



PETS2

Process Electron Tilt Series

user manual

Gwladys Steciuk, Institute of Physics of the CAS

Contributed: Lukas Palatinus, Jaromíra Hrdá.

LAST UPDATE FROM VERSION 2.2.20231114.1432, November 2023

Table of Contents

INTRODUCTION	4
A GETTING STARTED WITH PETS2	5
A.1. Requirements	5
A.2. Supported files	5
A.3. Installation	5
A.4. Create a new project	5
A.4.1 Creating a new project from a tilt series of frames using PETS2 GUI	5
A.4.2 Create a starting input PTS file manually	7
A.5. Open an older PTS project	9
B GRAPHICAL USER INTERFACE	9
B.1. The toolbar	10
B.1.1 File	10
B.1.2 Edit	12
B.1.2.a. The Frame dialog panel	12
B.1.2.b. The Settings panel	12
B.1.3 View	12
B.1.4 Help	13
B.2. Commands or function panel	13
B.2.1 Parameters	14
B.2.2 Peak search	15



B.2.3	Tilt axis-----	15
B.2.4	Peak analysis -----	16
B.2.5	Find unit cell and orientation matrix-----	17
B.2.5.a.	Find possible cells automatically-----	18
B.2.5.b.	Find unit cell manually -----	19
B.2.5.c.	Modify cell-----	21
B.2.5.d.	Refine cell -----	22
B.2.5.e.	Finish -----	23
B.2.6	Process frames for integration-----	23
B.2.6.a.	Intensity determination method -----	24
B.2.6.b.	Profile parameters for the integration -----	24
B.2.7	Optimize reflection profile-----	25
B.2.8	Optimize frame geometry -----	26
B.2.9	Finalize integration -----	28
B.2.9.a.	Files obtained-----	28
B.2.9.b.	Skip saturated reflections -----	28
B.2.9.c.	Intensity estimation for kinematical integration-----	29
B.2.9.d.	Integration parameters for kinematical integration -----	30
B.2.9.e.	Outlier detection limits for kinematical integration -----	30
B.2.9.f.	Frame scaling for kinematical integration -----	31
B.2.9.g.	Refine error model for kinematical integration-----	32
B.2.9.h.	Dynamical integration-----	33
B.2.10	Serial electron diffraction-----	33
B.2.10.a.	Introduction-----	33
B.2.10.b.	Available options -----	33
B.2.10.c.	How to proceed in PETS2-----	35
B.2.11	Generate a 3D map-----	37
B.2.12	Reciprocal-space sections-----	38
B.2.13	Write check files-----	39
B.3.	Main panel -----	40
B.3.1	Image data tab-----	40
B.3.1.a.	General frames' information of the toolbar -----	41
B.3.1.b.	General display options-----	41



B.3.1.c.	Image types -----	42
B.3.1.d.	General overlays accessible from the toolbar -----	43
B.3.1.e.	Specific Friedel pairs overlays to define manually the pattern center -----	44
B.3.1.f.	Beam stop overlay -----	45
B.3.2	Section images -----	46
B.3.3	Graph tab -----	47
B.3.3.a.	Peak search: pattern center -----	48
B.3.3.c.	Peak analysis: in-plane-distances/3D distances -----	49
B.3.3.d.	I/sigma in two shells -----	50
B.3.3.e.	Resolution graph -----	51
B.3.3.f.	Rocking curves -----	51
B.3.3.g.	Frame scales -----	52
B.3.3.h.	Tilt corrections and origin corrections -----	52
B.3.3.i.	Frame-by-frame distortions -----	53
B.3.3.j.	Profile parameters -----	54
B.3.3.k.	Normal probability plot -----	54
B.3.4	Cylindrical projection -----	55
B.3.5	Log files -----	56
B.3.6	3D panel -----	58
B.4.	Options panels -----	59
B.4.1	Indexing display options tab -----	59
B.4.1.a.	Axis bases -----	59
B.4.1.b.	View along an axis -----	60
B.4.1.c.	Unit cell display options -----	61
B.4.1.d.	Cloud display options -----	62
B.4.2	Image options tab -----	65
B.4.2.a.	General options -----	65
B.4.2.b.	Single frame options -----	66
B.5.	Console panel -----	67
C	BASIC PROCEDURE -----	75
D	KEYWORDS AND OPTIONS AVAILABLE IN THE PTS2 INPUT FILE -----	76
E	OUTPUT FILES -----	84
F	DEPENDENCY SCHEME -----	89



INTRODUCTION

PETS2 is a computer program for processing a series of diffraction images¹. It is intended for 3-dimensional electron diffraction data in continuous rotation mode (cRED, MicroED), stepwise mode with (PEDT) or without precession (ADT), and serial ED^{2,3}.

The original version of PETS was a console-based program with limited graphical capabilities. This manual describes version 2.0 with a graphical user interface and many new options.

PETS2 performs the following basic procedures: peak hunting, refinement of the position of the tilt axis, peak analysis (clustering and difference space generation), indexing, correction of the frame orientation and optimization of distortion parameters, integration of intensities, frame scaling, outlier rejection, integration of intensities for dynamical refinement, calculation of a 3D distribution of intensities in reciprocal space, and reconstructions of sections through the reciprocal space (also known as reconstructed precession images or unwarping).

This manual has – apart from the introduction – six parts. The first part describes how to get started with PETS2, from the installation to the creation of the initial input file. The second part is dedicated to the panels' descriptions and options. The third and fourth sections give all the keywords and commands recognized by PET2 and a list of all the output files created during the data reduction. Before the last part, we give a basic procedure model that should work for most normal/good-quality data. This manual is not a detailed guide for all cases. The procedure given in this manual is a starting point that may need adjustments depending on the data. Some data reductions of 3D ED data are already available as part of the JANA2020 cookbook (<http://jana.fzu.cz>). In the last section, the dependency scheme presents the interdependencies between options or procedures that influence output files and the upcoming steps.

CONTACT: PETS2 is under constant development and can thus suffer from occasional bugs and weird behavior. Don't hesitate to contact us with bug reports and feature suggestions.

Lukas Palatinus

Institute of Physics of the CAS, Na Slovance 2, Prague 182 21, Czechia

palat@fzu.cz



A GETTING STARTED WITH PETS2

A.1. Requirements

PETS2 is currently available as a Windows executable for 64-bit operating system. The graphic card must support OpenGL v4.0 or newer.

A.2. Supported files

At the moment, only diffraction stored as TIFF files are supported by PETS2. Any valid monochrome TIFF format is accepted.

A.3. Installation

PETS2 software and the documentation are available at <http://pets.fzu.cz/> (Figure A-1)

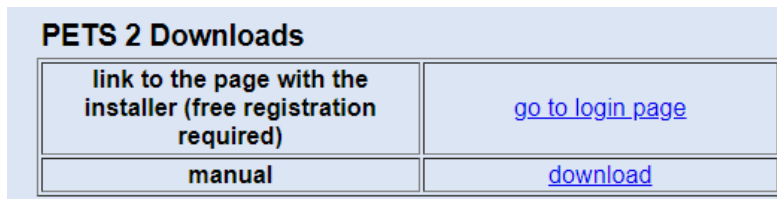


Figure A-1

The download page is <http://pets-login.fzu.cz>. You need to log in to access the download page and find the last version with a brief description of the updates. An installer PETS2_install.exe is downloaded by hitting the link "last version". By default, PETS2 is installed in "C:\Program Files\Pets2\pets2.exe". The PETS2 folder contains the executable and the minimal set of DLLs needed to run the program.

A.4. Create a new project

A.4.1 Creating a new project from a tilt series of frames using PETS2 GUI

Open PETS2; File/New;

A new dialog opens (Figure A-2)

Fill up the basic information: chose a project name, indicate the project directory and the directory where the series of frames are stored. The "initialize frame list from the directory" checkbox is checked by default.

Press NEXT;

Project name	example1	
Project directory	D:\work\2023\PETS2_manual\data\pyrite	Browse
Project frames' directory	D:\work\2023\PETS2_manual\data\pyrite\dp-100	Browse
<input checked="" type="checkbox"/> initialize frame list from the directory		

Figure A-2



In the new dialog, specify the project parameters (Figure A-3):

- The binning. This is not the binning used by the detector to store the frames, but the extra binning applied by PETS2.
- The wavelength (120 kV: $\lambda_{120} = 0.0335 \text{ \AA}$, 200 kV: $\lambda_{200} = 0.0251 \text{ \AA}$, 300 kV: $\lambda_{300} = 0.0196 \text{ \AA}$).
- The detector calibration in reciprocal angstrom per pixel (non-binned value).
- The geometry of the experiment: either precession (PEDT), static frame (ADT), or continuous rotation (cRED, MicroED).
- Tilt semiangle for continuous rotation data or precession angle for precession-assisted data (for static frame geometry, the precession angle = 0). Note: for continuous-rotation data, make sure to insert the tilt *seimangle*, i.e. half of the angular range spanned by each frame.

Figure A-3

Hit NEXT;

The list of frames is automatically generated (left panel Figure A-4). On the right panel of Figure A-4, the general information of the selected frame is given. At this stage, only the alpha-tilt has to be defined to start the data reduction. The other entries will be updated during the data reduction.

Figure A-4

To indicate the alpha tilt for all frames:

Press “Define alpha” (Figure A-5).

Indicate the alpha-tilt of the first frame and the tilt increment (angular step between frames);

Press OK;



The alpha angles are automatically generated for all the frames in the list (Figure A-5).
FINISH to create the initial PTS2 file.

Note: The data reduction will start with the ideal values of θ -tilt = 0 and $\Delta\omega$ = 0. They may be later optimized. The center of the frame will be determined later, as well as the intensity scale. The data set identifier is used in case several data sets are combined.

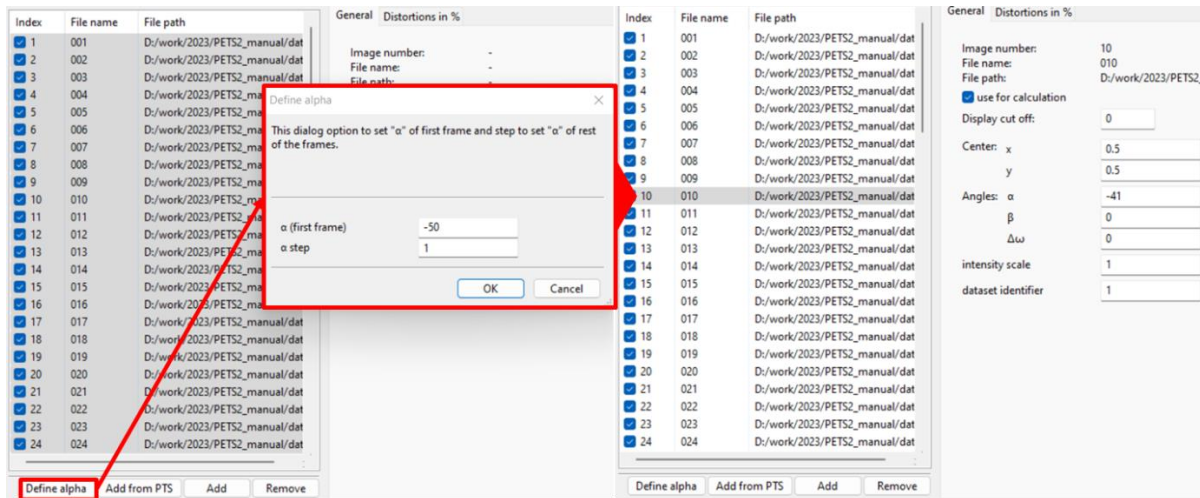


Figure A-5

If, for some reason, the list of frames is not properly generated when a new project is created, it can be done manually.

Select Add and go to the directory to select all the TIFF files of the data set.

File information can be edited manually by selecting the frame of interest.

To exclude a frame from the data reduction: uncheck the checkbox in front of the frame path on the left panel, or uncheck the checkbox "use for calculation" for the frame to exclude in the General dialog box (right panel in Figure A-5).

A.4.2 Create a starting input PTS file manually

The data reduction can also start from an initial input file containing (at least) a minimal set of instructions. It may be convenient to generate such file directly in the data-collection software and avoid the manual creation of new project in PETS2. The following information is needed to start (Figure A-6). Once the essential information is listed, save the file as a txt file or pts file. When you open it in PETS2 and save the project, a pts2 file will be created with all the other commands/parameters.



```

zeoliteA-crs6 - Notepad
File Edit Format View Help
lambda 0.0335

Aperpixel 0.001555

phi 0.50

omega 22.50

noiseparameters 3.5 38

reflectionsizesize 20

bin 2

imagelist
dp-050\001.tif -40.00 0.00
dp-050\002.tif -39.50 0.00
dp-050\003.tif -39.00 0.00
dp-050\004.tif -38.50 0.00
dp-050\005.tif -38.00 0.00
dp-050\006.tif -37.50 0.00
dp-050\007.tif -37.00 0.00
dp-050\008.tif -36.50 0.00
etc. etc.
endimagelist
Ln 3, Col 1 100% Windows (CRLF) UTF-8

```

Figure A-6

The keywords are case-sensitive. Their description follows:

- **lambda**: relativistic wavelength of the incident electrons in angstroms: 100kV = 0.0370 Å, 120 kV = 0.0335 Å, 200 kV = 0.0251 Å, and 300 kV = 0.0197 Å. This is a compulsory keyword.
- **Aperpixel**: the scale of the diffraction patterns given as the size of one pixel in reciprocal angstroms. This is a compulsory keyword.
- **omega**: orientation of the tilt-axis of the sample holder with respect to the positive horizontal axis of the image. It must be estimated either by calibration or by visual inspection of the series of images. It can also be determined and refined later in PETS. This is an optional keyword. If absent, a default value of 0 is used.
- **noiseparameters**: two parameters for the determination of $\sigma(I)$. The first value is $G\gamma$, the second is ψ . The uncertainty on each pixel γ is then calculated as $\sigma_2(p)=G\gamma p+\psi$. For more information, see Waterman, D. & Evans, G. (2010).⁴ This is an optional keyword. If absent, default values of 1 and 40 are used.
- **phi**: semi-angle in degrees for the precession or the continuous rotation used during the data collection. Phi can be zero for the static frame experiment, of course. This is a compulsory keyword.
- **reflectionsizesize**: diameter of the spots on the images in pixels. Used for peak search and integration, should be large enough to encompass the strong spots and small enough to avoid overlaps of neighboring spots. This is an optional keyword. If absent, a default value of 20 is used.
- **bin**: binning of the images prior to any treatment. Saves time, makes nicer pictures, and seems to make the whole analysis somewhat more robust. In most cases it is useful and recommended to use binning, if the experimental frames are larger than 1000x1000 pixels. This is an optional keyword. If absent, a default value of 1 is used.



- **imagelist – endimagelist:** multiline keyword. Each line contains one image. The format is “name of the picture with path” alpha [beta]. The beta angle is optional, set to zero, if absent. This is a compulsory keyword.

A.5. Open an older PTS project

In previous versions of PETS2, the output files were created in the same directory as the input file, and some files were present/absent. In newer PETS2 versions, the output files are, by default, created in a subdirectory “projectname_petsdata.” When an old PTS/PTS2 file is opened for the first time in the latest version, a message appears to inform that all the output files will be moved to a subdirectory (Figure A-7).

To continue with the newest PETS2 version, you must accept.

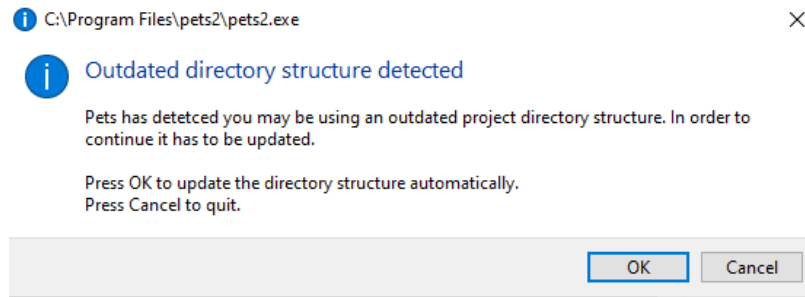


Figure A-7

B GRAPHICAL USER INTERFACE

The GUI is organized with several panels as shown below (Figure B-1). More layouts are available and the positions of the panels can be reorganized by dragging them by mouse.

The general description of the graphical interface will be done panel by panel.

The GUI has 4 main panels + the toolbar:

- the toolbar (purple)
- the command panel (red)
- the main panel with several graphical tabs (blue)
- the options panel (green)
- the console (yellow)
- the debug window (additional console window open in the background. This window must not be closed).

