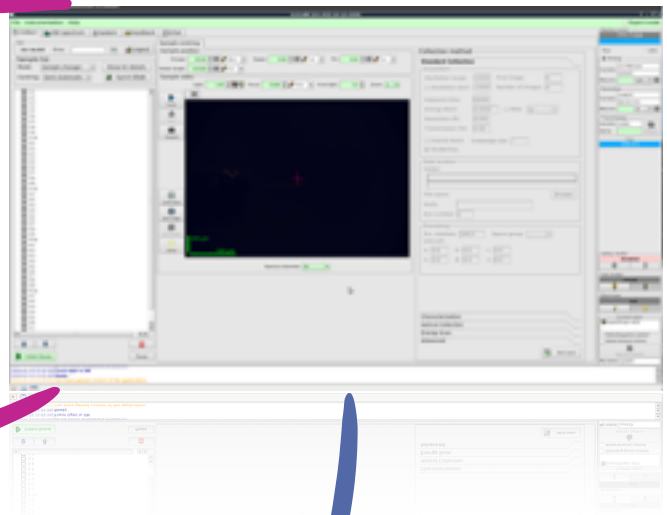
ESRF
The European Synchrotron

Sample information

ISPyB

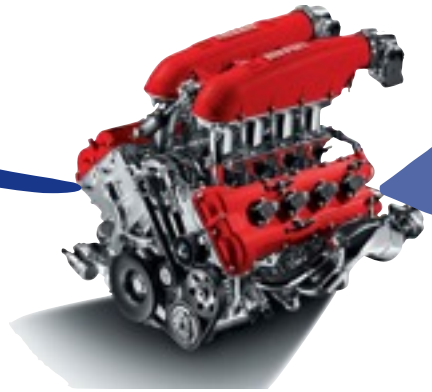
MXCuBE2

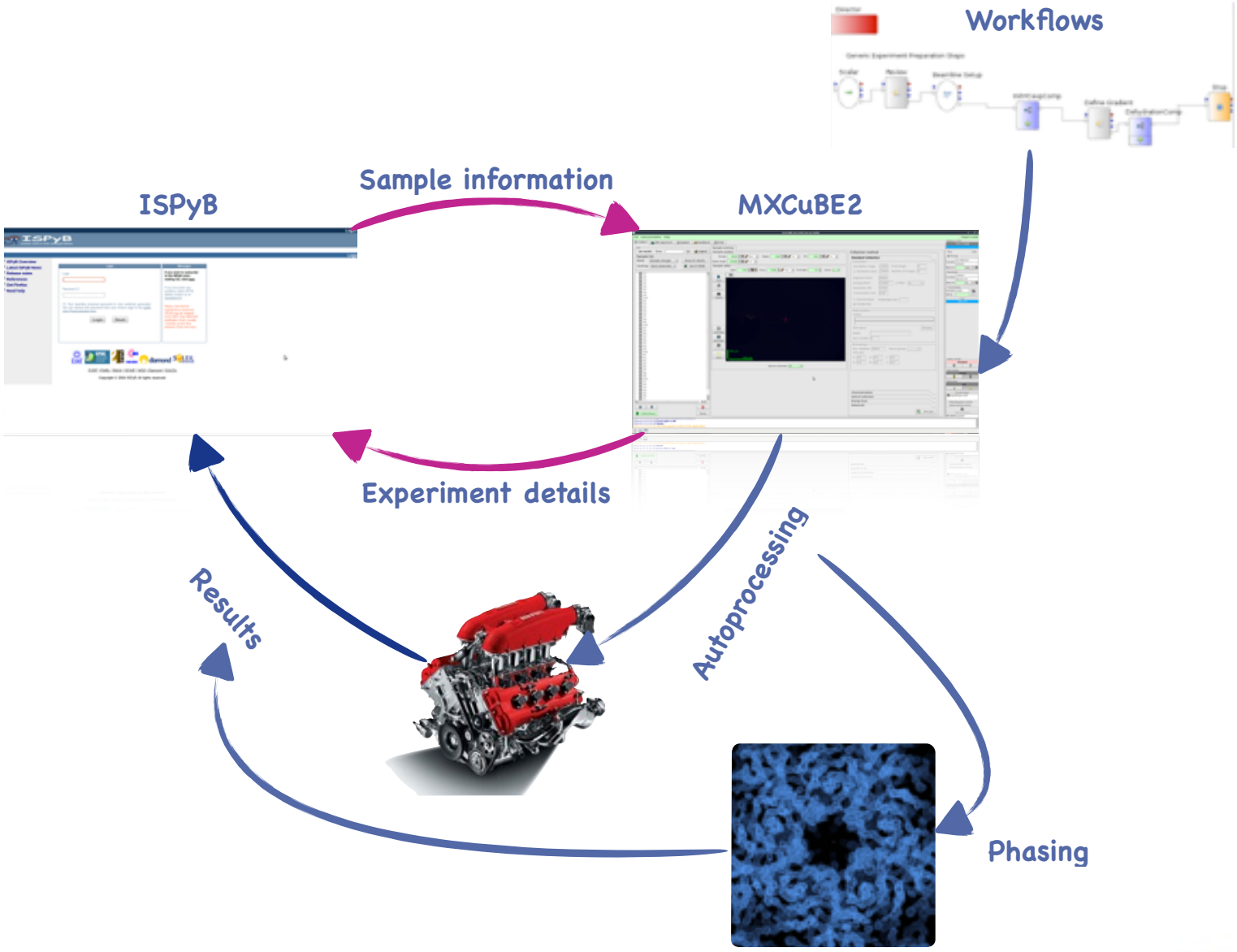


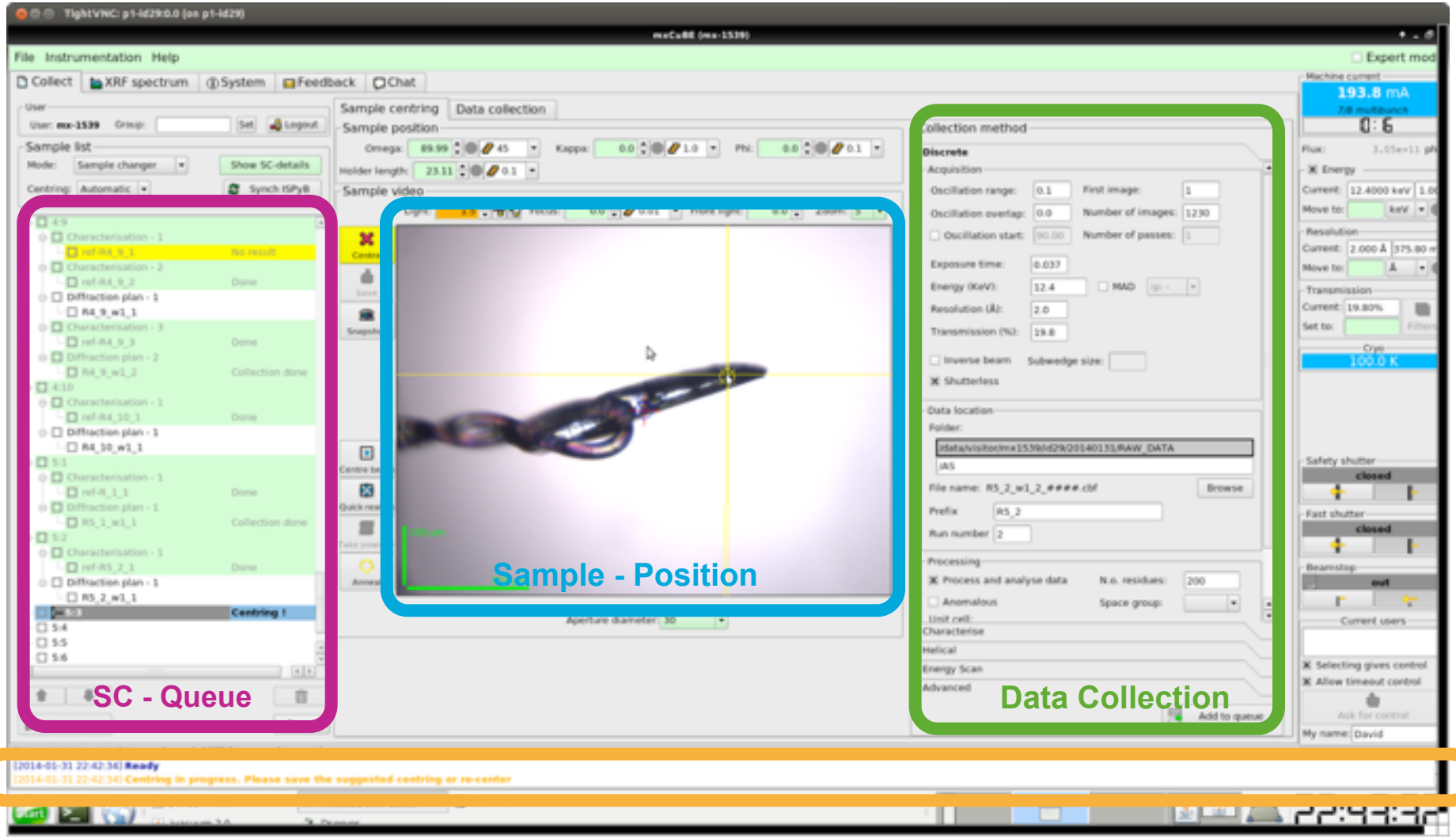
Experiment details

Results

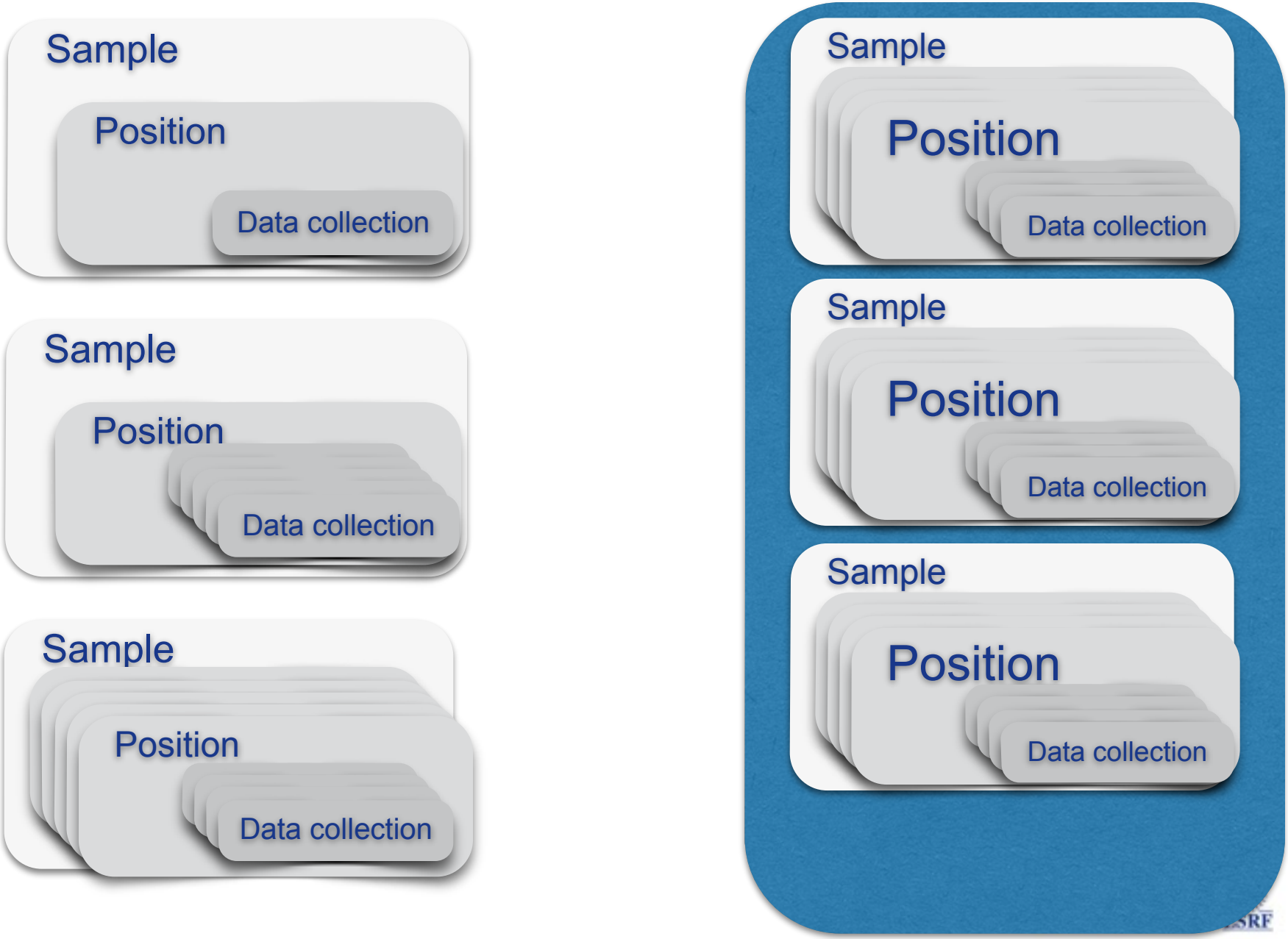
Autoprocessing




Workflows
Sample information
ISPyB
MXCuBE2
Experiment details
Results
Autoprocessing
Phasing


SC - Queue
Sample - Position
Data Collection

MXCUBE2


Sample
Position
Data collection
Sample
Position
Data collection
Sample
Position
Data collection
Sample
Position
Data collection
Sample
Position
Data collection
Sample
Position
Data collection

