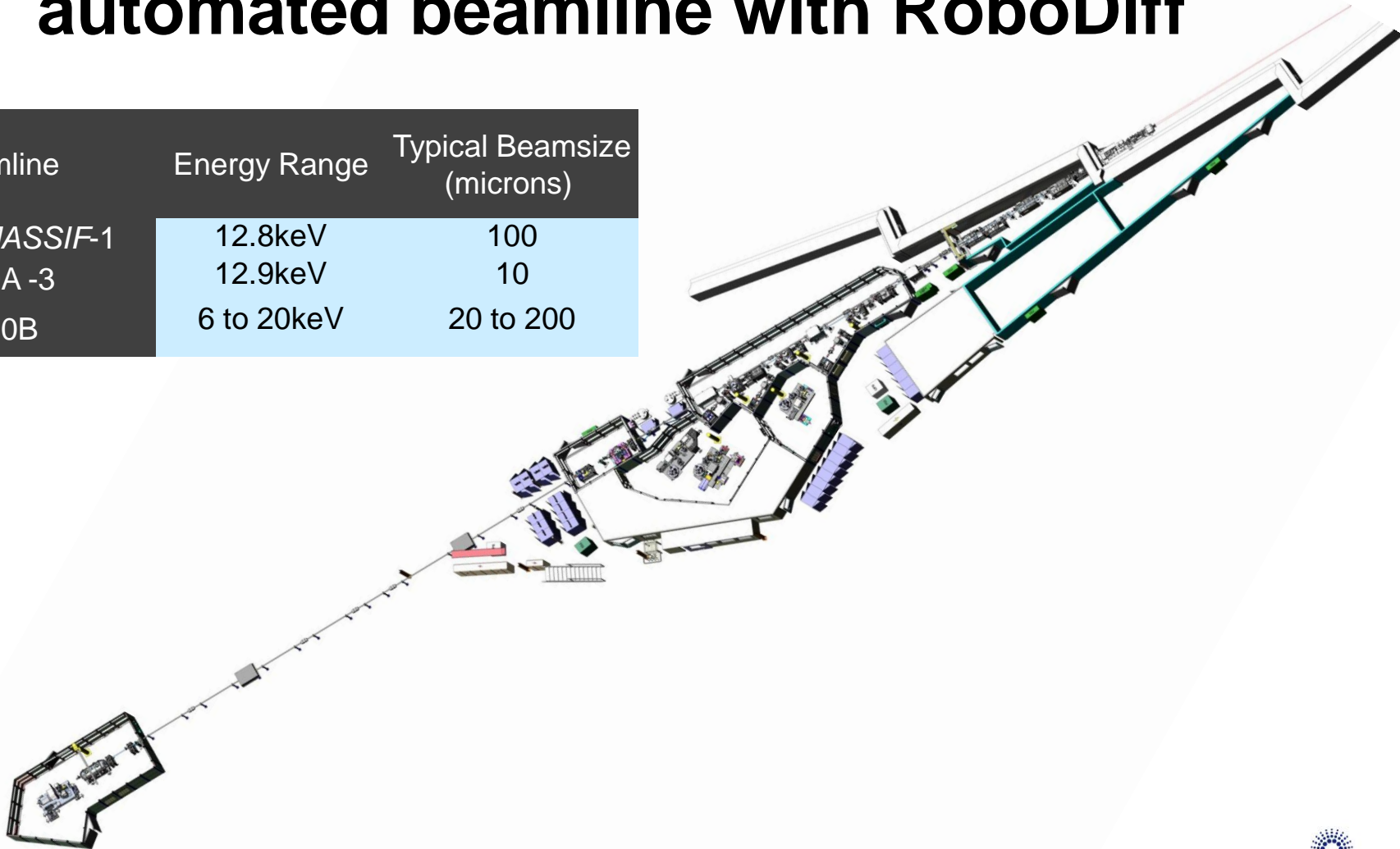
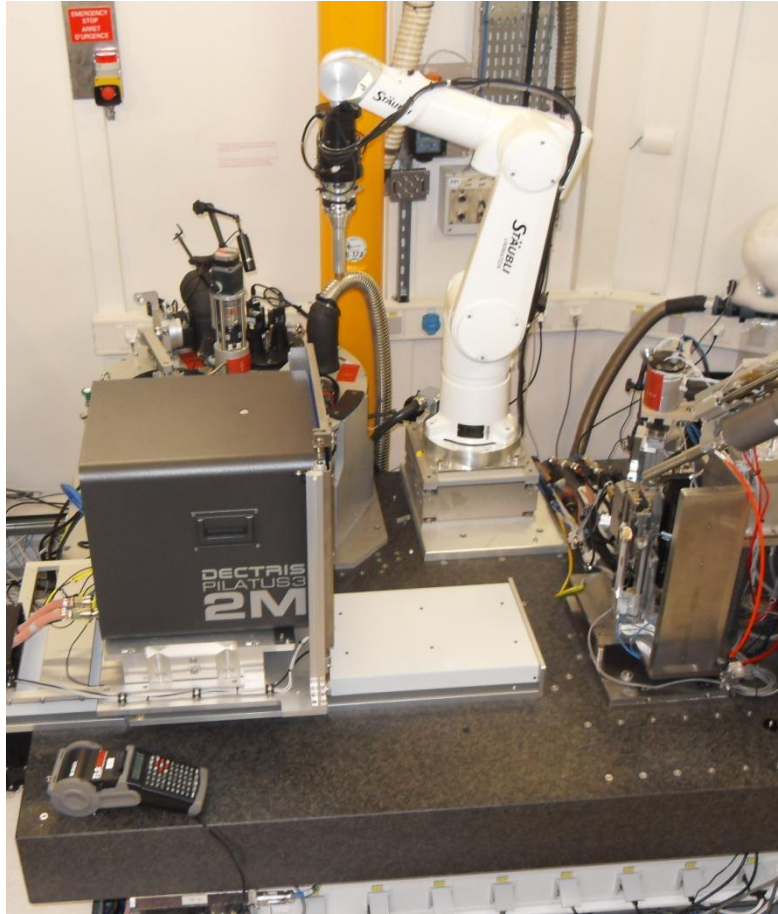


