Notes on converting 13-BMC single crystal data to CrysalisPro

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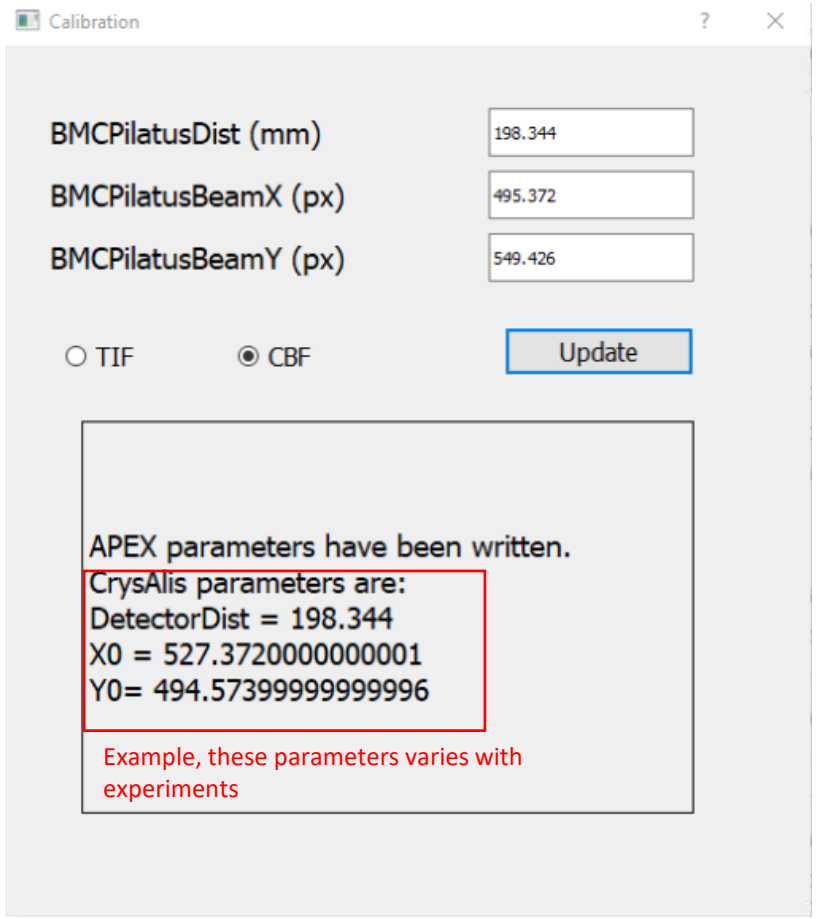
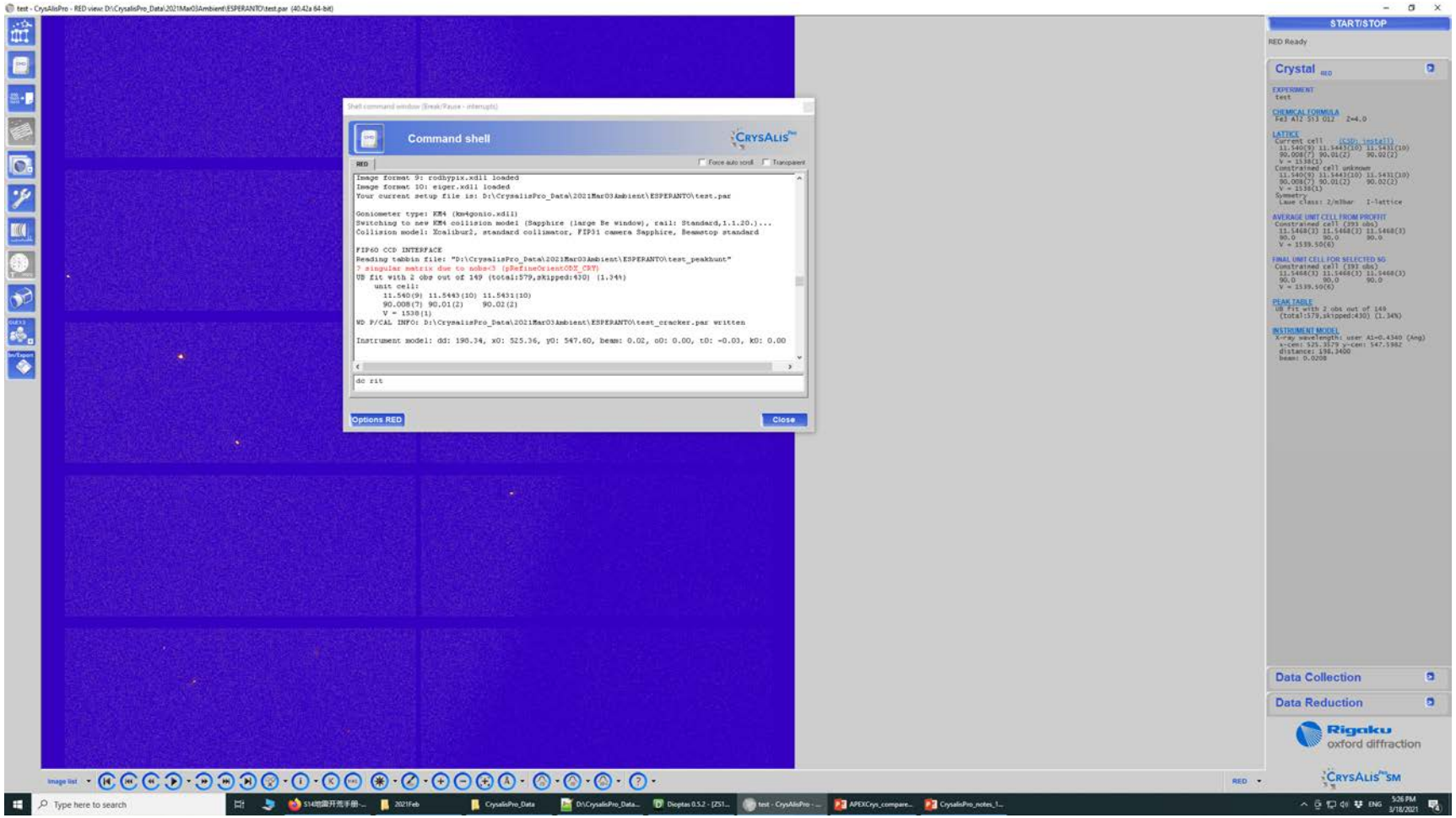
Information needed



