





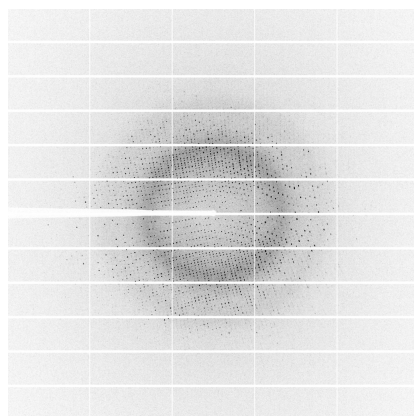
WHAT METADATA ARE NEEDED TO MAKE RAW DATA FROM ESRF MX BEAMLINES INTELLIGIBLE?

GORDON LEONARD
ESRF STRUCTURAL BIOLOGY GROUP

A MX EXPERIMENT



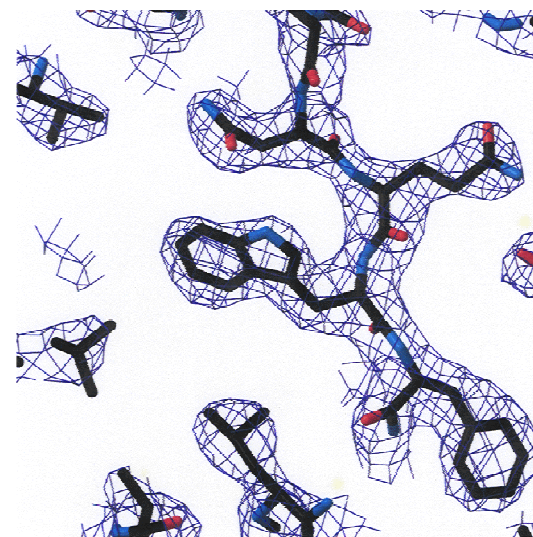
Crystal(s)



'raw' diffraction images



$h, k, l, I, \sigma(l)$

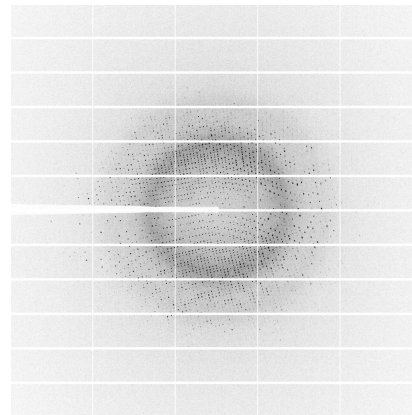


crystal structure

A MX DATA COLLECTION



Crystal(s)



'raw' diffraction images



$h, k, l, I, \sigma(I)$



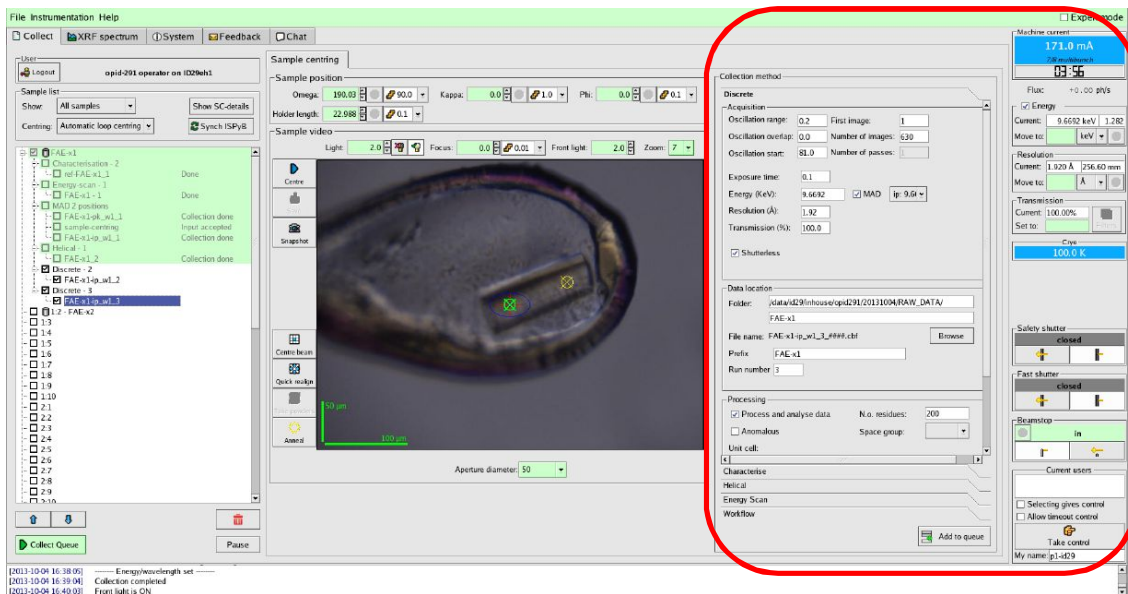
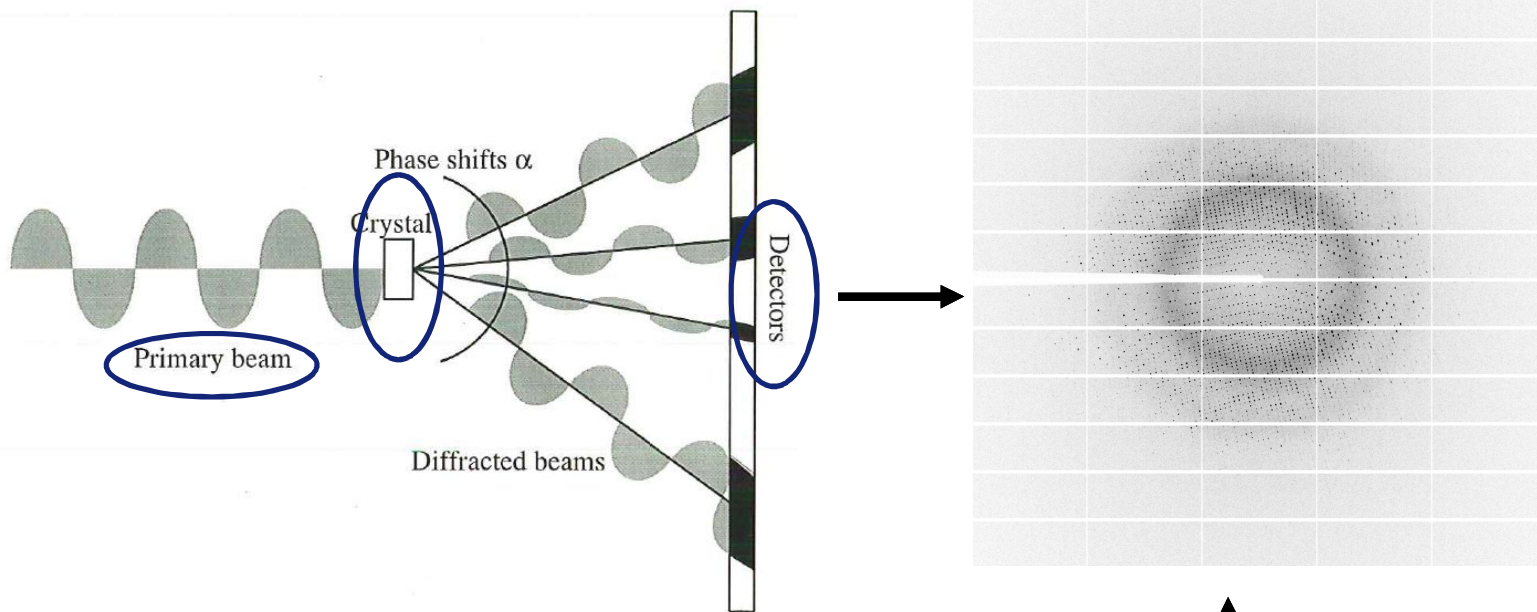
- 3rd generation MX-SR beamlines are extremely intense (ESRF ID29; $\sim 10^{13}$ photons/s in beam $50 \times 30 \mu\text{m}^2$ [HxV])
- Collection of a complete set of raw diffraction images from a given sample is extremely rapid (minutes/seconds/sub-second).
- To help users keep up with throughput most (all?) SR MX facilities provide automatic, experiment planning and execution as well as on-line, at beam-line 'autoprocessing'.
- Correct collection, use and archiving of metadata are required to (a) ensure correct results of autoprocessing; (b) allow off-line (re)processing after an experimental session.