# MASSIF 1, automated beamline with RoboDiff

Beamline	Energy Range	Typical Beamsize (microns)
ID30A / MASSIF-1	12.8keV	100
ID30A -3	12.9keV	10
ID30B	6 to 20keV	20 to 200





## “Hands-off” End Station :

Diamond monochromator and Be lenses

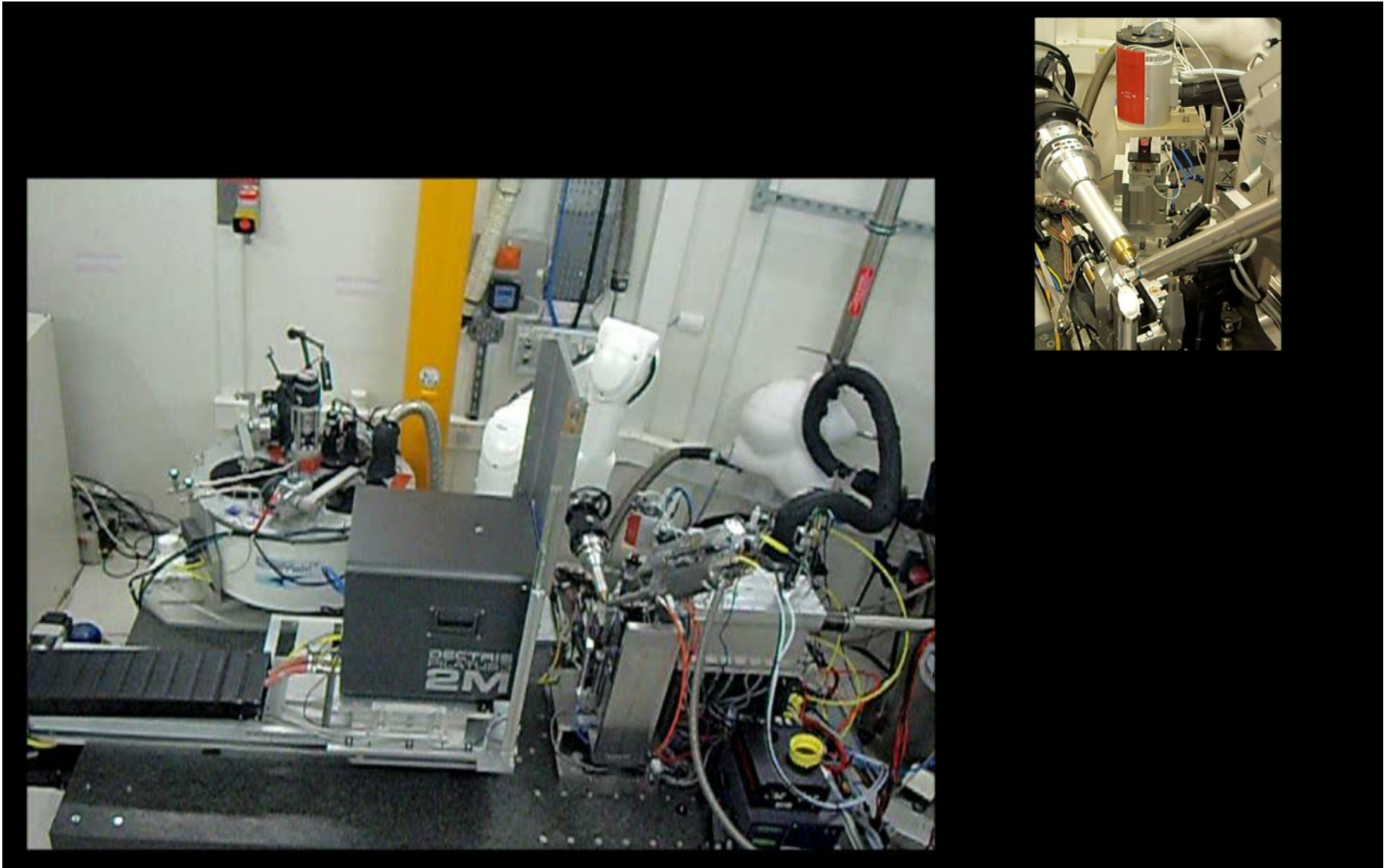
RoboDiff (Goniometer and Sample Changer)

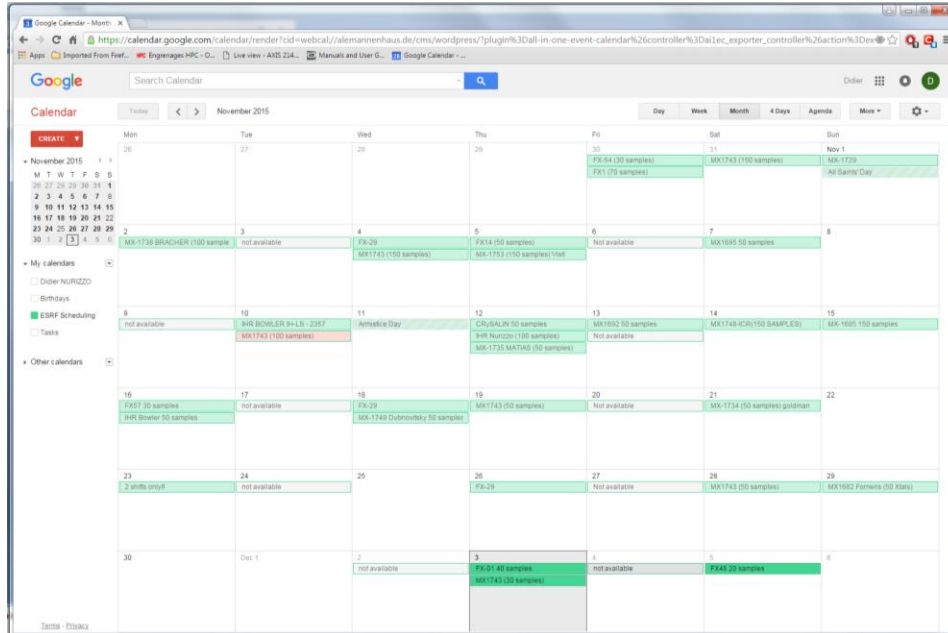
Pilatus3 2M

X-ray and rotation axis alignment

Automatic data Collection and processing

ISpyB integration





## Scheduling:

Shifts allocated to BAG

Book a slot on the MASSIF-1  
Google calendar

A form + invitation

Send crystals for slot

Samples will be processed  
within 3 working beam days  
of slot



# ROBODIFF AT MASSIF 1

**ISPyB** Home page to create and manage beamline

Lab-contacts | **Samples** | Prepare experiment | Data collection | Feedback | References | Help