- CrysAlis parameters from “Calibration” panel of BMC_Xtal
- Total phi-scan range, step size and exposure time for the cbf image sequences
- Total phi-scan range e.g.: start from 66, end in 116, then total range is 50 degs.

Start CrysalisPro



- Select a random project, then go to command shell, type “dc rit” then enter

Esperanto importer (1.0.6)

Input format

Known CrysAlisPro format DECTRIS/PILATUS cbf

Generic uncompressed image

Skip header bytes: 0 x= 1043 y= 981 Pixel type UNSIG SHORT (2 BYTES)

Frames info

Run digits 0 Separator None Frame 3 nameFFF.ext

D:\CrysalisPro_Data\test2\test_1_006_00001.cbf Browse

D:\CrysalisPro_Data\test2\test_1_006_00100.cbf Browse

Press after find files

Show header 1st | Show header last | Import data from headers | Run TC

Esperanto output

Images base name: test Run # 1

Rotation [deg]: 0 90 180 270 Mirror

Detector info, Auto-gap detection

Pixel size [mm]: 0.1720 x0= 527.4 y0= 494.6 > 99999.0 overflow

Use Auto-gap detection with value -1 Edit

Instrument info

Wavelength: User 0.43, 0.43, 0.43 Edit al1, al2, b Synchrotron: 0.4340 Edit lambda

Monochromator: MIRROR/SYNCHROTRON Polfact: 0.980 Edit polfact

Alpha, Beta [deg]: 50.0, 0.0 Edit

Omega0,Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 Edit

Detector dist. [mm]: 198.3 Edit Beam b2: 0.000 Edit

Gain: 1.0 Edit Thickn.: 4.0000mm Edit thk

Scan info

Scan type: Phi Omega= -0.0 Omega Phi= 90.0

Scan: start, step, exp: -25.0, 0.5, 2.0 Edit Theta= -0.0 Kappa= 0.0

Use frames in inverse order 1=last, 2=last-1... Scan scale err 1.000 Edit

Load | Save

Help | Cancel | OK

Del = 0, Nu = 0

X0 = Dioptas X0+32 pixel (for CrysalisPro square image pading)

Y0 = 1044 - Dioptas Y0

Use frames in inverse order

Start = -(phi-scan range)/2

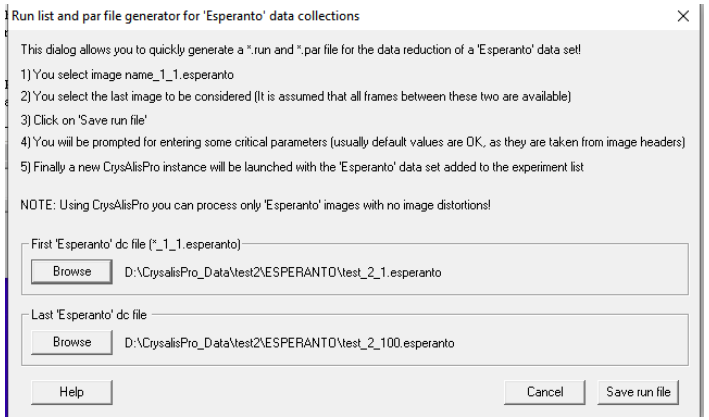
Uncheck “Thickn”

