## Reprocessing

# ISPyB

It is possible to reprocess the data with xia2 from within ISPyB with some (but not all) additional parameters. These jobs are run in addition to the auto processing.

From the Data Collections page, first click on the entry next to Group to access all sweeps for that data collection, and then click on the cog for the first sweep you want to include, to open the reprocessing window.

Proposals	cm28127 🗸	Projects	Unit Cell Search	Feedback	Help (Off)
Data Collections	for cm28127-3 or	n i19-1			
+ Assign Containers	Auto Processing 🕼 Visit Stats	📽 Users 🖪 Dewars 🛱 Sa	ample Changer 🌼 Reprocessing	& Beamline Status	
View All Data Co	ollections				
Data Collection Group					
	Beamline Status				
Log					
09:53:24 - New data collection 09:50:09 - New data collection 09:46:54 - New data collection	Suc18/Suc18_03_#####.cbf				^
00-49-59 New data collection	Qua10/Qua10 D1 ###### abf				~
					Search
Data Collections Grid Scans	Full Collections Auto Integra	ted Processing Errors So	creenings Edge Scans MCA	Spectra Robot Actions S	ample Actions Favourites
🖻 ☆ % 🗣0 🖿1	<b>8-07-2021 09:53:24 - </b>	uc18/Suc18_04_#####.cbf	r		
Sample: Suc18	Flux: NaN			30	-100 -50 0
Ω Start: -145.0°	Ω Osc: 0.20°				Spots Bragg
Ω Overlap: 0°	No. Images: 850	1999年1月1日日本		25 🕶	Res
φ: 240°	Resolution: 1.03Å			20	
Wavelength: 0.6889Å	Detector Distance: 160.0mm			15	
Detector 20: 30	Exposure: 0.200s			10	
Transmission: 0.60%	Beamsize: 0x0µm			19	State State State
Type: Standard				5	1.0
Comment:				0	200 400 600 800 1.5
Auto Processing				xia2	2 dials-aimless 🗸 xia2 dials 🗸
Downstream Processing				70.00	

Now click on the cog wheels for any other sweeps of data to be included – these will be added to the list in the Reprocess Data window.

By opening the sweeps in reverse order, e.g., 4,3,2,1, the results will be included with the results for the run at the top of the list, i.e., run 4 which allows for easier comparison with the auto processing results (for all data collected).

It is necessary to select which images are to be included from each sweep – either highlight (from left to right) on the plot or type the image numbers in the boxes. Clicking on the "+" button will autofill with the entire sweep.

January 2024

Reprocess Data		د
		🏵 Multi Crysta
Process Individually   Pipeline :	Xia2 DIALS V High Res :	Å   Space Group / Cell Options
Suc18_044 - Suc18/		+ x
Sample: Suc18	Ω Start: -145.0°, Osc: 0.20°	-125 -100 -75 -50 -25 0
Resolution: 1.03Å	Wavelength: 0.6889Å	20 10 10
Start 1 End 500	+	0 100 200 300 400 500 600 700 800 2.0
Suc18_033 - Suc18/		+ x
Sample: Suc18	Ω Start: -145.0°, Osc: 0.20°	-125 -100 -75 -50 -25 0
Resolution: 1.03Å	Wavelength: 0.6889Å	20 Spots - 1.0 10 Bragg 0.10
Start 100 End 550	+	0 Res 2.0
Suc18_02_2 - Suc18/		+ x
Sample: Suc18	Ω Start: -145.0°, Osc: 0.20°	-125 -100 -75 -50 -25 0
Resolution: 1.03Å	Wavelength: 0.6889Å	30 20 10 10 10 10 10 10 10
Start 1 End 850	<del>4</del> ·	0 100 200 300 400 500 600 700 800
Suc18_011 - Suc18/		+ x
Sample: Suc18	Φ Start: 0.0°, Osc: 0.20°	0 25 50 75 100 125 150 175 25
Resolution: 0.96Å	Wavelength: 0.6889Å	20 15 10 878001.0 87800 - 0.0
Start 1 End 900	<b>+</b>	5 0 100 200 300 400 500 600 700 800 900

Notes:

- Process Individually should be left unchecked
- Xia2-dials is the best pipeline but if it isn't working, the others can be tried
- The high resolution limit can be set in the High Res box, probably based on inspection of the auto processing results (see xia2.txt and merging-statistics.txt)
- Clicking on the "Space Group/Cell" button opens the option to input the known or expected information
- The "Options" button has one check box for small molecule this is checked by default for I19 data and should be left checked unless you are sure you know better

Reprocess Data	×
	Hulti Crystal
Process Individually   Pipeline : Xia2 DIALS V High Res : 0.8 A   Space Group / Cell Options	
Spacegroup:         P21         I a         7.8         b         8.7         c         10.9         α         90         β         103         γ         90	
Small Molecule	

At the bottom of the Reprocess Data window click on the "Integrate" button and a red message box should pop-up to show the job has been successfully submitted.

🖀 Home 🋗 Calendar 🕞 Logou	1 reprocessing job successfully submitted	iistics
» Data Collections » i19-1 » cm28127-3		

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Navigate to the Reprocessing window to check the job is progressing and see when it has completed.

tatus	Sample	DC	Process	Comments	Last Updated	Last Message	An	guments	
							Кеу	Value	
							d_min unit_cell	7.8.8.7.1	0.8 10.9,90,103,90
							spacegroup		P21
	0		1/1-0				small_molecule		true
¢.	Suc18 - Suc	Suc18_04_	Xia2 DIALS		23-07-2021 16:32	starting			
							Files		Image #
							/Suc18/Suc18_ /Suc18/Suc18_		1 - 500 100 - 550
							/Suc18/Suc18_		
							/Suc18/Suc18_		

The Reprocessing window is accessed from the line of Option buttons and shows a list of current and completed reprocessing jobs with any input commands set, i.e., resolution, unit cell information and which images were used. Click on the relevant line (the top line has the results for all included sweeps) under Files to be taken to the results of the processing job.

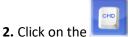
This will appear as another result in the Auto Processing section for that data collection. The  $\square$  indicates that this is a manually started reprocessing job rather than an auto processing job. At this point, all functions for the reprocessed job match those of the auto processing (see ???)

Sample: Suc18	Flux: Na	4					30	-125 -100 -7	5 -50 -25 0
Ω Start: -145.0°	Ω Osc: 0	20°						· · · · ·	Spots Bragg
Ω Overlap: 0*	No. Ima	es: 850					28		Res
φ: 240°	Resoluti	on: 1.03Å					15		
Wavelength: 0.6889Å	Detector	Distance: 160.0mm					10		
Detector 20: 30	Exposur	e: 0.200s						A CALLER COMPANY	a the second second second second
Transmission: 0.60%	Beamsiz	e: 0x0µm							
Type: Standard								100 200 300	400 500 600 700 800
	_	-		_	_	_	_	xia2 di	als-aimless ✔ xia2 dials unde
	Resolutio	n Spacegroup	o Mn≪l/si	g(i)> Rmea:	s Inner Rmeas Outer	Completeness	Cell	xia2 di	als-aimless 🛹 xia2 dials unde Status
to Processing data	Resoluti: 10.60 - 0.58	n Spacegroup P 121/m 1	> Mn <l si<br="">30.3</l>	g(i)> Rmea: 0.032	s Inner Rmeas Outer 0.082	Completeness 93.1	Cell 7.77 8.71 10.87 90.00 102.94 90.00	xia2 di	
to Processing data x multi-xia2 dials-aimless								xia2 di	Status
to Processing data x multi-xia2 dials-aimless x multi-xia2 dials	10.60 - 0.58	P 1 21/m 1	30.3	0.032	0.082	93.1	7.77 8.71 10.87 90.00 102.94 90.00	xia2 di	Status processing successful
to Processing data k multi-xis2 dials-aimless k multi-xis2 dials k multi-xis2 dials <b>2</b>	10.80 - 0.58 10.80 - 0.59 10.80 - 0.81	P 1 21/m 1 P 1 2/m 1	30.3 32.4	0.032	0.082	93.1 95.9	7.77 8.71 10.87 90.00 102.94 90.00 7.77 8.71 10.87 90.00 102.94 90.00	xia2 di	Status processing successful processing successful
Comment: to Processing data x multi-xia2 dials-dimites x multi-xia2 dials-g tx multi-xia2 dials-aimle pace Group A B	10.80 - 0.58 10.80 - 0.59 10.80 - 0.81	P 121/m 1 P 12/m 1 P 1211	30.3 32.4	0.032	0.082	93.1 95.9	7.77 8.71 10.87 90.00 102.94 90.00 7.77 8.71 10.87 90.00 102.94 90.00		Status processing successful processing successful
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o Processing data multi-xia2 dials-aimless multi-xia2 dials (multi-xia2 dials) x multi-xia2 dials-aimle x multi-xia2 dials-aimle	10 60 - 0 58 10 60 - 0 59 10 60 - 0 51 255 4x multi-xia2 dials 4 C α β γ 10 87 90.00 102.95 900 Observations Uniqu	P 1 21m 1 P 1 2/m 1 P 1 21 1 multi-xia2 dials C	30.3 32.4	0.032	0.082 0.065 0.047 CC Half Completene	93.1 95.9 100.0	7.77 8.71 10.87 90.00 102.94 90.00 7.77 8.71 10.87 90.00 102.94 90.00 7.77 8.71 10.87 90.00 102.95 90.00		Status processing successful processing successful processing successful 20Logs & Files Q Lookup C
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# **CrysAlis** Pro

