

Data Processing with iMosflm

launch the graphical interface

In the terminal, go in the appropriate directory :

```
cd data-oleron/RX/lyso-Gd-SAD
```

or

```
cd data-oleron/RX/lysozyme-renafobis/BM30A-2014-11-19
```

One directory contains data for the SAD phasing method, the other is for molecular replacement.

Create a directory for the processing :

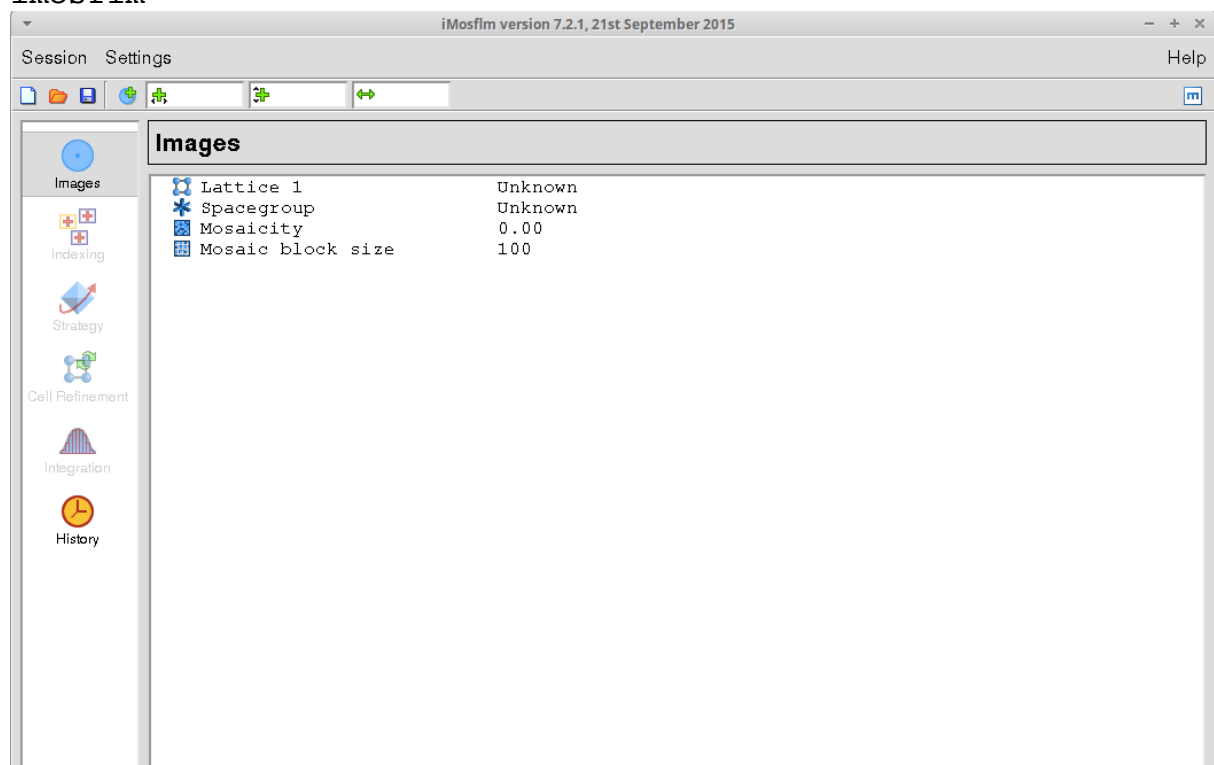
```
mkdir process
```

```
cd process
```

set up the CCP4 environment and launch iMosflm:

```
setccp4
```

```
imosflm
```