AT ESRF EXPERIMENT CONTROL IS THROUGH THE MXCUBE2 BCM

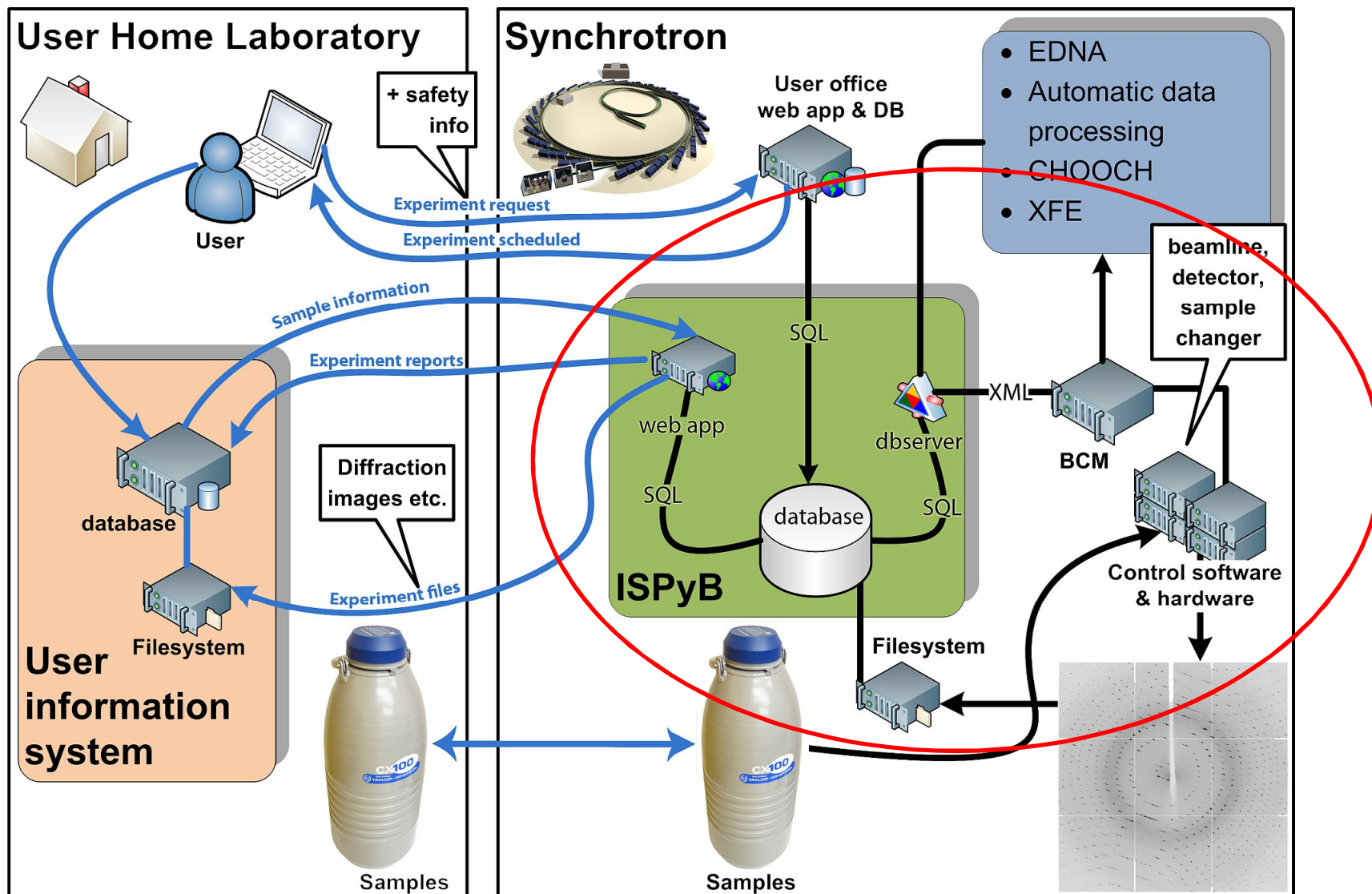
The screenshot displays the MXCUBE2 BCM control interface. On the left, a tree view shows the sample list with 'Discrete - 2' selected. The central panel shows a sample image with a scale bar of 100 μm and an aperture diameter of 50. The right panel contains acquisition parameters such as 'Oscillation range: 0.2', 'Energy (KeV): 9.6692', and 'Resolution (Å): 1.92'. A red circle highlights the 'Add to queue' button in the bottom right corner. A blue circle highlights the 'Collect Queue' button in the bottom left corner. A blue arrow points from the 'Collect Queue' button to the 'Add to queue' button.

D. de Sanctis & G. Leonard, in *Notiziario Neutroni e Luce di Sincrotrone* Vol. 19 (Consiglio Nazionale delle Ricerche, 2014), p. 24.
Gabadinho et al., (2010) *J. Sync. Rad.*, 17, 700-707

WHAT METADATA FOR A ESRF MX DATA COLLECTION/EXPERIMENT?