Download the raw images (a link to this information was sent out by the user office)

1. Open CrysAlisPro (version 38.41 or later) and any random project from the list



button, type dectris import in the box and press enter

In the window that pops up, browse to the dataset and select the first image.

Then set the file format: run digits should be 2, the separator is an underscore, and frame digits should be 5.

Check the last image is set correctly, then click on "Save run file".

Shell command window (Ctrl - interrupts)	×
Command shell	CRYSALIS <sup>Peo</sup>
RED	Force auto scroll Transparent
(compiled Apr 29 2019,15:20:48) Plugin 1: abs.odplugin loaded Plugin 2: odbench2.odplugin loaded Plugin 3: powder.xodplugin loaded Plugin 4: gral.xodplugin loaded Image format 1: sapphire.xdll loaded Image format 2: dectris.xdll loaded	Run list and aliases file generator for DECTRIS data collections       ×         This dialog allows you to quickly generate a *.run file and aliases file for the data reduction of a DECTRIS data set!       1. Select an image, by clicking 'Browse' button in group box First DECTRIS file, e.g. name1001.cbf         2. Choose whether instrument model will be loaded from selected image header or selected par file       3. Terminator format is automatically set, but you can change it if necessary
<pre>Image format 2: dectris.xdl1 ibaded Image format 3: pilatus.xdl1 loaded Image format 4: esperanto.xdl1 loaded Image format 5: marip.xdl1 loaded Image format 6: saxi.xdl1 loaded Image format 7: dtrek.xdl1 loaded Image format 8: rod.xdl1 loaded Image format 9: rodhypix.xdl1 loaded Image format 10: eiger.xdl1 loaded Image format 10: eiger.xdl1 loaded</pre>	4. Also the last image will be automatically found, but you can change it if necessary (if it is not automatically found) Note: It is assumed that all frames between these two are available     5. Save the file     • You will be prompted for entering some critical parameters (usually default values are OK, as they are taken from image headers)     • Finally a new CrysAlisPro instance will be launched with the DECTRIS data set added to the experiment list     NOTE: Using CrysAlisPro you can process only DECTRIS images from selected Pilatus detectors     First DECTRIS file (*0001.cbf )
Goniometer type: KM4 (km4gonio.xdll) Switching to new KM4 collision model	Browse       C:\Users\wcx62662\Documents\Data\sugar2\sugar2_01_00001.cbf         Image information: det. distance=160.00mm, wavelength=0.688900, x=814.0, y=734.7, Si thickness=0.320mm         2. Instrument model       Use par file information instead of image header
< dectris import	Browse n/a Par file information: n/a
Options RED	Terminator format Run digits  Separator Underscore '_'  Frame digits  5 nameRR_FFFF.cbf
	Last DECTRIS file Browse C:\Users\wcx62662\Documents\Data\sugar2\sugar2_04_00850.cbf
	Help Run TC Stoe STADIVARI Cancel Save run file

3. Check that values in the pop up window match those for the dataset and press OK

Parfile parameters ×	
Please enter parfile parameters: binning detector_distance wavelength centerx centery SiThickness_mm	
1 160.00 0.688900 814.00 734.71 0.32000	
OK Cancel	

**4.** Once the program has finished setting up the run file, select this experiment (it should be highlighted at the bottom of the list) and click on "Open selected" to open the dataset in a new instance of CrysAlis.