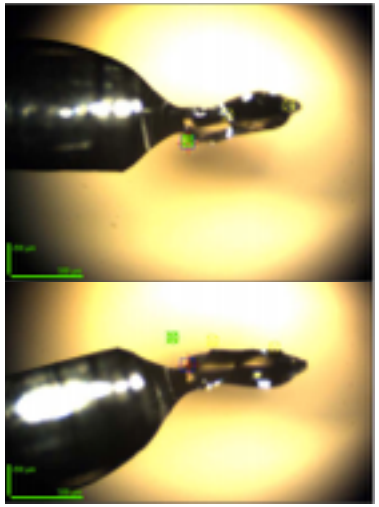
QUEUE

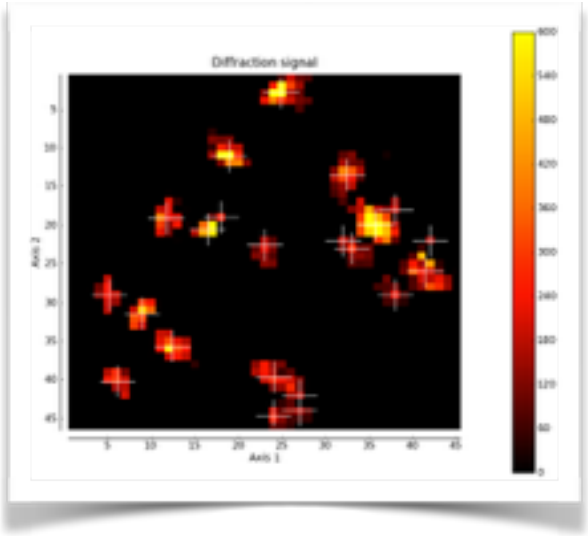
1. Standard Collection
2. Characterisation
3. Helical Data Collection
4. Energy Scan
5. Advanced

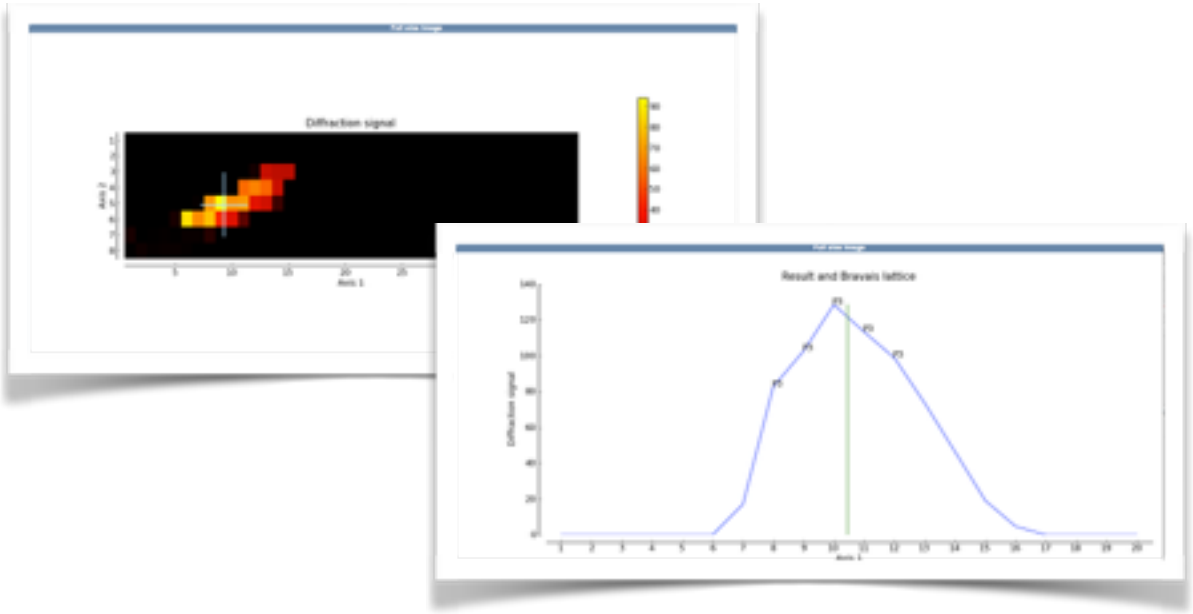
Powerful intuitive interface
Close integration with ISPyB
Enhancing automation
Robust abstraction level
Open to external experiment descriptors

This design permits:

Advance experiments: (ex.) MAD, multi positional MAD, multi kappa, raster & collect



