

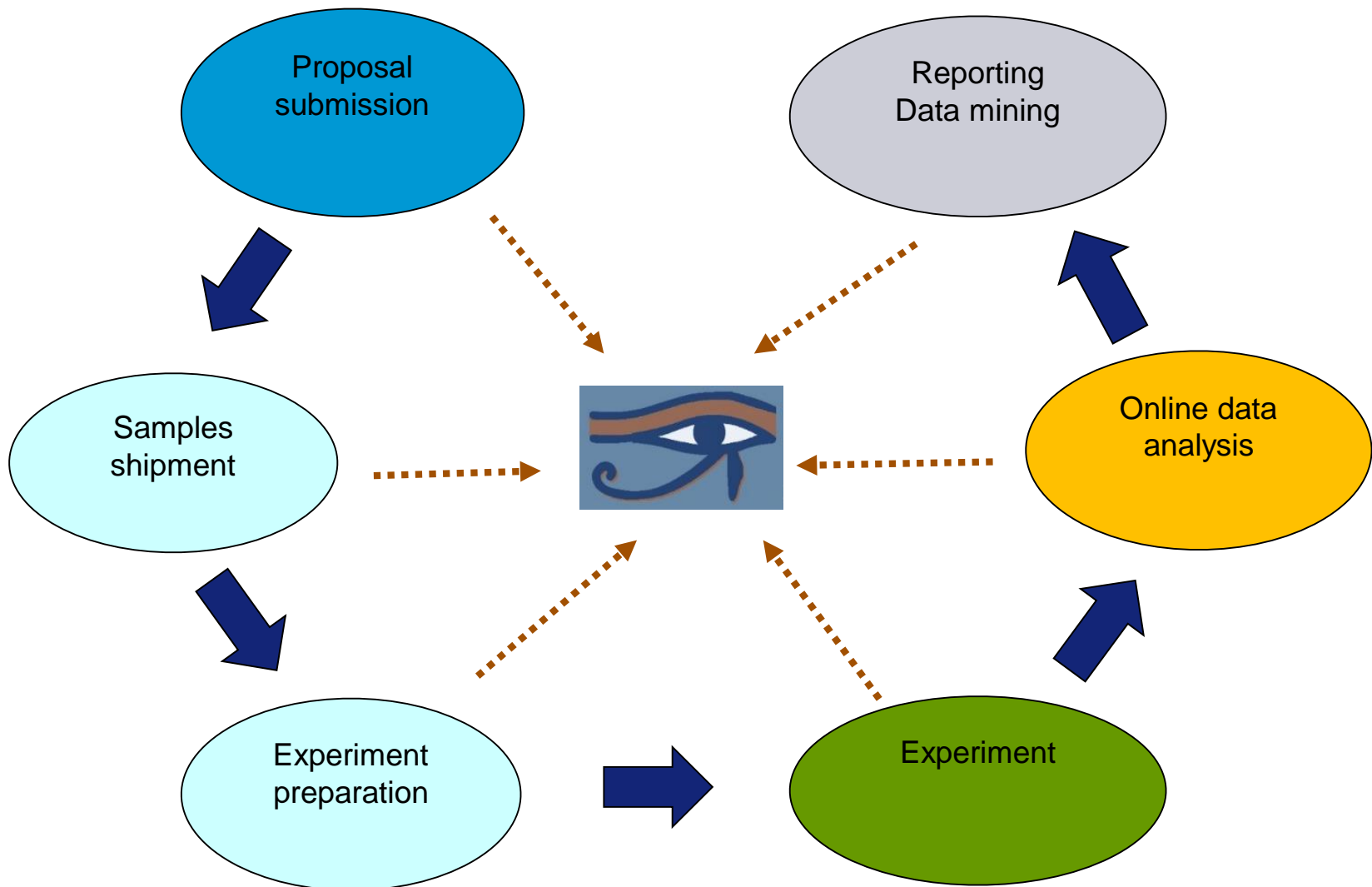
The ISPyB project: Introduction to new developers and partners

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- **What is ISPyB and why we need ISPyB**
- **History**
- **Facilities and collaborators**
- **The ISPyB environment – interaction with other systems**
- **Three techniques : MX, BioSAXS and CryoEM**
 - Sample tracking
 - Data acquisition
 - On-line data analysis
- **Collaboration**
 - Github
 - Releases
 - Developers VC

WHAT IS ISPYB : A LABORATORY INFORMATION MANAGEMENT SYSTEM



- **Simplifying experiment preparation & execution**
 - Connection with SMIS (proposal submission)
 - Sample shipment
 - Experiment preparation
- **Experiment reporting**
 - The course of the experiment can be followed by colleagues in real time
- **Real time experiment tracking & data analysis**
 - Sample characterisation
 - Automatic data processing
 - *Including download of processed data [h, k, l, I s(l) etc.]*
 - *Merged or unmerged*