Create  
 • Shipment  
 • Puck  
 • CSV upload  
 View  
 • Shipments  
 • Dewars  
 • Search  
 • Shipment  
 • Dewar

A Shipment consists of a set of Dewars which is sent from your home lab to the synchrotron via a courier company. Each dry shipping Dewar within the shipment is identified by a label (barcode or sticker). The dewars(s) contains a set of Containers (Pucks or cassettes). Containers (typically Pucks), contain Samples. A Sample Cassette Holder contains the Crystals.

Dewars Containers Samples

Tracking your shipment & contents (Dewars, toolboxes etc) allows you to follow the progress of your shipment from your home Lab to the ESRF. This feature also provides for:

- Generation of Dewar and shipment labels for sending your shipment by courier.
- Notification by email of your shipment arrival and departure from The ESRF. Returned shipment notifications also include the courier tracking number to allow you to track the shipment while in transit back to your home laboratory.
- Location of your shipment at The ESRF.

Laboratory (internal control)	Courier (date in ESRF / date in courier)	ESRF - Shores (date in Shore City)	ESRF - Beamline (Beamline ID)
Create shipment	Prepare Dewar with ICPs	Check in arrival at the ESRF	Check in arrival at the beamline
Send Dewar to courier	Shipment received	Shipment received	Shipment received
Shipment received back	Shipment received	Shipment received	Shipment received

**ISPyB** Home page to create and manage beamline

Lab-contacts | **Samples** | Prepare experiment | Data collection | Feedback | References | Help

### What you can do in the samples pages

Create

- New sample
- New crystal form
- Proteins and crystal forms
- Search
- Protein
- Sample
- Update Database

**View**

Proteins and crystal forms

To display all the proteins you have entered through samplesheets and the crystal forms associated. Click on a protein acronym to retrieve the list of all samples coming from this protein. Click on crystalForm space group to retrieve the list of all samples coming from this crystal form.

All samples

To display the list of all your samples. Click on edit to adapt/update sample parameters after experiment. Click on Diffraction plan to edit the diffraction plan parameters you want (By default the parameters you submitted through samplesheets are kept). Click on the sample name to have all the characteristics of this sample.

Search

Forms to search for a particular protein or a particular sample.

Update Database

If some protein acronyms are missing in the list when creating a sample, you can get them by updating ISPyB database.

ESRF | ESRF | BSLA | SEINE | HSD | SOLEIL  
 Copyright © 2004 ISPyB All rights reserved.

**ISPyB** Home page to create and manage beamline

Lab-contacts | Shipment | **Prepare experiment** | Data collection | Feedback | References | Help

Prepare your experiment:

1. Select the dewars you want for processing.
2. Fill the sample changer, assign a location for your containers (only required if not using Diamond codes).
3. Associate data collections to samples in mcCuB.

First step: Select the Dewars

```

    graph TD
        A[Select the Dewars] --> B[Fill the Sample Changer]
        B --> C[Link Samples with Containers]
    
```

Linking Samples to Data Collection: how does it help my experiment?

Linking Samples of your Shipment (sample descriptions) with Crystals in the Sample changer (physical samples) will allow you to associate the Data Collections made on these crystals to their Sample description. Then, you will be able to make Sample Ranking or to make reports that can be processed by your LISTS.

```

    graph TD
        A[Home Laboratory] --> B[Create & Fill Shipment]
        A --> C[Sample sent to the Facility]
        B --> D[Sample Descriptions]
        C --> E[Data Collection]
        D --> F[Linking Samples with Data Collections]
        E --> F
        F --> G[Sample Ranking]
        F --> H[Sample Reports]
    
```

ESRF | ESRF | BSLA | SEINE | HSD | SOLEIL  
 Copyright © 2004 ISPyB All rights reserved.

