

# Notes on converting 13-BMC single crystal data to CrysalisPro

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# Information needed

Calibration

BMCPilatusDist (mm) 198.344

BMCPilatusBeamX (px) 495.372

BMCPilatusBeamY (px) 549.426

☐ TIF ☒ CBF Update

APEX parameters have been written.

CrysAlis parameters are:

DetectorDist = 198.344

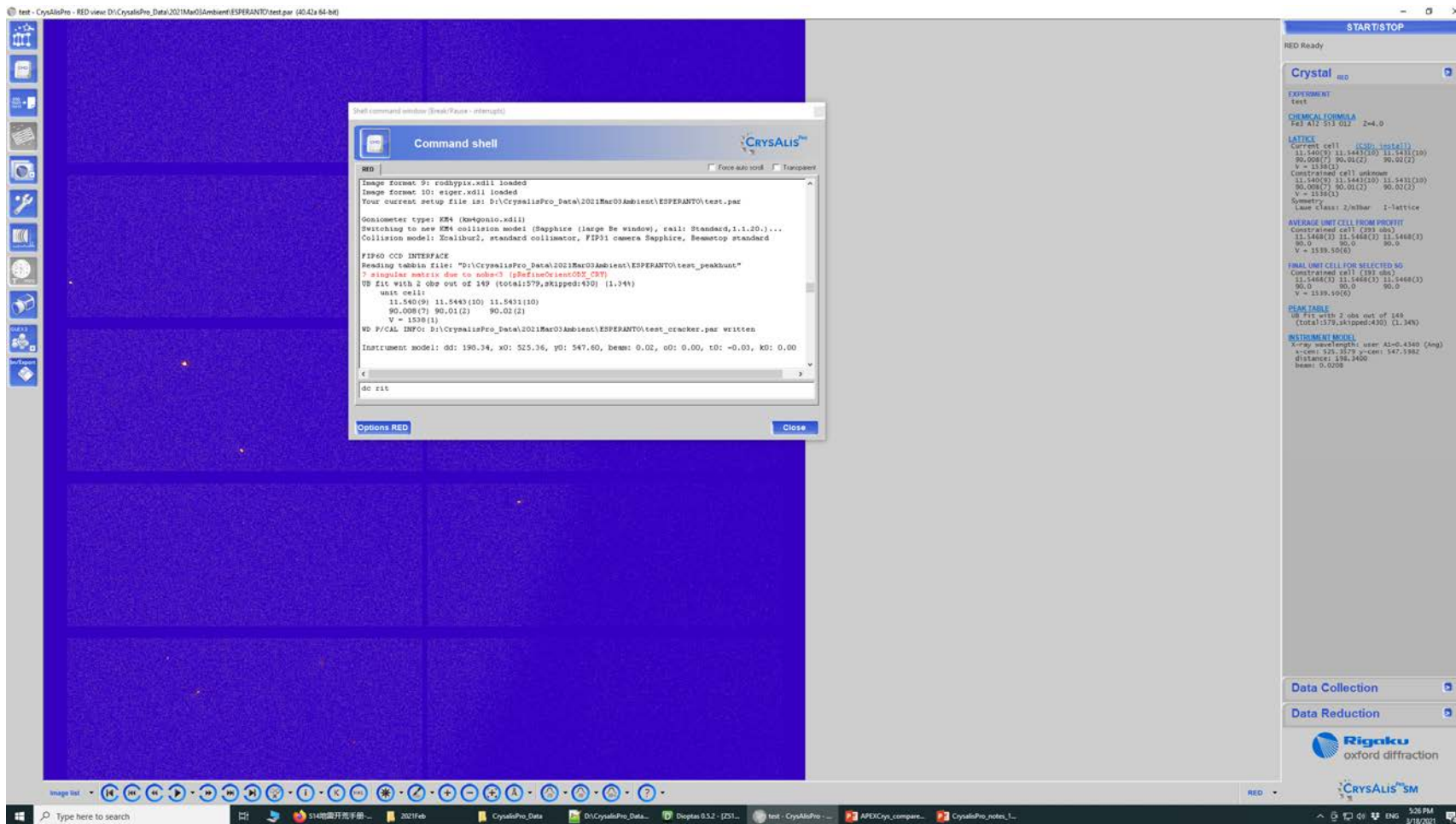
X0 = 527.37200000000001

Y0 = 494.57399999999996

Example, these parameters varies with experiments

- 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

Input format

☒ Known CrysAlisPro format DECTRIS/PILATUS cbf

☐ Generic uncompressed image

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

Frames info

Run digits: 0 Separator: None Frame: 3 name: FFF.ext

D:\CrysAlisPro\_Data\test2\test\_1\_006\_00001.cbf Browse

D:\CrysAlisPro\_Data\test2\test\_1\_006\_00100.cbf Browse

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 padding)

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.