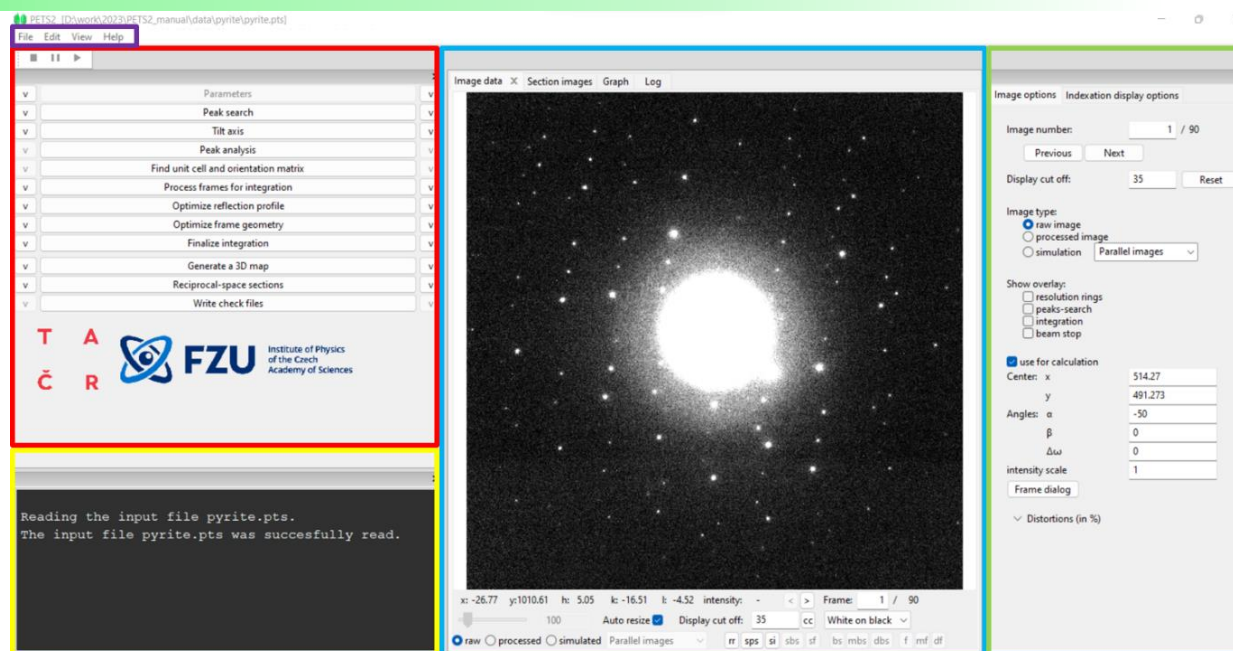


Figure B-1

On the top left of the window is the name and the path of the PETS2 job and the icons File/Edit/View/Help (Figure B-2)

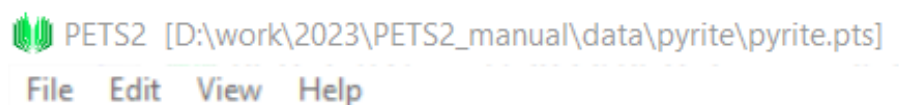


Figure B-2

B.1. The toolbar

B.1.1 File

Under File: New project/merge projects/Open project/Save project/Save as.../Quit: to create a new PETS2 project, open an existing one (pts or pts2 files), to save it or save As and Quit the current project (Fig.A). With File/New (Ctrl+N), the GUI opens a new window to create a new PETS2 project from scratch (from a series of frames). The complete procedure to create a new project is explained in section A.4. With Open (Ctrl +O) PETS2 can open existing PTS or PTS2 files (Figure B-3).

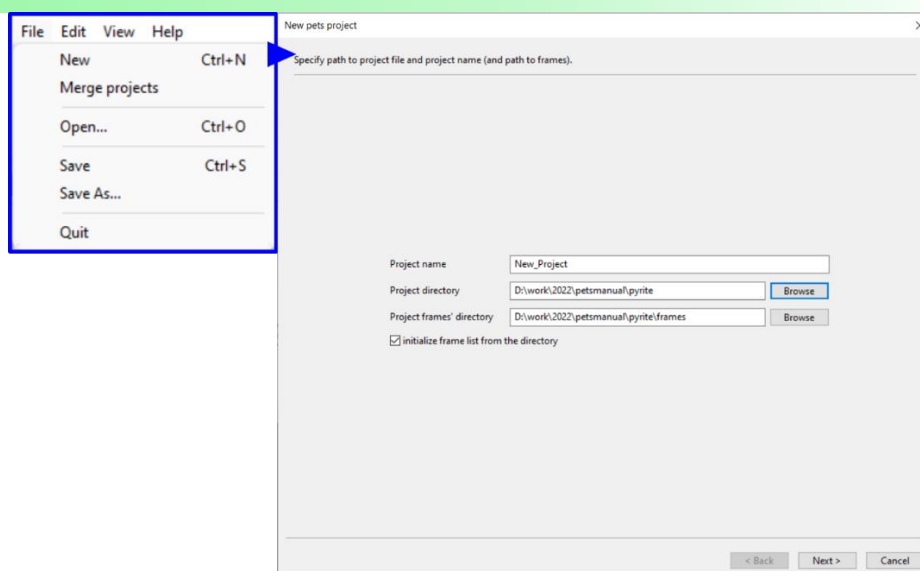


Figure B-3

Merge projects: PETS2 allows merging several projects to create one project containing all data. It is useful for beam-sensitive materials where only a few frames can be collected on each crystal. Merging several data is then necessary to achieve reasonable data completeness. Before merging several projects, a valid pts2 file must exist for each of them, and unit cell/orientation matrix must be defined (celllist file). Instructions on how to merge separated projects are given in the header of the window “Merge projects” (Figure B-4).

-Data sets collected with different camera lengths can be merged.

-Data with different geometries—continuous, precession, no precession, or different precession angles—cannot be merged.

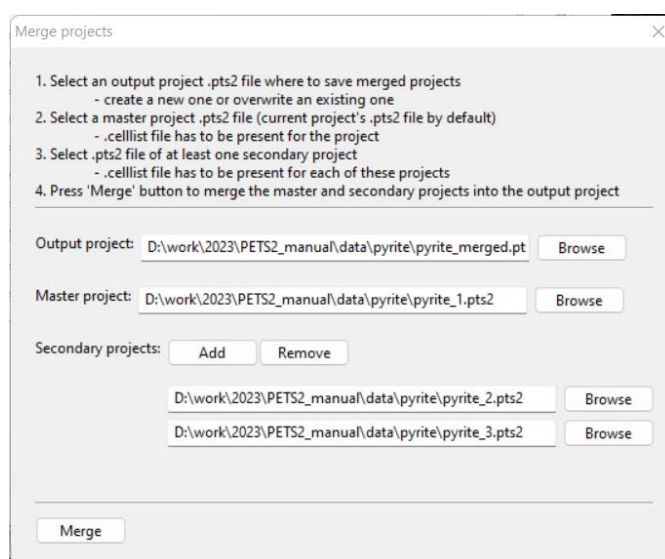


Figure B-4



B.1.2 Edit

Under Edit, two panels are accessible (Figure B-5): frame dialog and Settings

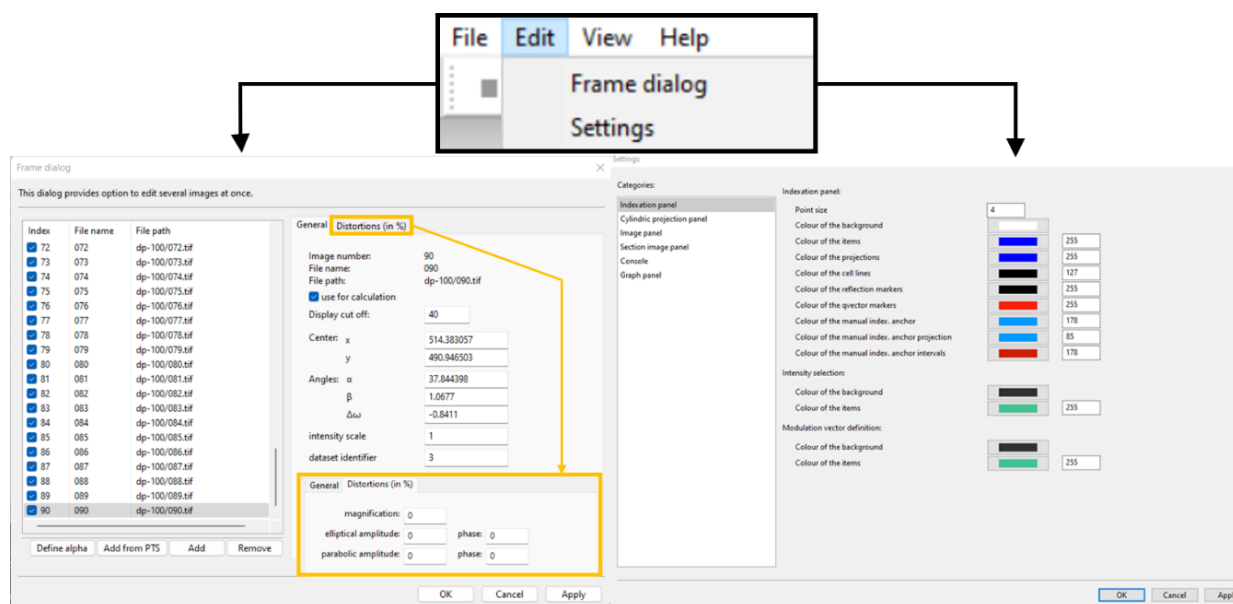


Figure B-5

B.1.2.a. The Frame dialog panel

This panel gives all information about the series of frames used in the project. It is also accessible from the Options panel/Image options panel. This panel will be described in detail in the Options panel sections.

B.1.2.b. The Settings panel

In that section, the colors, size of some items for the different panels, and the font size of the console can be adjusted. Settings to adjust are the colors of the indexing panel (3D panel and options), the cylindric projection panel, the Image panel, the section image panel, the console, and the Graph panel. The font can only be changed for the console (Figure B-5, right).

B.1.3 View

The View menu is summarized below (Figure B-6). It contains the items Main panel tabs, Panels, Tools/Layouts, Reset layout, Show tooltips.

- Main panel tabs menu. Using checkboxes to display or not the tabs of the Main panel: 3D panel/ Cylindric projection/Image data/Section images/Graph/Log
- Panels menu. Checkboxes are used to display or not the following panels: Commands/Options/Console/Main
- Tools: stop/start. Icons Stop/Start and Pause can also be found at the top of the Commands panel.
- Layouts, three default layouts are available: 1655x1150; 1800x1330; 2497x1008
- Reset layout: go back to the default layout.
- Show tooltips: check/uncheck that option to activate/deactivate tooltips in the GUI.

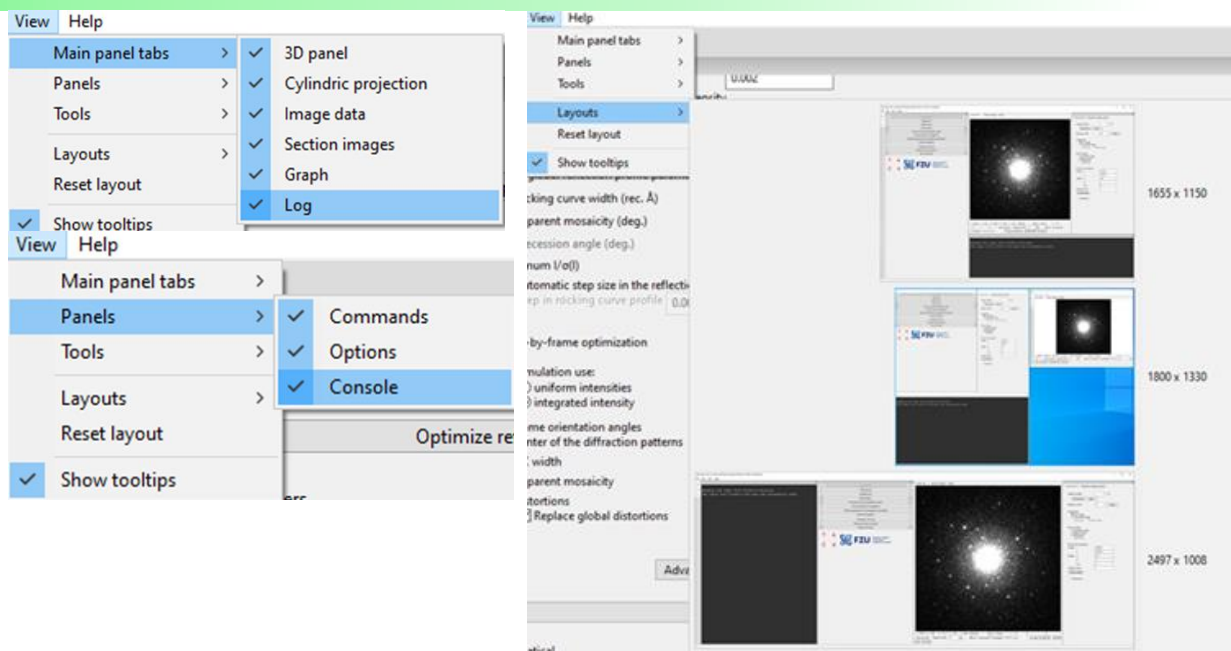


Figure B-6

B.1.4 Help

Software information, version number, logo etc. (Figure B-7).



Figure B-7

B.2. Commands or function panel

All the functions with their options for data reduction are available in that panel (Figure B-8). This section aims to introduce the graphical features and briefly describe the functions.

As explained previously, parameters related to a command are displayed by hitting one of the arrows \vee on each side of the main command button. To run the command, hit the main button.

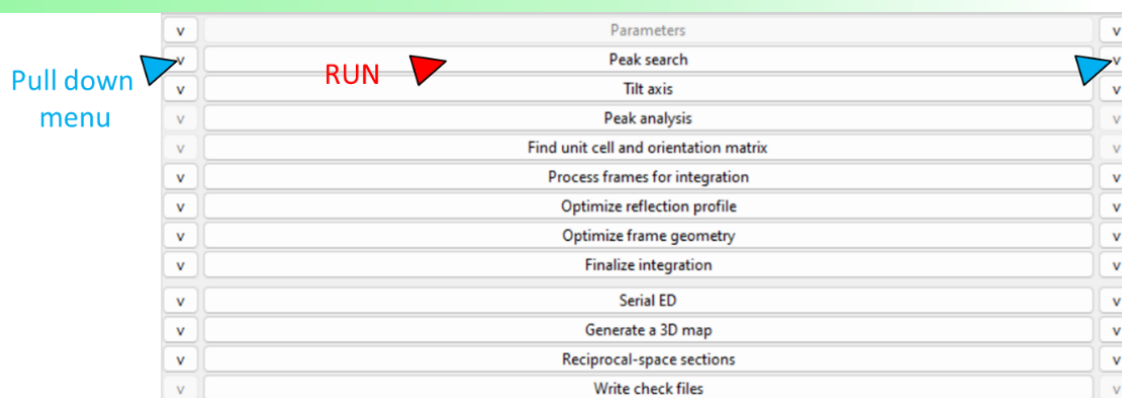


Figure B-8

B.2.1 Parameters

Open the options menu with the left or right arrow on each function button's side (Figure B-9, left). This menu shows the basic parameters of the experiment. The geometry of the 3D ED experiment can be set here (Figure B-9, right): static frames, continuous rotation, or precession. The other parameters needed to start the experiment are:

- The reflection diameter in pixels. The value is the binned one: the binning is set when a new PTS project is created or in the input pts/pts2 file. Used for peak search and integration, it should be large enough to encompass the strong spots, but small enough to avoid overlaps of neighboring spots.
- d^* values: the distances in \AA^{-1} in the pattern from the direct beam. Different values of maximum distances can be set for the peak search and the integration. The d^* minimum is the distance below which no peak is considered (for peak search and integration). By default, $\max d^* = 1.4 \text{ \AA}^{-1}$ and $\min d^* = 0.05 \text{ \AA}^{-1}$.
- The two detector noise parameters are detector specific. They are used to determine $\sigma(I)$.
- The detector saturation limit (detector dependent).
- Beam stop: if Yes, use the Main panel to define the BS manually from the first frame (see the Main panel section B.3 to see how to proceed), or "Browse" the xy coordinates (text file) of the beam stop's shape. When the BS coordinates are loaded, the BS outline is displayed on the frames and its position can be adjusted from the Main panel (see section B.3 Main panel for the explanations).
- Bad pixels. This option removes bad pixels during the data processing (detector dependent). To use this option, load a list of pixel coordinates x and y (text file). The coordinates are defined so that the upper-left pixel has coordinates 1,1.
- Mask ice rings. Check this box to avoid the peak search or the integration close to the ice rings positions. The default mask are two rings defined by their d^* values relative to the calibration constant used. The ice rings (green) can be visualized together with the resolution rings (pink) on the Image tab of the Main panel (Figure B-35).

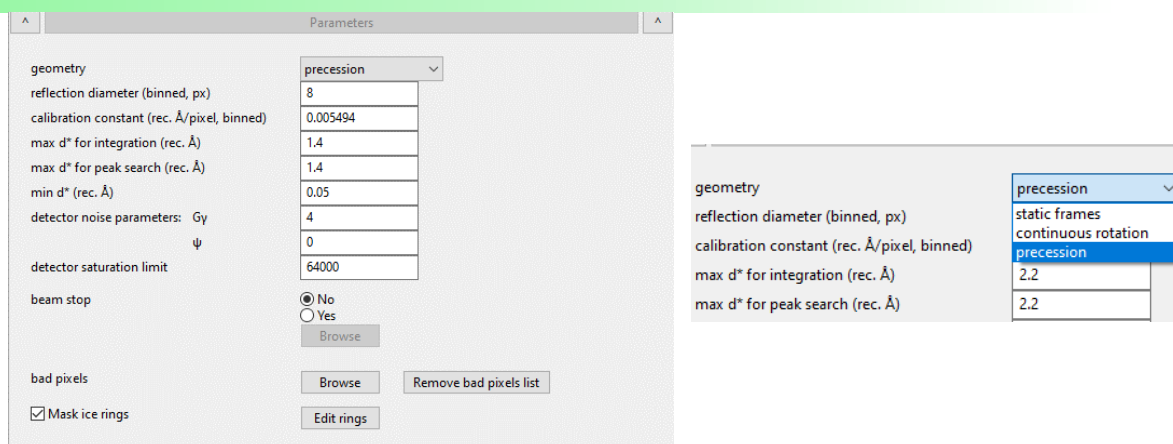


Figure B-9

B.2.2 Peak search

The parameters of this section are related to the frame center determination and the detection threshold $I/\sigma(I)$ (Figure B-10). The picture below shows the default setting.