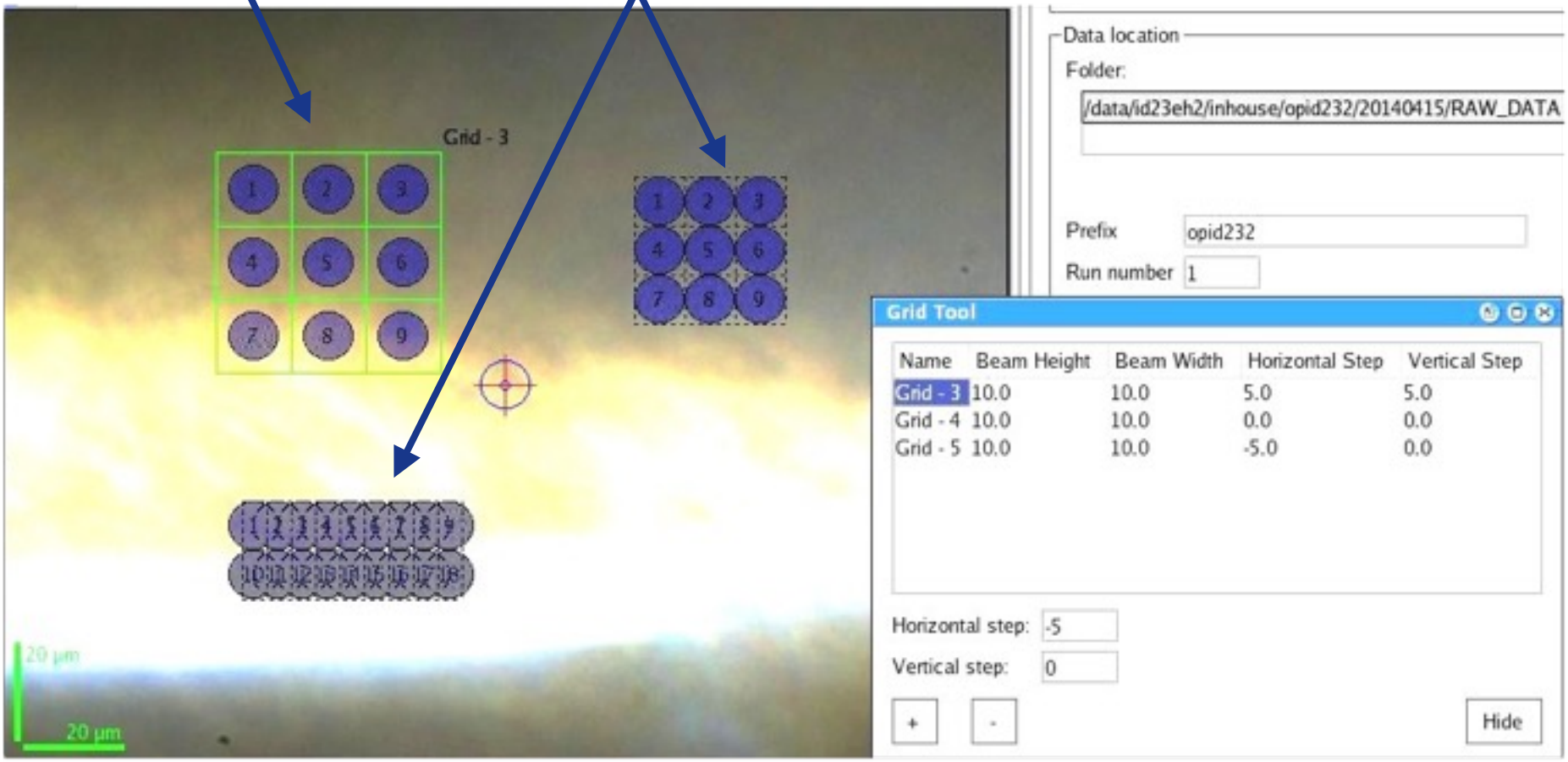

Diffraction signal
Axis 1
Axis 2


Diffraction signal
Result and Bravais lattice

- Fast meshes available via ICEPAP on all beamlines

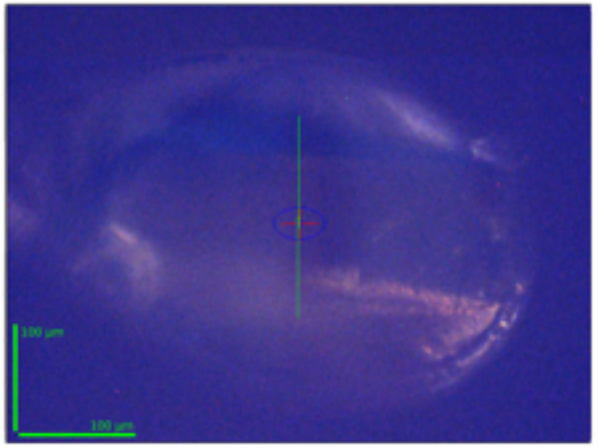
Discrete mesh

4dscan mesh

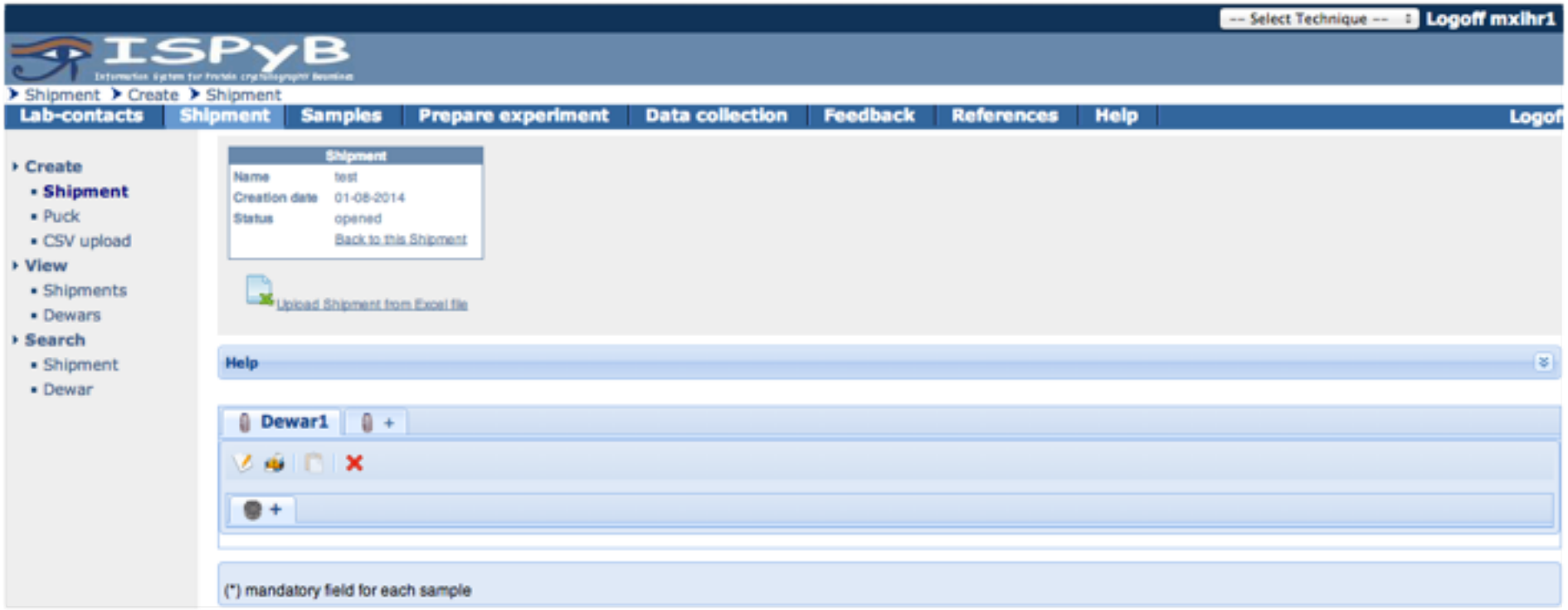


MXCUBE2 LATEST NEWS

- Use full dynamic range of OAV
- Getting more and more independent from SPEC
  - New beamlines are SPEC-free for what concerns data collection
  - ID29 on the way
  - More new application as Advanced Collection Methods
- MXCuBE collaboration growing: two new partners
  - ESRF, EMBL, SOLEIL, MAXLAB, BESSY, Global Phasing, ALBA and DESY
  - Plans for future development