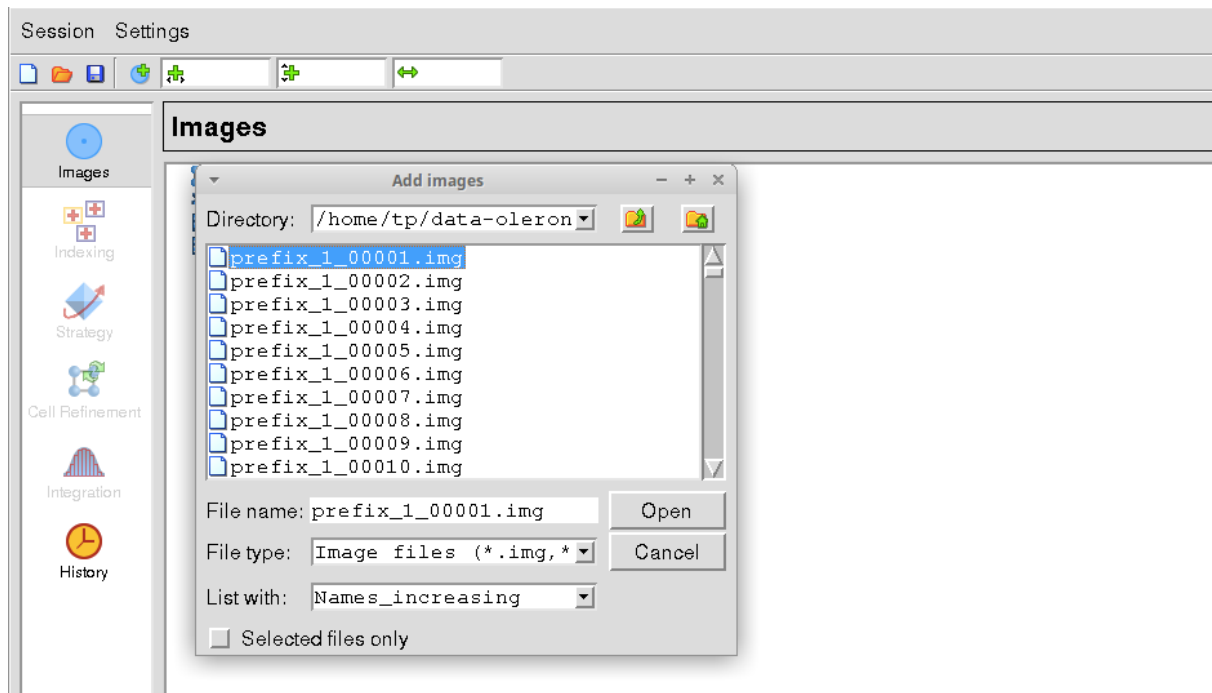
On the left side, you will find the different buttons that execute each step of data processing : images (select the images you will process), indexing (autoindexation in order to find possible cell parameters and possible spacegroup), cell refinement (optimize estimation of cell parameters), integration (get the intensity of all spots on all images). The strategy button is only useful when collecting data.

Indexation

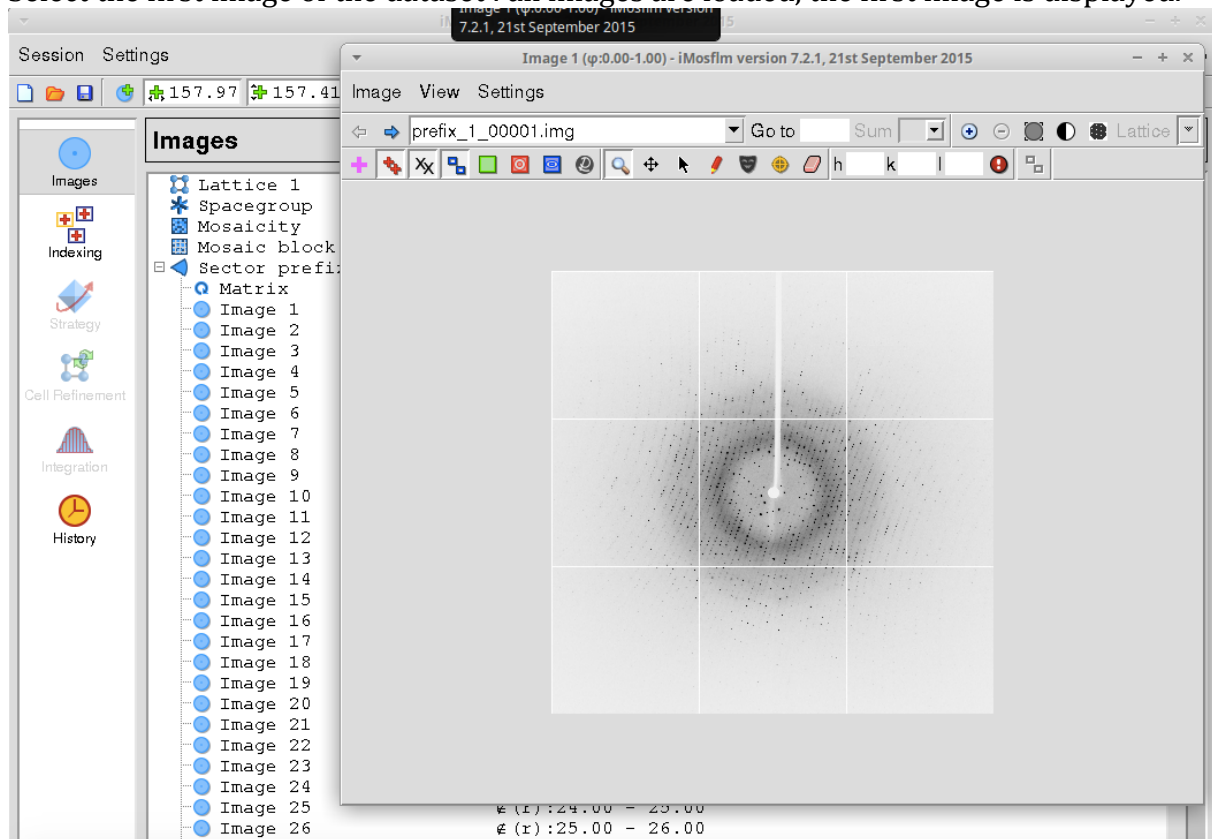
Select the images :