- Always accept center: if not checked, and the center moves by more than 1/8 of the reflection size, PETS2 asks to either accept the new center or enter manually new coordinates.
- Automatic initial beam coordinates: if PETS2 fails to find the center automatically, uncheck this checkbox and enter manually the center's coordinates or use the button "f", "mf" or "df" at the bottom of the Image data tab to manually determine Friedel pairs and the center. The option "f" (= define Friedel pairs), "mf" (= move one Friedel point) and "df" (= delete Friedel point) are active only when the option "automatic initial beam coordinates" is unchecked.

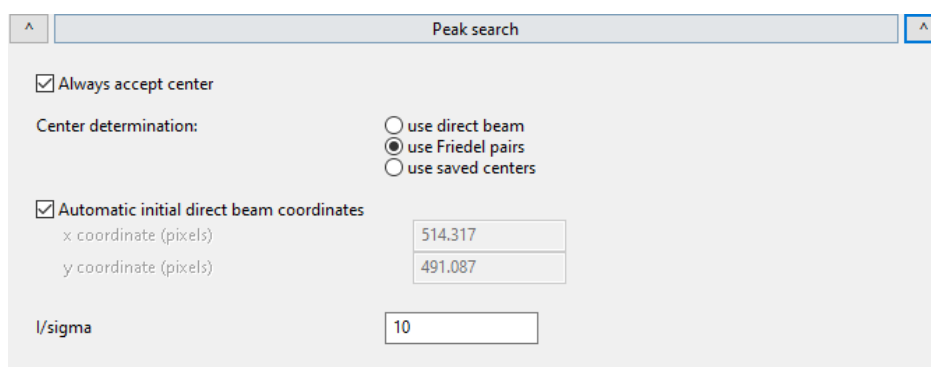


Figure B-10

B.2.3 Tilt axis

The ω angle omega (angle between the projection of the alpha-tilt axis on the image and the horizontal axis on the frame) depends on the microscope, the camera length, and the exact focusing conditions. Therefore, it cannot be precisely calibrated and may need to be optimized for each data set.

Two checkboxes indicate if the tilt axis position is refined globally (a 360-degrees scan) or/and more precisely with "refine tilt axis position ω " (Figure B-11). The sharper the projection becomes, the better. The details of how it works are beyond the scope of this tutorial. Still, you can quickly assess the quality of the data and accuracy of the parameters by looking at the cylindrical projection of the peak positions



shown by PETS2 during the refinement in the cylindrical projection tab of the Main panel. The angle ω can be manually changed, and the cylindrical projection replotted using the button “Replot”.

Another angle δ delta corresponds to the inclination of the alpha tilt-axis in the perpendicular direction of omega. The value can be refined too and should remain close to zero.

Figure B-11

B.2.4 Peak analysis

There is no option below that command. Running “Peak analysis” procedure will recreate the 3D cloud of reflections after clustering. Before running the peak analysis, the cor file (3D cloud without clustering) is the only 3D peak distribution available. After the clustering, three other peak lists are produced: the xyz, the clust, and the diff files.

PETS2 starts the analysis of the peak positions obtained in the peak hunting procedure. The first step analyzes distance distribution between peaks in the image plane. Then, a sorted plot of inter-peak distances is displayed in the Graph tab (red curve) with its derivative (green). For a good-quality data set, the red curve must contain distinct steps; consequently, the green curve has distinct peaks (Figure B-12).

Hit “Peak analysis (continue)”.

In the next step, an auto convolution of the diffraction pattern (difference space) is analyzed, and the groups of peaks in the auto convolution (clusters) are replaced by the cluster centers. Again, a distance distribution is displayed (Figure B-12, right screenshot), and clear-cut steps on the curve indicate a well-defined lattice.

Hit “Peak analysis (continue)”

The first step is finished and PETS2.0 prepared the files needed for unit cell determination and indexing.

At the end of this step, you should get the following message in the console:

```
Threshold for considering two peaks the same: 0.0046 reciprocal angstroms.
15928 peaks merged into 6362 clusters, 1670 with more than one peak.
Peak analysis successfully finished.
```

At the end of this procedure three files are produced: [jobname.xyz](#) contains the “cleaned” peak list, where individual peaks are replaced by the cluster centers. [jobname.diff](#) contains the difference vectors, and [jobname.clust](#) contains the list of cluster centers from the difference vectors.

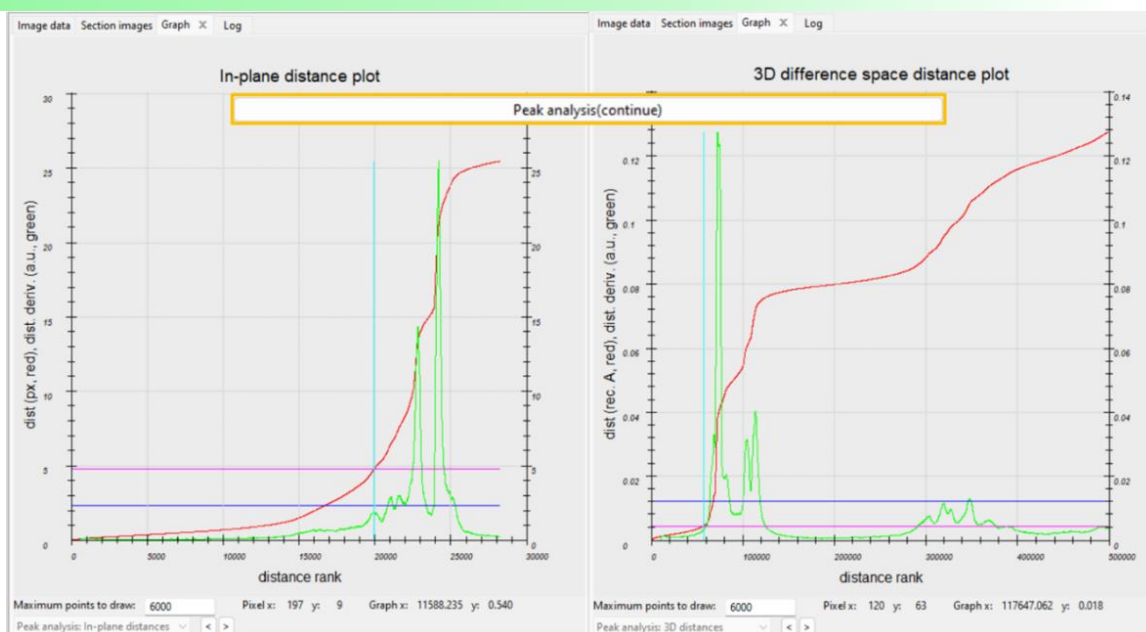


Figure B-12

B.2.5 Find unit cell and orientation matrix

Select that command to access the indexing panel. The Main panel tab switches to the 3D panel tab (with the 3D reciprocal space visualization, and the Options panel with “Indexation display options” is now activated. The basic indexing layout is shown in Figure B-13 with the list of functions on the left, the 3D panel, and the Options on the right-side panel.

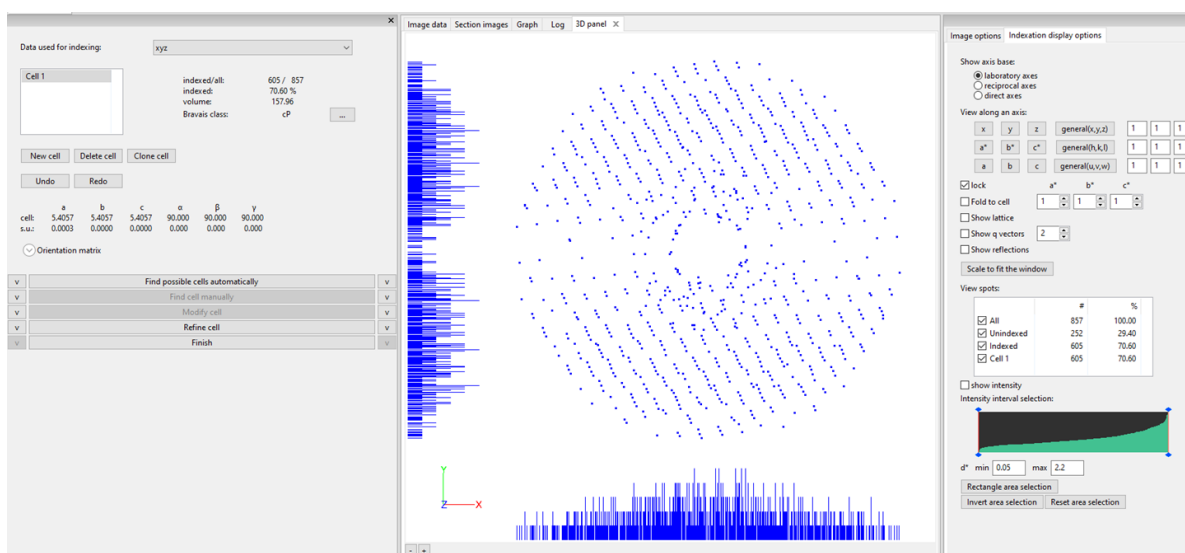


Figure B-13

On the left window, the Indexing panel contains a header and several functions to define (a) new unit cell(s), to modify it/them, clone and refine it/them.

The header contains first a pull-out menu of all the 3D reconstructions available (xyz, clust, diff, and cor files). The selected reconstruction is displayed in the 3D panel tab of the Main panel. The header also



contains a list of all unit cells defined with the basic information on the parameters, the crystal system, the centering, the unit-cell volume, the orientation matrix, and the statistic on how well the unit cell indexes the data. Five buttons are below the cell list: New cell, delete cell, clone cell, Undo, and Redo. Undo and Redo are there to cancel the previous action(s) and, eventually, change your mind again with Redo.

When the indexing panel is opened for the first time, A default Cell 1 is present with parameters 10 10 10 90 90 90.

To change the name of the cell, select the cell in the list to change, and click it once more (fast) with left mouse button.

Next to Bravais class, the icon “...” opens a new window where one can change the crystal system (a = triclinic, m = monoclinic, o = orthorhombic, t = tetragonal, r = rhombohedral, h = hexagonal, and c = cubic), and adjust the centering (standard or non-standard) (Figure B-14). As indicated in the picture, when you define a non-standard centering, the definition of each centering vector needs to be on a separate line. Each vector must have 3+ “number of modulation vectors” items.

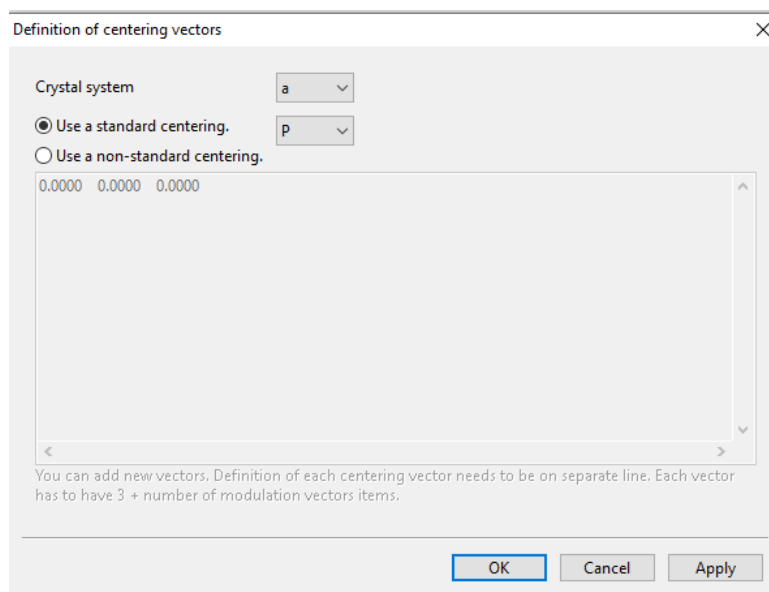


Figure B-14

Below the header is a list of functions and commands (Figure B-15).

v	Find possible cells automatically	v
v	Find cell manually	v
v	Modify cell	v
v	Refine cell	v
v	Finish	v

Figure B-15

B.2.5.a. Find possible cells automatically

Hit one of the arrows on each side of the command to access the parameters of that function (Figure B-16). Two main algorithms are available to search for the unit cell automatically: “from difference space” (default option) and “from triplets”.



Find possible cells automatically

☒ from difference space ☐ from triplets

Maximal d^* difference for indexing (rec.Å):

Angular tolerance for rec. direction (deg):

Maximal volume (\AA^3):

Symmetry search: tolerance for lengths (%):

tolerance for angles (deg):

	a	b	c	α	β	γ	V	Bravais	ind/all
1	5.402	5.403	5.408	90.012	90.022	90.073	157.814	cP	2092/2114

Figure B-16

“from difference space” is the default option and uses the clust file to determine distinct directions in reciprocal space. Make sure the clust reconstruction is meaningful and representative of the complete data before using that option (compare it with the cor file); otherwise, the automatic search will likely fail or find a sub-cell. The “from triplet” option is based on the selected 3D reconstruction (xyz, clust, dif, or cor file).

For both search options, further parameters can be adjusted.

- The **maximal d^* difference for indexing** (in reciprocal Å) is the error allowed between a reflection and the nearest lattice point position (defined by the orientation matrix and the lattice parameters).
- The **angular tolerance** is given in degree and only relevant when the “from difference space” is selected. Within this angle the different reciprocal directions are considered as one direction.
- The **maximum volume** allowed for the unit cell can only be changed when the “from triplet” option is selected.

The two tolerance options on the lengths and angles for the symmetry search are used to determine the possible crystal system and centering.

When the “Find possible cells automatically” command is hit, all the possible unit cells found by the algorithm will appear in the list with the corresponding parameters, the most likely Bravais system and the number of reflections indexed by this unit cell. The best cell will be automatically selected. In the simple case shown in Figure B-16, the algorithm found only one cubic unit cell. Sometimes, when the data are more ambiguous, the list can contain a lot of possible unit cells. In the worst case, when no unit cell is found, an error message appears in the console.

Two buttons are below the list of possible unit cells: rewrite current unit cell, and Add as a new unit cell.

B.2.5.b. Find unit cell manually

That section has the tools to manually define a new cell or modify a pre-existing one (Figure B-17). That section works hand and hand with the 3D panel and the “indexation display options” panel.

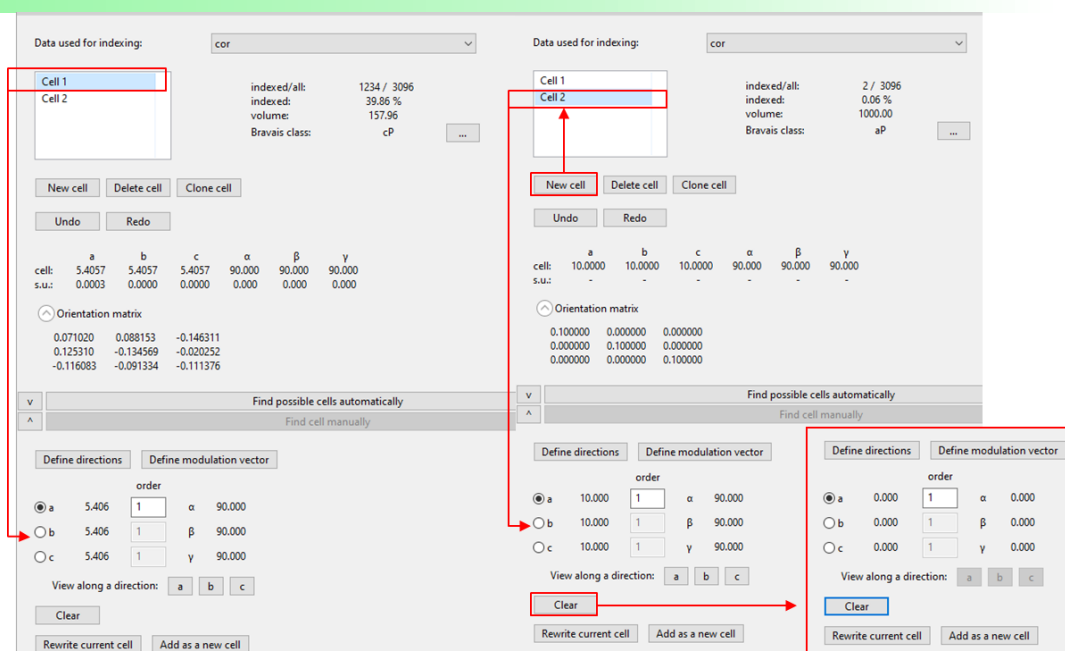


Figure B-17

Select a cell to modify manually in the cell list available or create a new one. By default, a new unit cell is created with parameters 10 10 10 90 90 90 and its parameters are loaded in the section “Find cell manually”. You can either “Clear” the existing parameters to start with 0 0 0 0 0 0, or start defining the parameters from the existing ones.

To define a parameter, turn the cloud of reflections in the 3D panel until a special orientation is found with one of the main lattice vectors in the plane of the projection, then activate the “Define directions” option. In the 3D panel, left click and drag the cursor to where you want to define a parameter, as shown below (Figure B-18). Adjust the order of the plane (i.e. the number reciprocal-lattice planes between the selected plane and the origin), if the automatic estimation does not provide a good value. Here the order should be 5 because the cursor was dragged through 5 interplanar spaces. To move the 3D cloud again and find a new direction, first, deactivate the “Define directions” button. Use the view along a direction (**a**, **b** or **c**) to help find new directions. When all the unit cell parameters are defined, hit “Rewrite current cell” to replace the previous parameters with the new ones in the header.