File | Instrumentation | Help

Collect XRF spectrum Log

User: mx1587 Group: Set Logout

Sample list  
 Mode: Sample changer  
 Centring: Fully Automatic

Sample centring  
 Sample position  
 Omega: 214.30  
 Chi: 0.00  
 Phi: 1.0  
 Tilt: 0.672  
 Tilt: 1.0  
 Tilt: 0.41

Sample video  
 Light: 0.79  
 Focus: 1.300  
 Front light: 0.00  
 Zoom: 3

Collection method  
 Standard Collection  
 Acquisition  
 Oscillation range: 1.0  
 First image: 1  
 Oscillation start: 214.30  
 Number of images: 4  
 Exposure time: 0.267  
 Energy (keV): 12.8483  
 Resolution (Å): 2.232  
 Transmission (%): 100.0  
 Data location  
 Folder: /usr/local/mx1587/1103/20141006/RAW\_DATA  
 File name: <acronym><name>\_1\_###.cbf  
 Prefix: <acronym><name>  
 Run number: 1

Machine current  
 171.6 mA  
 02:29

Flux  
 Energy: 12.8483 keV  
 Wavelength: 0.965 Å  
 Resolution: 2.232 Å  
 Current: 269.69 mA  
 Move to: A  
 Transmission: 100.00%  
 Set to: Filters

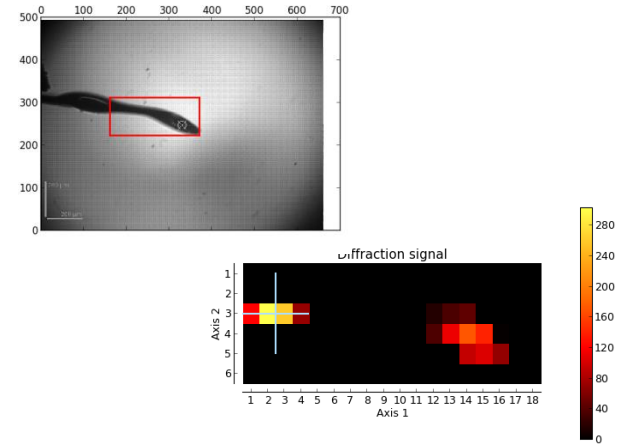
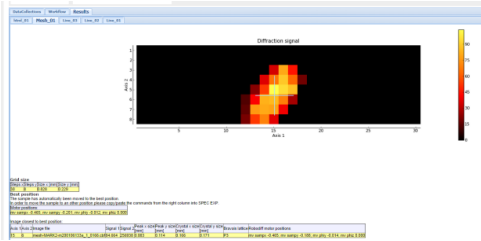
Safety shutter: opened  
 Fast shutter: closed  
 Beamstop: in  
 Current users: capak

2014-10-06 18:20:52 Workflow: Optimal strategy has been calculated and been transferred to the mcCuB queue.  
 2014-10-06 18:20:52 Workflow: Workflow finished successfully.

## User experiments linked to ISPyB

- Dewar tracking
- Safety coordination
- Data collection and processing
- File transfer

Image Profile	Run No	Experiment Type	Protein Acronym	Start time	# images	Experiment Parameters	Status	Space Group	Completeness	Resolution	Rayem (over/observed)	Unit_cell (a, b, c, alpha, beta, gamma)	Sample Ranking	Skip	Comments	Download additional files
SPB92-m20010111a	1	OSG		09-10-2014 12:02:19	940		🟢🟢🟢🟢	P 61	95.5-6.6 1.97-1.9 47.05-1.9	2.7	119.80, 119.80, 105.40 90.00, 90.00, 120.00					
sp19992-m20010113a	4	OSG		09-10-2014 12:01:12	4		🟢🟢🟢🟢	P 3	2.21		120.32, 120.32, 106.32 90.00, 90.00, 120.00					
sp19992-m20010113a	4	OSG		09-10-2014 12:00:26	40		🟢🟢🟢🟢									
sp19992-m20010113a	3	OSG		09-10-2014 11:59:36	40		🟢🟢🟢🟢									
sp19992-m20010113a	2	OSG		09-10-2014 11:58:50	40		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:58:12	30		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:57:52	30		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:57:31	30		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:57:10	30		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:56:50	30		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:56:29	30		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:56:08	30		🟢🟢🟢🟢									
sp19992-m20010113a	1	OSG		09-10-2014 11:55:54	30		🟢🟢🟢🟢									



ISPyB interface showing session information and data collection results. The 'Data collection' tab is highlighted in red.