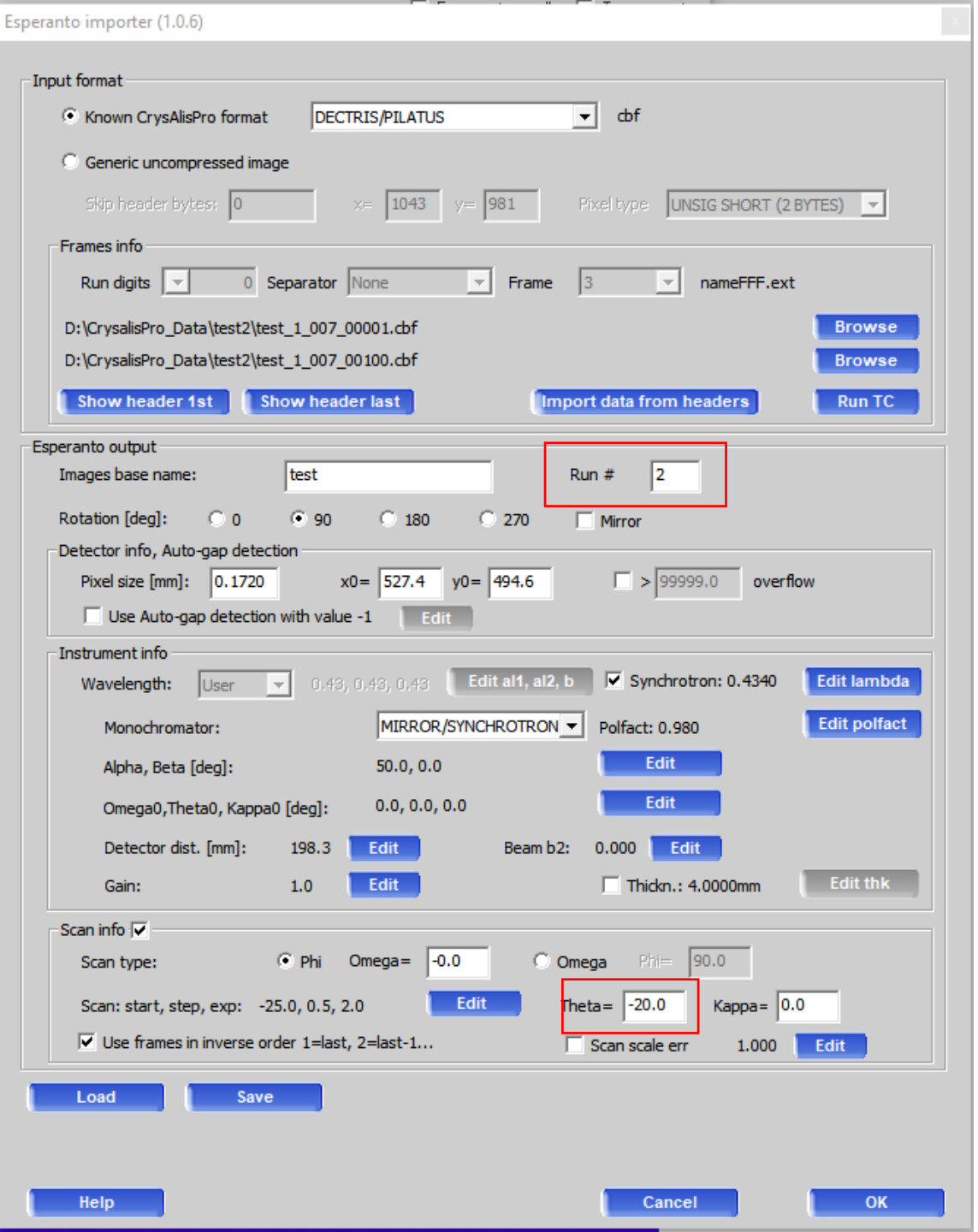
Remember to change your images base name, and Run#.

For (del =0, nu = 0), use them as Run#1.

If peak harvest still screw up, use “um i” command to update the detector info

After data conversion save run file for future use.