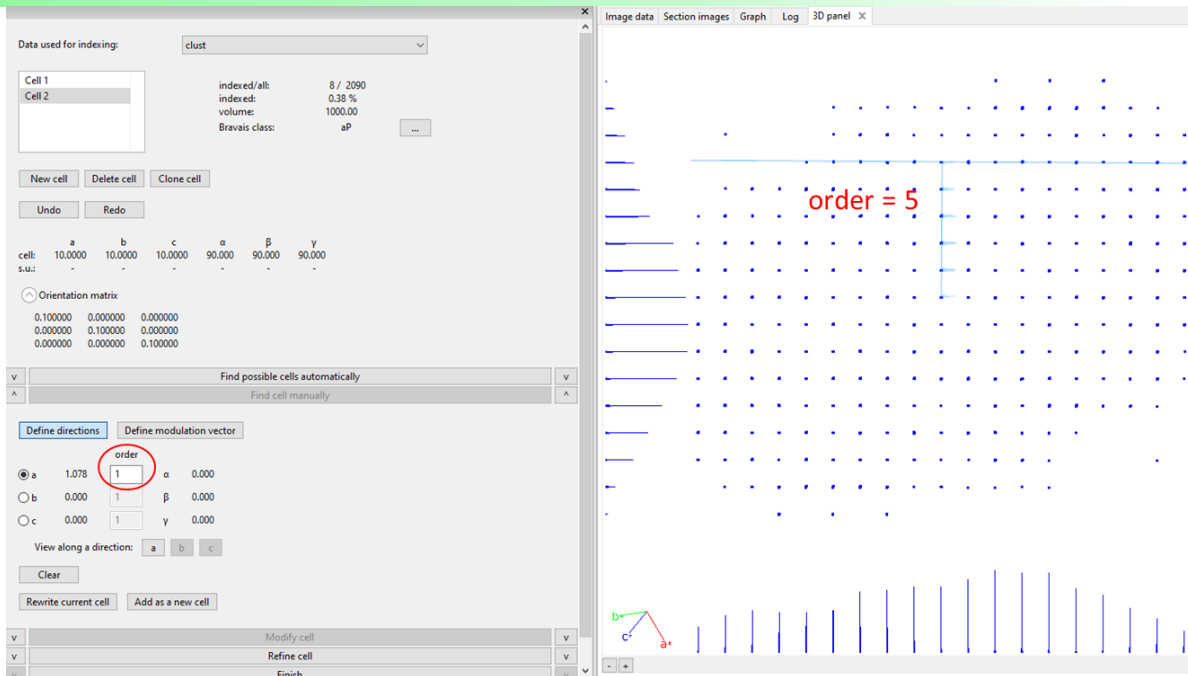


Figure B-18

B.2.5.c. Modify cell

In this section (Figure B-19), you can modify the selected unit cell by a matrix, reduce the cell by hitting “Reduce cell”, check if there is a centering with “Check centering” or look for a supercell with “Go to supercell”.

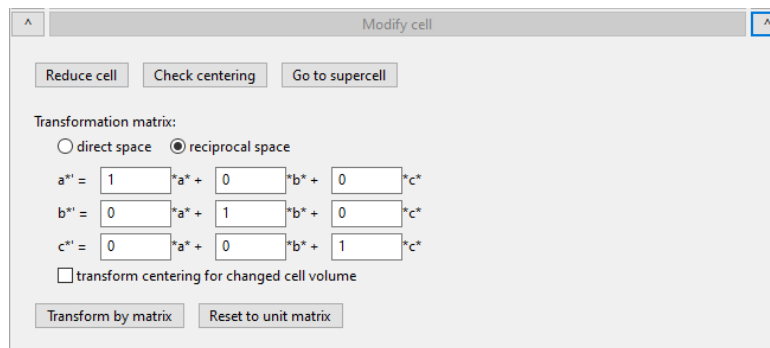


Figure B-19

With Check centering, the result is given in the console like in the example for the cubic pyrite:

```
Check centering: The centering cP was confirmed.
Unit cell is primitive and search for higher symmetry (centered) cell is going
on .....
Cell with higher symmetry was not found.
5.406 5.406 5.406 90.00 90.00 90.00 157.96 c P
7.645 7.645 9.363 90.00 90.00 120.00 473.88 h Robv
```

With “Go to supercell”, the result is given in the console like in the example for the cubic pyrite:

```
Sorry, no frequent fraction vector was found.
No suitable supercell was found.
```



To apply the transformation matrix, hit “Transform by matrix”. The matrix can be defined either in the direct space or in the reciprocal one.

To reset the matrix to unit matrix, press “Reset to unit matrix.”

If you are unhappy with the new cell after the transformation, go into the header and hit “Undo” below the cell list.

B.2.5.d. Refine cell

The section will allow you to refine the unit cell parameters and, optionally, the distortion parameters. (Fig. B19).

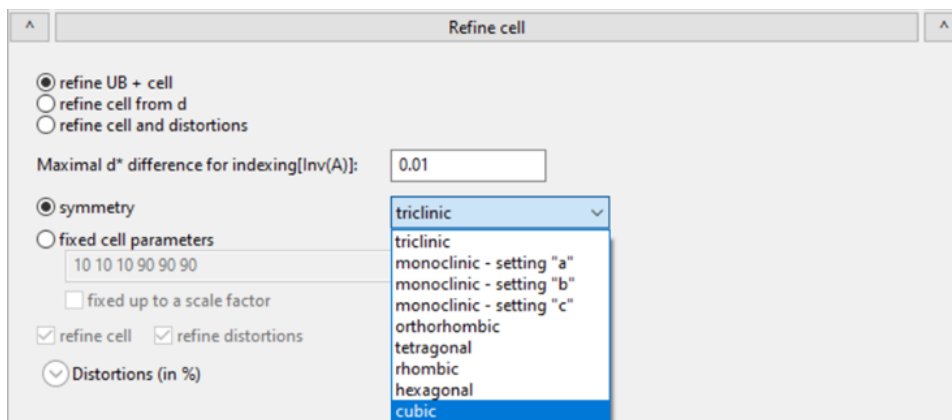


Figure B-20

Radio buttons are used to select one of the three refinement methods (Figure B-20);

- refine UB + cell (refinement against 3D reconstruction of the reciprocal space, recommended data cor and xyz),
- refine cell from d (refinement using only d spacing, recommended data cor and xyz), or
- refine cell and (global) distortions (refined within the 2D of the frames – minimizes the distance between predicted and observed peak position, only cor data are used). In that mode, both cell and distortions can be refined together or separately (checkboxes “refine cell” and “refine distortions”).

Just below, for all three methods, the indexing tolerance is defined as the “maximal d^* difference for indexing (in reciprocal Å).” The indexing tolerance is the same parameter as used in the automatic unit cell determination.

For both “UB+cell” and “cell and distortions”, the user has to select one option from:

- “symmetry”: will impose crystal system constraints on the unit cell parameters (see picture).
- “fixed cell parameters”: the unit cell will be transformed to be the same as you set OR, when the checkbox “fixed up to a scale factor” is selected, the refined unit cell will keep the same proportions as the indexed cell and get as close as possible using a scale factor. The “fixed up to a scale factor” is only accessible with the method “refine UB + cell” because the scaling would correlate with the distortion parameters (the magnification) with the method “Refine cell and distortions.”



No symmetry or fixed cell parameters can be imposed for the “refine cell from d” option at this moment.

Pull down the “Distortions” menu (Fig. B20). Two radio buttons are available to switch the display of the distortion values in percent or pixels. The pixel units are included mostly for historical reasons. They depend on the calibration constant, while the percentage values do not.

Two tabs are available with the distortion parameters:

- The standard mode is sufficient for most data sets.
- The Expert mode contains additional distortion components. Most of them are used for development purposes, and it is not recommended to mingle with them, unless you know well what you are doing.

The two pictures below (Figure B-21) show the same distortions parameters (in percentage) displayed in the “Standard” and the “Expert” modes. The radial $g \cdot S_g$ parameter is only meaningful for precession geometry. Detailed information about the distortions used in PETS2 is available in Brazda et al. (2022)⁵.

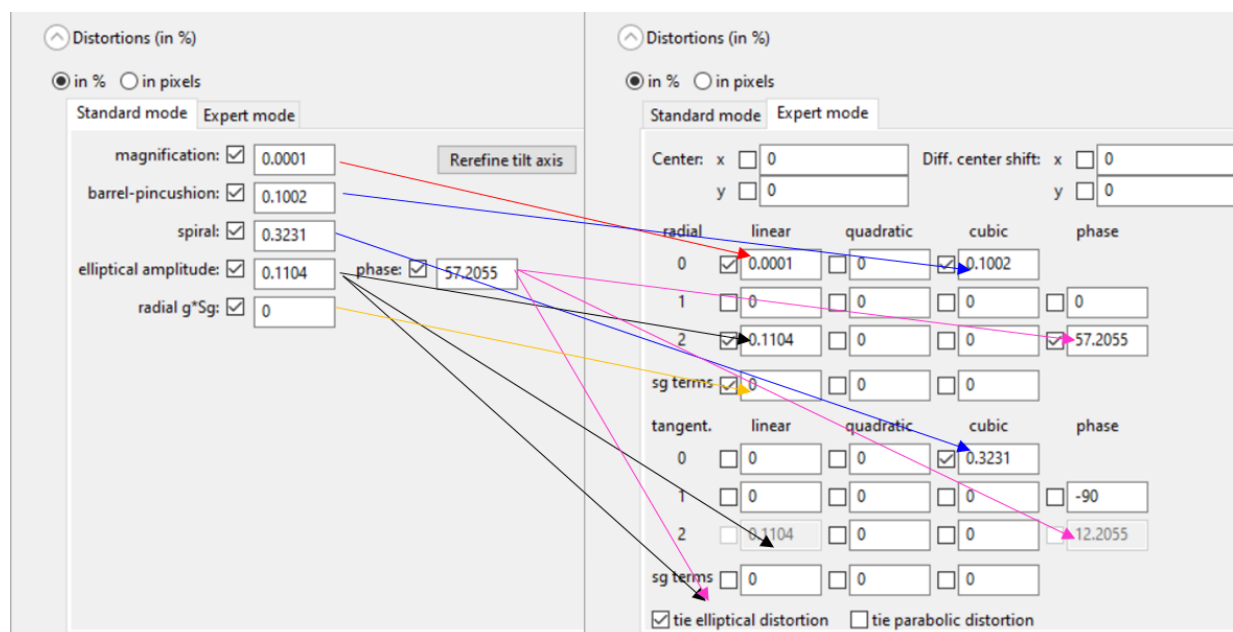


Figure B-21

An option “Rerefine tilt axis” is on the right side of the distortions panel. The tilt axis angle ω is usually optimized once more after determining the distortions parameters, especially if the spiral distortion changes significantly.

B.2.5.e. Finish

Press Finish to go back to the main commands panel and continue with the data reduction.

The last selected unit cell will be the active one in the rest of the data reduction.

B.2.6 Process frames for integration

Pull out the menu by hitting one of the arrows on each side of the function button to display the parameters (Figure B-22). Hit the command to start processing frames for integration.

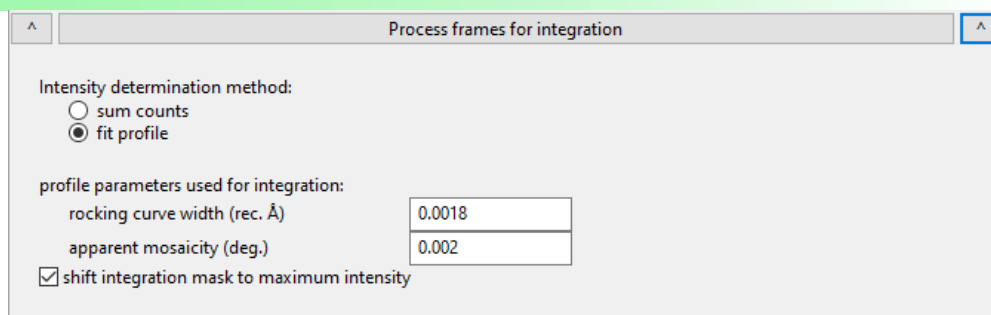


Figure B-22

This window has two sections:

B.2.6.a. Intensity determination method

Radio buttons are used to select either “sum counts” or “fit profile” methods. With sun count, the intensity is determined from the total counts measured inside the mask less the background. With “fit profile”, the average profile of reflections is defined during the “peak search” procedure from the strong reflections. This profile is later use in the integration, and it position (x , y) and intensity are refined for each reflection. For better results, the “fit profile” option should be used together with the “shift integration mask to maximum intensity” (at the bottom of the menu). For the “sum counts” option, the user can try with and without checking the shift option box. The “fit profile option” is slower than the sum option but usually provides (slightly) better results. The difference is especially important, if reflections on the frames overlap, for weak or saturated reflections.

B.2.6.b. Profile parameters for the integration

The two main profile parameters of the Rocking curve are used for integration: the rocking curve width (\AA^{-1}) and the apparent mosaicity (deg.). The Rocking curve is visible on the main panel in the Graph tab. Those two profile parameters are repeated in the “Optimize reflection profile and geometry” section. They are used to estimate the angular extent of the reflections (i.e. on how many frames the reflection is present)

The “shift integration mask to maximum intensity” allows the integration masks to be shifted a little from their ideal positions to reach the real position of the reflection (center of mass of the intensity).

As the process for integration runs, two graphs related to the data resolution are produced and displayed in the Graph tab.

- “Integration: Resolution” graph: for each frame the length of the maximum diffraction vector (d^* in reciprocal \AA) is given for 2σ , 3σ and 5σ .
- “ I/σ in two shells”: for each frame the mean I/σ is given for reflections with $d^* < 0.5 \text{ \AA}^{-1}$ (inner shell with lower resolution), and $d^* > 0.5 \text{ \AA}^{-1}$ (outer shell with higher resolution). The default threshold between the inner and outer shell is set to 0.5 \AA^{-1} and can be changed in the input pts2 file after the keyword “resshellfraction”.

See Sections B.3.3.d, and B.3.3.e for further details about the graphs.



B.2.7 Optimize reflection profile

Parameter	Value
<input checked="" type="checkbox"/> rocking curve width (rec. Å)	0.00106
<input checked="" type="checkbox"/> apparent mosaicity (deg.)	0.0403
<input type="checkbox"/> precession angle/tilt semiangle (deg.)	1.02
minimum $I/\sigma(I)$	5
<input type="checkbox"/> Automatic step size in the reflection profile	0.003

Replot

Figure B-23

This is where the global reflection profile parameters are displayed and can be optimized (Rocking curve or Camel plot) (see Figure B-23). They will influence the calculated rocking curve (see the red curve of the Rocking curve in the Graph tab Figure B-24).

3 parameters will influence the shape of the calculated Camel plot:

- The RC width (\AA^{-1}) (global value). This parameter can be refined.
- The apparent mosaicity (deg) (global value). This parameter can be refined.
- The tilt-semi angle or the precession angle (deg) depending on the geometry of the experiment – not refined.

2 parameters affect how the curve is displayed:

- The minimum $I/\sigma(I)$ is used to select the reflections involved in the Camel plot calculation.
- The Automatic step size in the reflection profile.

The parameters can be refined by pressing the command button. They may also be changed manually. After changing the parameters manually, use the Replot button to refresh the Rocking curve profile on the Graph tab.

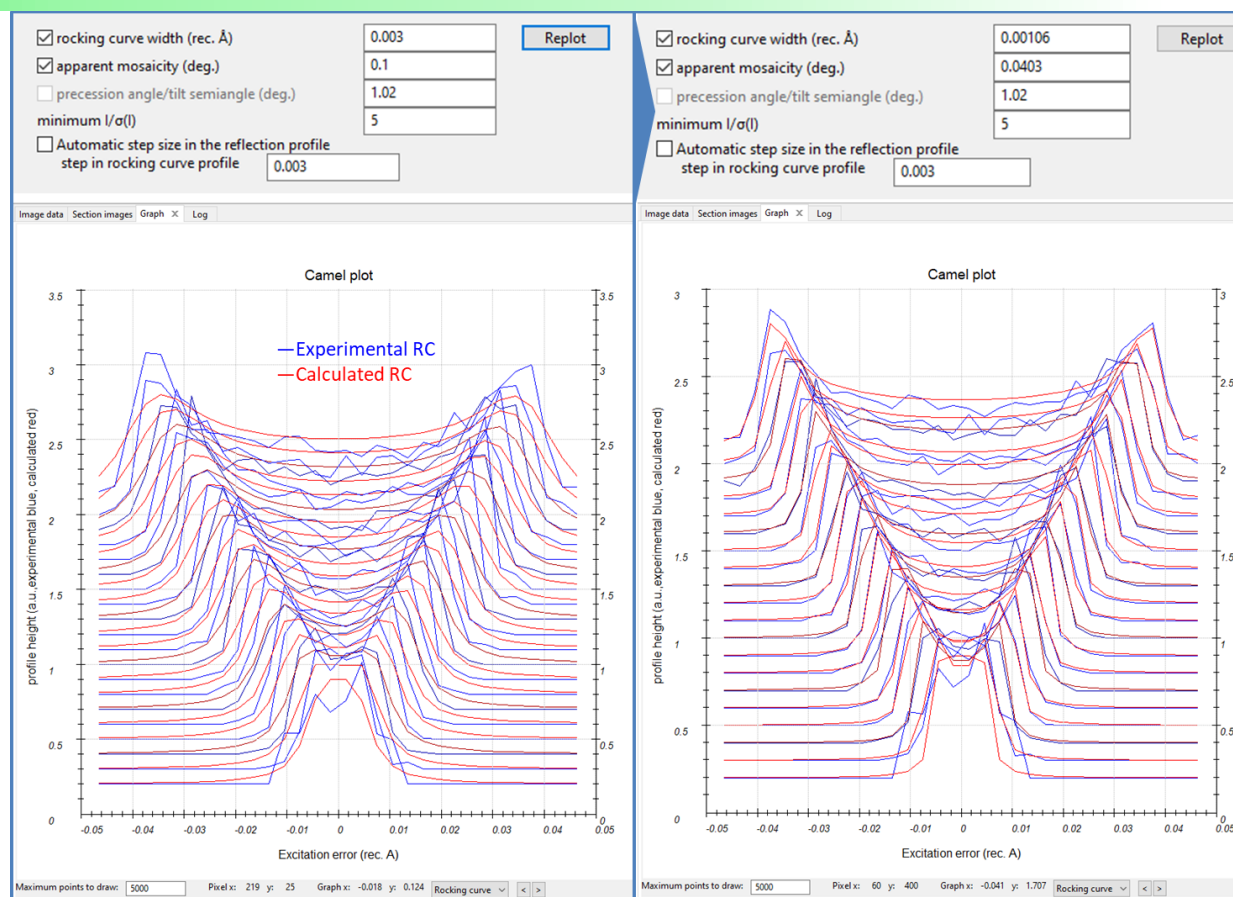


Figure B-24

B.2.8 Optimize frame geometry

This section will optimize the frame-by-frame geometry of the experiment, including orientation angles, center of the diffraction patterns, RC width and apparent RC mosaicity, and frame-by-frame distortions. Below are the default settings.