**Session Information:**  
 Local Contact: Didier Nurizzo/Helm Dorel  
 Comments: HiWond estimated data collection Device1 completed, Device2 (DVA) now processing.

**Session Statistics:**  
 Nb Collect: 1162  
 Nb Frame: 76  
 Nb Energy Scans: 0  
 Nb IOPictures: 0

**Reports:**  
 General report: [icon]  
 Screening report: [icon]  
 HiWond/HiWond report: [icon]

Equipment	Acronym	Image Profile	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Second Graph	Comments
SPB92	PHNX-m20010113a	SPB92-m20010113a	1	Nb diff images: 346 Nb images: 324 Nb scans: 22 Phi range: 0.25 Delta: 1.822 deg/2 Distances: 500.22 Å Resolution: 5.862 Å Total exposure: 65.82 s	HiWond EDS: 15.0 Screening: P 61 Completeness: [bar]					
SPB92	PHNX-m20010113a	SPB92-m20010113a	1	Nb diff images: 324 Nb images: 304 Nb scans: 20 Phi range: 0.25 Delta: 1.822 deg/2 Distances: 500.22 Å Resolution: 5.862 Å Total exposure: 58.19 s	HiWond EDS: 15.0 Screening: P 61 Completeness: [bar]					
SPB92	PHNX-m20010114b	SPB92-m20010114b	1	Nb diff images: 394 Nb images: 374 Nb scans: 24 Phi range: 0.25 Delta: 1.822 deg/2 Distances: 500.22 Å Resolution: 5.862 Å Total exposure: 112.69 s	HiWond EDS: 15.0 Screening: P 61 Completeness: [bar]					

Mesh scan:

Aperture 50µm

37% transmission

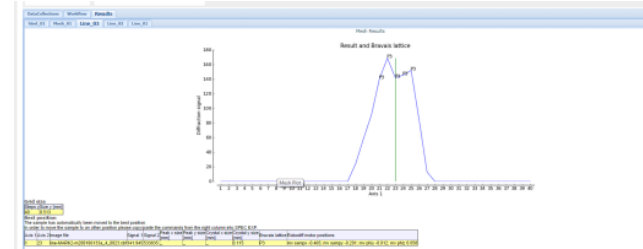
700µm for 30 images in 8s

300µm for 8 lines

Analyzed with Dozor

# ROBODIFF AT MASSIF 1

Image Profile	Run No	Experiment Type	Problem Acronym	Start time	# Images	Experiment Parameters	Status	Space Group	Completeness	Resolution	Rayton Clear (Clear/Default)	Unit_cell a, b, c	Sample Ranking	Skip	Comments	Download as PDF
img3092-m00104133a	1	OSC		09-10-2014 12:02:19	940		🟢🟢🟢	P 61	99-5.66 157-1.53 47.85-1.3	2.7	119.80, 119.80, 105.60 90.00, 90.00, 120.00	4.1				
img3092-m00104133a	4	OSC		09-10-2014 12:03:12	4		🟢🟢🟢	P 61		2.21	120.32, 120.32, 106.32 90.00, 90.00, 120.00					
img3092-m00104133a	3	OSC		09-10-2014 11:59:36	40		🟢🟢🟢									
img3092-m00104133a	2	OSC		09-10-2014 11:58:50	40		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:58:12	30		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:57:52	30		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:57:31	30		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:57:10	30		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:56:50	30		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:56:29	30		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:56:08	30		🟢🟢🟢									
img3092-m00104133a	1	OSC		09-10-2014 11:55:34	30		🟢🟢🟢									



Rotation Axis Alignment :

Aperture 50 $\mu$ m

100% transmission

2 scans (0/180 $^\circ$ ) 400 $\mu$ m for 40 images in 4s

Horizontal Alignment :