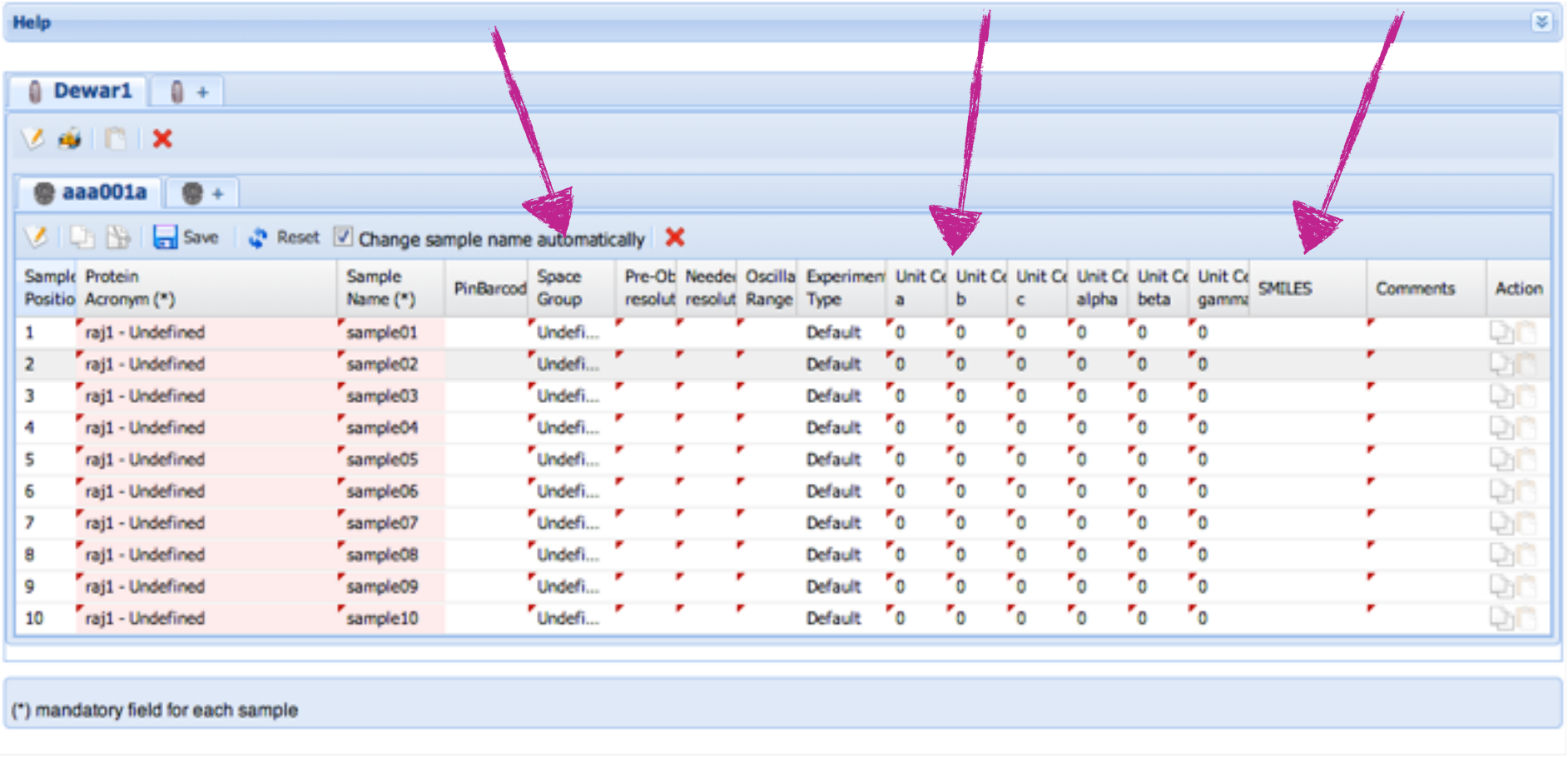


ISPYB: PREPARE EXPERIMENT



- A new web tool is available to fill the sample name and details for each sample in the sample changer - no need for xls file upload - can be done in a couple of minutes at the beamline

ISPYB: PREPARE EXPERIMENT


Help

Dewar1 +

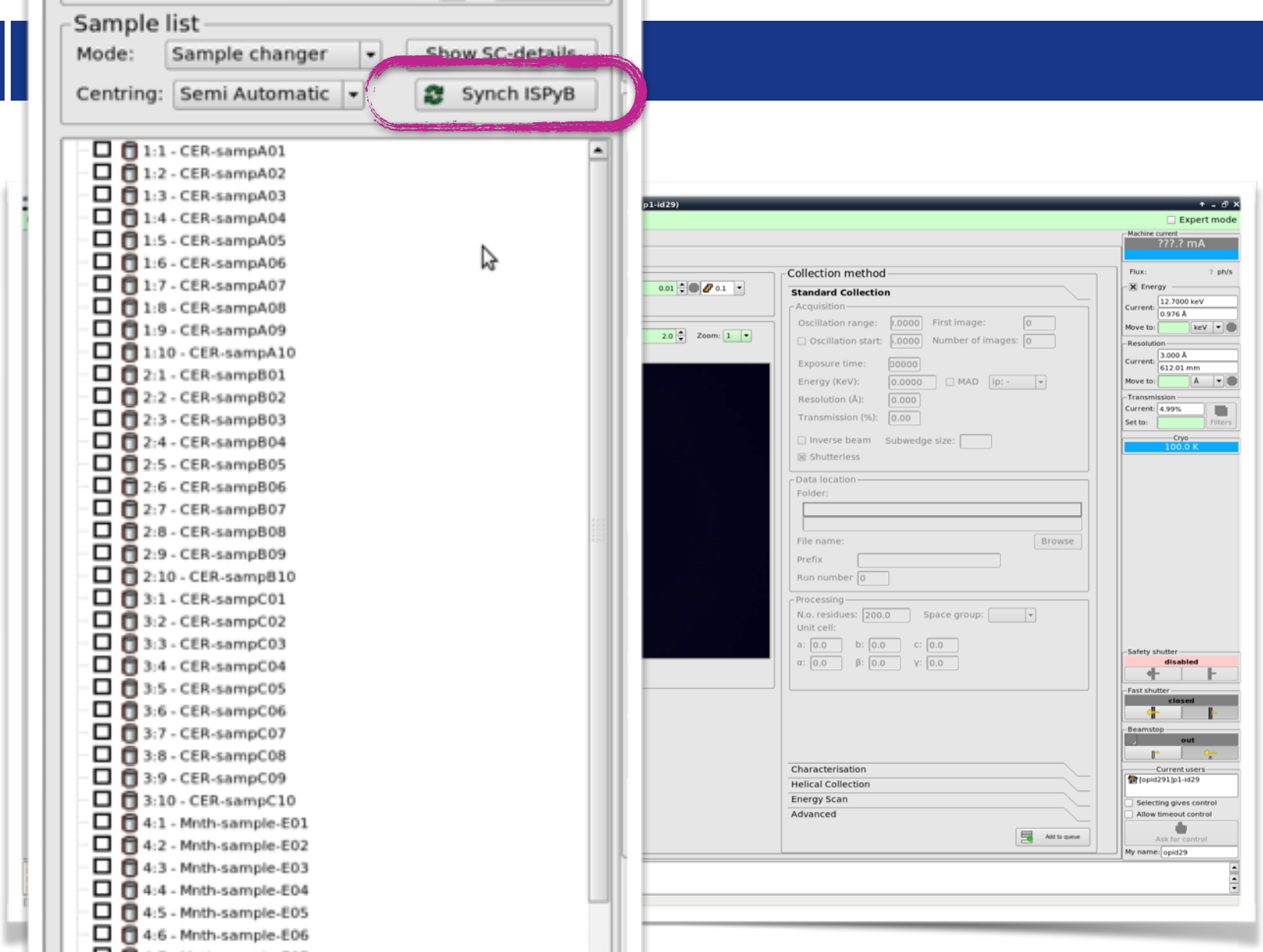
aaa001a +

Save Reset Change sample name automatically

Sample Positio	Protein Acronym (*)	Sample Name (*)	PinBarcod	Space Group	Pre-Ob resolut	Needec resolut	Oscilla Range	Experimen Type	Unit Ce a	Unit Ce b	Unit Ce c	Unit Ce alpha	Unit Ce beta	Unit Ce gamma	SMILES	Comments	Action
1	raj1 - Undefined	sample01		Undefi...				Default	0	0	0	0	0	0			
2	raj1 - Undefined	sample02		Undefi...				Default	0	0	0	0	0	0			
3	raj1 - Undefined	sample03		Undefi...				Default	0	0	0	0	0	0			
4	raj1 - Undefined	sample04		Undefi...				Default	0	0	0	0	0	0			
5	raj1 - Undefined	sample05		Undefi...				Default	0	0	0	0	0	0			
6	raj1 - Undefined	sample06		Undefi...				Default	0	0	0	0	0	0			
7	raj1 - Undefined	sample07		Undefi...				Default	0	0	0	0	0	0			
8	raj1 - Undefined	sample08		Undefi...				Default	0	0	0	0	0	0			
9	raj1 - Undefined	sample09		Undefi...				Default	0	0	0	0	0	0			
10	raj1 - Undefined	sample10		Undefi...				Default	0	0	0	0	0	0			