Session -> Add images

A file browser pops up : go in the img directory that lies beside the proces directory (../img)



Select the first image of the dataset : all images are loaded, the first image is displayed.



Check the diffraction quality, the resolution limit...

Before indexing, you will have to change a parameter that defines the geometry of the experimental setup :

Experiment settings

Experiment | **Detector**

Project: New Project

Crystal: New Crystal

Dataset: New Dataset

Title: Untitled

Beam position: X (mm): 157.98
Y (mm): 157.73

Crystal to detector distance (mm): 140.80

Beam divergence: X (°): 0.02
Y (°): 0.02

Wavelength (ϵ , Å): 0.9792

Wavelength dispersion (Å): 0.0002

Beam polarization: 0.95

Detector angle (2ϵ , °): 0.00

☒ Reverse direction of spindle rotation

Detector omega: 0.0

Invert X direction TRUE/FALSE: T

Close

Settings -> Experiment settings

Tick the « Reverse direction of spindle rotation.

Click the indexing button : it starts automatically, using 2 images

iMosflm version 7.2.1, 21st September 2015

Session Settings Help

157.98 157.73 140.80 5.00 10.0 0.51 0.71 0.00 20 252

Autoindexing

prefix_1_####.img: 1, 90

Image	ϵ range	Auto	Man	Del	> I/ ϵ (I)	Find	Use
1	0.00 - 1.00	1568	0	0	1147	☒	☒
90	89.00 - 90.00	1324	0	0	898	☒	☒
Total		2892	0	0	2045		

Lattice 1

Solution	Lat.	Pen.	a	b	c	$\epsilon^\pm$	ϵ''	$\epsilon^\pm$	$\epsilon(x,y)$	Nref	ϵ beam
1 (ref)	aP	0	37.0	79.2	79.2	90.0	90.1	90.0	0.22	1929	0.26 (0.2)
2 (ref)	mP	0	37.0	79.2	79.2	90.0	90.1	90.0	0.22	1923	0.26 (0.1)
3 (ref)	mP	0	37.0	79.2	79.2	90.0	90.1	90.0	0.21	1919	0.26 (0.1)
4 (ref)	mP	0	79.2	37.0	79.2	90.0	90.0	90.0	0.21	1914	0.25 (0.1)
5 (ref)	aP	0	37.0	79.2	79.2	90.0	89.9	90.0	0.22	1929	0.26 (0.2)
6 (ref)	oC	1	112.0	112.0	37.0	90.0	90.0	90.0	0.22	1903	0.25 (0.2)
7 (ref)	oP	1	37.0	79.2	79.2	90.0	90.0	90.0	0.21	1917	0.25 (0.1)
8 (ref)	mC	1	112.0	112.0	37.0	90.0	90.1	90.0	0.23	1914	0.25 (0.2)
9 (ref)	mC	1	112.0	112.0	37.0	90.0	90.1	90.0	0.23	1914	0.25 (0.2)
10 (ref)	tP	1	79.2	79.2	37.0	90.0	90.0	90.0	0.21	1914	0.25 (0.1)
11 (reg)	mC	98	37.0	162.7	79.2	90.0	90.0	90.0	-	-	-
12 (reg)	mC	98	162.7	37.0	79.2	90.0	90.0	90.0	-	-	-
13 (reg)	oC	98	37.0	162.7	79.2	90.0	90.0	90.0	-	-	-
14 (reg)	mC	98	37.0	162.5	79.2	90.0	90.1	90.0	-	-	-