#### January 2024

Name	Path	Created	Accessed
ovtidene 0	C:\Users\wcx62662\Desktop\HaloAlcs\TFE-210619\cytidene_te	Tue Jun 25 16:31:25 2019	Tue Jun 25 16:31:36 2019
1_TFE_6040bar_scre		Sun Jun 23 11:58:35 2019	Fri Jul 23 11:47:41 2021
	C:\Users\wcx62662\Desktop\HaloAlcs\TFE-210619\02_TFE_604	Sun Jun 23 13:31:01 2019	Wed Oct 02 18:22:36 2019
	C:\Users\wcx62662\Desktop\HaloAlcs\TFE-210619\04_TFE_604	Fri Oct 04 10:03:43 2019	Fri Oct 04 10:05:00 2019
	C:\Users\wcx62662\Desktop\HaloAlcs\TFE-210619\03 TFE 604	Fri Oct 04 10:42:59 2019	Thu Dec 19 12:49:48 2019
oos1_100_	C:\Users\wcx62662\Documents\Data\SW26636\beamstop_1007	Tue Feb 25 09:18:14 2020	Tue Feb 25 09:19:17 2020
oos4-100_	C:\Users\wcx62662\Documents\Data\SW26636\pos4-100	Tue Feb 25 09:47:42 2020	Tue Feb 25 09:47:57 2020
os11-100	C:\Users\wcx62662\Documents\Data\SW26636\pos11-100	Thu Mar 05 13:16:33 2020	Thu Mar 05 13:16:49 2020
os12-100	C:\Users\wcx62662\Documents\Data\SW26636\pos12-100	Thu Mar 05 14:47:30 2020	Thu Mar 05 14:47:50 2020
4_TFE_6040bar_50pe	C:\Users\wcx62662\Desktop\HaloAlcs\TFE-210619\04_TFE_604	Sun Jun 23 15:14:24 2019	Wed May 06 10:10:14 2020
oos4-100_	C:\Users\wcx62662\Documents\Data\SW26636\pos4-100-2	Thu Mar 12 12:38:00 2020	Thu Mar 12 12:38:00 2020
6_TFE_7141bar_100p	C:\Users\wcx62662\Desktop\HaloAlcs\TFE-210619\06_TFE_714	Wed May 06 16:41:12 2020	Mon May 11 15:50:50 2020
6_TFE_7141bar_100p	C:\Users\wcx62662\Desktop\HaloAlcs\TFE-210619\06_TFE_714	Tue May 12 11:04:18 2020	Tue May 12 11:04:48 2020
/3Sb2_P7_I2_5thP_30	C:\Users\wcx62662\Documents\Data\CY21726-12\MJR3055	Thu Jun 04 16:50:14 2020	Fri Jun 05 09:32:03 2020
/3Sb2_P7_I2_5thP_30	C:\Users\wcx62662\Documents\Data\CY21726-12\MJR3055-t2	Fri Jun 05 12:06:07 2020	Thu Jul 09 09:14:40 2020
rystal1_	C:\Users\wcx62662\Documents\Data\SW27107-1\crystal1	Mon Jul 13 11:25:45 2020	Mon Jul 13 11:26:00 2020
rystal3_	C:\Users\wcx62662\Documents\Data\SW27107-1\crystal3	Mon Jul 13 13:40:07 2020	Tue Jul 28 13:08:43 2020
rystal3_	C:\Users\wcx62662\Documents\Data\SW27107-1\crystal3-orth	Wed Aug 05 16:32:09 2020	running
04-4_1_	C:\Users\wcx62662\Documents\Data\Industry\Almac\SW21015	Thu Jan 28 15:31:04 2021	Thu Jan 28 15:38:18 2021
ugar2_	C:\Users\wcx62662\Documents\Data\sugar2	Thu Aug 05 16:23:47 2021	Thu Aug 05 16:23:47 2021

5. Click OK in the pop-up error box to set the basic settings

**6.** In the window that opens up, make sure Small Molecule is checked and then click on "Edit options". Check Single wavelength data red in the new window.

