)

Shipment

Name: uni\_1 Type: UNIPUCK Beamline: #Sample Changer: Status:

#	Protein Acronym	Sample Name	Crystal Form	Exp. Type	Pin BarCode	Pre-observed resolution	Needed resolution	Pref. Diameter	Number Of positions	Radiation Sensitivity	Required multiplicity	Required Completeness	Space Group	Smiles	Comments	Edit Crystal Form
1	N155H		P65 - (0 : 0 : 0   90 : 90 : 120)				0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
2	N155H		P65 - (0 : 0 : 0   90 : 90 : 120)				0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
3	N155H		P65 - (0 : 0 : 0   90 : 90 : 120)				0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
4	N155H		P65 - (0 : 0 : 0   90 : 90 : 120)				0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
5	N155HD		P21				0	0	0	0	0	0	P21			<a href="#">Edit Crystal Form</a>
6	N155H		P65 - (0 : 0 : 0   90 : 90 : 120)				0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
7	N155H		P65 - (0 : 0 : 0   90 : 90 : 120)				0	0	0	0	0	0	P65			<a href="#">Edit Crystal Form</a>
8																
9																
10																
11																
12																
13																
14																
15																
16																

S. Monaco - ISPyB meeting 17/01/17

[Remove](#) [Save](#) [Return to shipment](#)

# Shipments - 2

- Prepare experiment :
  - Simplification
  - Management of multiple sample changers of the ESRF SB beamlines

The screenshot displays the ExiMX web interface, titled "ExiMX Extended ISPyB for MX". The navigation bar includes links for Home, Shipments, Proteins and Crystals, Prepare Experiment (active), Data Explorer, Offline Data Analysis, and Help. A search bar for protein acronym and a login button for mx415@mx415 are also present.

The main content area is divided into two sections: "1 Select Shipment" and "2 Load Sample Changer".

**Loaded or to be Loaded on MiCube**

Shipment	Container	Barcode	Container type	Beamline	Sample Changer Loc...
exp1	CAK4 (3 samples)	ESP1210273	ADRAUG	C3B	
exp1	CAK5 (7 samples)	ESP1210271	ADRAUG	C3B	
SP-exonides	juak (10 samples)	ESP120324	SPMERUCK	CD-2	1
SP-exonides	juak (10 samples)	ESP120324	SPMERUCK	CD-3	
SP-exonides	juak (10 samples)	ESP120324	SPMERUCK	CD-2	
SP-exonides	juak (10 samples)	ESP120324	SPMERUCK	CD-2	
SP-exonides	juak (10 samples)	ESP120324	SPMERUCK	CD-2	

**ID30B (FlexHCD)**

The diagram shows a circular sample changer with 24 positions, numbered 1 to 24. Positions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, and 24 are shown. Positions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, and 24 are shown. Positions 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, and 24 are shown.

**Container** CAK4  
**SC Location** CAK4

Click on a sample changer location to state the desired

Unload all

# What's next for EXI-MX?

- MR pipelines results visualisation
- Reporting : extraction full & minimal reports
  - per session
  - per project
- Multiple pdb per protein for automatic MR
- Sessions page proper design
- Longer term (e.g.)
  - Offline pipeline for : “mesh & collect”
  - Ligand screening results in summary: probability to have a ligand bound?
  - Extraction of data on a project from various techniques (e.g. BIOSAXS, MX)



# ESRF Roadmap for the next 3M

## For EXI MX

- **January 17**: Validation of actual developments + mandatory little tools (e.g. manual expt annotations)
- **February 17**: “Test users” for feedback  
Collaboration ? – data on MX1816
- **March 17 onwards**:
  - Opening to all users of ESRF
  - New developments

# ISPyB – EXI/MX : a special thanks to

- Alejandro de Maria
- Sergio Gonzales
- Solange Delagenière
- Olof Svensson
- Marcin Wojdyr  
(DLS) for Uglymol
- All Automation Task Force members  
D. Van Stetten, M. Nanao, A. Mc Carthy (EMBL), M. Bowler (EMBL)
- Gordon Leonard