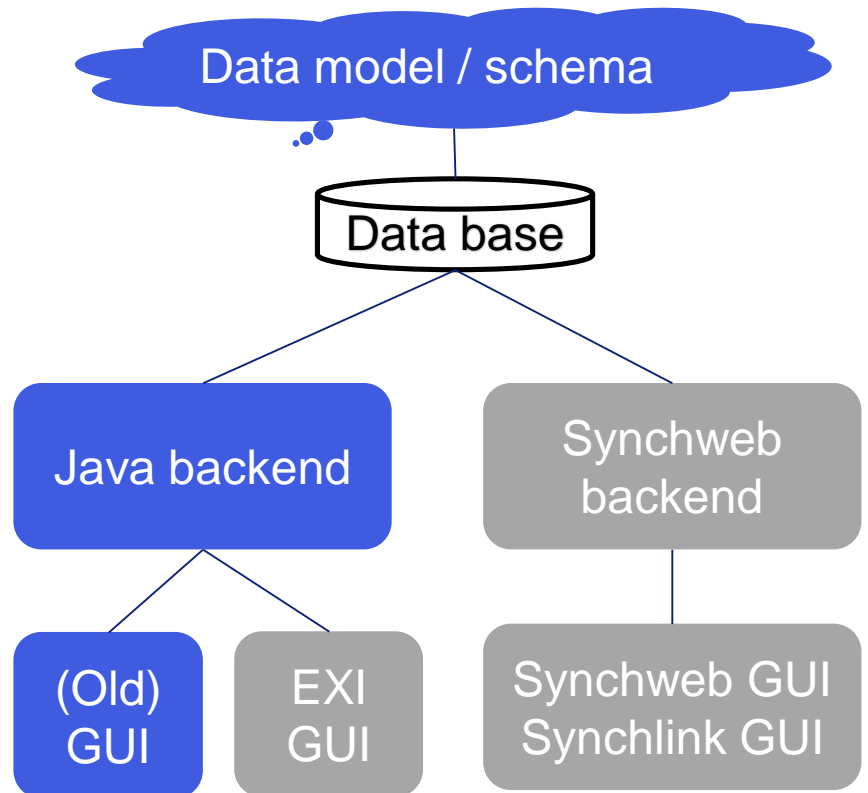
- **2001 - 2005:** Pxweb
Python/Zope, MySql
JSBG Project (ESRF/EMBL)
Experiment logging for MXPress users (FX users)
- **2005-2011:** ISPyB
Java/Struts/Jboss, Mysql
ESRF/Spine/Bioxhit and BM14/MRC/eHTPX collaboration
Pxweb features + new features + Dewar Tracking
- **2009:** Collaboration with Diamond (code sharing)
- **2012** Important upgrade :
ISPyB data model extensions (Autoprocessing, EDNA)
Jboss server 6.0, EJBs3
Web services to communicate with BLC (MXCube)
- **2012:** BioSAXS extension
Collaboration between ESRF, EMBL HH & DLS [BioSTRUCT-X]
- **2016** : Official collaboration extension
MOU (Memorandum Of Understanding) signed.

- **The ISPyB collaboration is about:**

- The database schema / data model
- The Java backend / API of web services

- **ISPyB GUIs :**

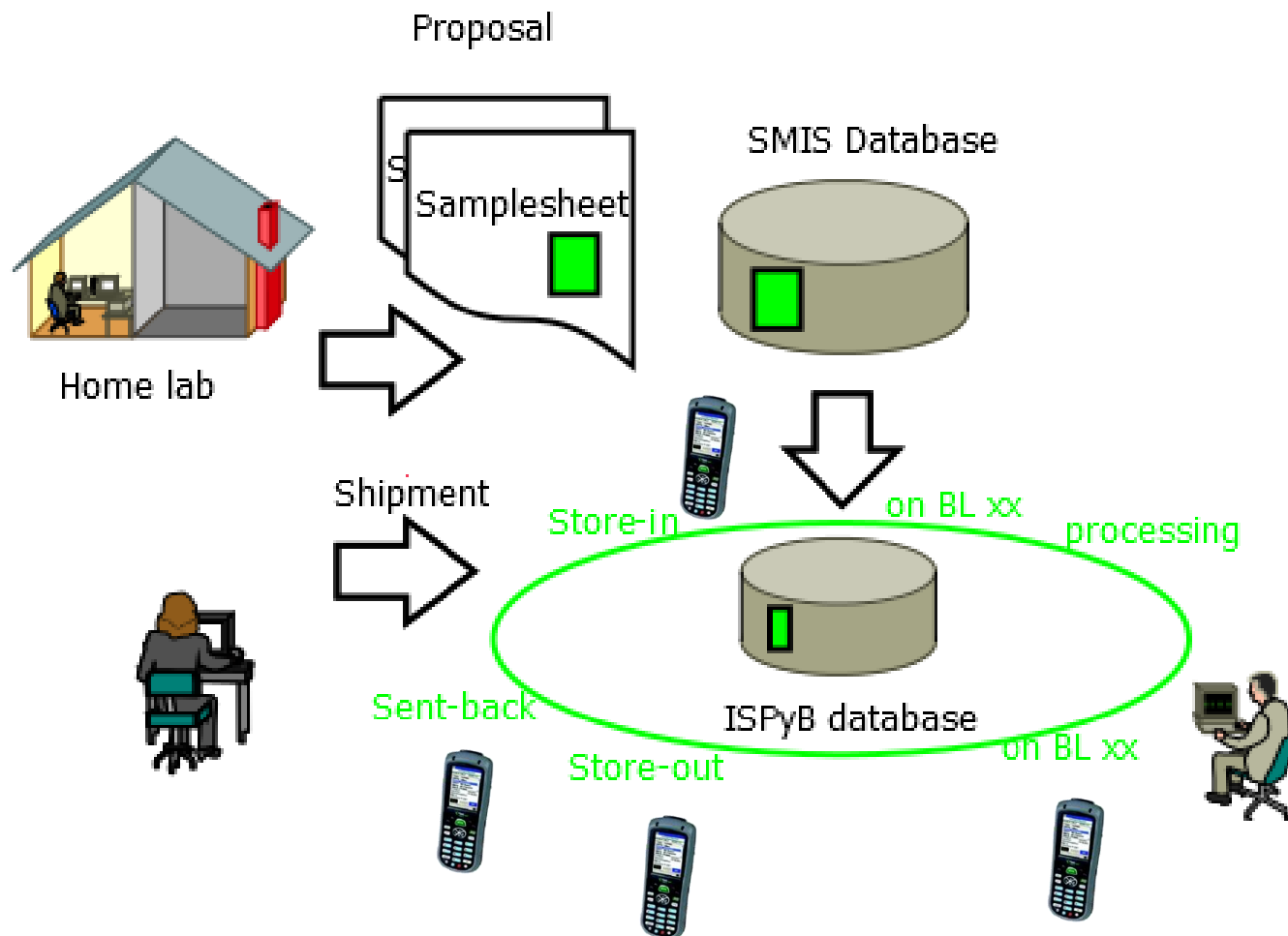
- **The official GUI** is part of the Java backend, however, it is in the process of being phased out
- The DLS GUIs **Synchweb** and **Synchlink** are not using the Java backend and are not part of the collaboration
- The **EXI** GUI developed at the ESRF and used by several facilities is using the Java backend and is not part of the collaboration