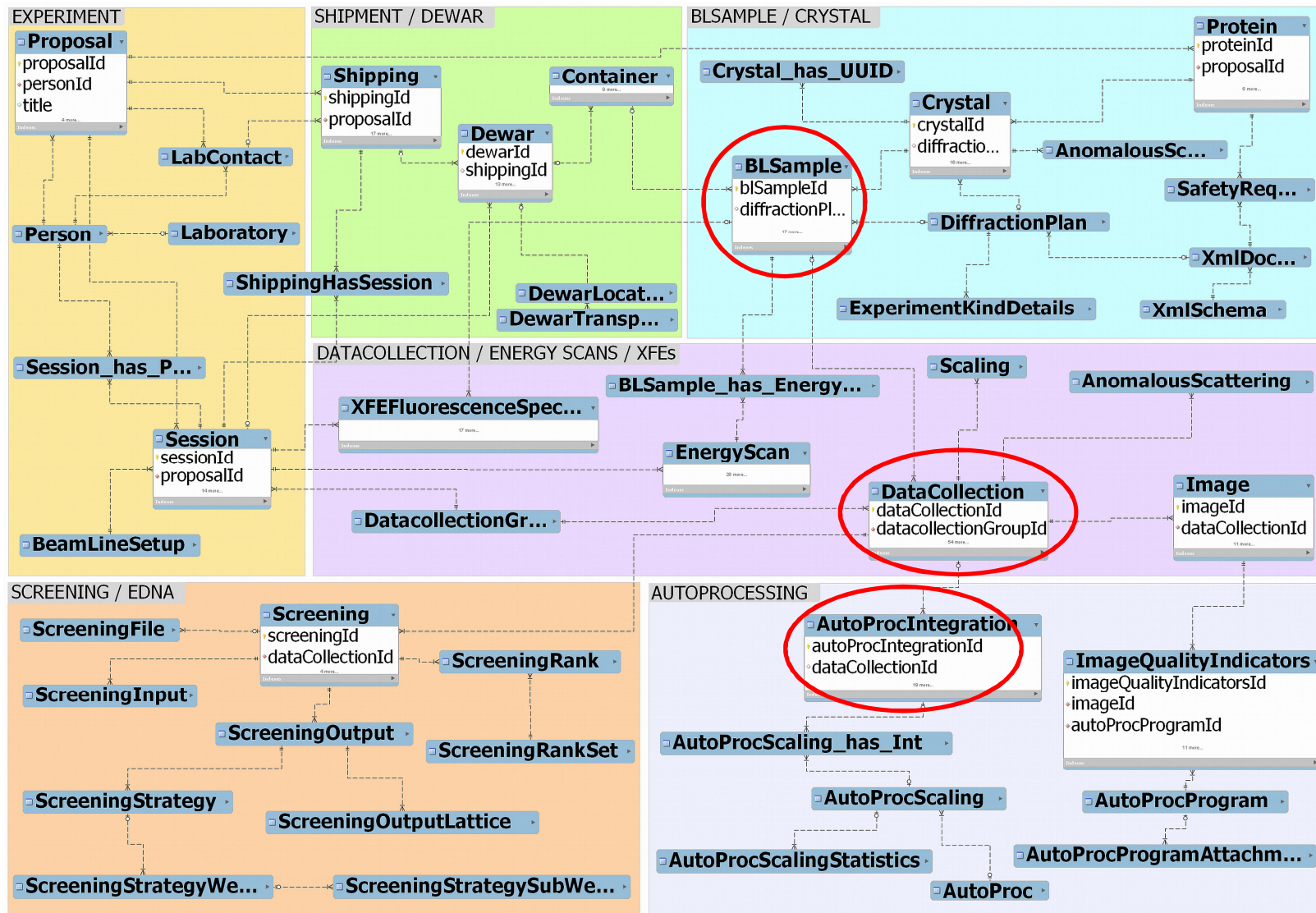


ALL METADATA FOR ESRF MX EXPERIMENTS ARE STORED IN ISPYB



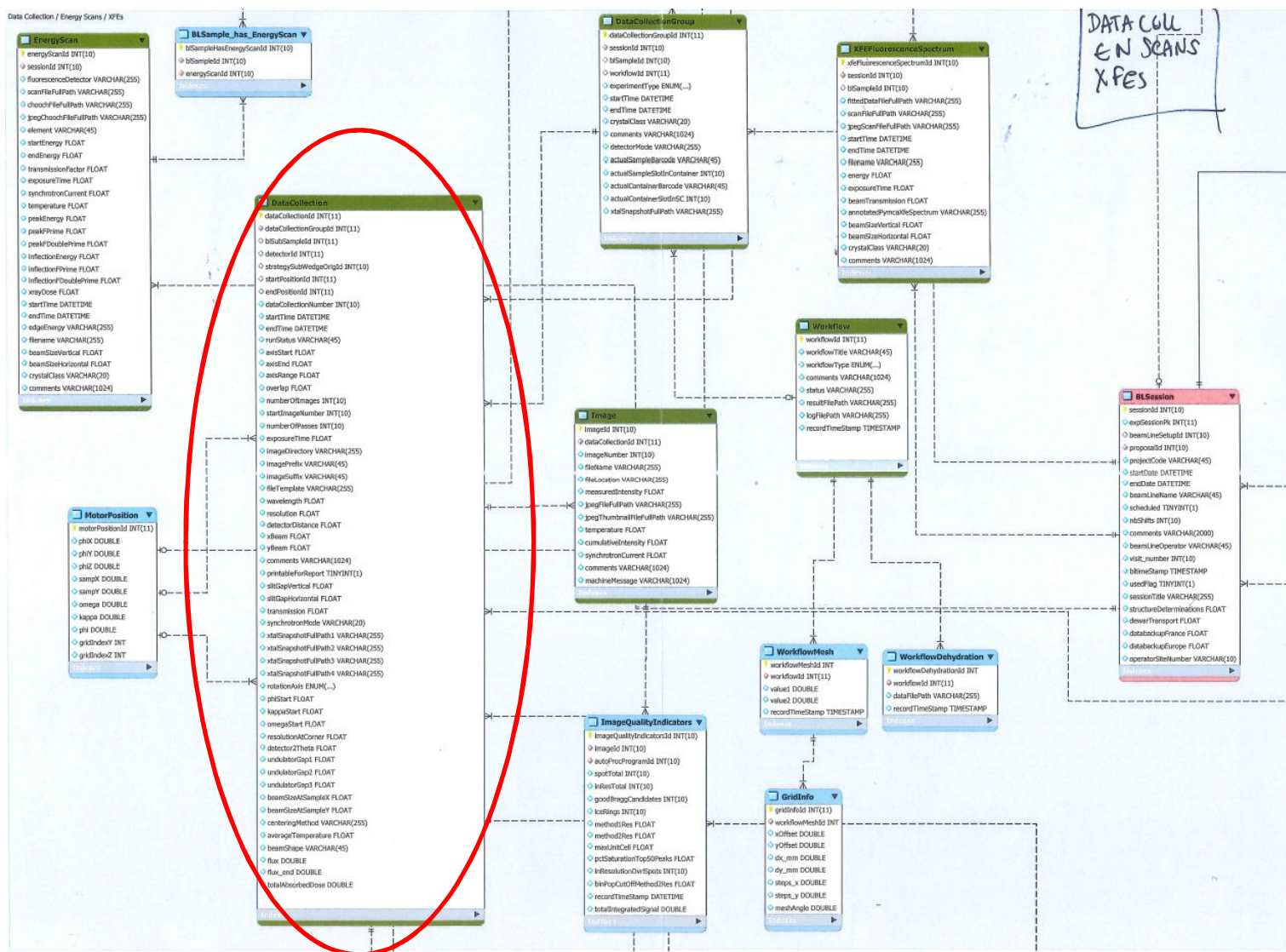
Delageniere, S. et al., (2011) *Bioinformatics* 27, 3186. doi:10.1093/bioinformatics/btr535.

ISPYB IS A METADATA CATALOGUE/LIMS WITH A MODULAR DATA MODEL