Run list and par file generator for 'Esperanto' data collections

This dialog allows you to quickly generate a \*.run and \*.par file for the data reduction of a 'Esperanto' data set!

- 1) You select image name\_1\_1.esperanto
- 2) You select the last image to be considered (It is assumed that all frames between these two are available)
- 3) Click on 'Save run file'
- 4) You will be prompted for entering some critical parameters (usually default values are OK, as they are taken from image headers)
- 5) Finally a new CrysAlisPro instance will be launched with the 'Esperanto' data set added to the experiment list

NOTE: Using CrysAlisPro you can process only 'Esperanto' images with no image distortions!

First 'Esperanto' dc file (\*\_1\_1.esperanto):

Browse D:\CrysAlisPro\_Data\test2\ESPERANTO\test\_2\_1.esperanto

Last 'Esperanto' dc file:

Browse D:\CrysAlisPro\_Data\test2\ESPERANTO\test\_2\_100.esperanto

Help Cancel Save run file

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: UNSIGNED SHORT (2 BYTES)

Frames info

Run digits: 0 Separator: None Frame: 3 name: FFF.ext

D:\CrysAlisPro\_Data\test2\test\_1\_007\_00001.cbf Browse

D:\CrysAlisPro\_Data\test2\test\_1\_007\_00100.cbf Browse

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

Esperanto output

Images base name: test Run # 2

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 a1, a2, 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 ☐ Thknn.: 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= -20.0 Kappa= 0.0

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

Load Save

Help Cancel OK

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.

Run list and par file generator for 'Esperanto' data collections

This dialog allows you to quickly generate a \*.run and \*.par file for the data reduction of a 'Esperanto' data set!

- 1) You select image name\_1\_1.esperanto
- 2) You select the last image to be considered (It is assumed that all frames between these two are available)
- 3) Click on 'Save run file'
- 4) You will be prompted for entering some critical parameters (usually default values are OK, as they are taken from image headers)
- 5) Finally a new CrysAlisPro instance will be launched with the 'Esperanto' data set added to the experiment list

NOTE: Using CrysAlisPro you can process only 'Esperanto' images with no image distortions!

First 'Esperanto' dc file (\*\_1\_1.esperanto)

Browse D:\CrysAlisPro\_Data\test2\ESPERANTO\test\_2\_1.esperanto

Last 'Esperanto' dc file

Browse D:\CrysAlisPro\_Data\test2\ESPERANTO\test\_2\_100.esperanto

Help Cancel Save run file

# Merge two detector positions

Edit datacollection runs (1.0.21) (Detector distance = 198.34mm)

Name of experiment: test

Data collection directory: D:\CrysAlisPro\_Data\test2\ESPERANTO

Total # of frames: 200  
DC frames: 200  
Ref frames: 0  
Image binning: 1x1

Disk space required for all runs (MB): 219.07  
Disk space required for todo runs (MB): 109.54  
Disk space available: 3374075.76  
Approximate data collection time: 0:58

Run list

Export Import  
Append

#run	type	start	end	width	time	omega	detector	kappa	phi	binning	#to do	#done
1	p	-25.000	25.000	0.500	1.996 + 1.996	0.000	0.000	0.000	-	image	100	100
2	p	-25.000	25.000	0.500	1.996 + 1.996	0.000	0.000	0.000	-	image	100	0

Type of run list  
☒ Data collection frame ☐ Reference frames

Run functions  
Edit Expand select  
Select to new Done number

New runs: Choose a scan type  
omega phi

Run list functions  
Global width Change theta Delete  
Global time Invert done runs Binning options

referred to:  
☐ all runs  
☒ selected runs

Collisions ? Clipboard Cancel OK

Editing data collection run #2 - scan type: phi

Scan axis: phi

User: Range:

Start (deg): -25.000 -360.000

End (deg): 25.000 360.000

Width (deg): 0.500 720.000

☐ Use inverse scanning direction

Run information

User: Range:

Detector (deg): -30.000 -93.000, 120.000

Kappa (deg): 0.000 -179.000, 179.000

Omega: 0.000 -180.000, 180.000

Exposure (s): 1.996 0.25000 - 838.80960

☐ Do a video snap after every frame  
☐ Overflow run - fast scan

Collision map:

Kappa

Omega

Test collision Redraw map Help OK

Edit datacollection runs (1.0.21) (Detector distance = 198.34mm)

Name of experiment: test

Data collection directory: D:\CrysAlisPro\_Data\test2\ESPERANTO

Total # of frames: 200  
DC frames: 200  
Ref frames: 0  
Image binning: 1x1

Disk space required for all runs (MB): 219.07  
Disk space required for todo runs (MB): 0.00  
Disk space available: 3374075.76  
Approximate data collection time: 0:58

Run list

Export Import  
Append

#run	type	start	end	width	time	omega	detector	kappa	phi	binning	#to do	#done
1	p	-25.000	25.000	0.500	1.996 + 1.996	0.000	0.000	0.000	-	image	100	100
2	p	-25.000	25.000	0.500	1.996 + 1.996	0.000	-20.000	0.000	-	image	100	100

Type of run list  
☒ Data collection frame ☐ Reference frames

Run functions  
Edit Expand select  
Select to new Done number

New runs: Choose a scan type  
omega phi

Run list functions  
Global width Change theta Delete  
Global time Invert done runs Binning options

referred to:  
☐ all runs  
☒ selected runs

Collisions ? Clipboard Cancel OK

- 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.

Peak hunting wizard (1.0.15)

**Peak hunting**

Run list, image type and image directory  
Run list: E:\CrysalisPro\BMC\_En\_test3\ESPERANTO\oen\_1\_014\_00  
Image dir: E:\CrysalisPro\BMC\_En\_test3\ESPERANTO \*.esperanto

#	type	start	end	width	exposure	omega	detector	kappa	phi	start	end
1	p	-170.00	170.00	1.00	0.50	0.00	-20.00	0.00	-	1,	240

Run list modification  
By default the whole experiment will be evaluated.  
To modify this behaviour edit the run list --> [Edit start num of selected run](#) [Edit end num of selected run](#)

☐ Automatic threshold and background detection (preferred) ☐ Traditional peak hunting ☒ **Smart peak hunting** ☐ 3D peak extraction

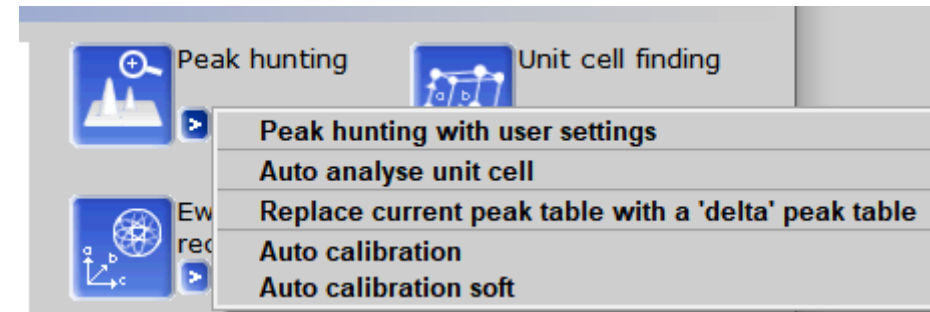
Peak finding control  
Threshold: 1000 7x7 average: 20  
Overwrite existing peak hunting table  
☒ Yes ☐ No

☐ Use background subtraction  
Background evaluation control -> 25 [Edit Re](#) 25 [Edit Fr](#)  
Binning for background evaluation: ☒ 1 ☐ 2 ☐ 4  
☒ Reduce background accumulation to SHORT type (saves memory)

Resolution limits  
☐ Skip peaks outside resolution limits  
d-value (Ång): inf-0.51  
2theta (deg): 0.00-50.04 [Edit res limits](#)

☐ Apply float correction n/a  
☐ Remove spikes ☒ weak ☐ strong

[Help](#) [Cancel](#) [OK](#)