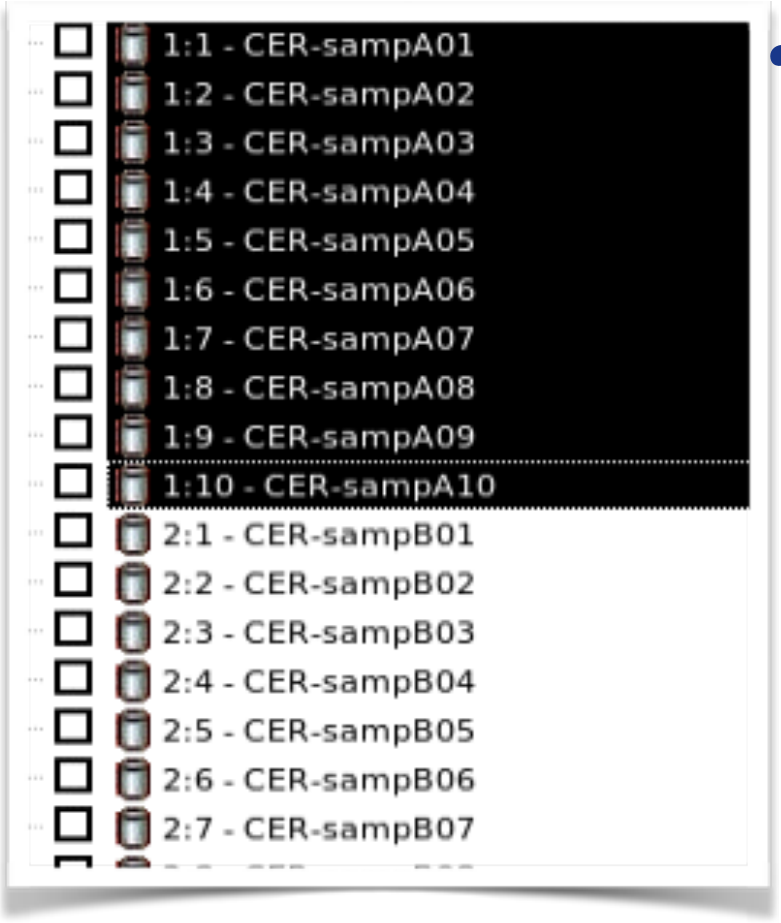
(*) mandatory field for each sample

- minimal information required but
  - space group unit cell can be specified
  - SMILES for ligand study (more later)

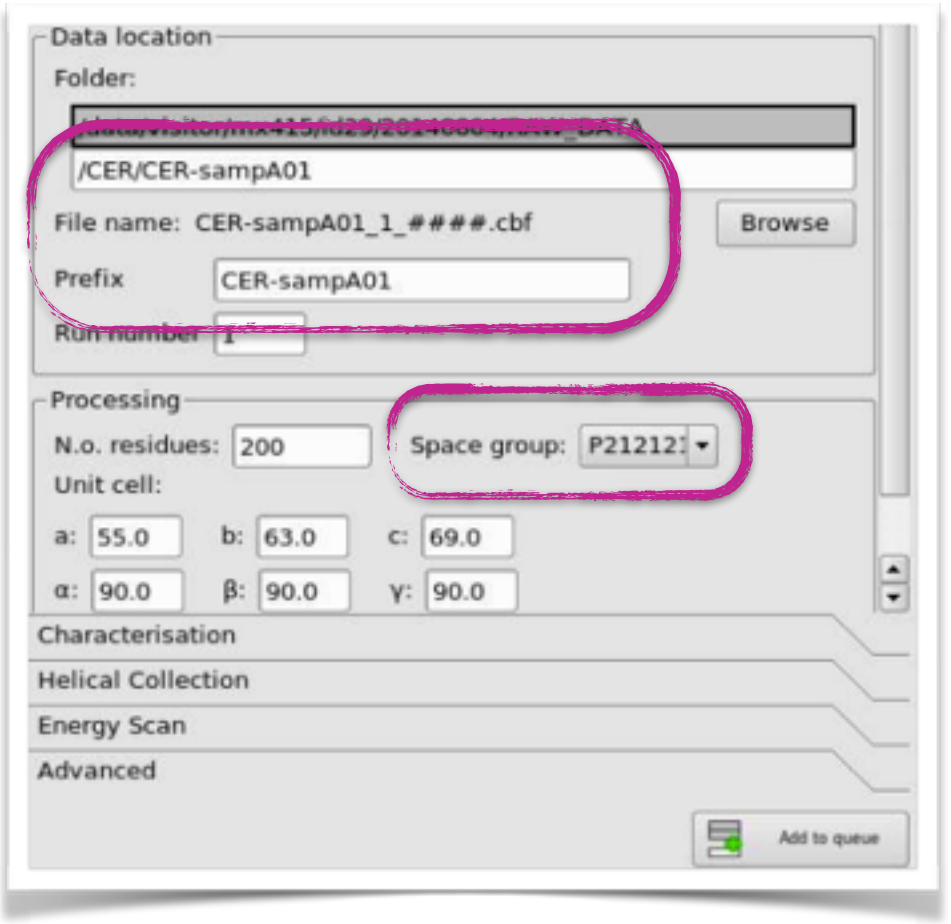

Sample list
Mode:
Sample changer
Show SC-details
Centring:
Semi Automatic
Synch ISPyB
1:1 - CER-sampA01
1:2 - CER-sampA02
1:3 - CER-sampA03
1:4 - CER-sampA04
1:5 - CER-sampA05
1:6 - CER-sampA06
1:7 - CER-sampA07
1:8 - CER-sampA08
1:9 - CER-sampA09
1:10 - CER-sampA10
2:1 - CER-sampB01
2:2 - CER-sampB02
2:3 - CER-sampB03
2:4 - CER-sampB04
2:5 - CER-sampB05
2:6 - CER-sampB06
2:7 - CER-sampB07
2:8 - CER-sampB08
2:9 - CER-sampB09
2:10 - CER-sampB10
3:1 - CER-sampC01
3:2 - CER-sampC02
3:3 - CER-sampC03
3:4 - CER-sampC04
3:5 - CER-sampC05
3:6 - CER-sampC06
3:7 - CER-sampC07
3:8 - CER-sampC08
3:9 - CER-sampC09
3:10 - CER-sampC10
4:1 - Mnth-sample-E01
4:2 - Mnth-sample-E02
4:3 - Mnth-sample-E03
4:4 - Mnth-sample-E04
4:5 - Mnth-sample-E05
4:6 - Mnth-sample-E06
4:7 - Mnth-sample-E07
4:8 - Mnth-sample-E08
4:9 - Mnth-sample-E09
4:10 - Mnth-sample-E10
5:1 - PFLU-SampD01
5:2 - PFLU-SampD02
Expert mode
Collection method
Standard Collection
Acquisition
Oscillation range:
First image:
Oscillation start:
Number of images:
Exposure time:
Energy (KeV):
MAD
Resolution (Å):
Transmission (%):
Inverse beam
Subwedge size:
Shutterless
Data location
Folder:
File name:
Browse
Prefix
Run number
Processing
N.o. residues:
Space group:
Unit cell:
Characterisation
Helical Collection
Energy Scan
Advanced
Add to queue
Machine current
???.? mA
Flux:
Energy
Current:
12.7000 keV
0.976 Å
Move to:
keV
Resolution
Current:
3.000 Å
612.01 mm
Move to:
Å
Transmission
Current:
4.99%
Set to:
Filters
Cryo
100.0 K
Safety shutter
disabled
Fast shutter
closed
Beamstop
out
Current users
[opid291]p1-id29
Selecting gives control
Allow timeout control
Ask for control
My name:
opid29