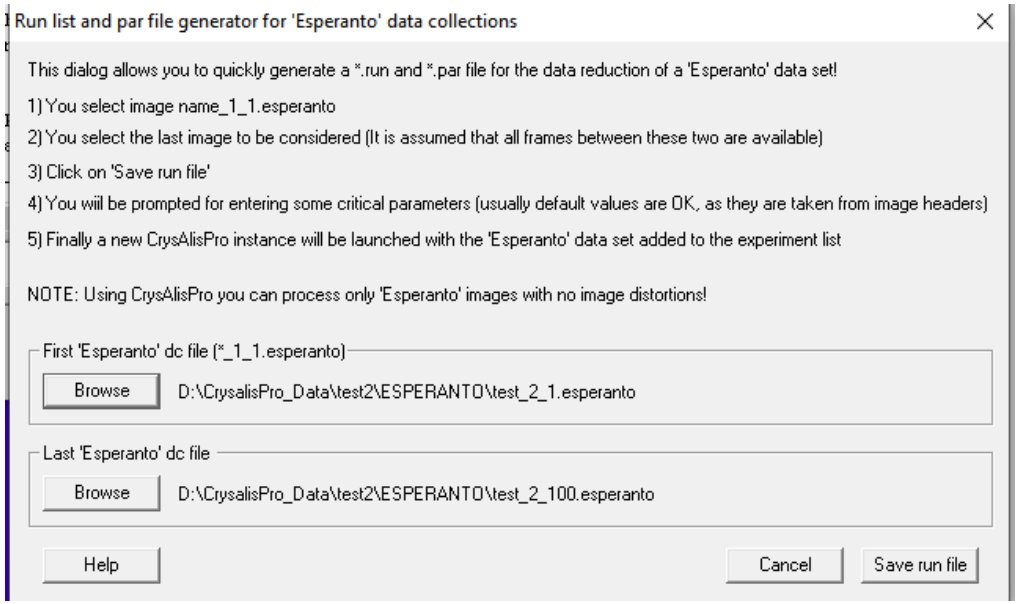




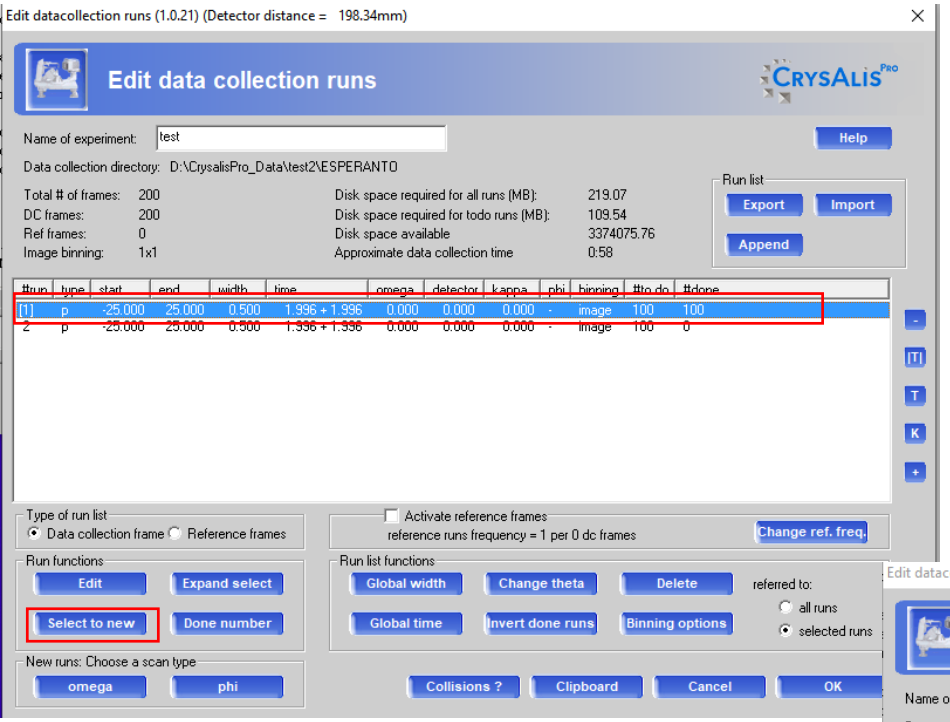
For data collected at non-zero del angle, Theta = - del, Other parameters should be the same as zero-del.

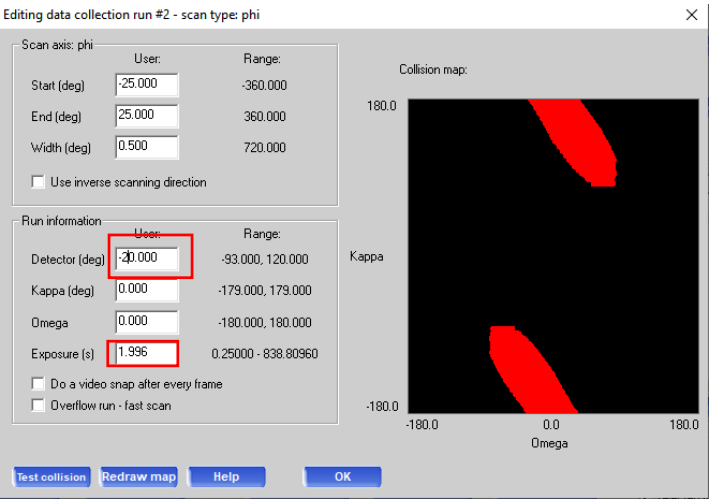
Remember to change the image base name and the run #

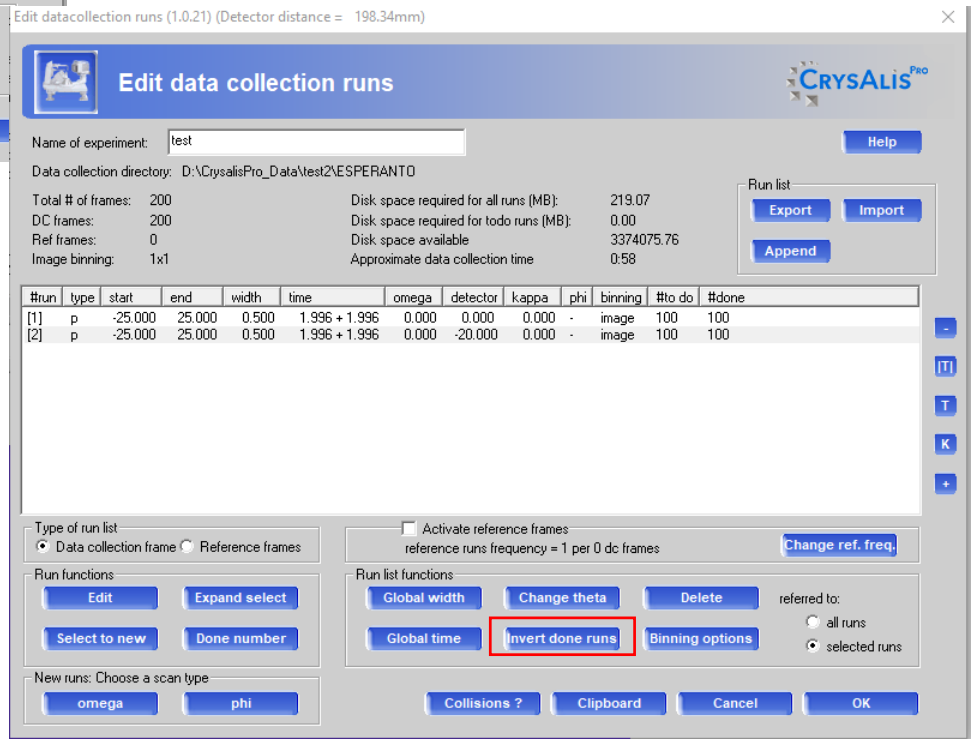
You don’t need to save run file for the second detector position of the same pressure point.