Lattices: Show Start beam search Show

Check the proposed cell parameters : what are the lengths ? the angles ?

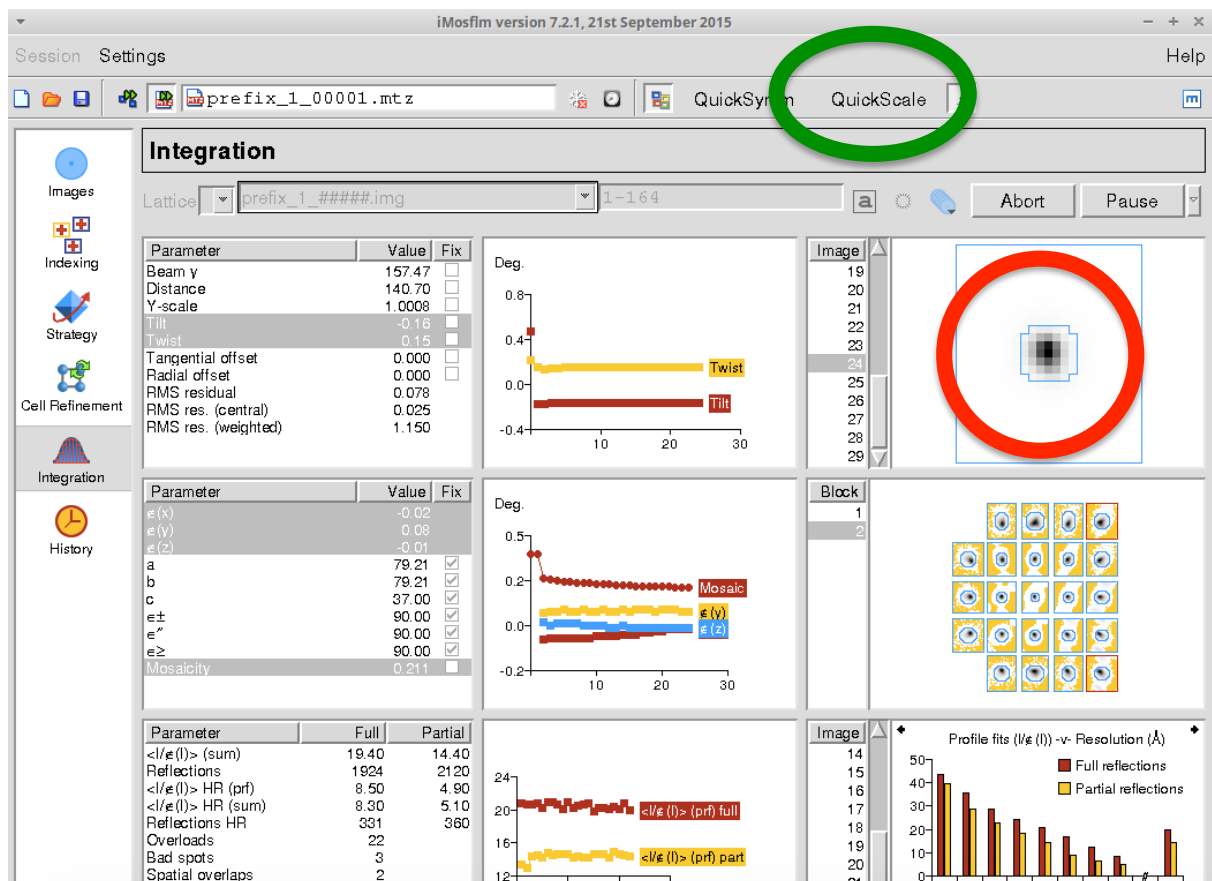
The default proposed symmetry (P4) can be used as a starting hypothesis.