Hit the command to start the optimization or

Pull down the menu (arrows) to set what to refine and adjust the parameters.

Checkboxes are used to select what is refined (blue area in Figure B-25). Possibly,

- The frame orientation angles (alpha and beta-tilts, $\Delta\omega$ axis),
- The centers of the diffraction patterns,
- The frame-by-frame RC width and apparent mosaicity, and
- Frame-by-frame distortions: the distortions that can be refined frame-by-frame are the magnification, the amplitude and the phase of the elliptical distortion, and the amplitude and the phase of the parabolic distortion.

By selecting “Replace global distortions” (blue area in Figure B-25), the three global distortions parameters that are also refined frame-by-frame (see in the “Find unit cell and orientation matrix”) will be replaced by the average values of the frame-by-frame optimization.



The optimization is based on a match between the experimental and simulated frames. For simulating the frames, either **uniform intensities** or **integrated intensities** may be used. Integrated intensities can only be used after a (reasonably successful) Finalize integration step (see section B.2.9.). If you are unsure about the data quality, use uniform intensities first and refine only the orientation angles and the center of the diffraction pattern before including distortions and/or RC parameters.

The refinement of the tilt-angles ($\Delta\alpha$, $\Delta\beta$ tilts, and $\Delta\omega$) can be stabilized using a smoothing method. The smoothing avoids outliers for frames with fewer reflections, for example.

With the polynomial method, the order corresponds to the order of the polynomial equation. In Figure B-26, order = 4 means that the curves with the correction of the angles are described with a polynomial function $Ax + Bx^2 + Cx^3 + Dx^4 + E$ with (A, B, C, and E constants). With the moving average option, the order corresponds to how many consecutive frames are used to smooth the curve (Usually from 5 to 10). The moving average method is a safer approach to start. “Reset to default” will reset the frame-by-frame optimization and go back to the “initial” values.

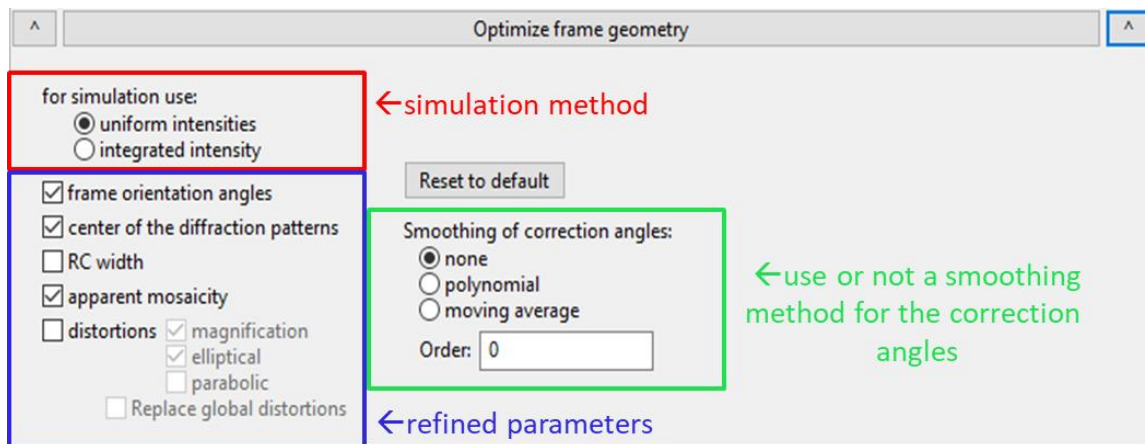


Figure B-25

During the optimization, different plots will be produced and visible in the Graph tab of the main panel:

- Tilt corrections plot
 - Origin correction plot
 - Frame-by-frame distortion plot
 - Profile parameters plot.
- (More information on the plots in the dedicated section B.3.3.)

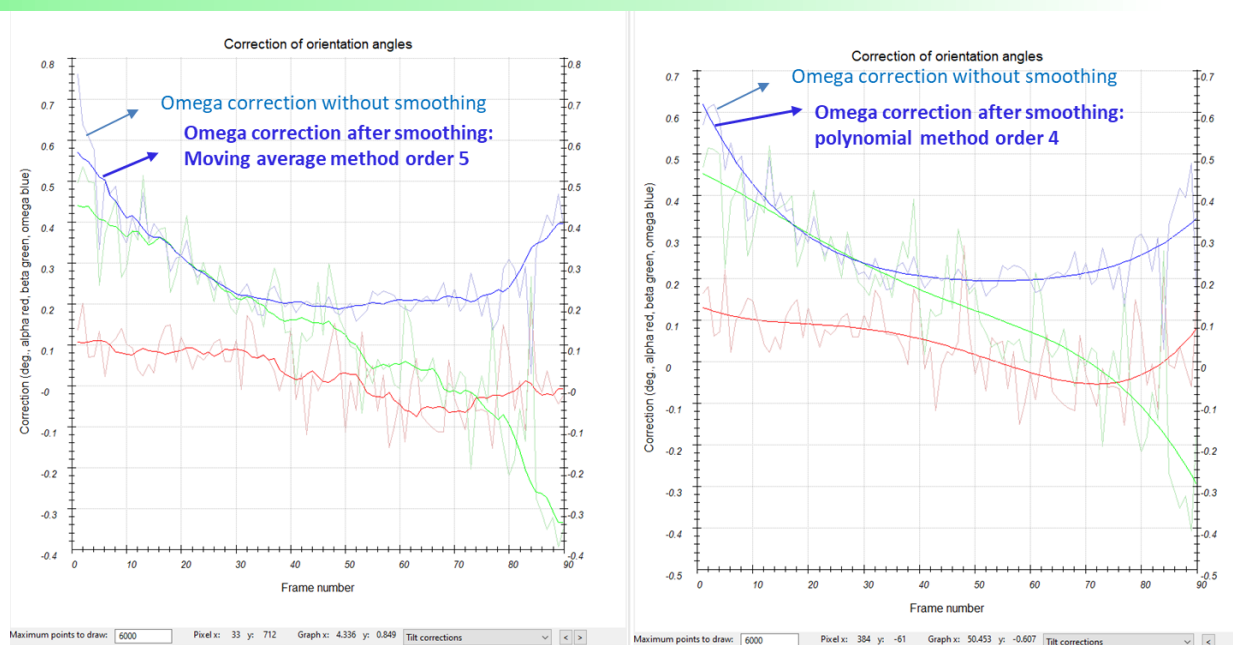


Figure B-26

B.2.9 Finalize integration

Hit the command to finalize the integration and get *hkl*-type files dedicated to structural analysis with the kinematical approximation (solution + kinematical refinement) or considering the dynamical theory of diffraction (dynamical refinement)^{6–8}. “kinematical” and “dynamical” are selected by checkboxes. Pull down the menu to access the options (Figure B-27).

B.2.9.a. Files obtained

The output files produced are listed below:

- Jobname.hkl. This file is a simple list of reflections $h\ k\ l\ (m\ n\ p)$ associated with their intensity and $\sigma(I)$ without a header. This file can be used in any software for solution and refinement, considering the kinematical approximation.
- Jobname.cif_pets. The same list as mentioned above with an additional header giving additional unit cell and experimental information. This type of file is only recognized by JANA2006/2020 (as far as we know).
- Jobname_dyn.cif_pets. File dedicated to the dynamical refinement in JANA2020 containing a header with unit cell and some experimental parameters. This file contains a list of reflections $hkl\ (mnp)$ with their intensity and $\sigma(I)$ for each (overlapping virtual) frame. See Palatinus et al. (2015a,b)^{6,7} and Klar et al. (2023)⁸ for more details.

B.2.9.b. Skip saturated reflections

The first option, “skip saturated reflections,” allows including or rejecting the saturated reflections in the output files. Saturated reflections should be included for the structure solution and dismissed for the refinements (kinematical or dynamical).



Geometry: precession

Finalize integration

☐ skip saturated reflections

☒ kinematical
 intensity estimation:

☒ fit profile
☐ integrate profile
☐ maximum intensity
☐ Bragg position

min. number of reflection measurements
 reflection width multiplier

integration parameters:

for profile fitting
 for symmetry averaging

Outlier detection limits:

for profile fitting
 for symmetry averaging

☒ frame scaling
 Laue class for scaling:
 Interframe correlation range:
 Interframe correlation weight:

☒ refine error model
 s_fac:
 s_b:
 s_add:

☒ dynamical
☒ apply frames scales to intensities

Geometry: continuous rotation/static frames

Finalize integration

☒ skip saturated reflections

☒ kinematical
 intensity estimation:

☒ fit profile
☐ integrate profile
☐ maximum intensity
☐ Bragg position

min. number of reflection measurements
 reflection width multiplier

integration parameters:

for profile fitting
 for symmetry averaging

Outlier detection limits:

for profile fitting
 for symmetry averaging

☒ frame scaling
 Laue class for scaling:
 Interframe correlation range:
 Interframe correlation weight:

☒ refine error model
 s_fac:
 s_b:
 s_add:

☒ dynamical
☒ automatic virtual frame parameters
 number of frames:
 step between frames:

☒ apply frames scales to intensities

Figure B-27

For each type of integration (kinematical or dynamical), parameters must be chosen and adjusted. However, default parameters should lead to reasonable results. The parameters related to kinematical integration are broken down into sections, as shown in Figure B-27

B.2.9.c. Intensity estimation for kinematical integration

There are 4 possible options to estimate the kinematical intensities and selected with the radio buttons.

- **Fit profile:** This option corresponds to the red dashed area in Figure B-28. The intensity of an hkl reflection is defined with the calculated Rocking curve profile on all the resolution range according to the data and the two RC parameters (sigma and moisaicity), and the value of the semi-angle or precession angle. The fit profile integration should produce the best results for medium to high-quality data.
- **Integrated profile:** the intensity of one reflection hkl is determined by the area (volume in 3D) defined by all the measurements for this reflection found in consecutive frames (blue area in Figure B-28).
- **Maximum intensity:** the value of the measurement with the highest intensity for one given hkl reflection is used as a global intensity for this reflection (yellow measurement in Figure B-28). Reserved for special cases, generally not recommended.
- **Bragg position:** The intensity of the hkl reflection is estimated from the closest measurement from the Bragg position (green measurement in Figure B-28). Reserved for special cases, generally not recommended.

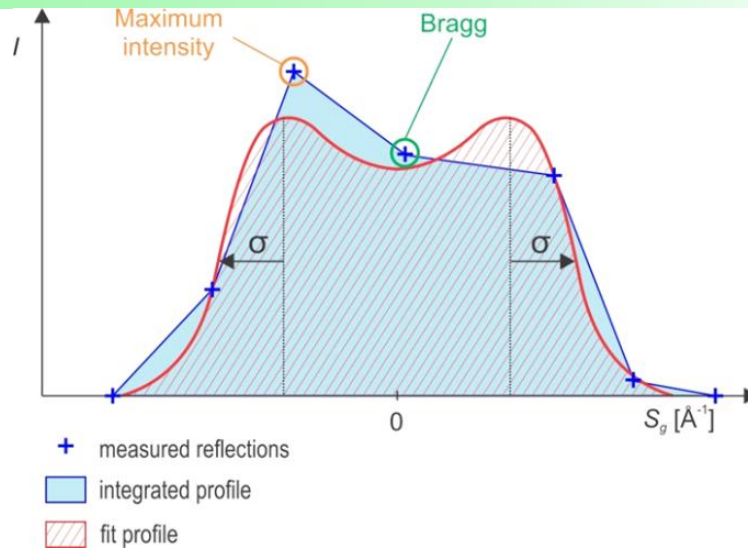


Figure B-28 Integration options illustrated with a basic Camel plot profile drawn for a sample reflection.

B.2.9.d. Integration parameters for kinematical integration

Two additional integration parameters that are kept to the default value most of the time:

- **The minimum number of reflection measurements** (default value 1): how many times a reflection hkl has to be present on consecutive frames to be considered in the integration. Increasing the number might improve the data quality, but it may reduce the data coverage, especially with data with large tilt steps.
- **Reflection width multiplier** (default value = 1): to extend the integration beyond the S_g limit set by the reflection profile.

B.2.9.e. Outlier detection limits for kinematical integration

Removing outliers is a new feature in PETS2. It relies on two parameters.

- **The outlier detection limit** is based on the profile fitting (default value: 1000). Limit for rejecting reflections with a too-large discrepancy between the intensity on a frame and the fitted profile. Relevant only for the fit profile option.
- **Outlier detection limit based on symmetry averaging** (default value: 1.5). Limit for rejecting reflections with too large discrepancy between its integrated intensity and the average of all symmetry-equivalent reflections. This parameter is active, and rejected outliers appear in red in the Normal probability plot in the Graph tab (Figure B-29). Setting a too low value might have a detrimental effect on data coverage.

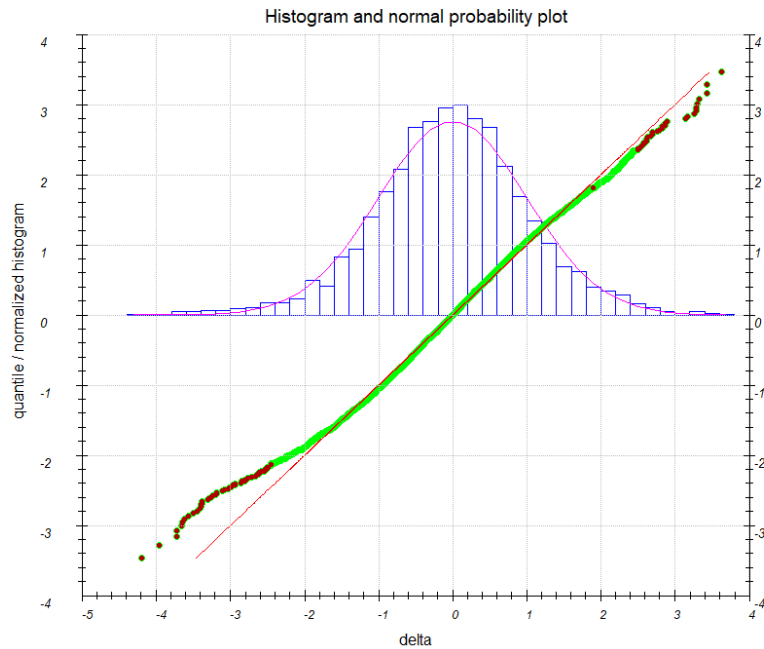


Figure B-29

B.2.9.f. Frame scaling for kinematical integration

When the frame scaling is checked, select the appropriate Laue class and set reasonable parameters for the interframe correlation range (typically from 3 to 6) and interframe correlation weight (typically 0.5-1).

-For unknown Laue class: select the option “**Auto**” in the top of the Laue class list. In that case, PETS2 will evaluate the Laue class to apply for the frame scaling. The “Auto” option, will be replaced by the best Laue class guess after “Finalizing integration”.

-**The interframe correlation range** corresponds to how many consecutive frames are considered around the frame to scale. To scale frames independently, set 0.

-**The interframe correlation weight** indicates how strongly the scales are forced to be close (1 = strong correlation). The scaling is only relevant for the kinematical integration. The result of the frame scaling is visible in the related graph below (Figure B-30).