Merge two detector positions



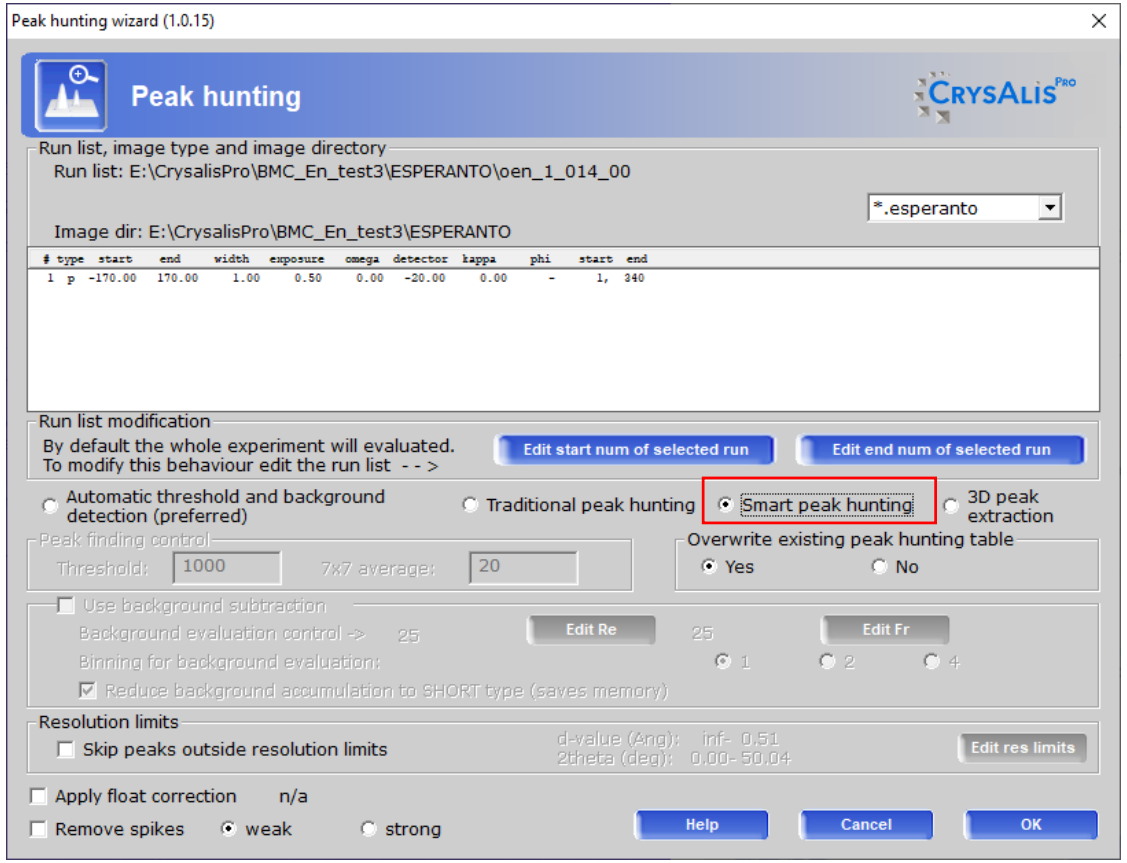


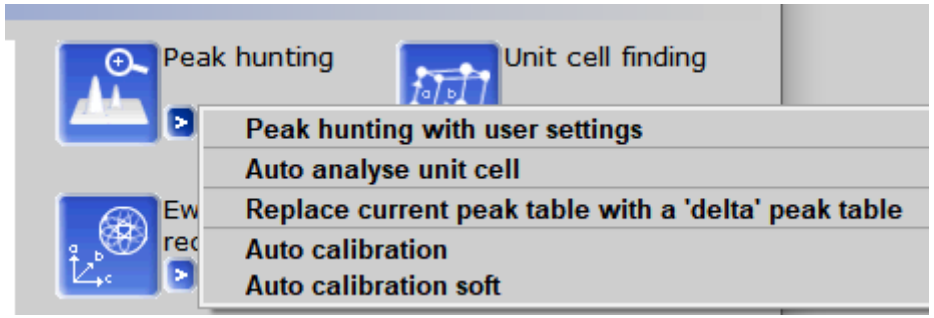


- Go to command shell, “dc editruns”, highlight the experiment, then click “select to new”
- Edit the second run so that the detector angle and the exposure is correct
- Then highlight the second run and “invert done runs” so that “#done” is the same as “#to do”

Peak hunting


- Now go to lattice wizard->peak hunting with user settings
- Usually use smart peak hunting.