- Part of the ISPyB collaboration
- Not part of the ISPyB collaboration

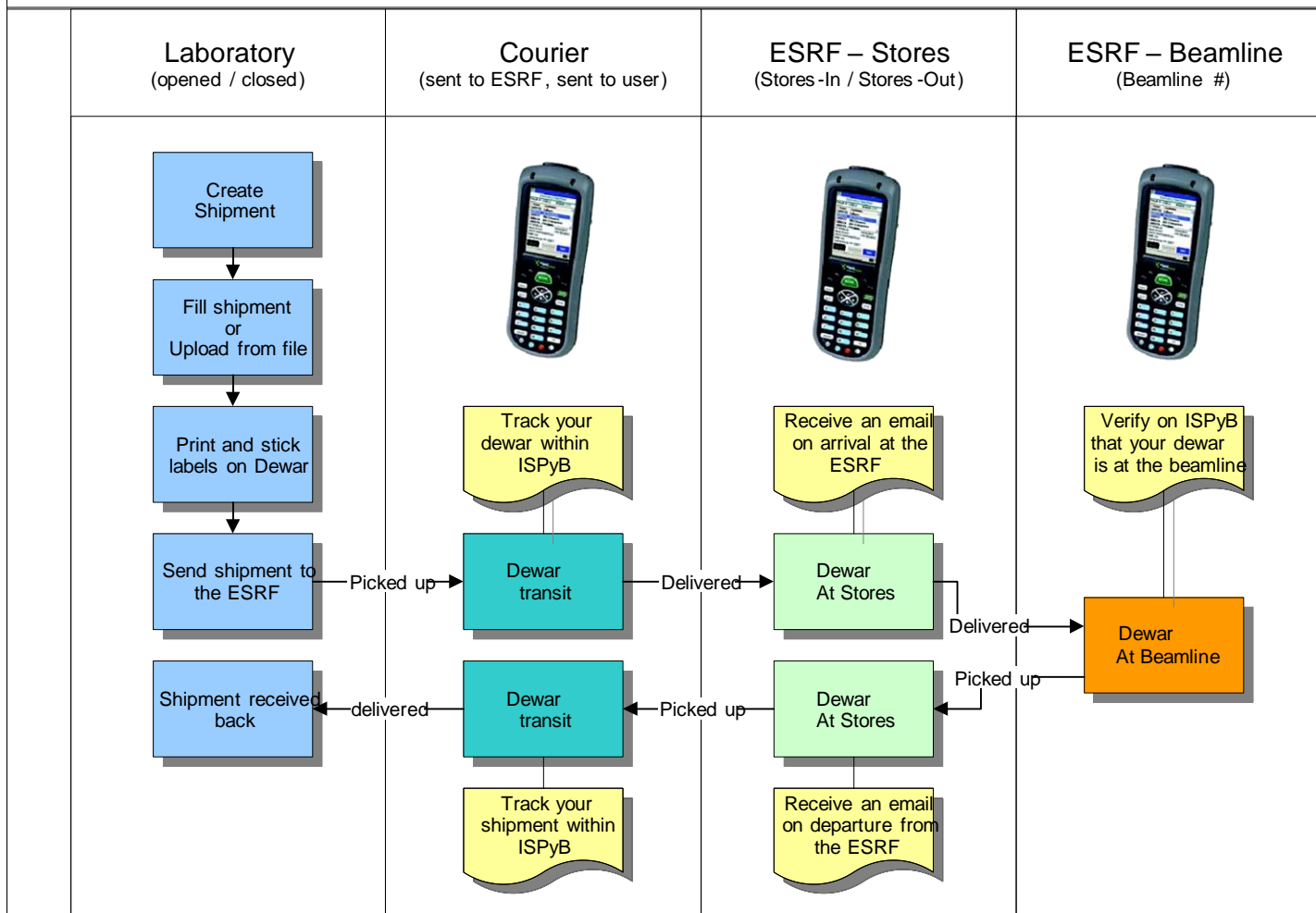
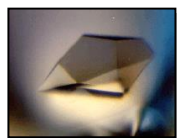
- **An ISPyB database is in production at the following facilities using the Java backend and EXI GUI:**
 - ESRF
 - Soleil
 - EMBL Hamburg
 - Max IV
 - Alba
- **An ISPyB database is in production at the following facility using the Synchweb backend and Synchweb / synchlink GUIs :**
 - DLS
- **The following facility and enterprise are participating in the collaboration:**
 - Global Phasing
 - Elettra
 - BESSY II