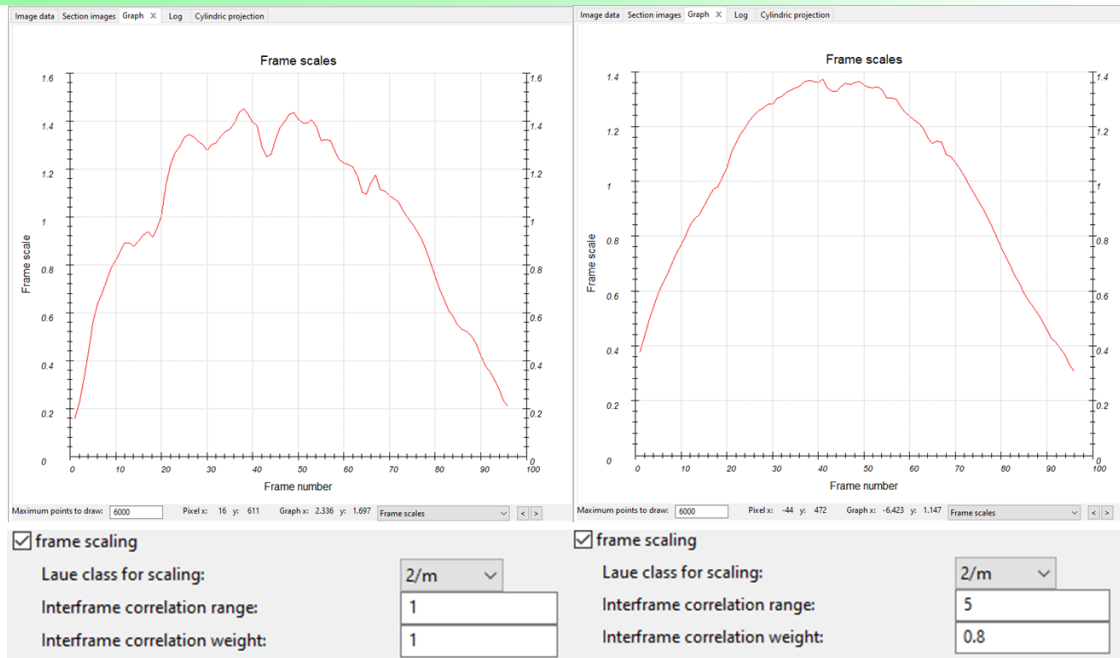


Figure B-30

B.2.9.g. Refine error model for kinematical integration

The error model is used to correct the $\sigma(I)$. The refinement finds optimal modifiers (s_{fac} , s_{b} , and s_{add}) of the counting-statistic $\sigma(I)$ to produce a normal distribution of residuals following the equation: $\sigma(I_{hkl})_{\text{corrected}} = s_{\text{fac}} \cdot \sqrt{\sigma(I_{hkl})_{\text{count}}^2 + s_{\text{b}}^2 \cdot I_{hkl} + s_{\text{add}}^2 \cdot I_{hkl}^2}$. The default values are $s_{\text{fac}} = 1$, $s_{\text{b}} = 0$ and $s_{\text{add}} = 0$. On the histogram and probability plot (Figure B-31), a satisfying refinement of the modifiers brings the green curve close to the perfect Gaussian distribution (= red curve). As a side effect, the optimization tends to decrease the number of observed reflections. For more information see Khouchen et al., 2023⁹.

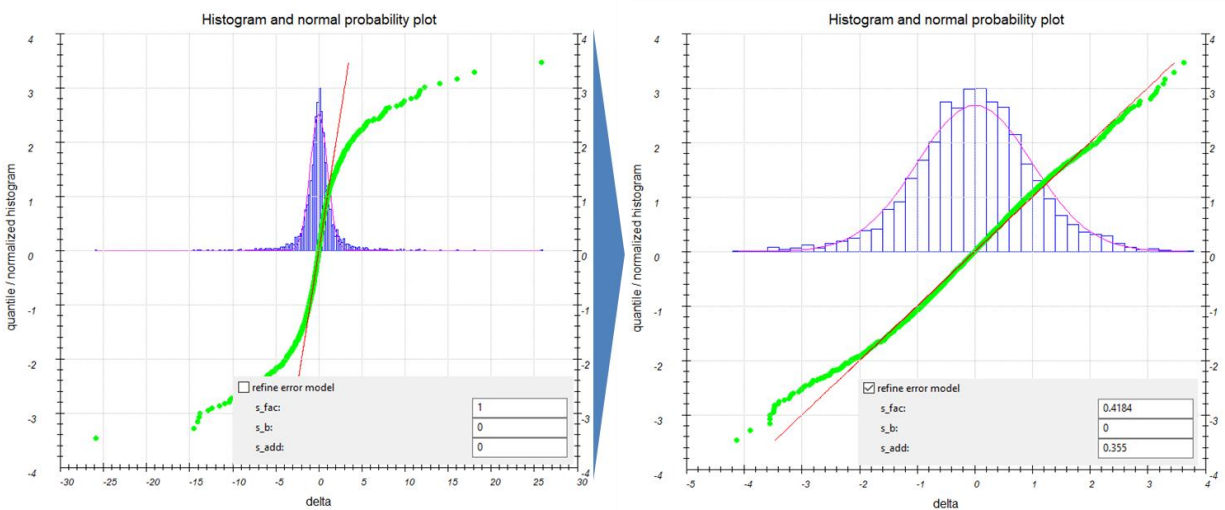


Figure B-31



B.2.9.h. Dynamical integration

-apply frames scales to intensities: For all kinds of data, the frame scaling can be applied to the dynamical frames by checking the box “apply frames scales to intensities”. When the scaling is applied in PETS2, the scaling later defined in JANA2020 frame by frame should be closer to a flat curve.

-automatic virtual frame parameters: For continuous rotation or static frame geometries, two additional options define how to merge consecutive frames to create overlapping virtual frames (*OVF*) (see Figure B-27).

By checking the box “automatic virtual frame parameters”, PETS2 will set the two following parameters automatically depending on the value of the tilt semi-angle.

- The “**number of frames**” is the number of frames merged to create one virtual frame.
- The second parameter called “**step between frames**” defines the increment between 2 virtual frames and, thus, the overlap between the *OVFs*.

Typically, real frames are merged to create *OVF* covering about 2.5-3 degrees. A safe overlap can be set to one third of that value. In the example in Figure B-27 on the right, the data are from continuous rotation and a $\Delta\alpha$ tilt of 1 degree. By merging 3 frames, each virtual frame covers 3 degrees with a 2-degree step between two frames, leading to an overlap of 1 degree.

B.2.10 Serial electron diffraction

Under development, contact us if you experience bugs. We strongly suggest saving at every step so as not to lose the progress of the data reduction in case the program crashes.

B.2.10.a. Introduction

REQUIREMENT: This option can be used when the **lattice parameters** and the **Laue class** are known.

FOR WHAT TYPE OF DATA? The serial electron diffraction data reduction can be used for electron diffraction frames with or without precession or with continuous rotation.

- collection of individual frames randomly oriented on different crystals for very beam sensitive materials (with or without precession).
- combination of several short tilt series (continuous rotation/precession/static geometry) which are individually insufficient to define the unit cell (no merging possible).
- combination of an incomplete data set for which the unit cell can be defined with additional individual randomly oriented frames from different crystals to complete the coverage.

B.2.10.b. Available options

Below is the basic description of the “Serial ED” parameters found when the menu below the command is pulled down.

Before doing anything with the “serial ED” command, make sure the expected Laue class is indicated as shown in Figure B-32.



The screenshot shows two windows from the PETS2 software. The top window, titled 'Finalize integration', contains various settings for data processing. A red box highlights the 'Laue class for scaling' dropdown menu, which is currently set to '2/m'. A red arrow with the number '1' points to this dropdown. The bottom window, titled 'Serial ED', contains settings for template matching. A red arrow with the number '2' points to this window. The 'Serial ED' window shows a 'template step' of 2.0000, a 'template resolution' of 1.0000, and a 'max. change of orientation' of 180.0000. It also has checkboxes for 'fine orientation refinement' and 'dynamical', and radio buttons for 'Use current orientation matrix' and 'Use these lattice parameters'. The 'Use these lattice parameters' option is selected, and a text box below it contains the values: 10.5080 9.4973 12.6256 90.000 95.236 90.000.

Figure B-32

The indexing of Serial ED data is based on template matching. This is why a Laue class, and a unit cell are needed to simulate frames. The simulation uses “uniform” intensities with a decay relative to the resolution.

Template step: by default, the template step is 2 degrees. This value should be enough for most experiments. For very sharp reflections where a small change in orientation brings a lot of change in the pattern the value can be decreased. For precession data, 2 degrees by default are usually sufficient, for small semi angle and continuous rotation data, a 1-degree step might be more reasonable. Note that the simulation will be more time-consuming with a smaller angle.

Template resolution: in reciprocal angstrom (\AA^{-1}). The default value is 1 \AA^{-1} . Increasing the resolution of the simulation will also slow down the process.

Maximum change of orientation: 180° (default value) will cover all the diffraction sphere. For higher symmetry, a smaller part of the simulated data can be used.

Fine orientation refinement: when the box is checked, the frame orientation is refined directly (20 000 templates are generated). It is useful in case of pseudo symmetry, with several closely matching orientations (set of best templates).

Unit cell: radio buttons are used to select either you already have an orientation matrix with “use current orientation matrix” (an existing cellist file from an older data processing), or if you start from scratch “use these lattice parameters”. In the latest case, indicate the expected lattice parameters.

Note: those lattice parameters are not saved!



B.2.10.c. How to proceed in PETS2

To start a new pets2 project with serial ED data, store all the collected frames in one directory even though they come from different crystals.

Open Pets2 and create a New project (File/New).

In the new window, name the project, indicate the project directory, and the project frames' directory. NEXT;

Fill information on the binning to apply, the wavelength, the calibration, the geometry, and the precession or tilt semiangle if any.

NEXT;

Figure B-33

Another window opens showing the list of frames, press OK. Frames are not expected to be a tilt series, so, we don't set angles.

As this pets2 project is created from scratch, once you are back to the main window, go into parameters and manually set a reasonable reflection diameter, the noise parameters, and the detector saturation limit. If you need to change the detector type (to remove the cross between the four quadrants of the cheetah asi detector for example), you must save, close the pets2 project and change the detector type directly in the pts2 input file.

Open PETS2 again.

Go into peak search parameters to adjust settings according to your experiment and run "peak search".

All peaks are collected as well as the d^* . At the end of this procedure, the graph showing the maximum resolution peak for each frame, as well as the graph showing the pattern center are given in the Graph tab of the Main panel (as usual).

Before going to the Serial ED command, set the Laue class in the parameters below the command "Finalize integration". Here we set 2/m.

Pull down the menu of parameters of the "Serial ED" command.

Set the parameters for the serial ED according to your data. In our example, we kept all parameters by default (Figure B-32) and we indicate the unit cell parameters as we start a new project.

Hit the command "Serial ED". The console gives the evolution of the simulation (Figure B-34).



```
Starting global orientation search
Template step: 2.0000
Template resolution: 1.0000
Laue class: 2/m
29%
```

```
Starting global orientation search
Template step: 2.0000
Template resolution: 1.0000
Laue class: 2/m
Analysing image nr. 96/ 96
Template matching finished.
```

Figure B-34

Do “Peak analysis” and go to “Find unit cell and orientation matrix” to check the 3D reconstruction and the success of the matching process. Add the centering if present and indicate the Bravais class.

Do not refine the cell now as the frames’ orientation might not be accurate at this stage.

Finish;

Go to the options in “Process frame for orientation”. Choose the intensity determination method (sum count of fit profile), set reasonable Rocking curve parameters for a first run ($RC\ width \approx 0.003\ \text{\AA}^{-1}$; *apparent mosaicity* $\approx 0.1\ \text{deg.}$) and the possibility to shift or not the integration masks.

At this stage, go to the Image data tab of the main panel, and select “si” to visualize the positions of the integration masks on the frames. The serial ED procedure might have failed to determine the orientation of some frames (usually when there are not enough reflections on the frame). In that case, remove those frames from the data reduction. To discard a frame, use the Image option panel and select “frame dialog”. Uncheck the box in front of the frames to remove from the data reduction as shown in Figure B-35.

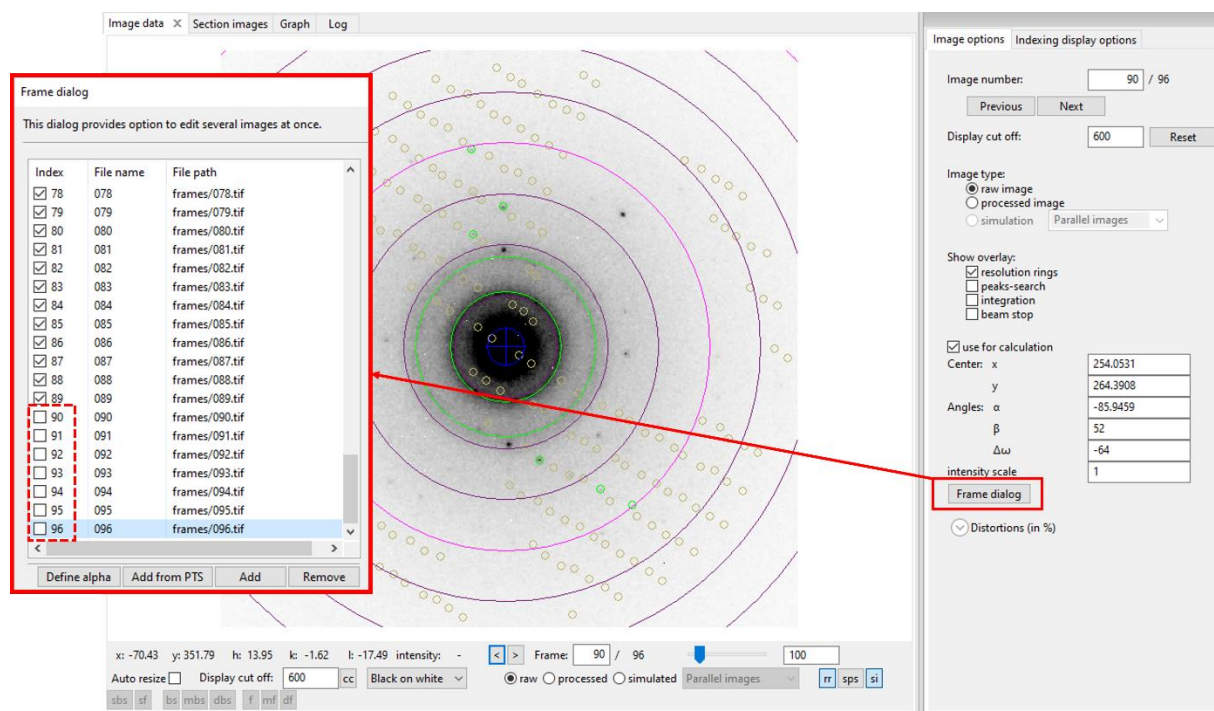


Figure B-35

Rerun “process frame for integration” without the badly indexed frames.

Adjust the reflection profile parameters as much as possible.



Pull down the menu of the command “Optimize frame geometry” and select “uniform intensities” as a simulation method and check the boxes “frame orientation angles” and “center of diffraction patterns” only. As the frames are not expected to be a tilt-series, do not use any smoothing method. The graph representing the correction of the correction angles can be chaotic and without trend.

Once the geometry is refined, process once more the frame for integration. The Rocking curves should get sharper as in the example below (Figure B-36).

To “Finalize integration” with the frame scaling, the interframe correlation range must be 0 as the frames are not a tilt-series. The scales are not correlated (see insert in Figure B-36).

The data set can be now processed as a normal tilt series data set. You can do a finer analysis, refine distortions, the unit cell or the geometry further.

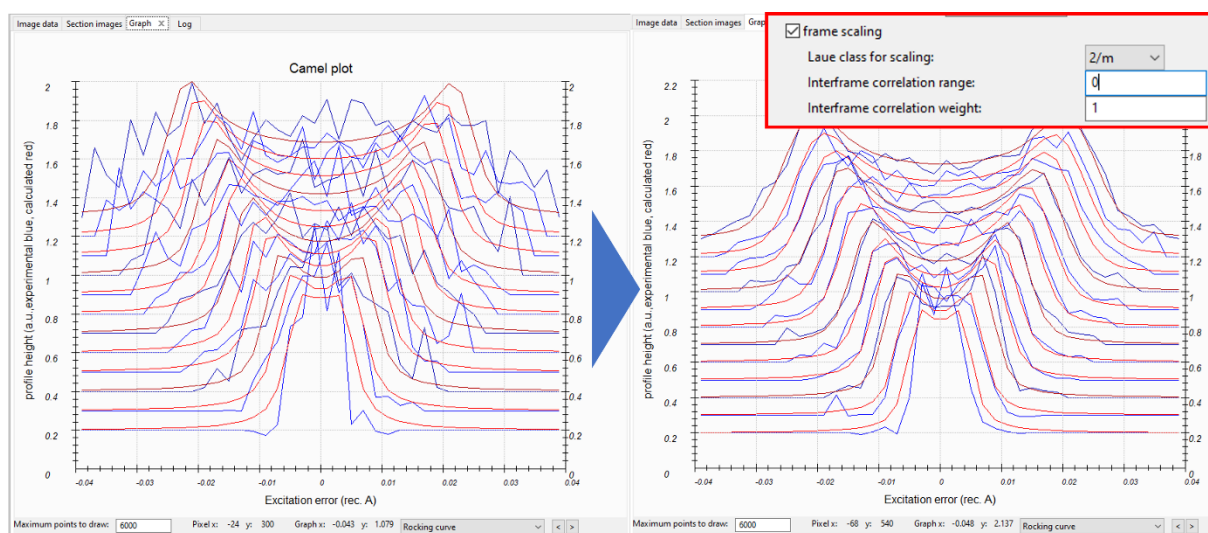


Figure B-36

B.2.11 Generate a 3D map

Hit the command to create a 3D map of the reflections with their associated intensities. Pull down the menu to adjust the pixel size and select one of the three available output file formats (Figure B-37).

The symmetry can be considered in the reconstruction according to the Laue class used for the frame scaling by checking the box.

By default, the background is subtracted from the 3D reconstruction but can be included by unchecking the checkbox. Including the background is necessary e.g. when the reconstruction is made for the analysis of diffuse scattering.

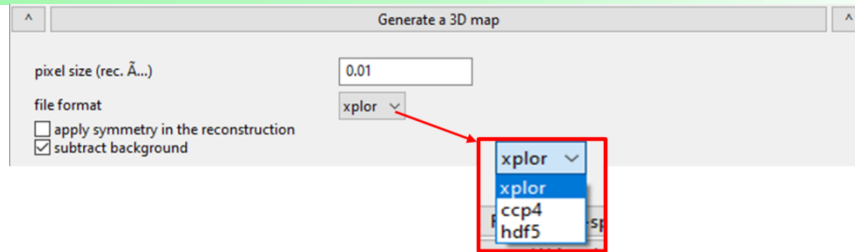


Figure B-37

B.2.12 Reciprocal-space sections

Hit the command to create the section or pull down the menu to access the options.