Click "OK" in both windows

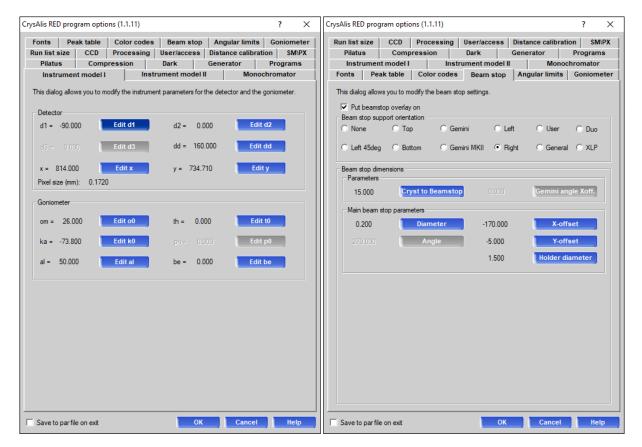
Note: For newer versions (42.49 onwards) there is an additional pop-up window which queries the min\_lattice setting – just press "OK" here and continue as above.

PX <ul> <li>Small Molecule</li> <li>Protein</li> </ul> attice finding? Usta reduction       Im lattice size: 120 Im lattice size: 120 Im lattice size: 120 Im lattice size: 120 Im lattice size: 120 Image: 120 <ul> <li>Protein</li> <li>Protein</li> </ul> intal collection / Strategy <li>Image: 120</li>	Deta collection / Strategy ✓ Use tab-based SM screening Use axes ✓ Symmetry axes first. ✓ Favour less runs in red alg KDS □ Denzo □ OTPEX: □ MOSFLM export during data collection 400 Max automode exposure time (sec) Overlap computation:
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Edit options         idit SM options (1.0.6)         Lattice finding / Data reduction         2       Min lattice         120       Max lattice         Use first delta peak table to attempt cell finding in auto-analysis         Smart background during reflection integration         Single wavelength data red         MRL deckin 30 peak analysis         Oropute completeness after data red         MTZ export data red for use in CCP4         Run space group taken into consideration         In the space group taken into consideration         In attacentrosymmetric       Chiral only	✓ Use tab-based SM screening     Use axes     G symmetry exes first     ✓ Favour less runs in red alg     XDS    Denzo    DTREX. MOSFLM export during data collect     400    Max automode exposure time (sec)
dit SM options (1.0.6)         Lattice finding / Data reduction         2       Mn lattice         120       Max lattice         Use first delta peak table to attempt cell finding in auto-analysis         Single wavelength data red         H4C, deckin 3D peak analysis during data red         20       Compute completeness after data red         MT2 export data red for use in CCP4         Run space group determination (GRAL) after data red         Lint space groups taken into consideration         Int space mouse taken into consideration	✓ Use tab-based SM screening     Use axes     G symmetry exes first     ✓ Favour less runs in red alg     XDS    Denzo    DTREX. MOSFLM export during data collect     400    Max automode exposure time (sec)
dit SM options (1.0.6)         Lattice finding / Data reduction         2       Mn lattice         120       Max lattice         Use first delta peak table to attempt cell finding in auto-analysis         Single wavelength data red         H4C, deckin 3D peak analysis during data red         20       Compute completeness after data red         MT2 export data red for use in CCP4         Run space group determination (GRAL) after data red         Lint space groups taken into consideration         Int space mouse taken into consideration	✓ Use tab-based SM screening     Use axes     G symmetry exes first     ✓ Favour less runs in red alg     XDS    Denzo    DTREX. MOSFLM export during data collect     400    Max automode exposure time (sec)
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Smart background during reflection integration         Single wavelength data red         HKL check in 30 peak analysis during data red         Zond cycle in 30 peak analysis         Compute completeness after data red         MIZ export data red for use in CCP4         Run space group determination (GRAL) after data red         Limit space group determination (GRAL) after data red         Limit space group taken into consideration         I increativesymmetric       C Chiral only	G Symmetry exes first.     C Long exis first.     Favour less runs in red alg     XDS Denzo DTREX MOSFLM export during data collect     400 Max automode exposure time (sec)
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H4L check in 3D peak analysis during data red     ✓ 2nd cycle in 3D peak analysis     ✓ Compute completeness after data red     MTZ export data red for use in CCP4     MTX export data red for use in CCP4     Limit space group determination (GRAL) after data red     Limit space groups taken into consideration	400 Max automode exposure time (sec)
And cycle in 3D peak analysis     Compute completeness after data red     MT2 export data red for use in CCP4     Run space group determination (GRAL) after data red     Limit space groups taken into consideration     Al inorcentrosymmetric C Chiral only	400 Max automode exposure time (sec)
Compute completeness after data red     MIZ export data red for use in CCP4     Run space group determination (GRAL) after data red     Limit space groups taken into consideration     G All noncentrosymmetric C Chiral only	
MTZ export data red for use in CCP4     Run space group determination (GRAL) after data red     Limit space groups taken into consideration     All increativosymmetric      Chiral only	Overlap computation:
Run space group determination (GRAL) after data red     Limit space groups taken into consideration     G All noncentrosymmetric     C Chirel only	
Limit space groups taken into consideration     G All noncentrosymmetric     C Chiral only	Complex approach: table with 9 cases: dd vs scan width
All noncentrosymmetric     Chiral only	
	Simplified approach: 1 case: current dd vs scan width
Use prediction uncertainty for integration mask size adjustment	Skip strategy reference frames (if darks are time-triggered)
	100.0 Default completeness goal (%)
Data reduction during data collection after 25 # of frames	
Restart full auto analysis during data collection:	2.0 I/sig criterion for max. resolution prediction
after 1/2 of data     of after 2/3 of data     of at the end of DC	Append fast phi run in case of overflows
	F HPAD native: Use run list sorting with scan inversion for fast experiment
Launch shape generation after movie	DC JETSHADOW (to visualize beforehand use 'beamstop mask')
Enable fast UB search during SM-screen [up to peaks] 400	
Use external process RED during data collection (64bit only)	Use JetShadow Edit parameters
External concurrent data red External pre-exp auto-analysis	
DC CRYSTALHOLDER SHADOW	
Use CrystalHolderShadow Edit parameters diameter: 1.00, height: 2.00	Default OK