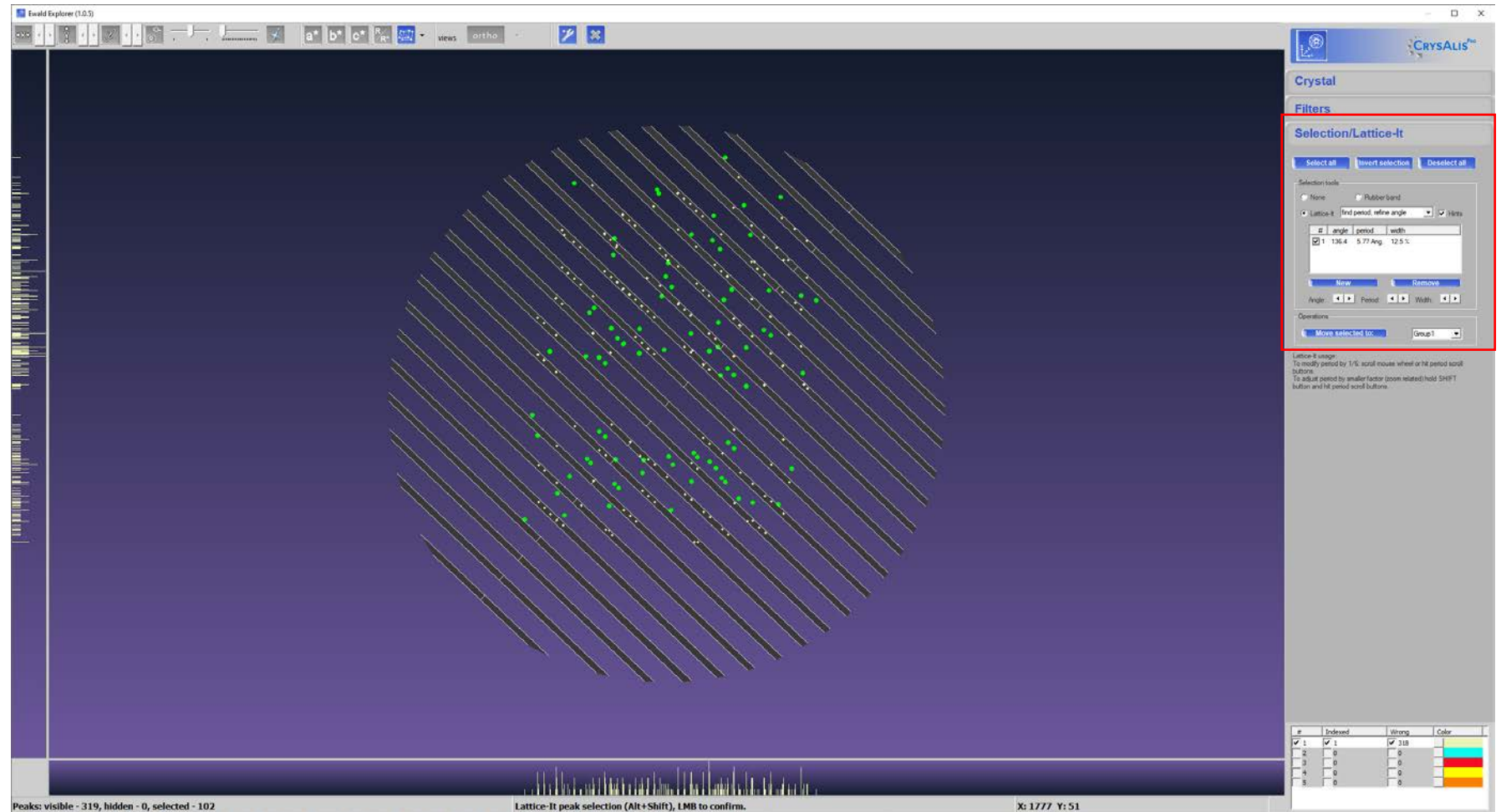
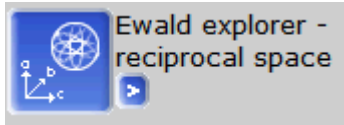
Play with other peak hunting settings if smart hunting doesn't give you enough peaks



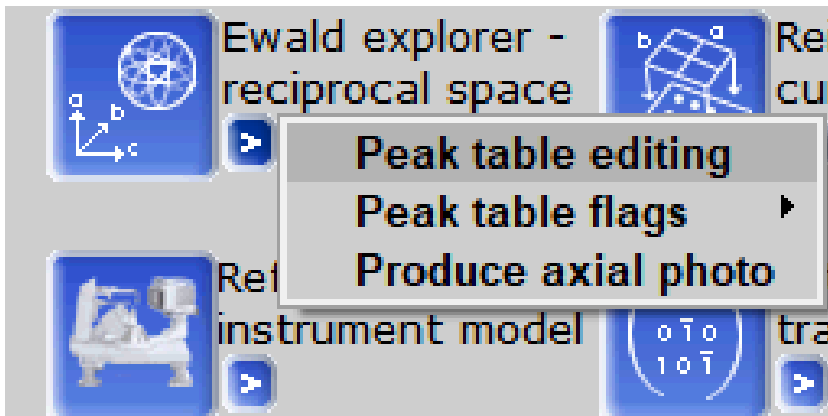
# Find lattice

Use lattice-it to select the outliers

Go to Ewald explorer







Move all outliers to g2

Go to Ewald explorer-> peak table editing

Remove all g2 peaks.