SYNC SAMPLES

ISPyB Sample names



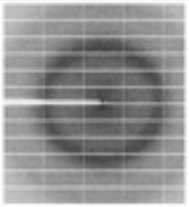
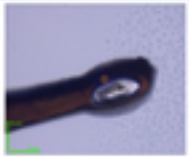
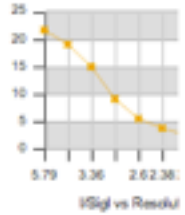
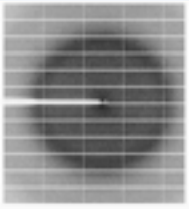
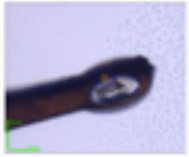
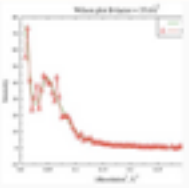
Data Collection



ISPYB: RESULTS

Session

Save Comments | View All DataCollection | Expand All | Collapse All | Clear Grouping

Experiment Type	Acronym Sample nam	Image Prefix	Run#	Parameters	Results	Image Thumbnail	Crystal snapshot	Graph	Comments
11-07-2014 (1 Item)									
OSC	AtFuT1-gdpfuc02	AtFuT1-gdpfuc02_w	1	*Nb images:* 2230 *Exp. time:* 0.04 s *Phi range:* 0.10 ° *Flux:* 2.03E11 ph/sec *Detector resolution:* 2.1... *Transmission:* 21.47 *Wavelength:* 0.976 Å *Total expo time:* 82.51 s	EDNA dp GrenADES fp GrenADES pp *Space Group:* P 1 21 1 *Completeness:*				
Start time: 17:11:01 11-07-2014 (1 Item)									
Characte...	AtFuT1-gdpfuc02	ref-AtFuT1-gdpfuc02	1	*Nb images:* 2 *Exp. time:* 0.04 s *Phi range:* 1.00 ° *Flux:* 8.89E11 ph/sec *Detector resolution:* 2.3... *Transmission:* 100.00 *Wavelength:* 0.976 Å *Total expo time:*	Indexing Strategy *Space Group:* P2 *Unit Cell:* *a, b, c:* 87.99, 85.53, 150.55 *Oα, Oβ, Oγ:* 90.00, 96.31, 90.00 *Mosaicity:* 0.02 Å *Ranking Resolution:* 2.16 Å				

Experiment parameters | Beamline parameters | Characterisation parameters | Characterisation results | AutoProcessing

Characterisation Results (EDNA log file)

Data collection info

Data collection date	2014/Jul/11 17:11:28.631
Image prefix	ref-AtFuT1-gdpfuc02_1
Directory	/data/id23eh1/inhouse/mxihr1/20140711/RAW_DATA/AtFuT1/AtFuT1-gdpfuc02

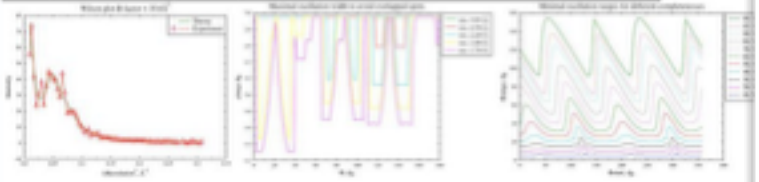
Diffraction Plan

Forced space group	Anomalous data	Aimed multiplicity	Aimed completeness	Aimed I/sigma at highest res.	Aimed resolution (Å)
	False	4.00	0.99	2.00	0.50

Collection plan strategy (RADDOSE log file , BEST log file)

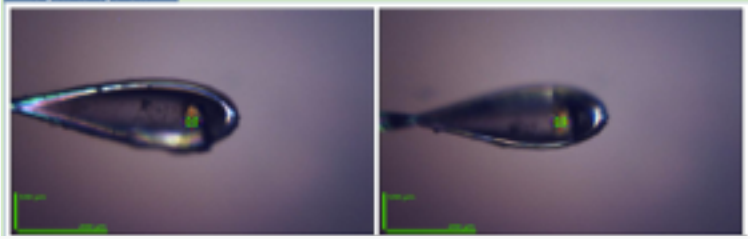
Resolution limit is set by the radiation damage

Wedge	Subwedge	Start (°)	Width (°)	No images	Exp time (s)	Max res (Å)	Rel trans (%)	Distance (mm)
1	1	129.00	0.10	2250	0.04	2.16	21.54	458.51



Indexing summary: Selected spacegroup: P2

Crystal Snapshots



Main Output Parameters

Overall:

Overall Resolution:	49.91-1.94 Å
Overall Completeness:	96.8%
Overall I over Sigma:	8.7
Overall Rsymm:	8.9%
Overall Multiplicity:	4.1

Outer Shell:

Outer Shell Resolution:	2.01-1.94 Å
Outer Shell Completeness:	75.9%
Outer Shell I over Sigma:	0.9
Outer Shell Rsymm:	108.9%
Outer Shell Multiplicity:	3.1

Unit Cell:

Unit Cell A:	87.9 Å
Unit Cell B:	85.8 Å
Unit Cell C:	150.6 Å
Unit Cell Alpha:	90.0 °
Unit Cell Beta:	96.22 °
Unit Cell Gamma:	90.0 °