SAMPLE TRACKING



SAMPLE TRACKING

ISPyB Dewar Tracking



Multi techniques summary view (EXI GUI)

ExiMX Extended ISPyB for MX_{BETA} Version: 5.16 Released: 20190227 ESRF

Home Shipment Prepare Experiment Proteins and Crystals **NEW** Data Explorer Manager Help SMIS search by protein acronym Log out svensson

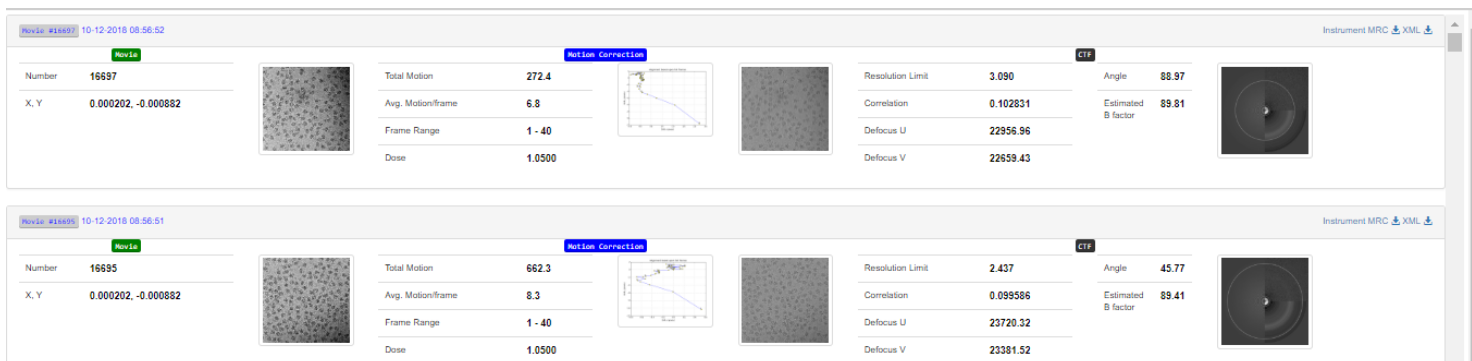
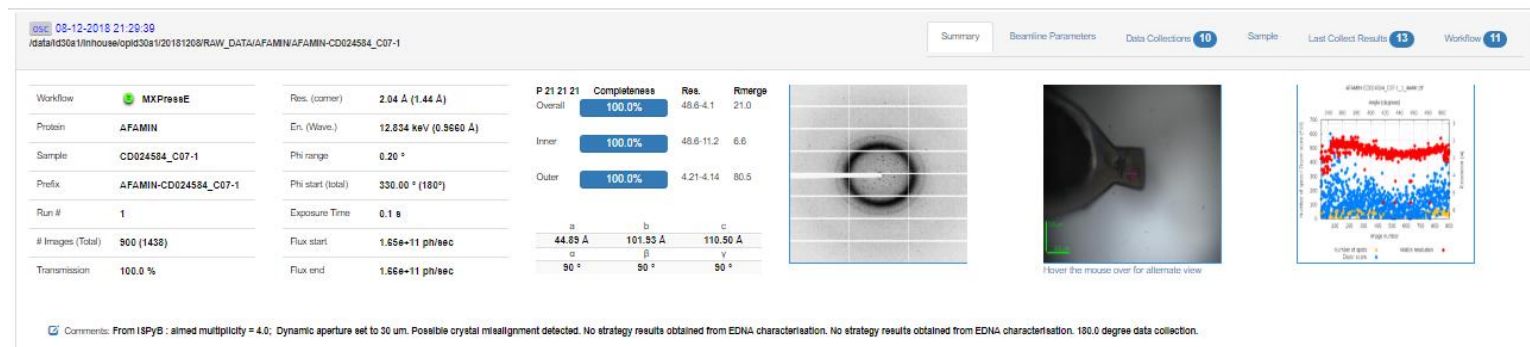
Home