Peak table editing (1.0.10)

Peak table editing

CRYSTALIS<sup>Pro</sup>

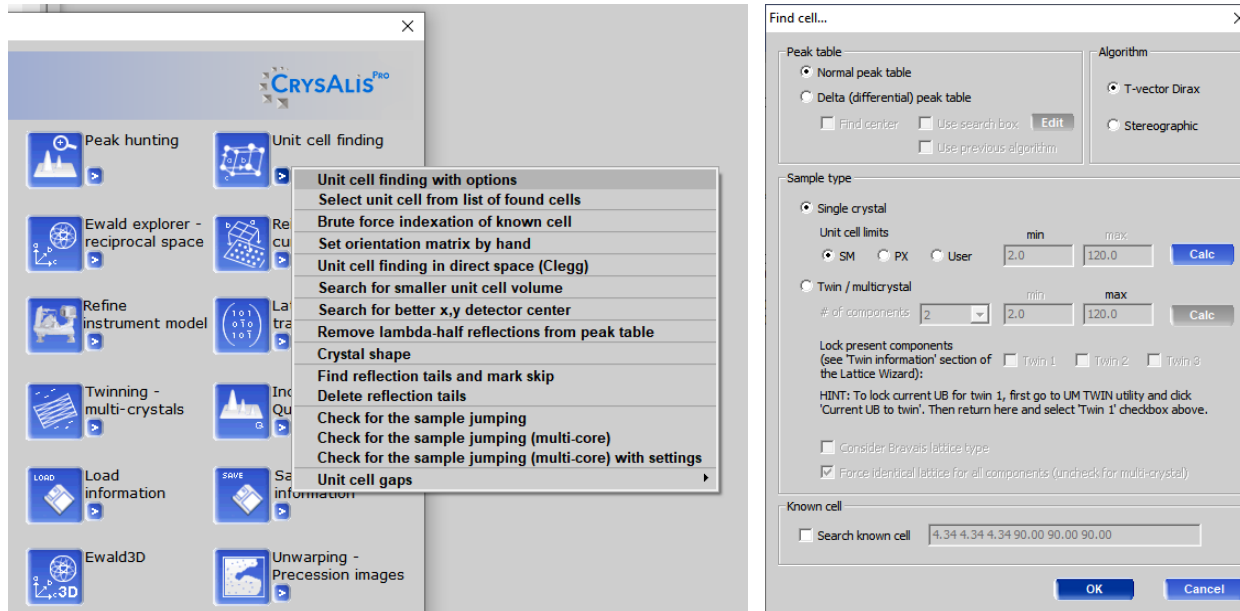
number	h	k	l	x	y	z	d	intensity	flag	prof pts
21	-0.249	-1.797	-1.000	-0.02462	-0.17969	-0.10193	2.08602	2808	wi g2	1
30	-0.177	-1.748	-1.544	-0.01772	-0.17477	-0.15440	1.85570	3779	wi g2	1
26	-0.132	-1.331	-1.701	-0.01321	-0.13306	-0.17010	2.00592	19679	wi g2	1
25	0.000	-2.589	-2.277	-0.01120	-0.25892	-0.22769	1.25806	204592	wi g2	1
24	0.000	-2.277	2.585	-0.00510	-0.22773	0.25646	1.26524	244452	wi g2	1
21	0.657	1.537	-0.591	0.04572	0.15373	-0.05909	2.44755	5548	wi g2	1
19	1.293	1.395	3.537	0.12934	0.13953	0.35369	1.08064	138707	wi g2	1
17	0.518	1.000	1.762	0.05180	0.05025	0.17616	2.12121	2767	wi g2	1
16	0.000	-1.171	-2.000	-0.01090	-0.11715	-0.20203	1.85632	7638	wi g2	1
14	0.653	1.359	1.000	0.06535	0.13590	0.09179	2.45840	9266	wi g2	1
13	1.000	0.381	-4.000	0.10050	0.03806	-0.38976	1.07345	134393	wi g2	1
12	-0.264	-3.375	2.637	-0.02637	-0.33753	0.26372	1.01129	6360	wi g2	1
10	1.200	1.000	-3.727	0.12005	0.09180	-0.37265	1.07925	76200	wi g2	1
8	0.610	1.000	-1.729	0.06097	0.09522	-0.17290	2.10071	3375	wi g2	1
6	-0.741	-4.000	-0.234	-0.07412	-0.38947	-0.02341	1.09278	29741	wi g2	1
5	-0.540	-2.000	1.000	-0.05297	-0.19871	0.10838	1.86512	2565	wi g2	1
219+	0.839	-1.553	-0.583	0.08386	-0.15521	-0.05831	2.33474	7068	wis gl	1
218+	0.617	-1.166	1.000	0.06171	-0.11659	0.10403	2.58240	20223	wis gl	1
215+	0.691	-1.650	0.468	0.06912	-0.16497	0.04677	2.34755	6055	wis gl	1
213+	1.277	-1.265	-2.732	0.12770	-0.12654	-0.37324	1.04760	2051	wis gl	1
212+	1.136	-1.843	2.678	0.11362	-0.18434	0.26784	1.26008	5270	wis gl	1