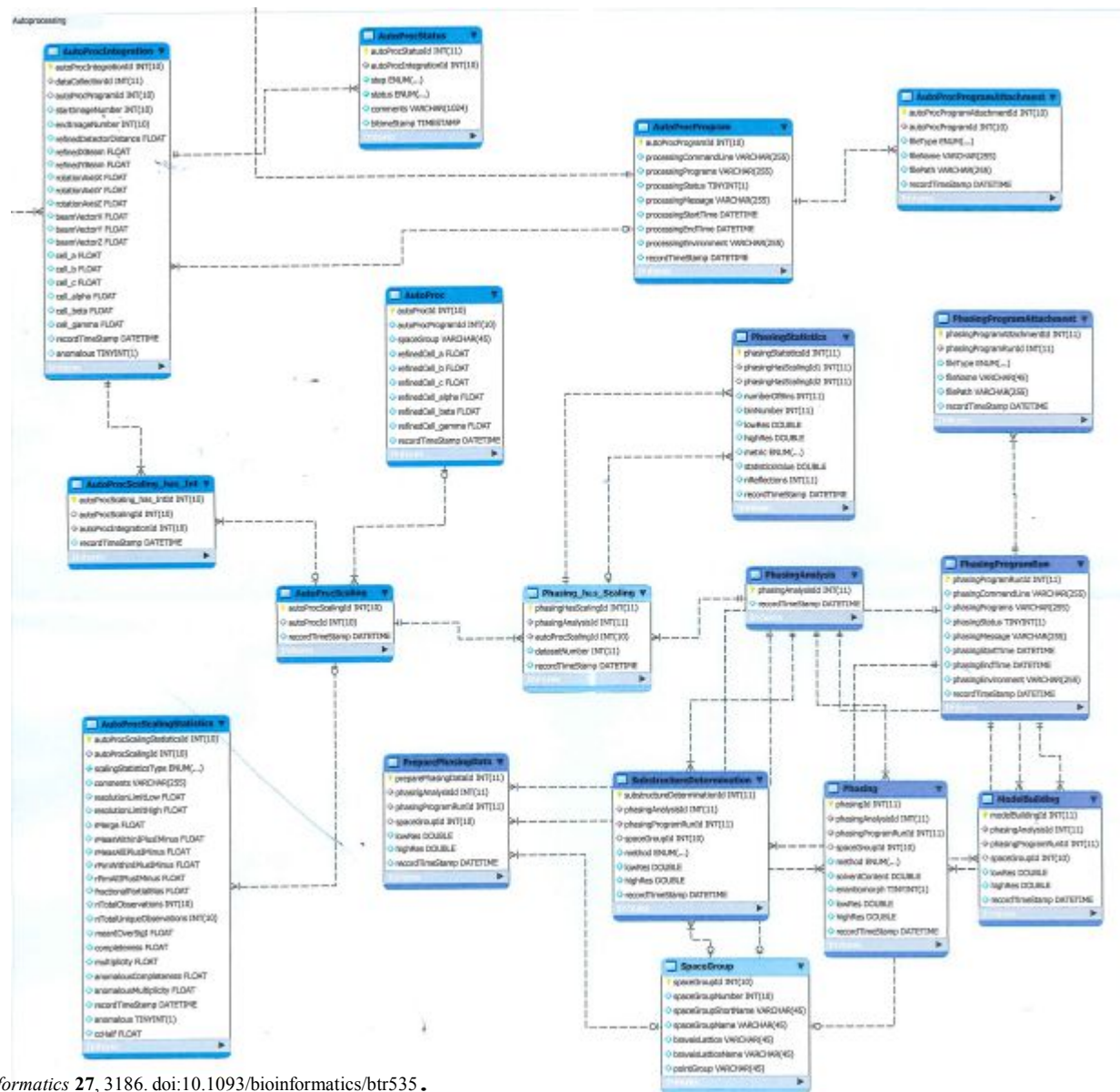
Delageniere, S. et al., (2011) *Bioinformatics* 27, 3186. doi:10.1093/bioinformatics/btr535.

THE ISPYB 'DATA COLLECTION' MODULE



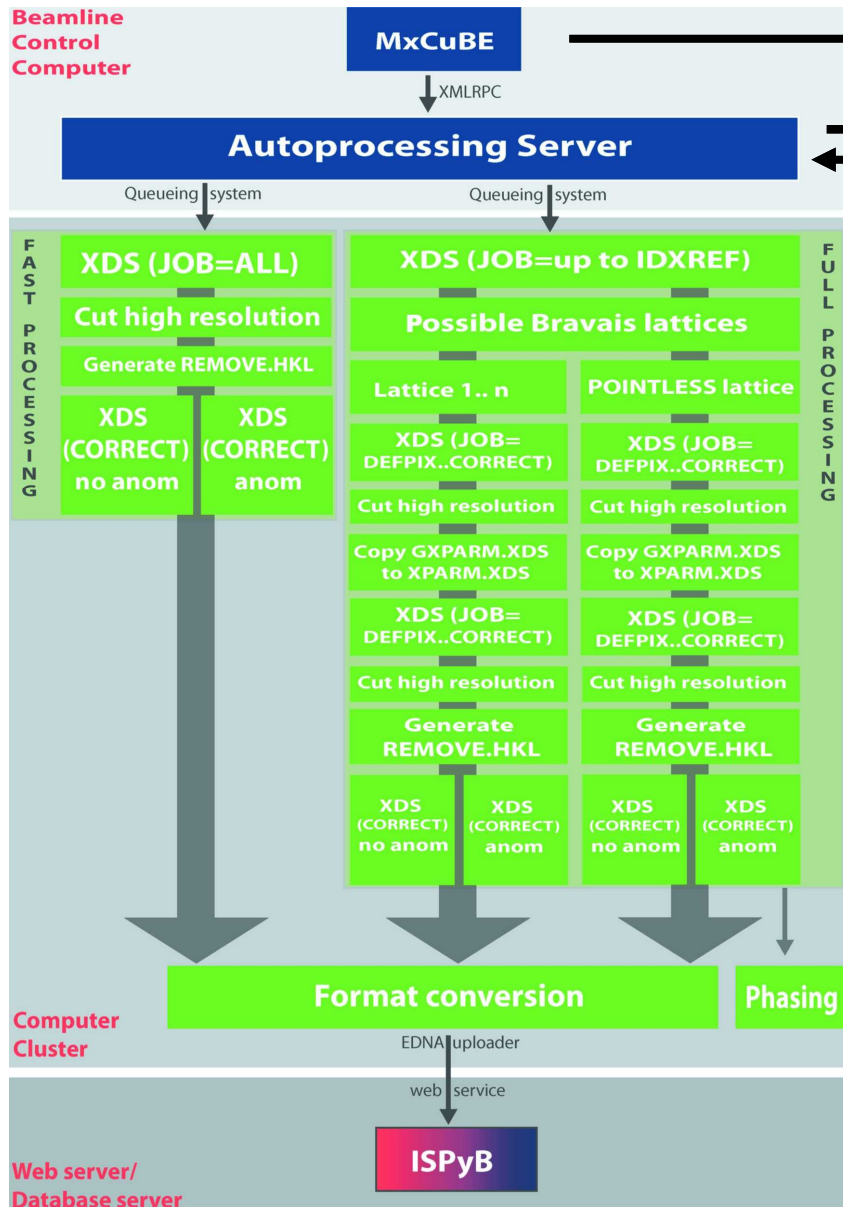
Delageniere, S. et al., (2011) *Bioinformatics* 27, 3186. doi:10.1093/bioinformatics/btr535.