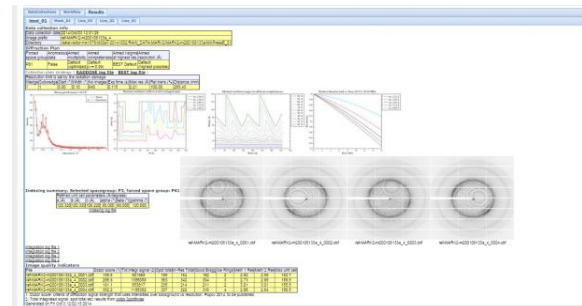
Aperture 50 $\mu$ m

80% Attenuation

1 scan (90 $^\circ$ ) 500 $\mu$ m for 40 images in 5s

# ROBODIFF AT MASSIF 1

Image Profile	Run No	Experiment Type	Protein Acronym	Start time	# Images	Experiment Parameters	Status	Space Group	Completeness	Resolution	Rayton Score (Overall)	Unit Cell a, b, c	Sample Ranking	Skip	Comments	Download as Image File
img59892-m200106113a	1	OSC		09-10-2014 12:02:19	940		●●●●	P 61	99.99% 99.99%	50 - 5.66 1.97 - 1.9 47.85 - 1.9	2.7 139.0 4.1	119.80, 119.80, 105.60 90.00, 90.00, 120.00				
img59892-m200106113a	4	OSC		09-10-2014 12:03:12	40		●●●●	P 61	99.99% 99.99%	2.21		120.32, 120.32, 106.32 90.00, 90.00, 120.00	95			
img59892-m200106113a	4	OSC		09-10-2014 12:03:26	40		●●●●									
img59892-m200106113a	3	OSC		09-10-2014 11:59:36	40		●●●●									
img59892-m200106113a	2	OSC		09-10-2014 11:59:50	40		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:59:12	30		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:57:52	30		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:57:31	30		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:57:10	30		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:56:50	30		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:56:29	30		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:56:08	30		●●●●									
img59892-m200106113a	1	OSC		09-10-2014 11:55:34	30		●●●●									



EDNA characterisation:

Aperture 50 $\mu$ m

100% transmission

4 images 90° apart 1° / 0.267s

Analyzed with Dozor, Best / Labelit/Mosflm including crystal size



more than 15,000 samples collected since September 2014

Image Prefix	Run No	Experiment Type	Problem Acronym	Start time	# Images	Experiment Parameters	Status	Space Group	Completeness	Resolution	Rayson	Unit Cell	Sample Ranking	Skip	Comments
39892-m20106113a	1	OSC		09-10-2014 12:02:19	940		OK	P 61	99.5%	50 - 5.66 157 - 1.9	139.0 47.85 - 1.9	119.80, 119.80, 105.60 90.00, 90.00, 120.00	1		
39892-m20106113a	4	OSC		09-10-2014 12:01:12	4		OK	P 3	99.5%	2.21	120.32, 120.32, 106.32 90.00, 90.00, 120.00	2			
39892-m20106113a	4	OSC		09-10-2014 12:00:26	40		OK								
39892-m20106113a	3	OSC		09-10-2014 11:59:36	40		OK								
39892-m20106113a	2	OSC		09-10-2014 11:59:36	40		OK								
39892-m20106113a	1	OSC		09-10-2014 11:58:12	30		OK								
39892-m20106113a	1	OSC		09-10-2014 11:57:52	30		OK								
39892-m20106113a	1	OSC		09-10-2014 11:57:31	30		OK								
39892-m20106113a	1	OSC		09-10-2014 11:57:10	30		OK								
39892-m20106113a	1	OSC		09-10-2014 11:56:50	30		OK								
39892-m20106113a	1	OSC		09-10-2014 11:56:29	30		OK								
39892-m20106113a	1	OSC		09-10-2014 11:56:08	30		OK								
39892-m20106113a	1	OSC		09-10-2014 11:55:34	30		OK								

Experiment parameters | Baseline parameters | **AutoProcessing**

AutoProcessing Summary (Click on an entry for more details)

Method	Point Group	Cell A	Cell B	Cell C	Cell Alpha	Cell Beta	Cell Gamma
Anomalous: OFF (Friedel pairs merged) (2 Items)							
EDNAproc	P 61	119.8	119.8	105.6	90	90	120
fastarc	P 6	119.8	119.8	105.6	90	90	120
Anomalous: ON (Friedel pairs unmerged) (2 Items)							
EDNAproc	P 61	119.8	119.8	105.6	90	90	120
fastarc	P 6	119.8	119.8	105.6	90	90	120

RSymm threshold in lower shell:  / Sigma threshold in lower shell:  **View Data Collection Statistics:**