Buttons: Delete, Up, New, Edit, Down, Reject, Copy to clip, Exit sorted, Help, Exit

hkl format: ☒ integer ☐ fractional

Coordinates: ☐ angles ☒ cartesian ☐ detector

# 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.

Select unit cell from list of found cells (1.0.1)

Solution	% Indexed	Niggli	Priority	Cell						Vpr	Vr
1	100.000	3	10	5.75	5.76	5.76	89.94	90.00	89.44	190.78	190.78
2	100.000	5	11	11.49	11.53	11.52	89.95	89.45	90.00	763.01	1526.01
3	100.000	1	12	11.53	11.52	11.49	90.56	90.00	90.06	381.57	1526.26
4	100.000	12	9	8.14	8.14	9.94	90.27	89.61	119.73	572.35	572.35
5	100.000	12	9	8.14	8.14	19.88	90.27	89.61	119.73	1144.70	1144.70
6	100.000	18	7	16.29	16.30	11.49	89.61	89.61	90.05	1526.33	3052.66
7	100.000	21	6	12.85	12.88	5.76	90.23	90.38	90.17	953.25	953.25

# Refine instrument model

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

Goniometer-Area-Detector-Model - LS (1.0.6)

**Refine model**

CRYSTALIS<sup>Pro</sup>

Refinement control  
Cycles: 10  
Levenberg-Marquardt: 0.00000

Refinement weights  
Diffraction: 1.00000  
hk1: 1.00000  
Spot position: 1.00000  
Ewald sphere: -1.00000

☐ Automatic selection of parameters

Crystal (lattice contents a, b, c,  $\alpha$ ,  $\beta$ ,  $\gamma$ ; rotation r1, r2, r3; wobbling w1, w2, w3)

LAT\_AAA  
ANG\_909090

☒ a = 11.4948 Edit a ☐ b = 11.4948 Edit b ☐ c = 11.4948 Edit c  
☐  $\alpha$  = 90.000 Edit  $\alpha$  ☐  $\beta$  = 90.000 Edit  $\beta$  ☐  $\gamma$  = 90.000 Edit  $\gamma$   
☒ r1 = -77.761 Edit r1 ☒ r2 = 49.560 Edit r2 ☒ r3 = -99.232 Edit r3  
☐ w1 = 0.000 Edit w1 ☐ w2 = 0.000 Edit w2 ☐ w3 = 0.000 Edit w3

☒ Goniometer  
☒ b2 = 0.00000 Edit b2 ☐ b3 = 0.00000 Edit b3 ☐  $\alpha$  = 50.00000 Edit  $\alpha$  ☐  $\beta$  = 0.00000 Edit  $\beta$   
☐ o0 = 0.00000 Edit o0 ☒ t0 = 0.00000 Edit t0 ☐ k0 = 0.00000 Edit k0 ☐ p0 = 0.00000 Edit p0

☒ Detector  
☒ d1 = 0.00000 Edit d1 ☒ d2 = 0.00000 Edit d2 ☐ d3 = 0.00000 Edit d3  
☒ x0 = 527.40000 Edit x0 ☒ y0 = 549.40000 Edit y0 ☐ dd = 198.34000 Edit dd

Help  
Cancel  
OK

# 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.