THE ISPYB 'AUTOPROCESSING' MODULE



Delageniere, S. et al., (2011) *Bioinformatics* 27, 3186. doi:10.1093/bioinformatics/btr535.

AUTOMATIC MX DATA ANALYSIS AT ESRF



```

JOB= ALL      !JOB= DEFPIX XPLAN INTEGRATE CORRECT
DATA_RANGE= 1 1220
SPOT_RANGE= 1 31
SPOT_RANGE= 580 610
BACKGROUND_RANGE= 1 4

!masking non sensitive area of Pilatus
UNTRUSTED_RECTANGLE= 487 495 0 2528
UNTRUSTED_RECTANGLE= 981 989 0 2528
UNTRUSTED_RECTANGLE=1475 1483 0 2528
UNTRUSTED_RECTANGLE=1969 1977 0 2528
UNTRUSTED_RECTANGLE= 0 2464 195 213
UNTRUSTED_RECTANGLE= 0 2464 407 425
UNTRUSTED_RECTANGLE= 0 2464 619 637
UNTRUSTED_RECTANGLE= 0 2464 831 849
UNTRUSTED_RECTANGLE= 0 2464 1043 1061
UNTRUSTED_RECTANGLE= 0 2464 1255 1273
UNTRUSTED_RECTANGLE= 0 2464 1467 1485
UNTRUSTED_RECTANGLE= 0 2464 1679 1697
UNTRUSTED_RECTANGLE= 0 2464 1891 1909
UNTRUSTED_RECTANGLE= 0 2464 2103 2121
UNTRUSTED_RECTANGLE= 0 2464 2315 2333
TRUSTED_REGION=0.0 1.41 !Relative radii limiting trusted detector region

!correction tables to compensate the misorientations of the modules

X-GEO_CORR= ../x_geo_corr.cbf
Y-GEO_CORR= ../y_geo_corr.cbf

MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT= 3
!STRONG_PIXEL= 3.0
OSCILLATION_RANGE= 0.1000
STARTING_ANGLE= 144.0
STARTING_FRAME= 1
X-RAY_WAVELENGTH= 0.97625
NAME_TEMPLATE_OF_DATA_FRAMES= ../rory_w1_1_?????.cbf !CBF
DETECTOR_DISTANCE= 218.61
DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE= 0.0 OVERLOAD= 1048500

SENSOR_THICKNESS=1.00
ORGX= 1234.63 ORGY= 1254.24
NX= 2463 NY= 2527
QX= 0.1720 QY= 0.1720
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 7000 30000

DIRECTION_OF_DETECTOR_X-AXIS= 1.0 0.0 0.0
DIRECTION_OF_DETECTOR_Y-AXIS= 0.0 1.0 0.0
ROTATION_AXIS= 1.0 0.0 0.0
INCIDENT_BEAM_DIRECTION= 0.0 0.0 1.0
FRACTION_OF_POLARIZATION= 0.99
POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0
!AIR= %.8f

SPACE_GROUP_NUMBER= 0
UNIT_CELL_CONSTANTS= 0 0 0 0 0
INCLUDE_RESOLUTION_RANGE= 50.0 0.0
!STRICT_ABSORPTION_CORRECTION=TRUE

REFINE (INTEGRATE)= BEAM ORIENTATION CELL
MAXIMUM_NUMBER_OF_PROCESSORS= 16
    
```

DATA PROCESSING AND ANALYSIS IN ISPYB

The screenshot shows the ISPyB web interface. At the top, there is a navigation bar with 'Proposals', 'Shipment', 'Feedback', 'Dashboard', and 'Update ISPyB database'. Below this, there are three panels for 'Selected Session', 'Selected DataCollectionGroup', and 'Selected DataCollection'. The 'Selected Session' panel shows 'Proposal: opid291', 'Start Date: 22-07-2015', and 'BeamLine: ID29'. The 'Selected DataCollectionGroup' panel shows 'Start Time: 22-07-2015 15:38:27' and 'Experiment Type: OSC'. The 'Selected DataCollection' panel shows 'Start Time: 22-07-2015 15:38:28', 'Image Prefix: rory_w1', and 'Run Number: 1'. Below these panels, there are tabs for 'Experiment parameters', 'Beamline parameters', and 'AutoProcessing'. The 'AutoProcessing' tab is active, showing an 'Autoprocessing Summary' table. The table has columns for 'Method', 'Point Group', 'Cell A', 'Cell B', 'Cell C', 'Cell Alpha', 'Cell Beta', and 'Cell Gamma'. There are two sections: 'Anomalous: OFF (Friedel pairs merged) (7 Items)' and 'Anomalous: ON (Friedel pairs unmerged) (7 Items)'. At the bottom, there are input fields for 'RSymm threshold in lower shell' and 'I/Sigma threshold in lower shell', with an 'Update' button.

This screenshot shows the 'Experiment parameters' tab of the ISPyB interface. It lists various parameters for the experiment, including 'Img directory', 'Img prefix', 'Nb of images', 'Run no.', 'Start Time', 'End Time', 'Type of experiment', 'Wavelength', 'Energy', 'Phi start', 'Oscillation range', 'Overlap', 'Exposure Time', 'Total Exposure Time', 'Estimated Total Absorbed Dose', 'Number of passes', 'Detector Distance', 'Resolution at edge', 'Resolution at corner', 'Xbeam', 'Ybeam', 'Kappa', and 'Phi'. The 'Experiment comment' field is empty.

This screenshot shows the 'Beamline parameters' tab of the ISPyB interface. It lists various parameters for the beamline, including 'Synchrotron name', 'Synchrotron filling mode', 'Beamline name', 'Undulator types', 'Undulator gaps', 'Beam transmission', 'Slit gap Hor', 'Slit gap Vert', 'Detector type', 'Detector name', 'Detector manufacturer', 'Detector mode', 'Detector pixel size Hor', 'Detector pixel size Vert', 'Focusing optics', 'Monochromator type', 'Beam shape', 'Flux', 'Flux end', 'Beam size at sample Hor', 'Beam size at sample Vert', 'Beam divergence Hor', 'Beam divergence Vert', and 'Polarisation'.

Delageniere, S. *et al.*, (2011) *Bioinformatics* 27, 3186. doi:10.1093/bioinformatics/btr535.

DATA PROCESSING AND ANALYSIS IN ISPYB

ISPyB
Information system for protein crystallography beamlines

Data collection

Proposals | Shipment | Feedback | Dashboard | Update ISPyB database

Selected Session
Proposal: opk0291
Start Date: 22-07-2015
BeamLine: ID29

Selected DataCollectionGroup
Start Time: 22-07-2015 15:38:27
Experiment Type: OSC

Selected DataCollection
Start Time: 22-07-2015 15:38:28
Image Prefix: rory_w1
Run Number: 1

Experiment parameters | Beamline 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) (7 Items)							
parallelproc	P 21 21 21	60	63.9	69.5	90	90	90
EDNAproc	P 21 21 21	60	63.9	69.5	90	90	90
fastproc	P 2 2 2	60	63.9	69.5	90	90	90
parallelproc	P 2 2 2	60	63.9	69.5	90	90	90
parallelproc	P 1 2 1	59.9	63.9	69.5	90	89.9	90
parallelproc	P 1 2 1	63.9	60	69.5	90	90	90
parallelproc	P 1	59.9	63.9	69.5	90	90	90
Anomalous: ON (Friedel pairs unmerged) (7 Items)							
parallelproc	P 21 21 21	60	63.9	69.5	90	90	90
EDNAproc	P 21 21 21	60	63.9	69.5	90	90	90
fastproc	P 2 2 2	60	63.9	69.5	90	90	90
parallelproc	P 2 2 2	60	63.9	69.5	90	90	90
parallelproc	P 1 2 1	59.9	63.9	69.5	90	89.9	90
parallelproc	P 1 2 1	63.9	60	69.5	90	90	90
parallelproc	P 1	59.9	63.9	69.5	90	90	90

RSymm threshold in lower shell: I/Sigma threshold in lower shell:

Main Output Parameters

Overall:
Overall Resolution: 100.7-1.34 Å
Overall Completeness: 98.6%
Overall I over Sigma: 15.3
Overall Rsymm: 4.4%
Overall Multiplicity: 4

Outer Shell:
Outer Shell Resolution: 1.9-1.34 Å
Outer Shell Completeness: 97.6%
Outer Shell I over Sigma: 1.5
Outer Shell Rsymm: 71.6%
Outer Shell Multiplicity: 4.2

Unit Cell:
Unit Cell A: 60.0 Å
Unit Cell B: 63.9 Å
Unit Cell C: 69.5 Å
Unit Cell Alpha: 90.0°
Unit Cell Beta: 90.0°
Unit Cell Gamma: 90.0°

Files

Download

XDS | XSCALE | SCALA/AIMLESS | SCALEPACK | TRUNCATE

Input Files:
XDS.INP

Output Files:
GXPARM.XDS

Correction Files:
x_geo_corr.cbf
y_geo_corr.cbf

Files

Download

XDS | XSCALE | SCALA/AIMLESS | SCALEPACK | TRUNCATE

Input Files:
scala_noanom.inp

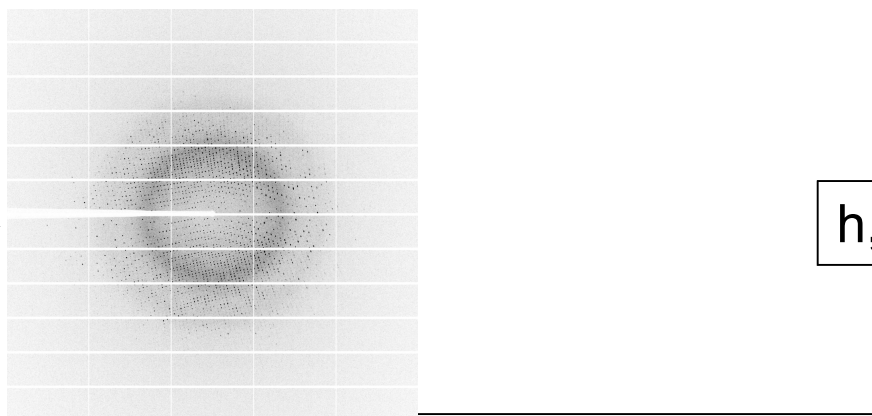
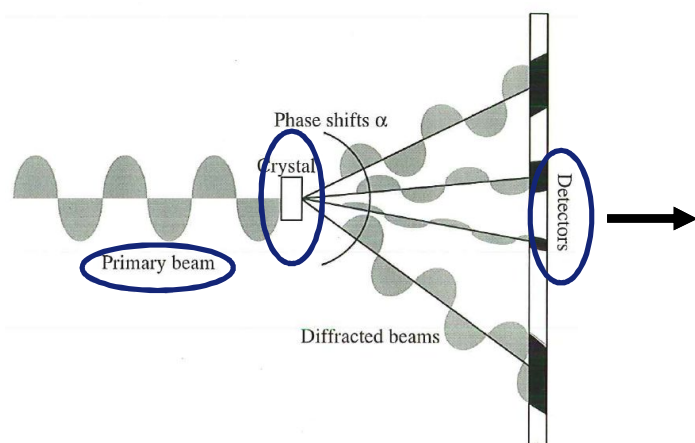
Log Files:
merged_noanom_XSCALE.LP

I/Sigma vs Resolution | Completeness vs Resolution | R-factor vs Resolution | CC/2

Resolution (Å)	I/Sigma
2.89	40
2.29	32
2	25
1.82	18
1.69	12
1.59	8
1.51	6
1.44	4
1.39	3
1.34	2

Delageniere, S. et al., (2011) *Bioinformatics* 27, 3186. doi:10.1093/bioinformatics/btr535.

REPROCESSING OF ESRF MX DATA



$h, k, l, I, \sigma(I)$



```

JOB= ALL      1JOB= DEFFIX XPLAN INTEGRATE CORRECT
DATA_RANGE= 1 1220
SPOT_RANGE= 1 31
SPOT_RANGE= 580 610
BACKGROUND_RANGE= 1 4

!masking non sensitive area of Pilatus
UNTRUSTED_RECTANGLE= 487 495      0 2528
UNTRUSTED_RECTANGLE= 981 989      0 2528
UNTRUSTED_RECTANGLE=1475 1483     0 2528
UNTRUSTED_RECTANGLE=1969 1977     0 2528
UNTRUSTED_RECTANGLE= 0 2464 195 213
UNTRUSTED_RECTANGLE= 0 2464 407 425
UNTRUSTED_RECTANGLE= 0 2464 619 637
UNTRUSTED_RECTANGLE= 0 2464 831 849
UNTRUSTED_RECTANGLE= 0 2464 1043 1061
UNTRUSTED_RECTANGLE= 0 2464 1255 1273
UNTRUSTED_RECTANGLE= 0 2464 1467 1485
UNTRUSTED_RECTANGLE= 0 2464 1679 1697
UNTRUSTED_RECTANGLE= 0 2464 1891 1909
UNTRUSTED_RECTANGLE= 0 2464 2103 2121
UNTRUSTED_RECTANGLE= 0 2464 2315 2333
TRUSTED_REGION=0.0 1.41 !Relative radii limiting trusted detector region

!correction tables to compensate the misorientations of the modules
X-GEO_CORR= ../x_geo_corr.cbf
Y-GEO_CORR= ../y_geo_corr.cbf

MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT= 3
!STRONG_PIXEL= 3.0
OSCILLATION_RANGE= 0.1000
STARTING_ANGLE= 144.0
STARTING_FRAME= 1
X-RAY_WAVELENGTH= 0.97625
NAME_TEMPLATE_OF_DATA_FRAMES= ../rory_w1_1_?????.cbf !CBF
DETECTOR_DISTANCE= 218.61
DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE= 0.0 OVERLOAD= 1048500

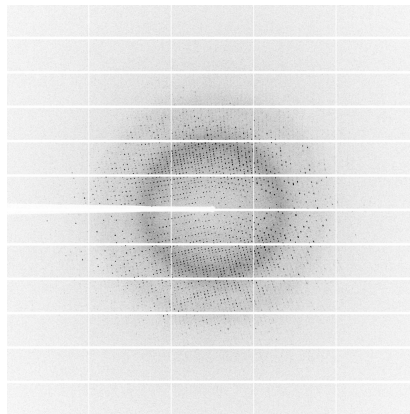
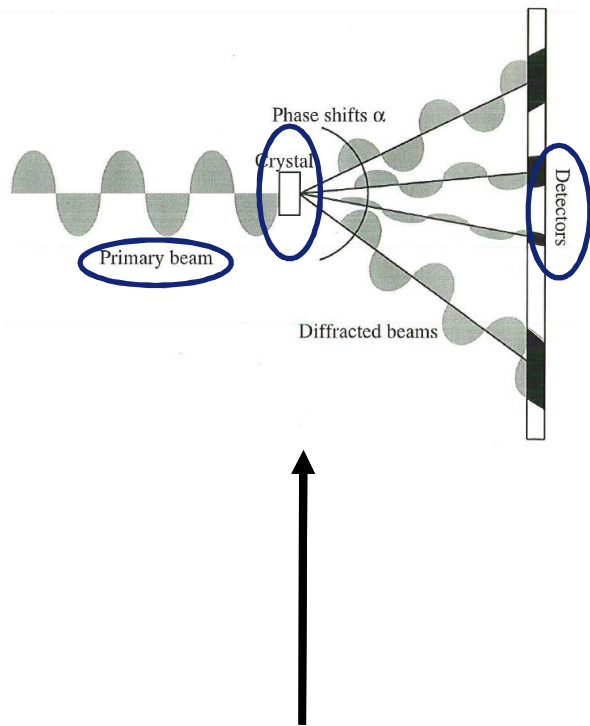
SENSOR_THICKNESS=1.00
ORGY= 1234.63 ORGX= 1254.24
NX= 2463 NY= 2527
QX= 0.1720 QY= 0.1720
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 7000 30000

DIRECTION_OF_DETECTOR_X-AXIS= 1.0 0.0 0.0
DIRECTION_OF_DETECTOR_Y-AXIS= 0.0 1.0 0.0
ROTATION_AXIS= 1.0 0.0 0.0
INCIDENT_BEAM_DIRECTION= 0.0 0.0 1.0
FRACTION_OF_POLARIZATION= 0.99
POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0
!AIR= %8E

SPACE_GROUP_NUMBER= 0
UNIT_CELL_CONSTANTS= 0 0 0 0 0 0
INCLUDE_RESOLUTION_RANGE= 50.0 0.0
!STRICT_ABSORPTION_CORRECTION=TRUE

REFINE(INTEGRATE)= BEAM ORIENTATION CELL
MAXIMUM_NUMBER_OF_PROCESSORS= 16
    
```