Choose a Date Choose a period of time enter search term (proposal or title) search by local contact

☐ BM29 ☐ ID23-1 ☐ ID23-2 ☐ ID29 ☐ ID30A-1 ☐ ID30A-2 ☐ ID30A-3 ☐ ID30B ☐ BM30A ☐ CM01 Filter by term (proposal or title) or comment

Start	Beamline	A-form	Proposal	Local Contact	MX			BIOSAXS			EM		Comments
					En. Scans	XRF	Samples	Tests	Collects	Calibration	SC	HPLC	
08-12-2018	ID23-1		OPID231				1	2					Session created by the BCM
08-12-2018	ID30B		OPID30b				3	5					Session created by the BCM
08-12-2018	ID30A-1		OPID30a1	BOWLER M			95	66	363				MXPressE Afamin and FADH
07-12-2018	CM01		MX2136	EFFANTIN g			1		11			11	
07-12-2018	ID30A-1		MX2068	BOWLER M			55	34	255				
07-12-2018	BM29		MX2079	BRENNICH M						3	22	3	
07-12-2018	ID30B		MX1977	SOLER LOPEZ M				56	20				
07-12-2018	ID30A-3		MX2083	FLOT D				11	1042				
07-12-2018	ID23-2		MX1997	ZUBIETA C				218	37				

EXAMPLE OF MX, BIOSAXS AND CRYOEM RESULTS DISPLAY (IN EXI)



EXAMPLE OF ON-LINE DATA ANALYSIS RESULTS (MX IN EXI)

08-12-2018 21:29:39

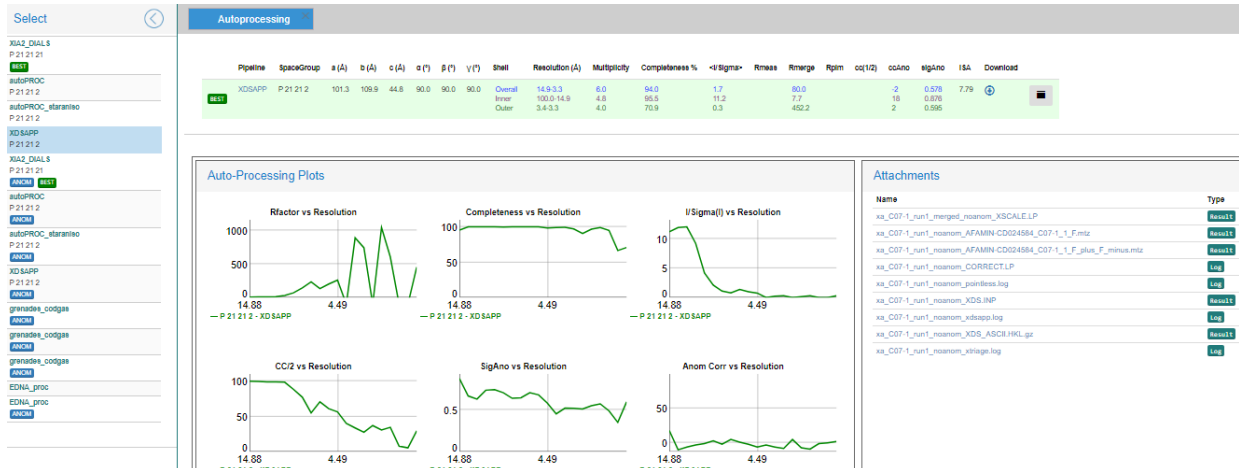
/data/d30a1/inhouse/opid30a1/20181208/RAW_DATA/AFAMIN/AFAMIN-CD024584_C07-1