**7.** Click on **1** and then "Options RED" in the bottom left of this window and edit the values in the Instrument Model I and Beamstop tabs.

	Older versions	More recent versions
Instrument Model I	Beamstop	Beamstop
d1 = -90	support orientation = right	support orientation = leave as default
om = 26	diameter = 0.2	diameter = 0.5
ka = -73.8	x-offset = -170	x-offset = -170
	y-offset = -5	y-offset = -2
		holder diameter=0.5



Click "OK" in this window and then close the CMD window.

**8.** Click forward through an image using *solution* along the bottom row and you should see the changes take effect.

Edit the beamstop parameters as required.

Use CrysAlis Pro as normal.

Notes:

- Do make sure you edit the instrument model correctly, all 3 values need updating, otherwise you won't get nice lattices.
- The general advice is to work up your best-looking dataset first and refine the instrument model parameters on that. Then use this par file (with this instrument model) on the less good datasets.
- NOTE: It may be necessary to use CrysAlis Pro index the data, but better processing results are often obtained by using this information and reprocessing with DIALS.

## DIALS

For more information about running DIALS, check the website: https://dials.github.io/index.html

Reprocessing jobs using xia2 / DIALS can be submitted directly using the command line. This is a more manual procedure, and a suitable directory structure needs to be created by hand.

The first step is to navigate to the *processing* directory within the visit folder as this is the only place with write access.

Open a terminal window and, if not already done, type module load i19 and press *enter*. This should direct you to your current visit directory, e.g.: /dls/i19-1/data/2024/cm37266-1 as well as enable DIALS to work.