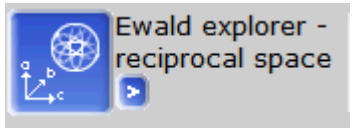




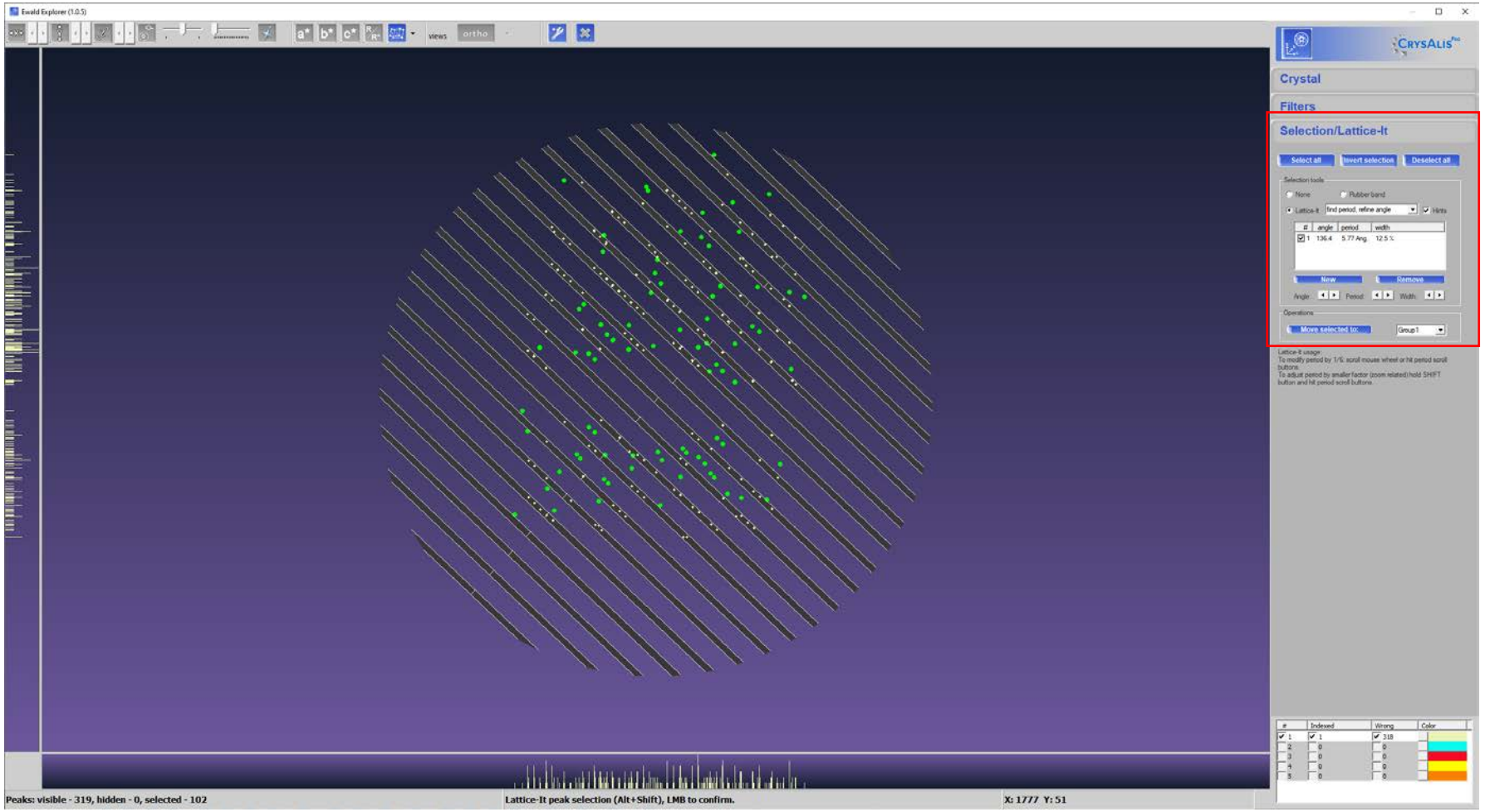
Play with other peak hunting settings if smart hunting doesn’t give you enough peaks