Summary

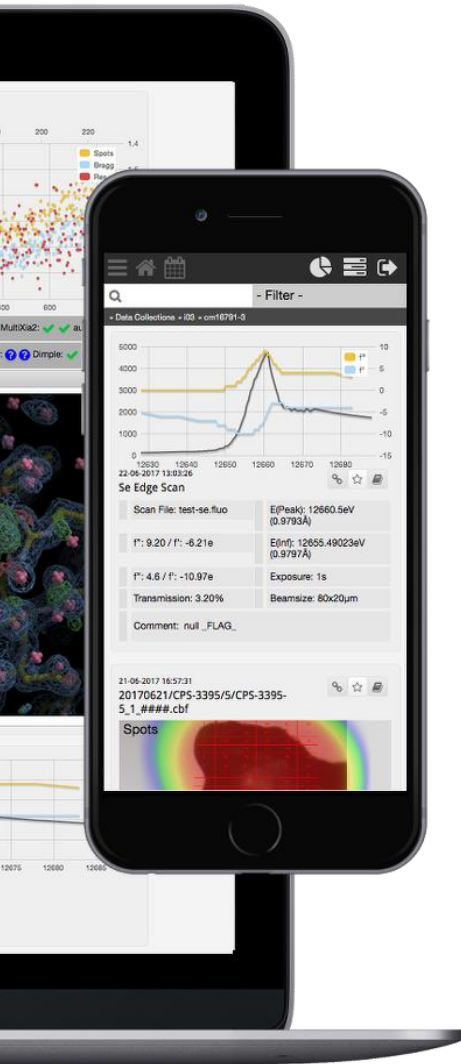
Beamline Parameters

Data Collections

	Pipeline	SpaceGroup	a (Å)	b (Å)	c (Å)	α (°)	β (°)	γ (°)	Shell	Resolution (Å)	Multiplicity	Completeness %	<I>/Sigma>	Rmeas	Rmerge	Rpim	cc(1/2)	ccAno	sigAno	ISA	Download		
BEST	XIA2_DIALS	P 21 21 21	44.9	101.9	110.5	90.0	90.0	90.0	Overall Inner Outer	48.6-4.1 48.6-11.2 4.2-4.1	6.1 5.5 6.8	100.0 100.0 100.0	4.9 13.9 1.4	21.0 6.6 80.5	100 100 90						4		
	autoPROC	P 21 21 21	101.5	110.0	44.5	90.0	90.0	90.0	Overall Inner Outer	74.6-5.7 74.6-15.4 5.8-5.7	6.0 5.0 5.6	99.8 96.0 100.0	10.2 18.3 2.3	11.5 6.2 71.5	100 100 90						4		
	autoPROC_staraniso	P 21 21 21	101.5	110.0	44.5	90.0	90.0	90.0	Overall Inner Outer	74.6-3.8 74.6-12.0 4.0-3.8	6.1 5.5 5.9	84.8 98.1 44.4	6.4 18.4 1.3	21.9 7.2 127.3	100 100 60						4		
ANOM	XDSAPP	P 21 21 21	101.3	109.9	44.8	90.0	90.0	90.0	Overall Inner Outer	14.9-3.3 100.0-14.9 3.4-3.3	6.0 4.8 4.0	94.0 95.5 70.9	1.7 11.2 0.3	80.0 7.7 452.2			-2 18 2	0.578 0.876 0.595	7.79			4	
	XIA2_DIALS	P 21 21 21	44.9	101.9	110.5	90.0	90.0	90.0	Overall Inner Outer	48.6-4.2 48.6-11.3 4.3-4.2	3.4 3.7 3.6	99.7 100.0 96.5	5.1 14.0 1.6	20.2 6.7 76.7	100 100 90						4		
	autoPROC	P 21 21 21	101.5	110.0	44.5	90.0	90.0	90.0	Overall Inner Outer	74.6-5.7 74.6-15.4 5.8-5.7	3.5 3.6 3.1	99.7 95.0 100.0	10.4 18.5 2.4	11.3 6.2 70.1	100 100 90						4		
ANOM	autoPROC_staraniso	P 21 21 21	101.5	110.0	44.5	90.0	90.0	90.0	Overall Inner Outer	74.6-3.8 74.6-11.9 4.0-3.8	3.5 3.7 3.6	83.3 98.1 41.9	6.5 16.6 1.3	21.7 7.0 131.9	100 100 60						4		
	XDSAPP	P 21 21 21	101.3	109.9	44.8	90.0	90.0	90.0	Overall Inner Outer	14.9-3.3 100.0-14.9 3.4-3.3	3.3 3.4 2.2	94.5 94.9 69.9	1.3 9.7 0.3	74.3 7.6 364.8			4 19 22	0.595 0.952 0.667	7.66			4	
	granades_codgas											TIMEOUT											
ANOM	granades_codgas											TIMEOUT											