Now type: cd processing

Create a suitably named directory for the processing files to be written in, e.g.: mkdir SampleA And then enter the directory: cd SampleA

Use of DIALS to run processing step-by-step is not covered here, but there is an example of how to do it here: https://dials.github.io/documentation/tutorials/small\_molecule\_tutorial.html

#### Useful things to know:

The up arrow

Press this once to redo the command above

Repeated pressing will scroll through previous commands (to save quite a lot of tedious typing) TAB key

If enough information is already included, TAB will autocomplete instructions (saving tedious typing) Double TAB will give the options available from whatever is input

Copy and Paste must be done via the right mouse button Everything is case sensitive

### xia2

The easiest way to invoke a DIALS processing job is to run xia2 as all of the steps are run sequentially automatically.

The basic xia2 command is: xia2 small\_moleule=true /dls/i19-1/data/2024/cm37266-1/SampleA

where:

xia2 - runs a xia2 processing job
small\_moleule=true - tells DIALS to run a small molecule processing job, which means things like cell
errors are calculated
/dls/i19-1/data/2024/cm37266-1/SampleA - path to where the images are stored.

Various additional instructions can now be added to this command – see the table for some of the most common ones.

Action	xia2 Instruction
Include space group and unit cell (both	space_group=
must be used together)	unit_cell="a b c α β γ"
	OR
	unit_cell=a,b,c,α,β,γ
Maximum resolution cutoff	d_min=
Choose a different indexing method	index.method=
	index.method=real_space_grid_search (normally the most
	robust method)
Set a threshold so only the strongest	sigma_strong=
reflections are used for indexing	(default value is 3)
absorption correction	absorption_level=
	choose from low/medium/high as most appropriate
Select which images should be included,	image=path/to/images/image_XX_00001.cbf:first:last
for example to omit images which look	OR
to have radiation damage	copy over an automatic.info file produced for the same
	dataset and edit the images required in this file - save as
	edit.info
	include xinfo=edit.xinfo
Can help integration complete	scan_varying=false
Will make the job complete even if the	failover=true
processing doesn't work for all sweeps	

#### So, an example command may look like:

xia2 small\_moleule=true sigma\_strong=15 index.method=real\_space\_grid\_search space\_group=P21 unit\_cell="7.72 8.68 10.82 90 103 90" /dls/i19-1/data/2024/cm37266-1/SampleA

#### shelxt

Manually running xia2 processing does not include the structure solution step. If desired, shelxt can be run on the xia2 output files.

Navigate to where the files are: cd DataFiles type shelxt shelxt to run shelxt

It is possible to include the correct (expected) atom types by editing the atom types listed in the shelxt.ins file using gedit shelxt.ins

### **Files**

The manual xia2 processing results are not incorporated into ISPyB so must be viewed (use gedit to open files from the terminal) within the file system – useful files can be found in the following locations.

#### Main folder:

xia2.txt xia2.html

#### DataFiles subdirectory:

Shelxt.ins and shelxt.hkl, plus any output files from running shelxt Xia2.cif

#### LogFiles subdirectory: AUTOMATIC\_DEFAULT\_NATIVE\_merging-statistics.txt

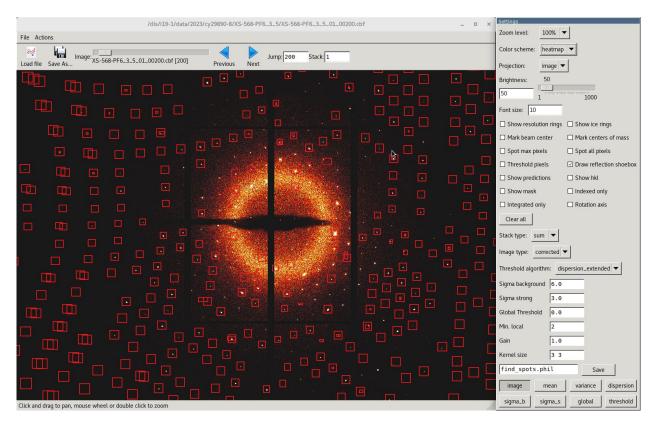
## **Viewing Images**

dials.image\_viewer can be opened using the files produced from the various processing steps. A matching pair of .refl and .expt files are required.

If the auto processing has completed, then the files corresponding to the final stage reached (scaling) are written to the DataFiles folder:

AUTOMATIC\_DEFAULT\_scaled.refl AUTOMATIC\_DEFAULT\_scaled.expt

From DataFiles, type (dials.ima TAB) dials.image\_viewer AUTOMATIC\_DEFAULT\_scaled.refl AUTOMATIC\_DEFAULT\_scaled.expt



By opening the images this way, knowledge of the indexing is read in so having the options checked will show how well the indexing has been done, for example.