REPROCESSING ESRF MX DATA



```
##CBF: VERSION 1.5
# CBF file written by CBFlib v0.8.0

data_image_0

_array_data.header_contents
;
# Detector: PILATUS3 6M, S/N 60-0128, ESRF ID29
# 2015/Jul/22 15:38:43
# Pixel_size 172e-6 m x 172e-6 m
# Silicon sensor, thickness 0.000320 m
# Oscillation_axis omega
# Excluded_pixels: badpix_mask.tif
# Chi 0.0000 deg.
# Angle_increment 0.1000 deg.
# Polarization 0.99
# file_comments
# N_oscillations 1220
# Beam_xy (1234.63, 1254.24) pixels
# Exposure_time 0.020000 s
# Phi 0.0020 deg.
# Energy_range (0, 0) eV
# Start_angle 144.0000 deg.
# Detector_distance 0.218607 m
# Detector_Offset 0.0000 m
# Alpha 0.0000 deg.
# Flat_field: (nil)
# Threshold_setting 7620 eV
# Exposure_period 0.020950 s
# N_excluded_pixels: = 321
# Kappa 0.0020 deg.
# Tau = 0 s
# Transmission 6.63615401085
# Detector_2theta 0.0000 deg.
# Flux 37000000000.0
# Count_cutoff 1048500
# Trim_directory: (nil)
# Wavelength 0.976250 A
;

_array_data.data
;
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
  conversions="x-CBF_BYTE_OFFSET"
Content-Transfer-Encoding: BINARY
X-Binary-Size: 6227375
X-Binary-ID: 0
X-Binary-Element-Type: "signed 32-bit integer"
X-Binary-Element-Byte-Order: LITTLE_ENDIAN
Content-MD5: e0W4qPa17GzzVnqt118A==
X-Binary-Number-of-Elements: 6224001
X-Binary-Size-Fastest-Dimension: 2463
X-Binary-Size-Second-Dimension: 2527
X-Binary-Size-Padding: 128
```

$h, k, l, l, \sigma(l)$



```
#Basic definitions
scanner PILATUS
synchrotron polar 0.99
dispersion 0.0002
divergence 0.090 0.003
genf genfile.gen

#Better have them
wavelength 0.976250
distance 218.61
beam 212.36 215.73

#Just a guess
mosaic 0.5

#Files
directory /data/1429/inhouse/opid291/20150722/RAW_DATA/roxy
template roxy_xl_1_###.cbf
extension cbf
image 1
go
```

METADATA IN ISPYB

Experiment parameters	Beamline parameters	AutoProcessing
Img directory:	/data/id29/inhouse/opid291/20150722/RAW_DATA/roxy	
Img prefix:	roxy_w1	
Nb of images:	1220	
Run no:	1	
Start Time:	22-07-2015 15:38:28	
End Time:	22-07-2015 15:39:16	
Type of experiment:	OSC	
Wavelength:	0.97625 Å	
Energy:	12.7 keV	
Phi start:	144 °	
Oscillation range:	0.1 °	
Overlap:	0 °	
Exposure Time:	0.02 s	
Total Exposure Time:	24.4 s	
Estimated Total Absorbed Dose:		
Number of passes:	1	
Detector Distance:	218.61 mm	
Resolution at edges:	1.30 Å	
Resolution at corner:	1.07 Å	
Xbeam:	212.36 mm	
Vbeam:	215.73 mm	
Kappa:	0	
Phi:	0	
Experiment comment:		

+

Experiment parameters	Beamline parameters	AutoProcessing
Synchrotron name:	ESRF	
Synchrotron filling mode:	7/8 multibunch	
Beamline name:	ID29	
Undulator types:	IVU21c_GAP U35a_GAP	
Undulator gaps:	9.55 mm 50.0 mm	
Beam transmission:	7 %	
Slit gap Hor:	500 µm	
Slit gap Vert:	200 µm	
Detector type:	PIXEL	
Detector name:	Pilatus3_6M	
Detector manufacturer:	DECTRIS	
Detector mode:	Unbinned	
Detector pixel size Hor:	0.172 mm	
Detector pixel size Vert:	0.172 mm	
Focusing optics:	Toroidal mirror	
Monochromator type:	Si(111)	
Beam shape:	ellipse	
Flux:	3.7e+11 photons/sec	
Flux end:	3.7e+11 photons/sec	
Beam size at sample Hor:	50 µm	
Beam size at sample Vert:	30 µm	
Beam divergence Hor:	104 µrad	
Beam divergence Vert:	6 µrad	
Polarisation:	0.99 °	

+

```
JOB= ALL !JOB= DEPIX XPLAN INTEGRATE CORRECT
DATA_RANGE= 1 1220
SPOT_RANGE= 1 31
SPOT_RANGE= 580 610
BACKGROUND_RANGE= 1 4

!masking non sensitive area of Pilatus
UNTRUSTED_RECTANGLE= 487 495 0 2528
UNTRUSTED_RECTANGLE= 981 989 0 2528
UNTRUSTED_RECTANGLE=1475 1483 0 2528
UNTRUSTED_RECTANGLE=1969 1977 0 2528
UNTRUSTED_RECTANGLE= 0 2464 195 213
UNTRUSTED_RECTANGLE= 0 2464 407 425
UNTRUSTED_RECTANGLE= 0 2464 619 637
UNTRUSTED_RECTANGLE= 0 2464 831 849
UNTRUSTED_RECTANGLE= 0 2464 1043 1061
UNTRUSTED_RECTANGLE= 0 2464 1255 1273
UNTRUSTED_RECTANGLE= 0 2464 1467 1485
UNTRUSTED_RECTANGLE= 0 2464 1679 1697
UNTRUSTED_RECTANGLE= 0 2464 1891 1909
UNTRUSTED_RECTANGLE= 0 2464 2103 2121
UNTRUSTED_RECTANGLE= 0 2464 2315 2333
TRUSTED_REGION=0.0 1.41 !Relative radii limiting trusted detector region

!correction tables to compensate the misorientations of the modules
X-GEO_CORR= ../x_geo_corr.cbf
Y-GEO_CORR= ../y_geo_corr.cbf

MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT= 3
!STRONG_PIXEL= 3.0
OSCILLATION_RANGE= 0.1000
STARTING_ANGLE= 144.0
STARTING_FRAME= 1
X-RAY_WAVELENGTH= 0.97625
NAME_TEMPLATE_OF_DATA_FRAMES= ../roxy_w1_1?????.cbf !CBF
DETECTOR_DISTANCE= 218.61
DETECTOR= PILATUS MINIMUM_VALID_PIXEL_VALUE= 0.0 OVERLOAD= 1048500

SENSOR_THICKNESS=1.00
ORGX= 1234.63 ORGY= 1254.24
NX= 2463 NY= 2527
QX= 0.1720 QY= 0.1720
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 7000 30000

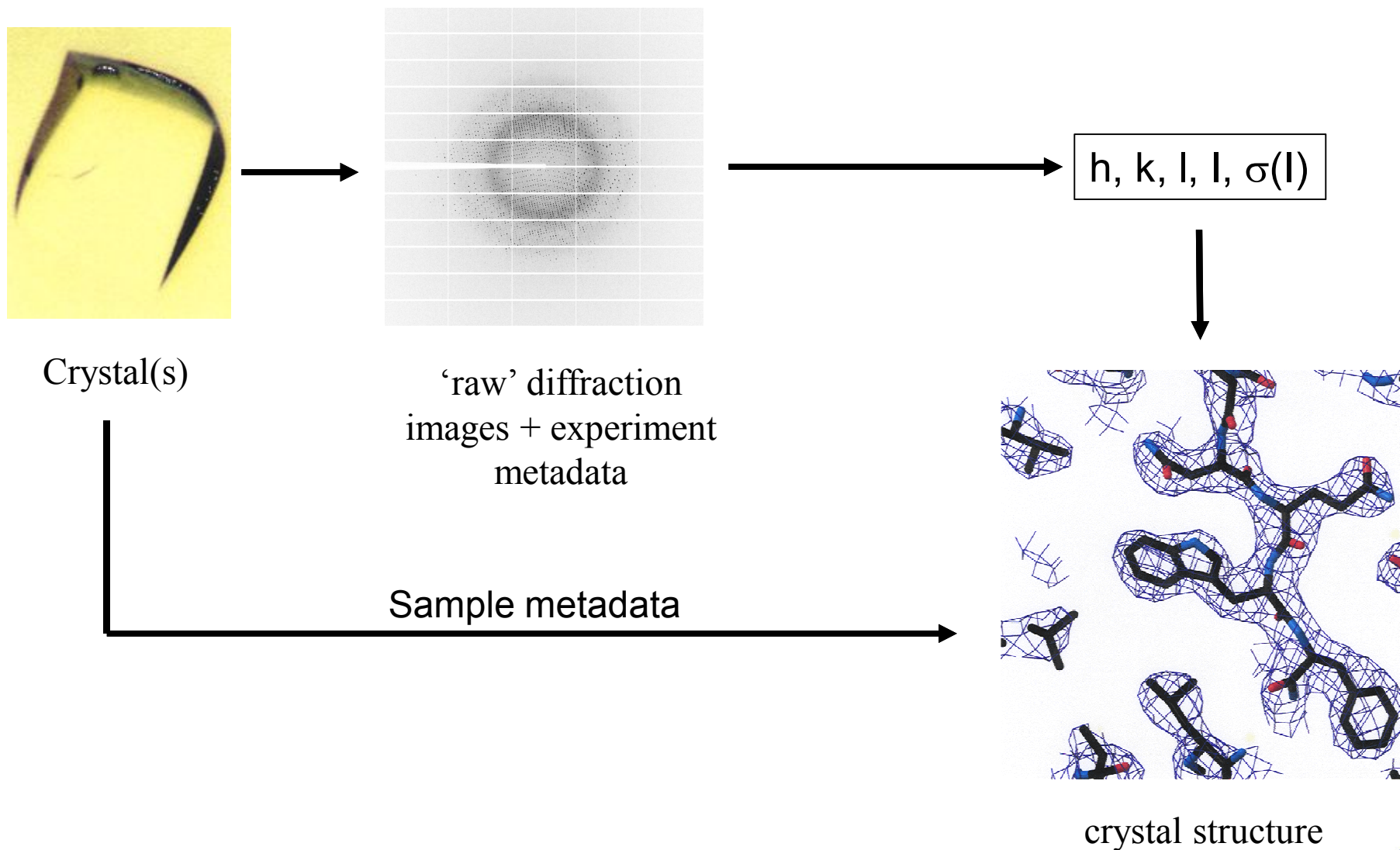
DIRECTION_OF_DETECTOR_X-AXIS= 1.0 0.0 0.0
DIRECTION_OF_DETECTOR_Y-AXIS= 0.0 1.0 0.0
ROTATION_AXIS= 1.0 0.0 0.0
INCIDENT_BEAM_DIRECTION= 0.0 0.0 1.0
FRACTION_OF_POLARIZATION= 0.99
POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0
!AIR= %.8f

SPACE_GROUP_NUMBER= 0
UNIT_CELL_CONSTANTS= 0 0 0 0 0
INCLUDE_RESOLUTION_RANGE= 50.0 0.0
!STRICT_ABSORPTION_CORRECTION=TRUE

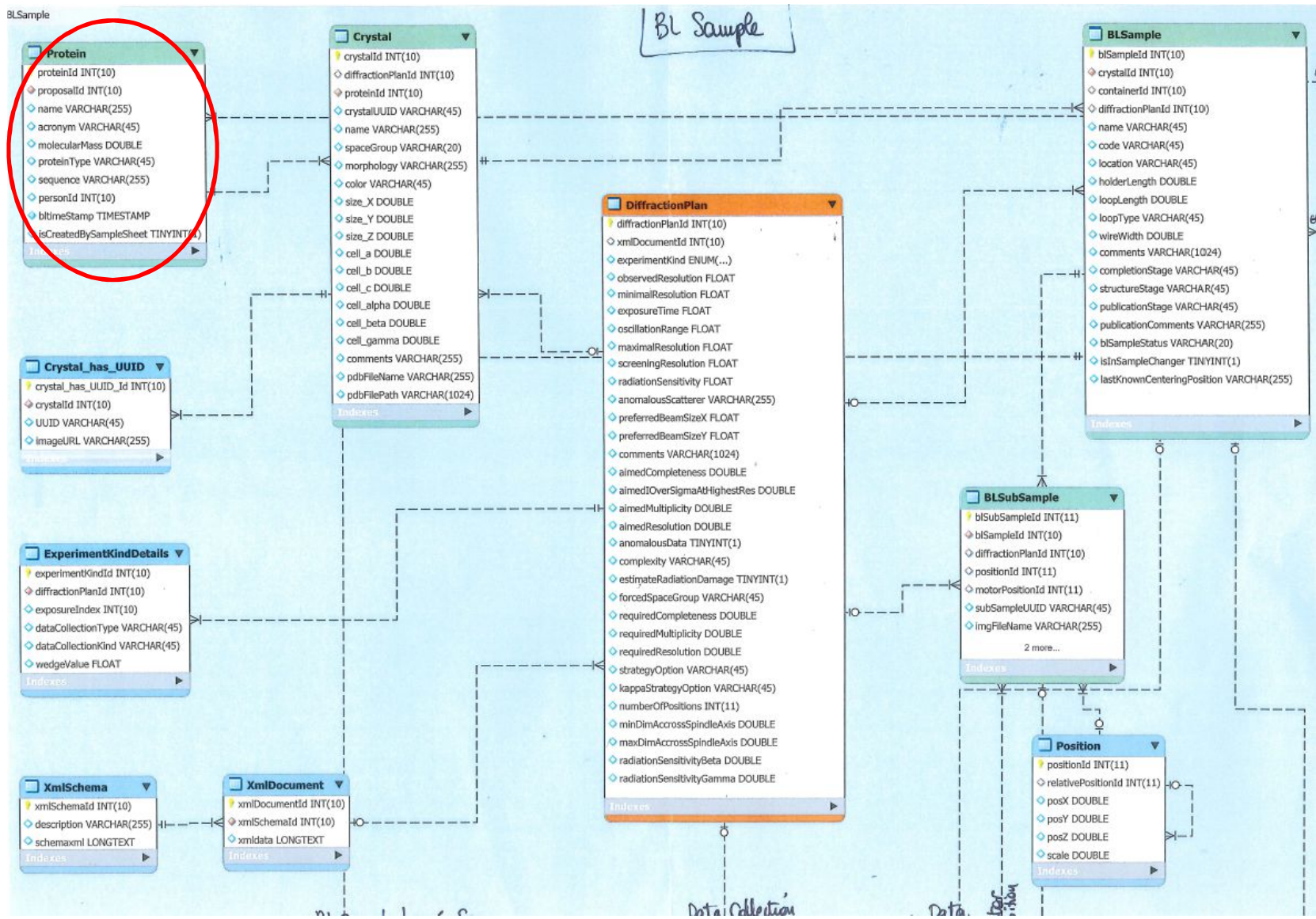
REFINE (INTEGRATE)= BEAM ORIENTATION CELL
MAXIMUM_NUMBER_OF_PROCESSORS= 16
```