ISPYB AT DLS : AUTO-PROCESSING RESULTS DISPLAY IN SYNCHLINK AND SYNCHWEB



21-11-2015 15:10:10 - 20151121/lys/Lys_Nov15_3_1_####.cbf

Sample: [Lys_Nov15_3](#) Flux: 4.91e+11

Ω Start: 89.0° Ω Osc: 0.15°

Ω Overlap: 0° No. Images: 9000

Resolution: 1.45Å Wavelength: 0.9763Å

Exposure: 0.030s Transmission: 100.00%

Beamsize: 50x20µm Type: SAD

Comment: (-51,427,-248) EDNAstrategy4: subWedge:1Aperture: Medium_FLAG_

Auto Processing Fast DP: ☒ Xia2: ☒ ☒

Fast DP ☒ XIA2 3dii ☒ XIA2 3d ☒ DIALS

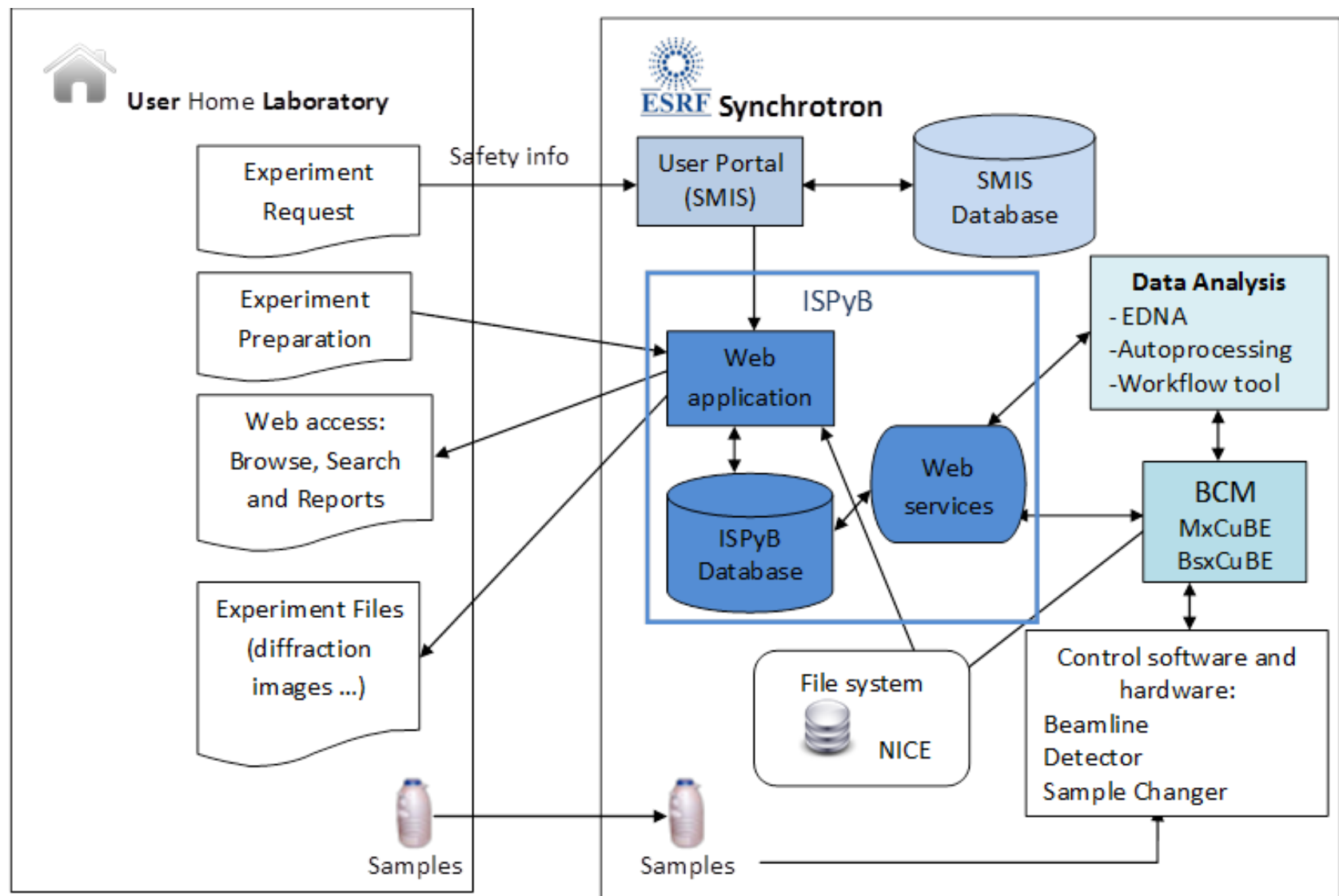
Beam Centre	X	Y
Start	215.61	208.50
Refined	215.74	208.69
Δ	-0.13	-0.19