In the frames displaying window, you can now load any images, and predicted spots for this rotation angle will be displayed.

Integration and scaling

Hit the integration buttons : all images from the dataset are selected. Hit the process button , get a cup of coffee while the computer works for you.

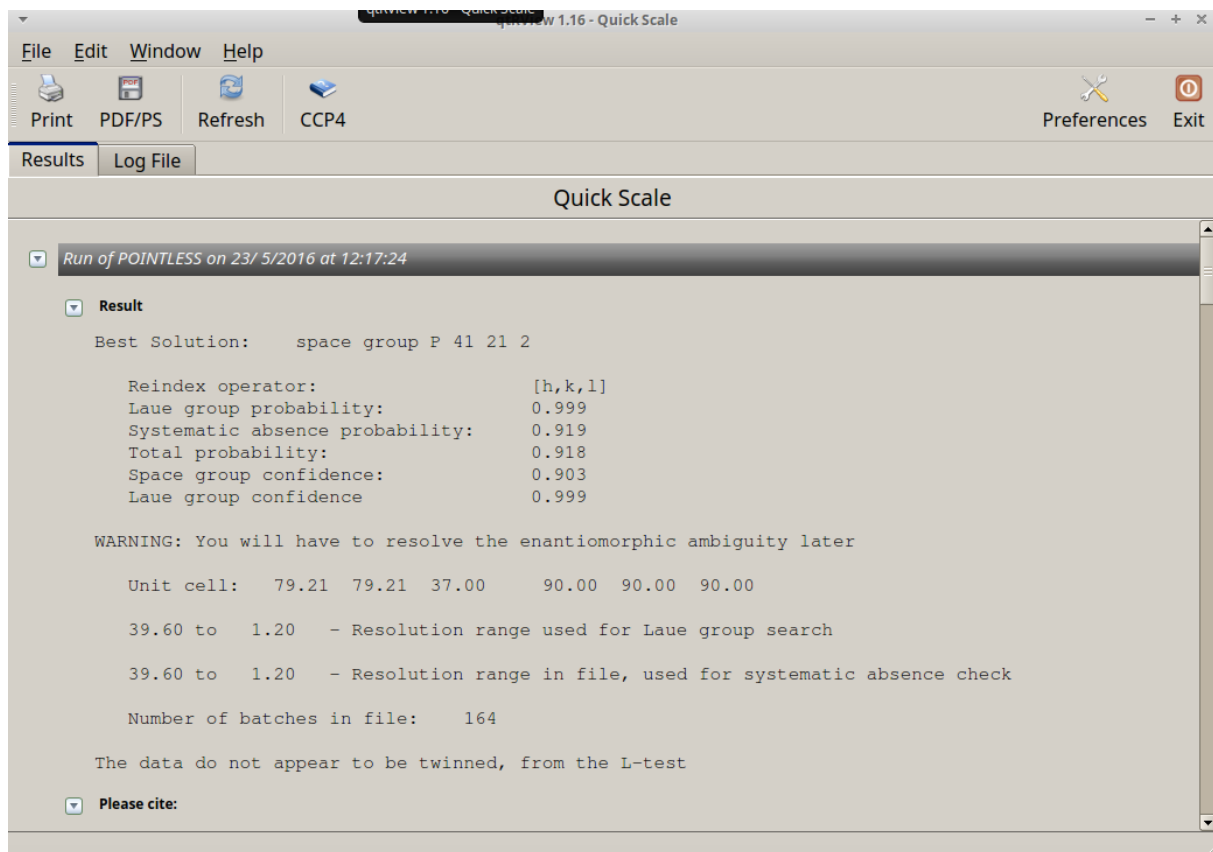
Keep an eye on the central profile (red circle) :



If something goes wrong, you will see it quickly !

When processing is finished, we can validate our hypothesis about symmetry, and scale and merge our data : click the QuickScale button (green circle above). Get another cup of coffee.

When scaling is finished, a new window pops up, where you can check what happens.



What is the proposed spacegroup ?

What does the Table 1 looks like ?

Are we ready for phasing ?