In this section, radio buttons are used to select:

- The **standard** set: The standard set of reciprocal-space sections is defined according to the Bravais class previously selected in the indexing section and displayed in the Status bar at the bottom of the PETS2 window. It includes all the necessary sections to determine the symmetry for a given Bravais system.
- The **user-defined** set: this option allows the user to create or modify the set of user-defined sections. The user-defined set is either the one defined by the standard set if the sections were created previously using that option or the basic set ($hk0$, $hk1$, $hk2$, $h0l$, $h1l$, $h2l$, $0kl$, $1kl$, $2kl$, $3kl$) if the sections were not created beforehand with the standard option. The sections can be displayed and edited by hitting the button “Define set”.

In the picture example (Figure B-38), the sections useful for a cubic system were first created with the option “standard set” using the Bravais class cP (cubic, P -centered). The corresponding set was written in PETS2 input file, and it became the pre-defined set.

Each user-defined section is specified by a name and nine numbers representing three vectors. The first vector lies in the section plane and will be horizontal in the section. The second vector defines the plane orientation. The third vector specifies the origin of the section plane. For example, the line “ $hk3\ 1\ 0\ 0\ 0\ 1\ 0\ 0\ 0\ 3$ ” defines a section named $hk0$, where the horizontal direction will be $1\ 0\ 0$, the second vector in the plane will be $0\ 1\ 0$, and the plane will contain point $0\ 0\ 3$.

When the option “apply symmetry in reconstruction” is checked, the missing wedge will be compensated as much as possible according to the Laue class selected in the section “Finalize integration”. Note that the Laue class will be used to create sections even if the frame scaling checkbox is unchecked to finalize the integration” (Figure B-38).

The sections are displayed in the main panel in the “Section images” tab.

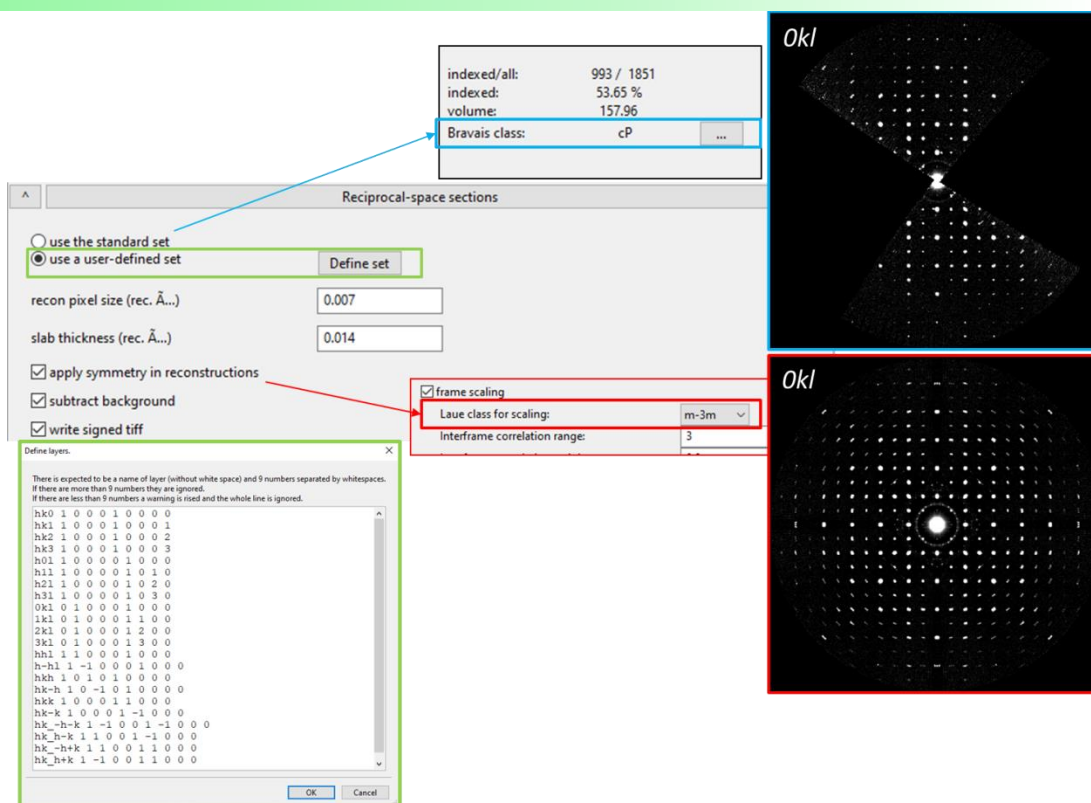


Figure B-38

Two parameters are linked to the reciprocal-space layers reconstruction. The two values are expressed in reciprocal angstroms.

- The first is the pixel size (recon pixel size) in the reconstruction.
- The second, slab thickness, is the half-thickness of the slab around the exact layer position that is projected onto the layer.

Taking a too small pixel size and/or too small slab thickness leads to “holey” reconstructions, where some pixels do not have any intensity. The default value for pixel size is equal to the value of the pixelsize keyword, default for the slab thickness is 2*pixelsize.

B.2.13 Write check files

This section is available only for development purposes and does not contain any function useful for the regular use of the program.



B.3.1.a. General frames' information of the toolbar

From left to right:

- The x and y coordinates (pixels) of the point where the cursor is placed (red area in Figure B-40).
- The corresponding h k l indexes (when a unit cell has already been defined) (red area in Figure B-40).
- The intensity of the point where the cursor is placed (red area in Figure B-40).
- The frame number/total number of frames in the data set with two arrows $<$ and $>$ to go to the previous and the next frames (in the blue area in Figure B-40).

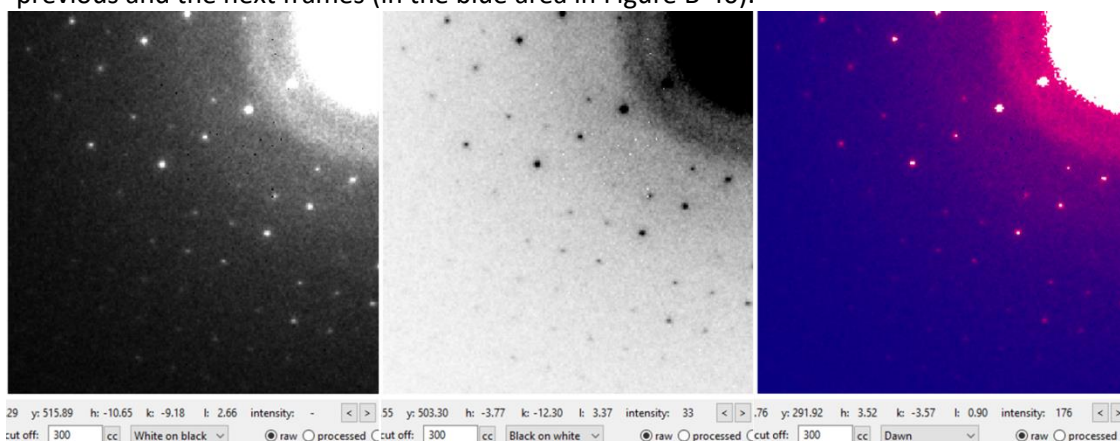


Figure B-41

B.3.1.b. General display options

- A **zoom scale** with a slider linked to a box with the zoom value (Figure B-40, blue). The slider and the zoom value are activated when “auto-size” is unchecked. The zoom can also be changed by scrolling up or down with the cursor in the Image data tab.
- “**Display cut-off**”: to change the contrast of the picture (Figure B-40, blue areas). To use the automatic cut off value, hit “cc” (= calculated cut-off) next to the “Display cut-off” value.
- Frames can be displayed using three **color modes** (Figure B-41): white on black, black on white, or dawn.

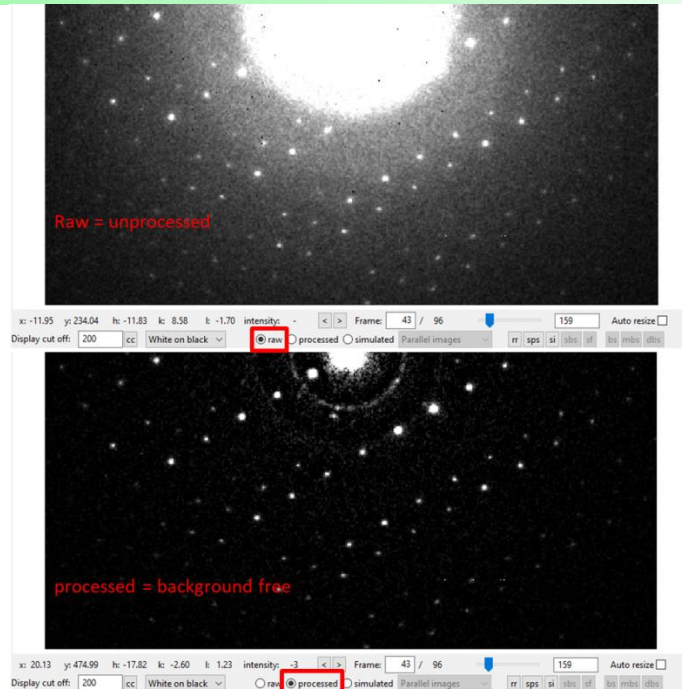


Figure B-42

B.3.1.c. Image types

Three **image types** that can be selected either with radio buttons in the toolbar of the “Image data” tab, or with radio buttons in the “Image options” tab (see yellow areas in Figure B-40): the raw images (Fig. B36 up), the processed ones (Fig. B36, down) and the simulated ones obtained after the geometrical optimizations (Fig. B37).

- **Raw images** = unprocessed TIFF files (Figure B-42).
- **Processed images** = background-subtracted images (Figure B-42).
- **Simulated images** show the calculated images during the frame-geometry optimizations (angles and center). To visualize the simulated data, the three displaying options are presented in Fig. B37.

-**Parallel images**: The processed and the simulated images are displayed next to each other (see the purple area in Fig. B37),

-**Simulation only**: The simulated frames (see the blue area in Figure B-43),

-**Combined images**: The combined view shows a superposition of the calculated and the experimental images (see the green area in Figure B-43). The green color corresponds to the calculated intensities higher than the observed ones. The pink color is the observed intensity higher than calculated ones, and the white parts correspond to the perfect overlap of both.

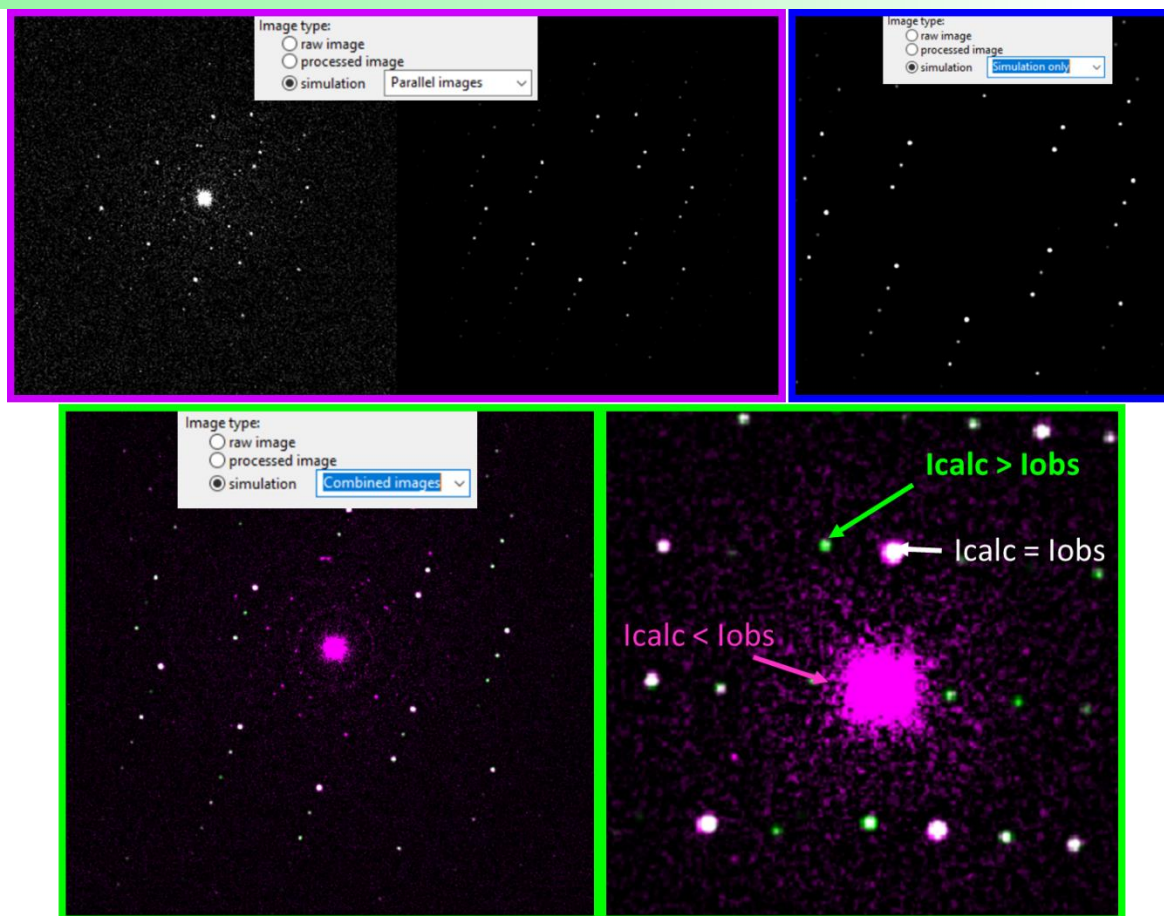


Figure B-43

B.3.1.d. General overlays accessible from the toolbar

- **rr** = to display the resolution rings on the frames (pink). The first thick ring corresponds to 1 \AA^{-1} (highlighted in pink in Figure B-40). The resolution rings can also be activated from the “Image option tab”. “rr” is also used to display the mask for ice rings (green in Figure B-35) if checked in “parameters”. In that case, green rings will appear together with the pink resolution ring (Figure B-35).
- **sps** = show peak search to display the points (green circles) where reflections are detected above the detection threshold $I/\sigma(I)$ during the peak search procedure (Figure B-44, left). The option sps is accessible via an icon in the toolbar of the “Image data” tab or via a check box “Peak-search” in the “Image options” tab.
- **si** = show integration to show the integration masks (Figure B-44, right). For each frame, the reflection positions are predicted using the current orientation matrix, the centering, and the profile parameters. Then, the intensity at each predicted reflection position is determined. During the process, PETS2 shows an image in the processing (si) of each frame with an overlay of circles (green or brown). A circle means the reflection is integrated and the circle is green when the reflection intensity is significant (for $I > 3\sigma(I)$). You can use the icon “si” at the bottom of the Image data tab or the check box “integration” in the “Image option tab”.

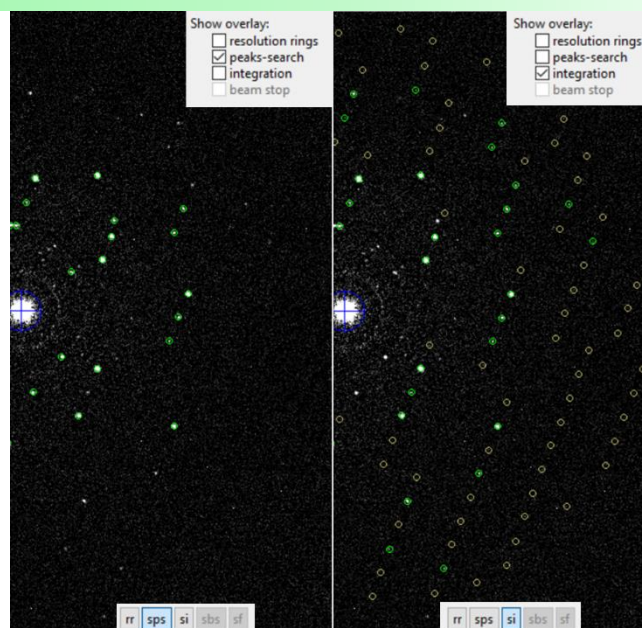


Figure B-44

B.3.1.e. Specific Friedel pairs overlays to define manually the pattern center

The Friedel pairs overlays are activated in the toolbar when the “Automatic initial direct beam coordinates” box is unchecked in the Options of the “Peak search” command. Drawing Friedel pairs is a help to manually determine the center with reasonable accuracy.

- **sf** = show defined Friedel pairs: activated when the automatic detection of the center is unchecked.
- **f** = define Friedel pairs. Hit “f”, and then use the cursor to select pairs of reflections either by clicking on both or by clicking on the first one and then dragging the cursor toward the second point (Figure B-45). You can define as many pairs as wanted to make the center determination more accurate.
- **mf** = move one Friedel point. This option helps to correct the position of the points (see Figure B-45). Click on the point to move on and drag it to its new position.
- **df** = delete Friedel point. To delete one or several Friedel point(s), select an area to remove, as shown in Figure B-45.



Several options are specifically related to the Beam stop in the toolbar.



- 45



- **bs** = create a new beam stop. When BS “yes” is selected in the “Parameters” options (commands panel) without a loaded file with the BS coordinates, you can manually define a BS through the Image data panel options. In Fig. B40, first Press bs to activate the creation of a new BS (step A), and click on the frame to create as many points as needed to describe the mask’s shape (B, C, D). The x and y coordinates of each point are stored in the pts2 file.
- **mbs** = move the beam stop. Hit the icon and move the beam stop mask by clicking directly on frame and dragging the BS to its new position (Figure B-47, left).
- **dbb** = delete beam stop. Delete a few points or all the beam stop by selecting the area to delete (Figure B-47, right).