Space Group	A	B	C	α	β	γ
P 4 2 2	77.97	77.97	37.46	90.00	90.00	90.00

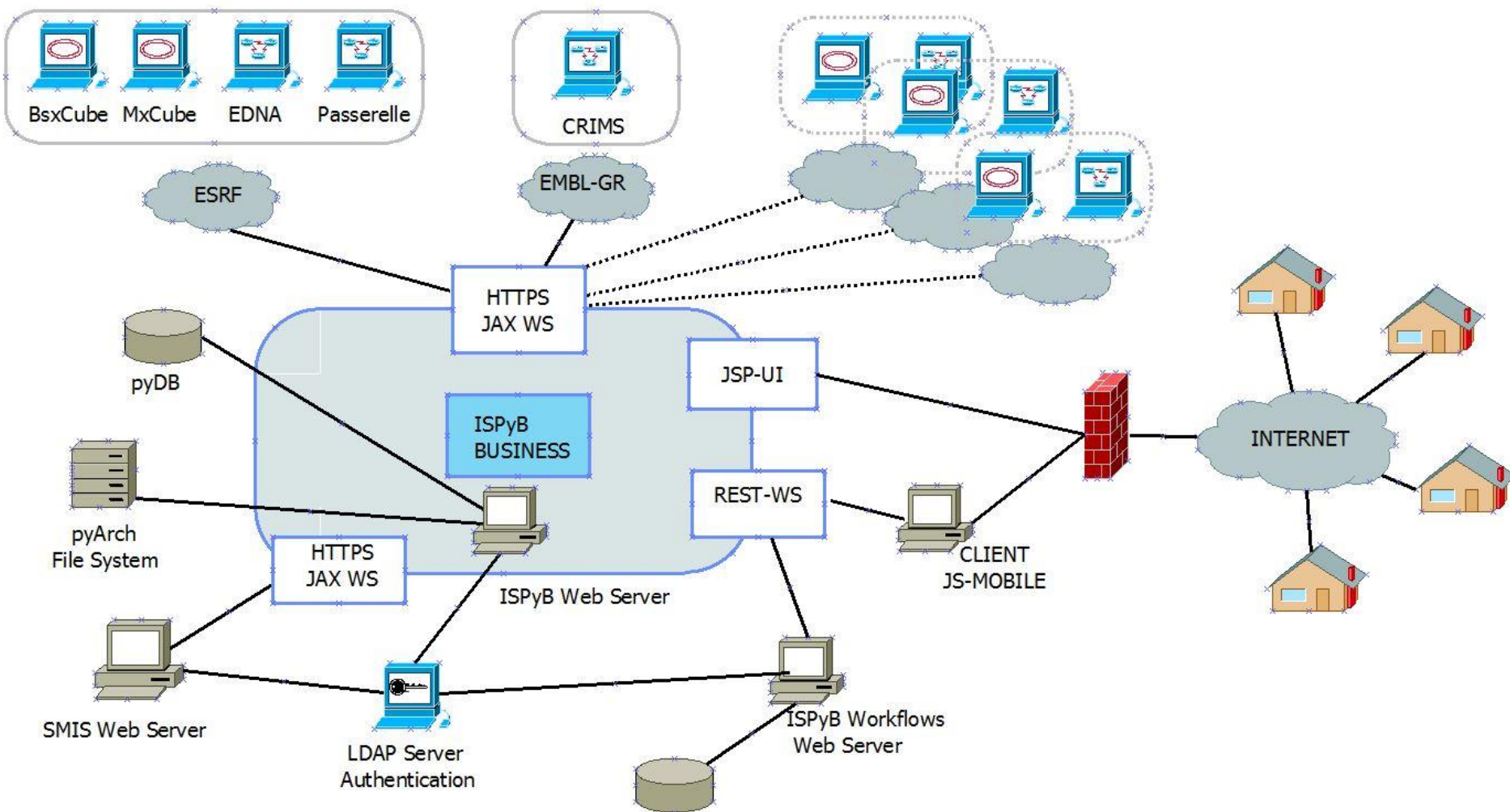
Shell	Observations	Unique	Resolution	Rmeas	I/sig(I)	CC Half	Completeness	Multiplicity	Anom Completeness	Anom Multiplicity	CC Anom
overall	943912	10754	1.83 - 27.57	0.114	45.9	100.0	99.8	87.8	99.6	47.3	17.6
outerShell	58826	765	1.83 - 1.87	0.972	5.2	87.9	98.2	76.9	95.2	41.1	-21.9
innerShell	9238	158	8.16 - 27.57	0.051	93.7	100.0	97.8	58.5	100.0	43.6	27.9

Downstream Processing Fast EP: ☒ Dimple: ☒ MrBUMP: ☒

THE ISPYB ENVIRONMENT



ISPYB @ ESRF: CURRENT ARCHITECTURE



- **The ISPyB project web page is located at :**
 - <https://ispyb.github.io/ISPyB>
- **The source code of the ISPyB project are located at :**
 - <https://github.com/ispyb/ISPyB>
This site also contains the ISPyB issue tracker :
<https://github.com/ispyb/ISPyB/issues>
- **Other resources available on github :**
 - <https://github.com/ispyb/ispyb-database-modeling>
Documentation and issues related to the ISPyB database datamodel
 - <https://github.com/ispyb/EXI>
The EXI ISPyB user interface – not part of the ISPyB collaboration

- The master branch of <https://github.com/ispyb/ISPyB> is considered to be stable
- The latest official release is a tag of the master branch :
 - <https://github.com/ispyb/ISPyB/releases>
- An ISPyB release has two or three version numbers :
 - **X.Y** or **X.Y.Z**
 - **X** and **Y** are major versions.
An increase of **X** implies deep changes of the ISPyB internal structure
An increase of **Y** means a change of the API
 - The latest release as of March 12th 2019 is **5.16**.

- **A collaboration meeting is organized every 6 month in different facilities:**
 - February 2017 : ESRF
 - June 2017 : Soleil
 - February 2018 : Global Phasing / DLS
 - September 2018 : Elettra / Trieste
 - March 2019 : Max IV / Lund
 - Second half 2019 : ?
- **A developers video conference is organized on the first Monday every month. The organizing facility is changed once a year :**
 - 2017 : DLS
 - 2018 : ESRF
 - 2019 : ?

FINAL WORD ABOUT MANPOWER

- The ISPyB collaboration is lacking manpower.
- The ISPyB developments are mainly done by the ESRF and the DLS
- The DLS has most manpower dedicated to ISPyB, however, as the DLS uses a different backend and GUI it is not straightforward for other facilities to take advantage of DLS' developments.

**A big thank to all
ISPYB developers
and collaborators!**