### **Reciprocal Lattice Viewer**

It is possible, from the file system, to open the reciprocal lattice viewer to include reflections from all sweeps of data collected. Navigate (cd) to the directory DEFAULT/NATIVE/SWEEP1/index. Although the folder is SWEEP1, the results from indexing all sweeps are actually here.

If you have collected 4 sweeps of data, then the indexing results are numbered 17, but choose whichever files are titled indexed (dials.rec TAB) dials.reciprocal\_lattice\_viewer 17\_indexed.expt 17\_indexed.refl

It is possible see which reflections come from which sweep (they are different colours) by selecting the appropriate Experiment ID's and to see which reflections have been indexed or not.

It is also possible to overlay the unit cell and see how well that fits.

				/0	ils/i19-1	/data/202	4/cm3726	i6-1/proc	essing/SA	B/DEFAU	LT/NATI\	/E/SWEE	P1/index/	17_inde>	ced.refl									- 1	• ×
High resolution: 0.95	4	:	4	1		1	•	•	٠	•	*	4	<b>3</b> *	4	*	•	*		:	٠	÷			:	-
Min Z 0	* *	÷.	÷	÷.	* •		•	*	-			*		*				*		*			-		-
Max Z 900		*	ŧ	*			*	÷	*		*						*			*		2			
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Max Pixels 1000000 *	<u>*</u>	1	÷.	ų,	1				*		*		*			*						*			
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Max partiality 0.000	*	÷.		1	÷.	*	÷.	*		*			***	*	*	*	*					•			
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Show beam vector		•	•	*	*	•	1	, T	*		•		*		*	*	*		*	*		*			
Show reciprocal cell	*	•				*	-	*	÷	*	: • k	*		*	*		*		*				*		-
Label nearest point	*	•	*	•	:	ŧ	:	÷.	*		*		• 4-	4	*	*		*				*		•	
Invert rotation axis	-	1	-	*	÷	+ +	ě.	*	٠	*	4	*	•	4	*	*	*				*		•	•	
Show in crystal frame	*	•	*	-	*	÷.	*		*	+	*		-	*	*	*	*	*		*		*		÷	*
Beam centre panel 0		*		*		-	•	1	*		*		** b*	•	*	4	*	*	*			•		•	
Beam centre (mm) 127.37 * 148.36 *	*		:	•	*		- 1	2	*	:		*	-		*	*		ę ÷			1		•		•
Marker size: 25	•	*	•	-	*		*	-	4	÷.	*	•	*		*	*	4	* *		*		\$ \$		4 \$	•
all indexed unindexed integrated		*	•	-	•	*		*	÷.	*	ŧ	÷	*	•	* *	*	*		*		*	•			
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	:	+				•	•	*	1	*	*	1	-	1	-	1	4	*	*		•	:	•	+	•
Model view matrix: [0.9959, 0.0589, 0.0691, 0.0000, 0.0239, 0	0.5645, -0.8	8251, 0.	0000, -0.	0876, 0.8	233, 0.5	608, 0.000	0, 0.0000,	0.0000,	4740880.	5000, 1.00	[000]														

If indexing has failed then look, instead, at the matching pair of files called xx\_strong.refl and xx\_strong.expt as this may give some useful insight.

## **Radiation Damage**

If you are concerned about radiation damage and want to check for evidence, there is a damage analysis tool (dials.dam TAB)

dials.damage\_analysis DataFiles/AUTOMATIC\_DEFAULT\_scaled.{expt,refl}

Then open the resulting file by typing: firefox dials.damage\_analysis.html &

Look at the Rcp vs dose plot to check where the line veers off and then use this as a guide as to where to cut the data for the next reprocessing job.

## **Auto Processing**

It is possible to look at the results from the auto processing in the same way as for the manual processing, but it is important to note that most of the files required are only available for 1 week after data collection.

They can be found within tmp/zocalo and the file structure here matches the way the data was collected. The results from all auto processing jobs can be found here, including the screen19 output.