Files

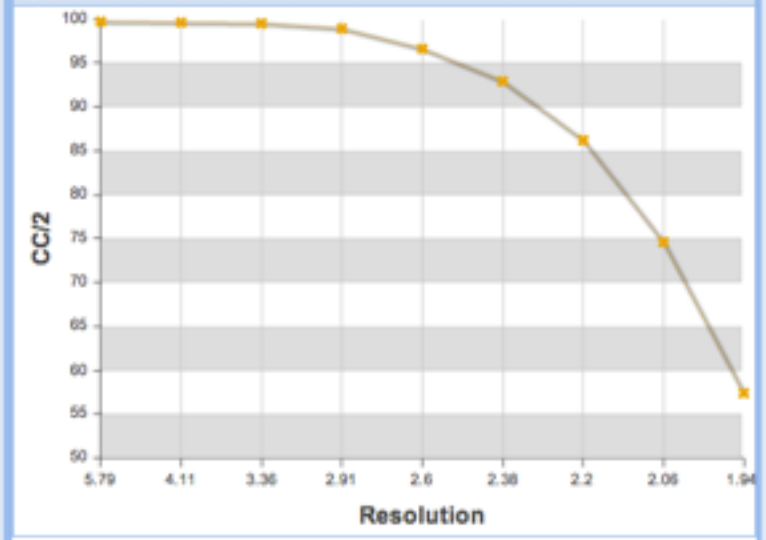
Download

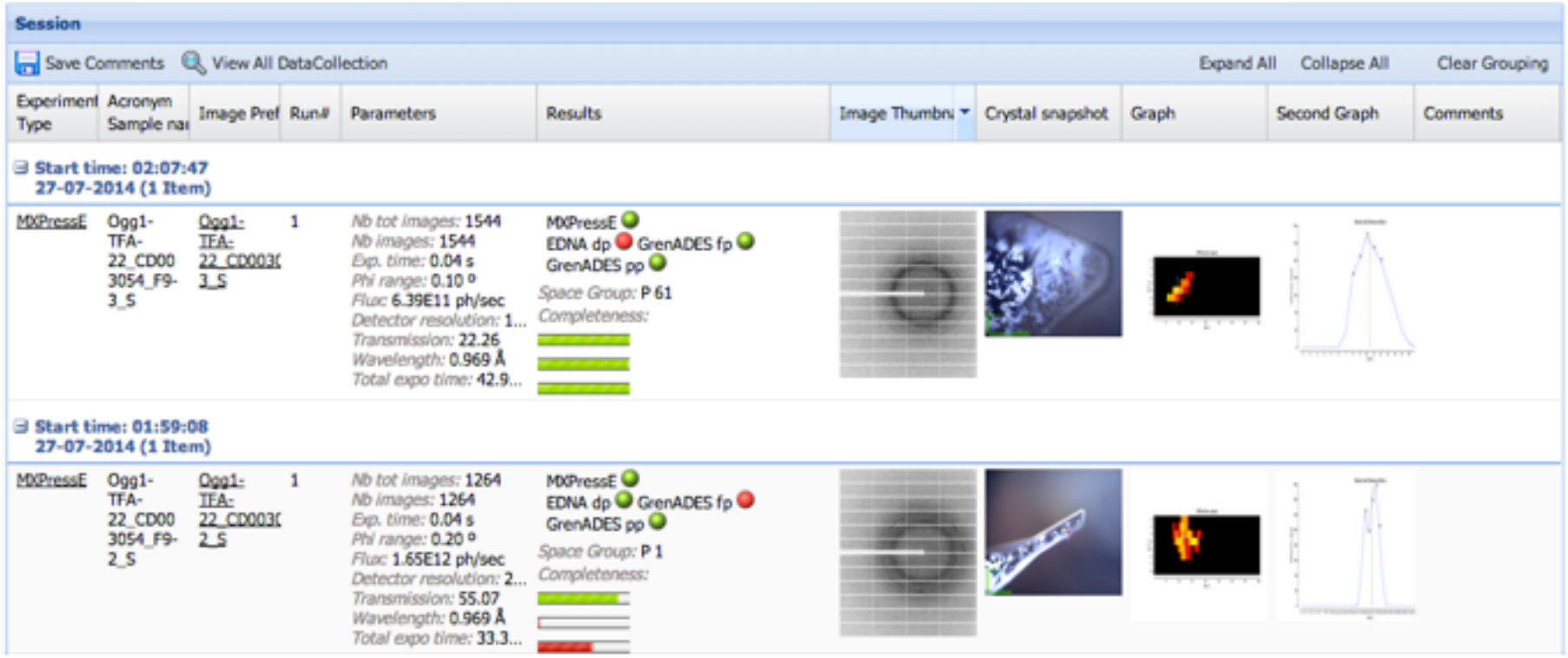
XDS | XSCALE | SCALA/AIMLESS | SCALEPACK | TRUNCATE

Log Files:

- AtFuT1-gdpfuc02_w1_run1_merged_anom_XSCALE.LP
- AtFuT1-gdpfuc02_w1_run1_unmerged_anom_XSCALE.LP
- AtFuT1-gdpfuc02_w1_run1_merged_noanom_XSCALE.LP
- AtFuT1-gdpfuc02_w1_run1_unmerged_noanom_XSCALE.LP

...tion | Completeness vs Resolution | R-factor vs Resolution | CC/2 vs Resolution




Session
Save Comments
View All DataCollection
Expand All
Collapse All
Clear Grouping
Experiment Type
Acronym Sample na
Image Pref
Run#
Parameters
Results
Image Thumbn
Crystal snapshot
Graph
Second Graph
Comments
Start time: 02:07:47
27-07-2014 (1 Item)
MXPressE
Ogg1-TFA-22_CD003054_F9-3_S
Ogg1-TFA-22_CD003(3_S
1
Nb tot images: 1544
Nb images: 1544
Exp. time: 0.04 s
Phi range: 0.10 °
Flux: 6.39E11 ph/sec
Detector resolution: 1...
Transmission: 22.26
Wavelength: 0.969 Å
Total expo time: 42.9...
MXPressE
EDNA dp
GrenADES fp
GrenADES pp
Space Group: P 61
Completeness:
Start time: 01:59:08
27-07-2014 (1 Item)
MXPressE
Ogg1-TFA-22_CD003054_F9-2_S
Ogg1-TFA-22_CD003(2_S
1
Nb tot images: 1264
Nb images: 1264
Exp. time: 0.04 s
Phi range: 0.20 °
Flux: 1.65E12 ph/sec
Detector resolution: 2...
Transmission: 55.07
Wavelength: 0.969 Å
Total expo time: 33.3...
MXPressE
EDNA dp
GrenADES fp
GrenADES pp
Space Group: P 1
Completeness:

- Autoprocessing
- New cluster being installed during User meeting
  - EDNAdp
    - Fast autoprocessing in best SG
    - If SG and Unit cell are given runs in these
    - Check data quality with phenix.xtriage
    - If pdb is given runs DIMPLE
  - Grenades
    - Fast autoprocessing
    - Parallel autoprocessing
      - In best multiple space groups
      - If SG is given runs _also_ in this
      - Triggers AutoSAD if anomalous signal is detected
      - Triggers AutoMR if same SG and unit cell are found in PDB
      - Triggers MR if pdb is given

- Advanced (Workflows)
  - Make complicated tasks simple to perform with minimal user input
    - MASSIF-1
    - Kappa
    - X-ray centring/mesh
    - ….
  - Just moved to a new platform: improved reliability and monitoring
  - Among latest development:
    - MAD
    - Interleaved MAD
    - HCA - multicrystal data collections

- MXCuBE2
  - Start work on web platform
  - Integrate latest developments
    - Multi-axis goniometer
    - beam definition
    - Minimize SPEC dependency

- ISPyB
  - A lot of ideas are on the pipeline. ISPyB is and will be the central platform. Short term plans include:
    - Evolve ISPyB to latest layout
    - Add sequence and make use of it
    - Report results for phasing
    - Define data collection (wished) plans beforehand
    - Add reprocessing functionalities
    - Introduction of new sample tracking tools (TAG)

- Autoprocessing (EDNAdp + Grenades) and Workflows
  - Complete integration of the pipeline
    - Phasing results into ISPyB
    - Add reprocessing functionalities
    - Multicrystal analysis (TAG)
    - Hierarchical cluster analysis
    - Eiger detector data reduction

- Software development is crucial for better science at MX beamlines
  - mesh, MXCuBE2 MAD/Multipos, kappa, …
  - We do not have more resources than the minimum