**Main Output Parameters**

Overall:  
 Overall Resolution: 100.0-1.95 Å  
 Overall Completeness: 98.9%  
 Overall I over Sigma: 17.67  
 Overall Rsymm: 4.3%  
 Overall Multiplicity: 5.3

**Outer Shell:**  
 Outer Shell Resolution: 2.02-1.95 Å  
 Outer Shell Completeness: 91.4%  
 Outer Shell I over Sigma: 1.04  
 Outer Shell Rsymm: 128.5%  
 Outer Shell Multiplicity: 4.4

**Unit Cell:**  
 Unit Cell A: 119.8 Å  
 Unit Cell B: 119.8 Å  
 Unit Cell C: 105.6 Å  
 Unit Cell Alpha: 90.0 °  
 Unit Cell Beta: 90.0 °  
 Unit Cell Gamma: 120.0 °

Files  
 Download  
 XDS XSCALE SCALA/ADRES SCALEPACK TRUNCATE  
 Input Files:  
 XDS.INP  
 XDS.OUTPUT  
 Output Files:  
 QUPARAM.XDS

ISPyB

Lab contacts | **Shipment** | Samples | Prepare experiment | Data collection | Feedback | References | Help

View last sessions | View all sessions | Search data collections

Session Information  
 Local Context: Order Runstep/Hub Bond  
 Comments: HiRes estimated data collection Device2 completed, Device2 now processing

Session Statistics  
 Nb Collect: 1182  
 Nb Frame: 76  
 Nb Energy Scans: 0  
 Nb IFFPackets: 0

Reports  
 General report  
 Screening report  
 HiRes/HiRes/HiRes report

Experiment Type	Acronym	Sample Name	Image Prefix	Run#	Parameters	Results	Image Thumbnail	Crystal Inset	Graph	Second Graph	Comments
EDNAproc	PHN2-m20106113a	39892-m20106113a	39892-m20106113a	1	All run images: 354 All images: 354 PHN2: 354 All: 354 Resolution: 100.0-1.95 Å Completeness: 98.9% Rsymm: 4.3% Total input time: 65.82 s	HiRes OK EDNA OK Space Group: P 61 Completeness: 98.9% Rsymm: 4.3%					
EDNAproc	PHN2-m20106113a	39892-m20106113a	39892-m20106113a	1	All run images: 354 All images: 354 PHN2: 354 All: 354 Resolution: 100.0-2.28 Å Completeness: 98.9% Rsymm: 4.3% Total input time: 138.19 s	HiRes OK EDNA OK Space Group: P 61 Completeness: 98.9% Rsymm: 4.3%					
EDNAproc	PHN2-m201061145	39892-m201061145	39892-m201061145	1	All run images: 354 All images: 354 PHN2: 354 All: 354 Resolution: 100.0-2.41 Å Completeness: 98.9% Rsymm: 4.3% Total input time: 152.69 s	HiRes OK EDNA OK Space Group: P 61 Completeness: 98.9% Rsymm: 4.3%					

Data processing:

EDNA / Fast / Parallel processing

Molecular replacement / Rigid body (Dimple)

Fragment Analysis (Smiles)

## Contact

Deborah Davison (deborah.davison@esrf.fr)  
Matthew Bowler (mbowler@embl.fr)  
Didier Nurizzo (nurizzo@esrf.fr)

## Engineering Unit

Pascal Theveneau  
Werner Schmidt  
Carole Clavel

## Electronics Unit

Ricardo Hino  
Jose-Maria Clement  
Hervé Gonzalez

## Structural Biology Group

David Von Stetten  
Daniele de Sanctis  
Stéphanie Malbet Monaco  
Christoph Mueller-Dieckmann  
Gordon Leonard

Nicolas Guichard  
Mario Lentini  
John Surr  
Thierry Giraud  
Hugo Caserotto  
Julien Soudarin  
Fabien Dobias

## Beamline Control Unit

Matias Guijarro  
Antonia Beteva  
Sebastien Petitdemange

## Data Analysis Unit

Olof Svesson

## EMBL

Matthew Bowler  
Max Nanao  
Andrew  
McCarthy  
Florent Cipriani  
Gergely Papp

# ROBODIFF AT MASSIF 1