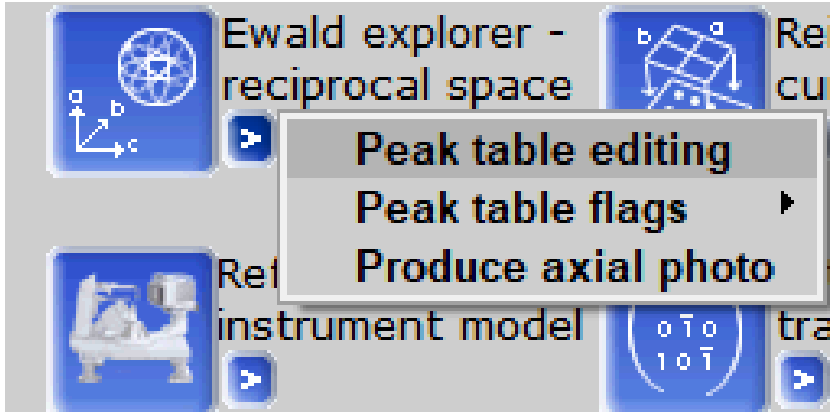
Find lattice

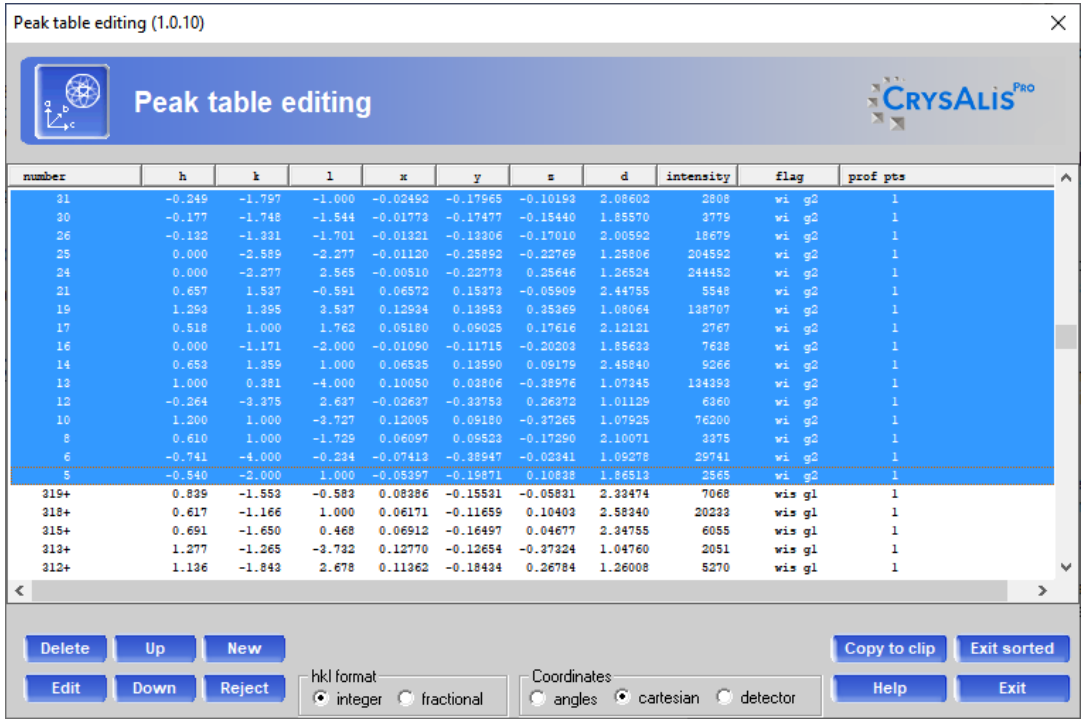
Go to Ewald explorer



Use lattice-it to select the outliers





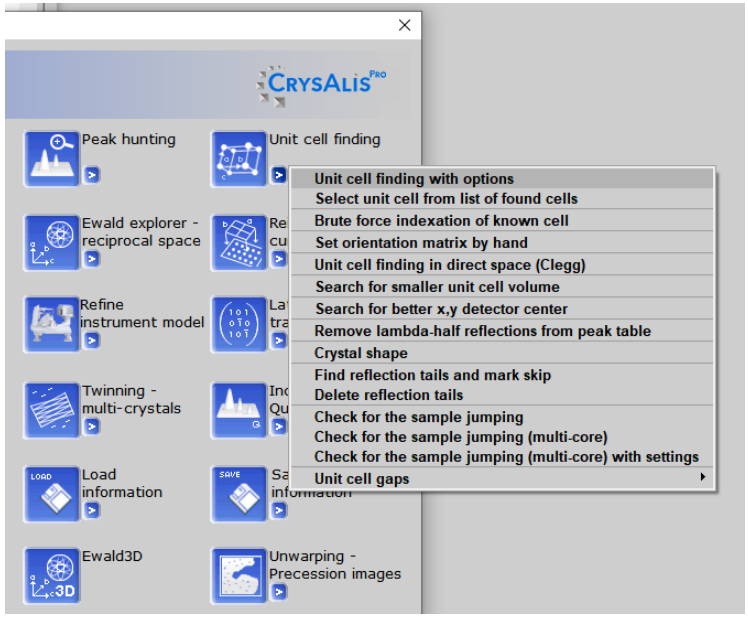


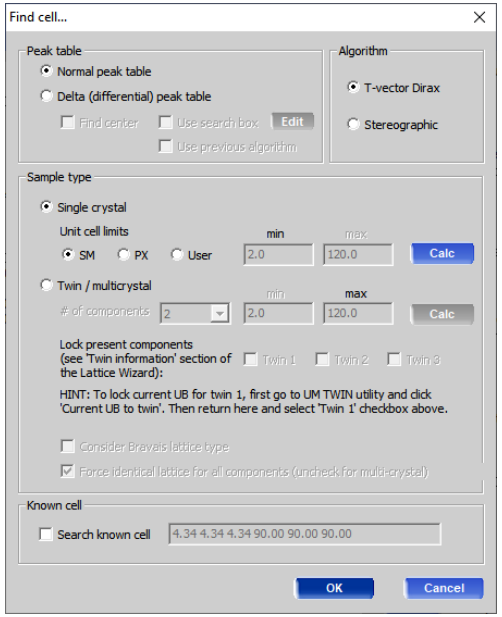
Move all outliers to g2

Go to Ewald explorer-> peak table editing

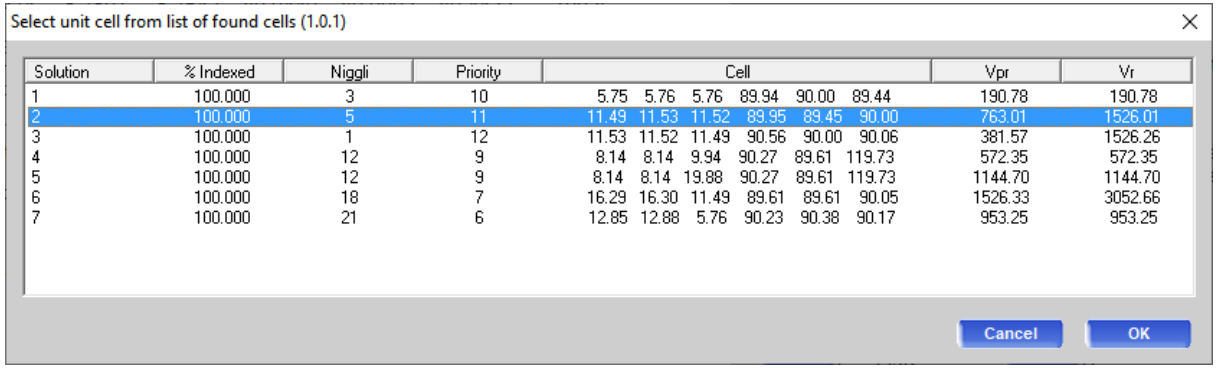
Remove all g2 peaks.

Find unit cell



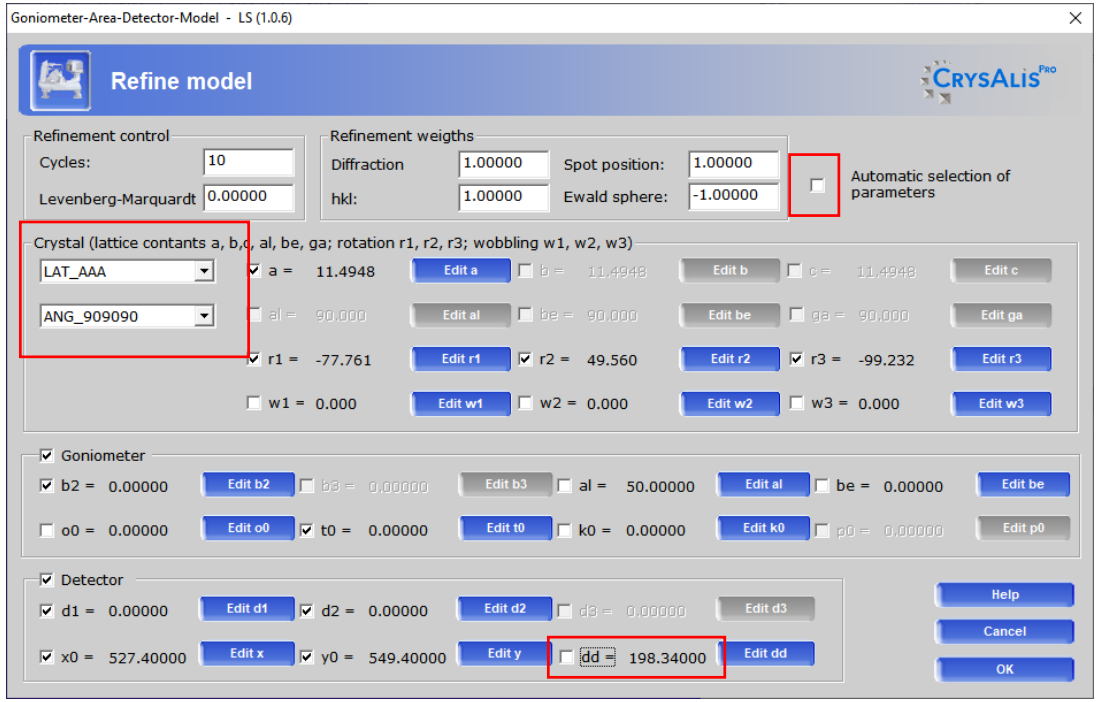


- Go to unit cell finding, then unit cell finding with options
- Find unit cell automatically, or search known cell
- If the correct cell is not found, select the correct one from list of found cells.



Refine instrument model

- Uncheck automatic selection of parameters
- Select the correct lattice type
- Uncheck dd



Ready for integration

- Now you should have the correct unit cell.
- Next step please refer to integration and find space group manual by Dr Stella Chariton.