- Metadata from data collection experiment reasonably well archived in ISPyB and available to experimenter/beamline managers etc.
- But, raw images themselves not available long term (i.e. > 6 months) for (re)analysis.

WHAT ABOUT METADATA FOR SAMPLE(S)?

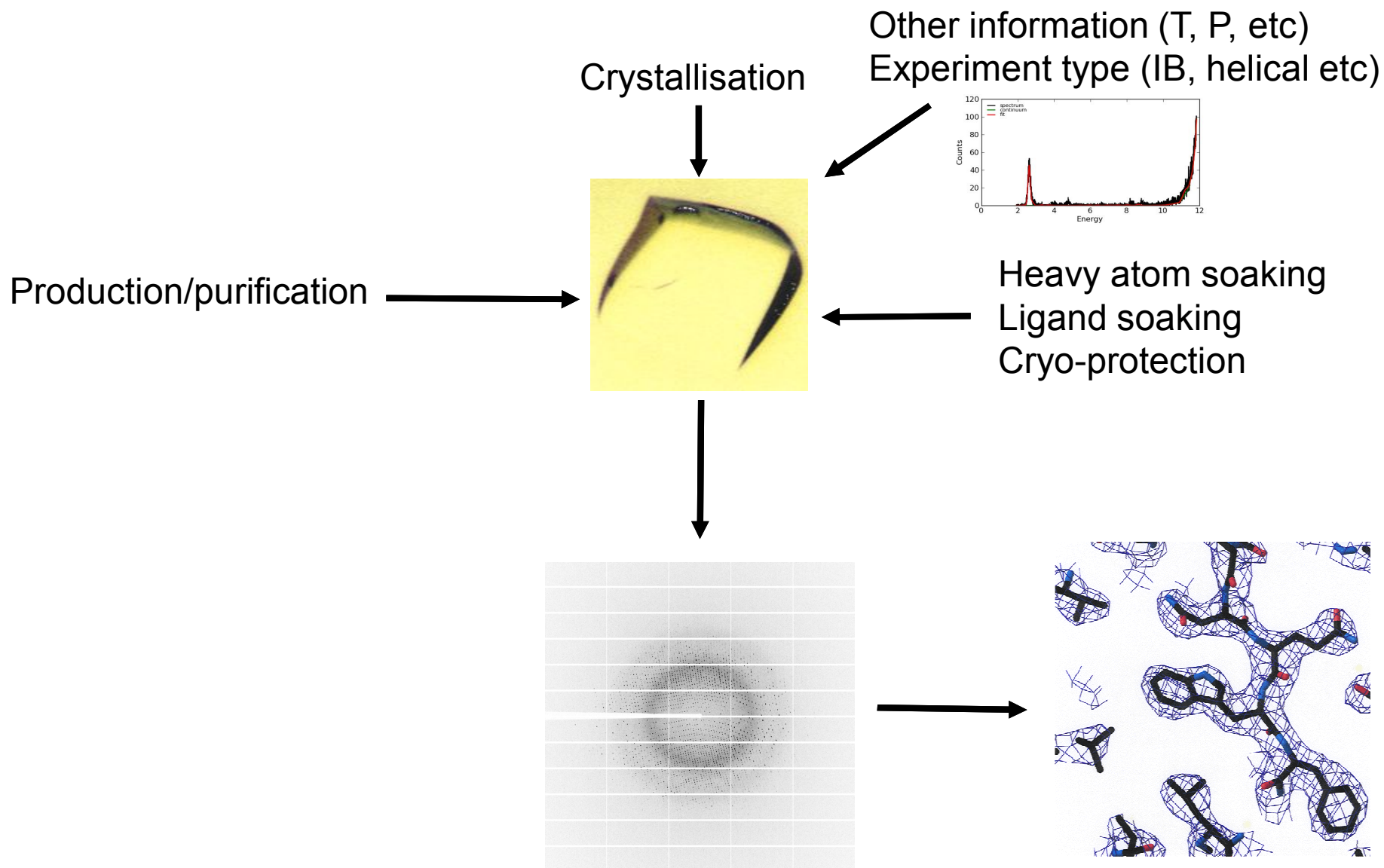


SAMPLE METADATA IN ISPYB

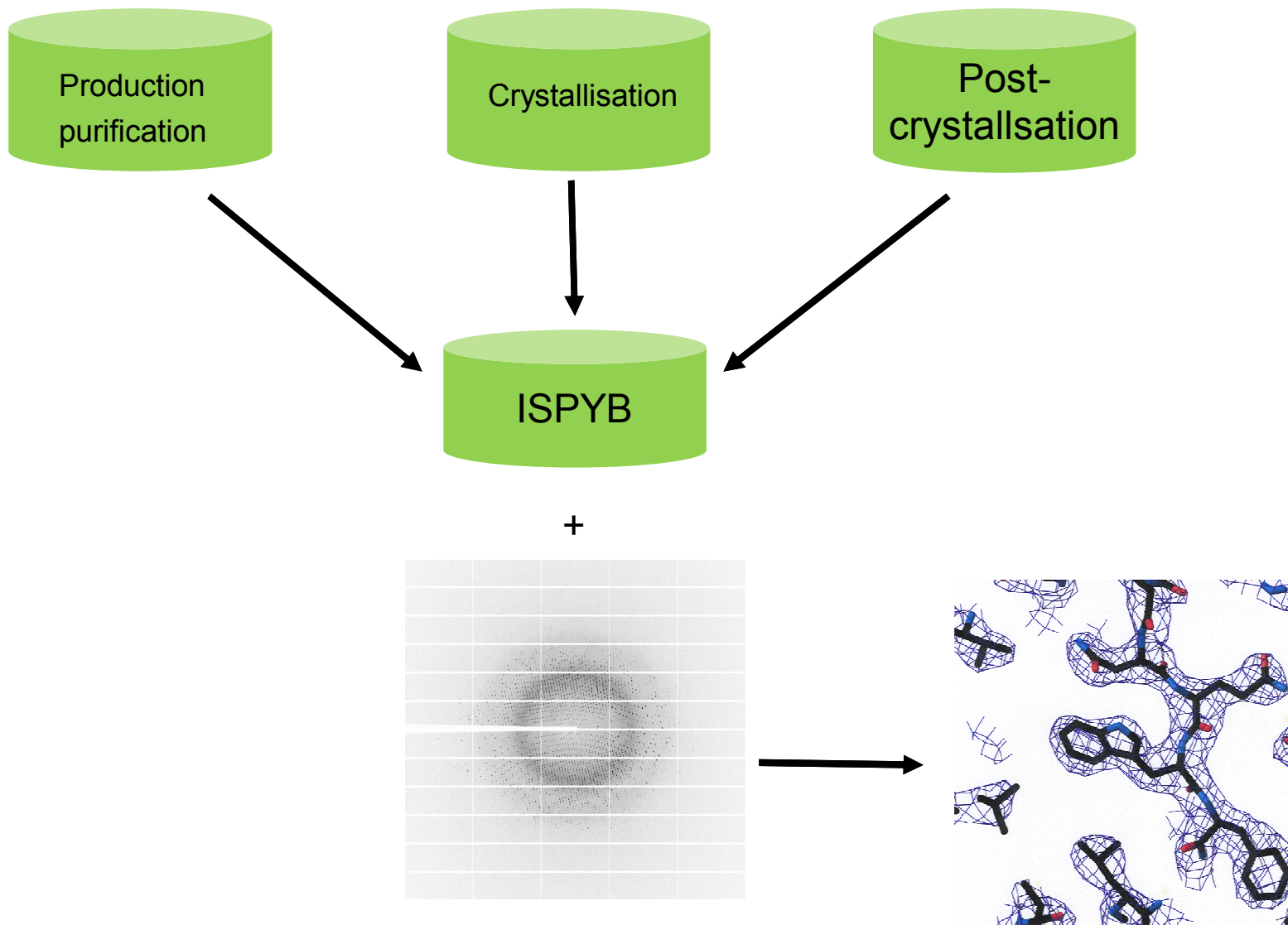


Delageniere, S. et al., (2011) *Bioinformatics* 27, 3186. doi:10.1093/bioinformatics/btr535.

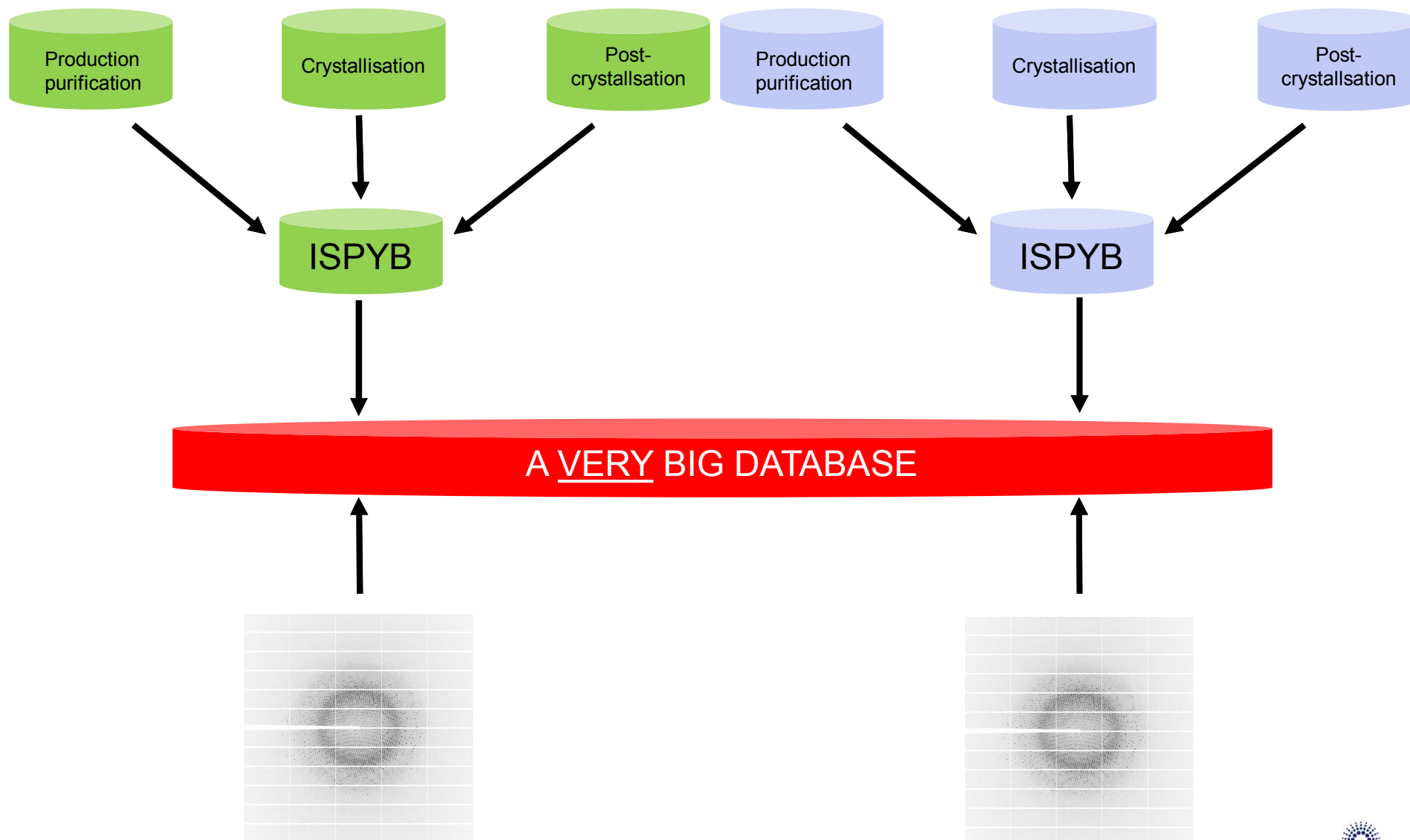
WHAT EXTRA SAMPLE METADATA MIGHT BE NEEDED?



ISPYB NEEDS CONNECTED TO OTHER DATABASES/LIMS AND TO RAW IMAGES



EACH SR SITE HAS ITS OWN 'ISPYB'



CONCLUSIONS

- **The metadata required in order to make raw data from ESRF MX beamlines intelligible are not extensive and are archived in ISPyB**
 - Describes the experiment carried out on a given sample
 - Enables users to understand what happened during autoprocesing
 - Enables reprocessing of raw images by users (limit to time these are held in ESRF central storage)
- **To make raw images fully intelligible for 'non-owners' further metadata are needed**
 - Sample production/purification
 - Crystallisation
 - Post-crystallisation
 - etc....
 - Requires linking of ISPyB and other databases (i.e. CRIMS, etc)
- **Each SR site has own version of ISPyB**
 - Should we have a centralized ISPyB where metadata for ALL SR-based MX experiments could be archived?

CONCLUSIONS

Thanks for your attention