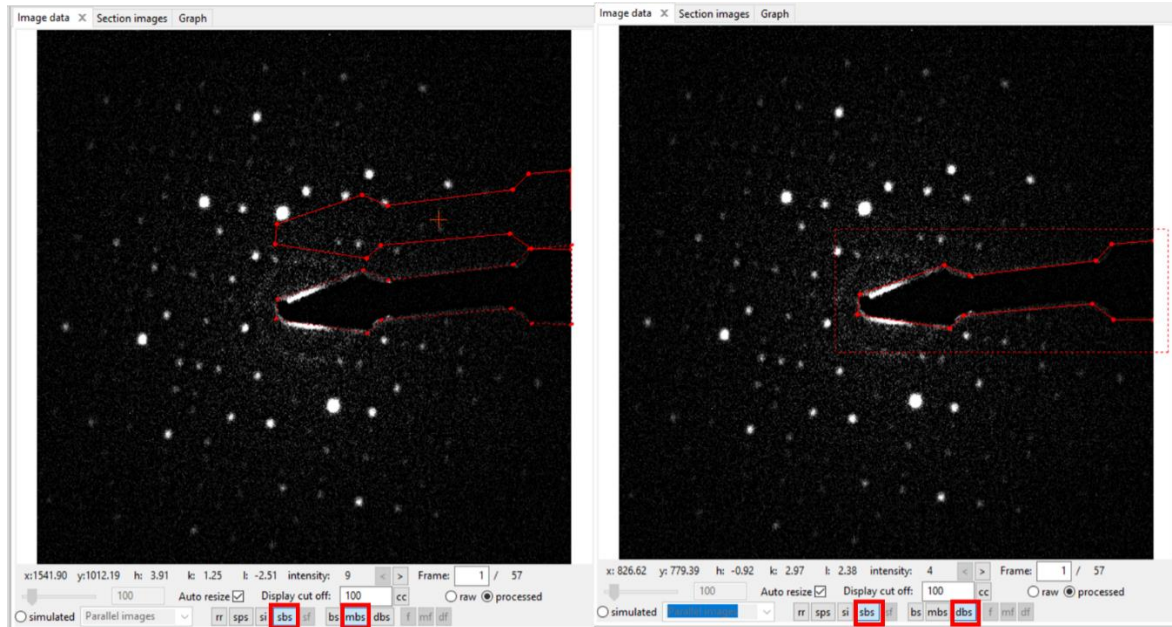


Figure B-47

B.3.2 Section images

The “Section images” tab contains sections of the reciprocal-space reconstructed after hitting the command “reciprocal-space” sections.

At the bottom of the tab there is a pull-down menu to select the section to display (Figure B-48, left), the **cut-off**, the **zoom** (automatic or not) and the coordinates expressed either with the x and y (pixel) or with the *hkl* indexes.

The icon **gr** = grid displays the lattice as an overlay on the sections.

By placing the cursor on one reflection (red arrow in Figure B-48, right), its *hkl* indices and its corresponding intensity are given in the information bar (red area in Figure B-48, right).

As for the main panel, the cut-off can be adjusted and applied to all sections by hitting “apply to all sections”.

The command “**save sections**” will save all sections simultaneously in png format considering the current cut-off value. Those sections are stored in a folder `jobname_petsdata\sections\png`.

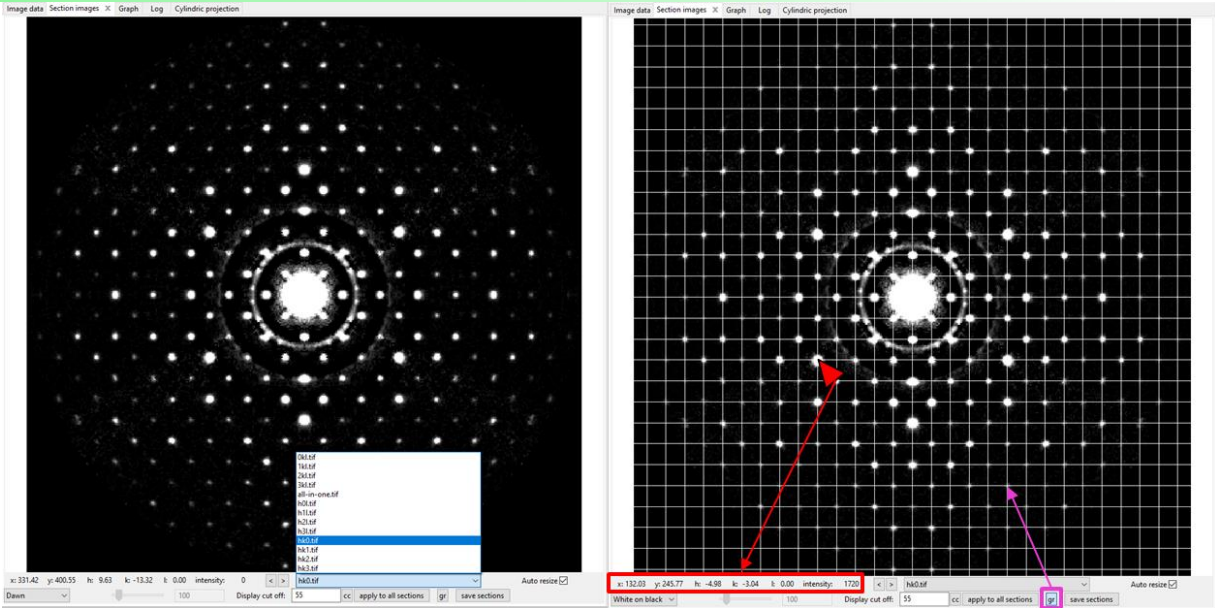


Figure B-48

B.3.3 Graph tab

All the Graphs produced during the data processing are given in this tab.

Below is a list of all graphs generated by PETS2 during the data reduction. To go from one graph to another, use the drop-down menu located at the bottom of the Graph tab or the arrow on the right of the menu (see Figure B-49).

Graph	Corresponding step
Peak search: pattern centers	Peak search
Peak search: Maximum resolution	Peak search
Peak analysis: In-plane distances	Peak analysis
Peak analysis: 3D distances	Peak analysis
I/sigma in two shells	Process frames for integration
Rocking curve	Process frames for integration/
	Optimize reflection profile and geometry
Integration: Resolution	Process frames for integration
Frame scales	Finalize integration
Normal probability plot	Finalize integration
Tilt corrections	Optimize reflection profile and geometry
Origin corrections	Optimize reflection profile and geometry
Frame-by-frame distortions	Optimize reflection profile and geometry
Profile parameters	Optimize reflection profile and geometry

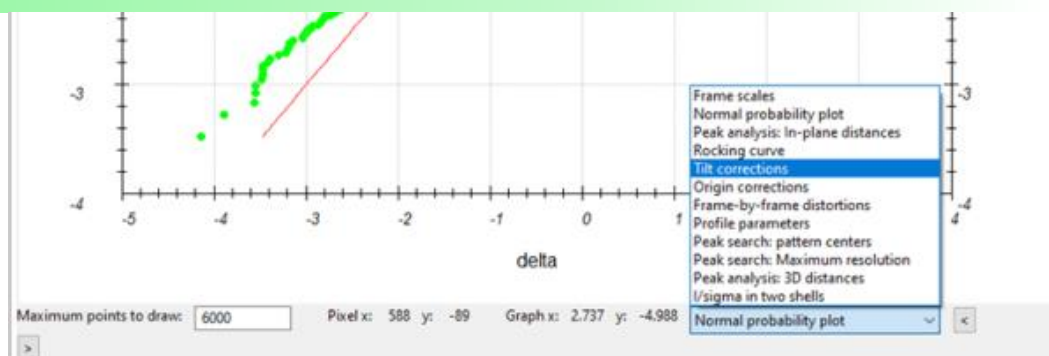


Figure B-49

Note: At this stage of the software development, graphs are available in the Graph tab as long as the PETS2 project is open. When an older PETS2 project is re-opened, some graphs can easily be regenerated (the RC curves, the cylindrical projection with the “replot” button). However, most of them are lost until the corresponding step is re-run. The detail of the previous data processing with the corresponding graphs is anyway given in the log files.

TIPS:

- To save an image the graphs, click right on the Graph tab you want to save and select **“Save graph as....”**.
- To report a bug related to the display of the graphs, click right on the graph and select **“Print debug info to console”**. The information generated in the console panel will only be useful for the developers.

B.3.3.a. Peak search: pattern center

This graph shows the x and y shift of the direct beam frame-by-frame with respect to the initial value of the center (determined automatically or manually) (Figure B-50).

The x (red) and the y (green) shifts are represented in pixels.

This graph is produced during the Peak Search procedure.

To see to what frame and or value corresponds to one point of the graph: place the cursor on the point of the graph; its x = frame number and y = shift value are given below the graph in the information bar (see example in Figure B-50, left).

B.3.3.b. Peak search: Maximum resolution

This graph (see Figure B-50, right) reports for each frame, the peak with the maximum resolution found above the detection threshold during the peak search procedure (I/sigma). This graph helps to have a quick overview of the data resolution frame-by-frame, the possible decay of the crystal, the thickness evolution, etc. It depends on:

- The data resolution.
- The d* max (data processing resolution) sets for the peak search (here the default value 1.4 \AA^{-1}).
- The I/sigma value (5 in that example).



Figure B-50

B.3.3.c. Peak analysis: in-plane-distances/3D distances

See section B.2.4.

In the first step, all reflections measured on subsequent frames are clustered, and the centers of the clusters are used instead of individual peak positions. For this step, the limit for the clusters must be determined. Next, the program shows a plot of inter-peak distances sorted from the shortest to the longest to check that the program did it correctly (Figure B-51, left). If everything works fine, you should see a clear jump in the distances (red curve in the plot) accompanied by a peak in the derivative (green curve in the plot).

In the next step, PETS2 calculates the difference vectors between the peaks. Then the same clustering procedure is applied to the group of difference vectors, and again a plot of distances is shown for checking the correctness of the choice. The jump in the second plot is usually even sharper than in the first plot (Figure B-51, right), unless the data contain signal from more than crystal, in which case the second plot may be rather fuzzy without clear sharp peaks.

On each graph the blue line is the limit for detecting a significant increase in the derivative line. Thus, the first intersection of the blue line with the green line is the point from which the algorithm detects the onset of the first jump. The light blue vertical line is the position in the distance ranking then defines the limit for the clustering - this is the most important line that really defines the limit for the clusters. It is this line that you can change by clicking in the plot. The horizontal purple line is placed at the intersection of the vertical light blue, and the red curve, and it shows on the y axis the distance threshold that is used for the clustering.

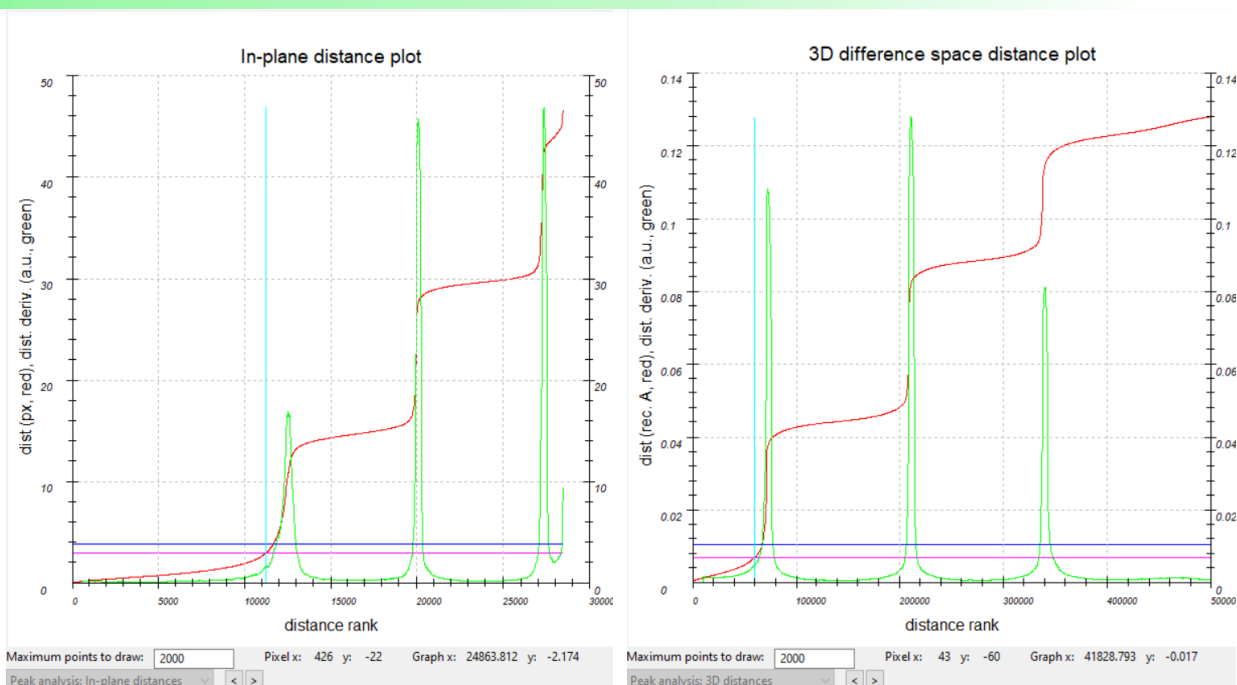


Figure B-51

B.3.3.d. I/σ in two shells

For each frame, this graph shows the mean $I/\sigma(I)$ of what are called the inner (red curve) and the outer shells (green curve) (Figure B-52). The shell below d^* integration*threshold is considered the inner shell (by default, threshold = 0.5 \AA^{-1}). The default limit between inner and outer shell for the calculation of average I/σ can be changed in the input PETS2 file after the keyword “resshellfraction”. It does not influence the integration steps but is a way to visualize the attenuation of the resolution. The graph is created during the “process frame for integration”.

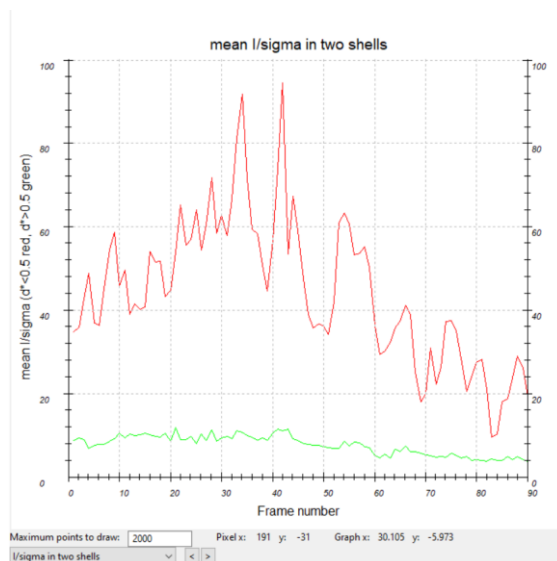


Figure B-52



B.3.3.e. Resolution graph

The “Integration: Resolution” graph: for each frame the length of the maximum diffraction vector (d^* in reciprocal Å) is given for 2σ (red in Figure B-53), 3σ (green in Figure B-53) and 5σ (blue in Figure B-53). This graph is the easier way to follow the resolution decay in the data set. The graph is created during the “process frame for integration”.

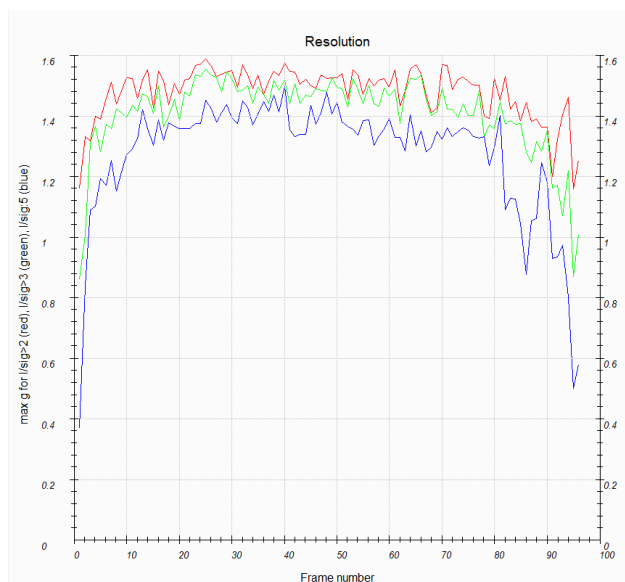


Figure B-53

B.3.3.f. Rocking curves

At the end of the integration process, the camel plots (rocking curves profiles) are displayed (data/ experimental - blue, fit/ calculated - red) (Figure B-54). Because of the specific shape (one or two humps), the curve is called the “the camel” and the plot of rocking curves is “the camel plot”. On the horizontal axis of the plot is the excitation error of the reflections (i.e., the deviation from perfect Bragg condition). Each curve shows an average rocking curve of reflections in one resolution shell, starting from 0.2-0.3 Å⁻¹ in steps of 0.1 Å⁻¹. Notice the splitting of the humps for precession data ((Figure B-54, right). The splitting will increase with the increase of the precession angle. For continuous rotation or static frame experiments, the camel plot shows a single hump ((Figure B-54, left).

Three parameters found in the section “Optimize reflection profile and geometry” (inset in the figure B47) will directly influence the quality of the fit (red): The rocking curve width, the apparent mosaicity, and what is called the precession or tilt semi-angle. On the other hand, the minimum $I/\sigma(I)$ and the step size in the reflection profile are two display parameters that won’t influence the quality of the fit and the integration result.

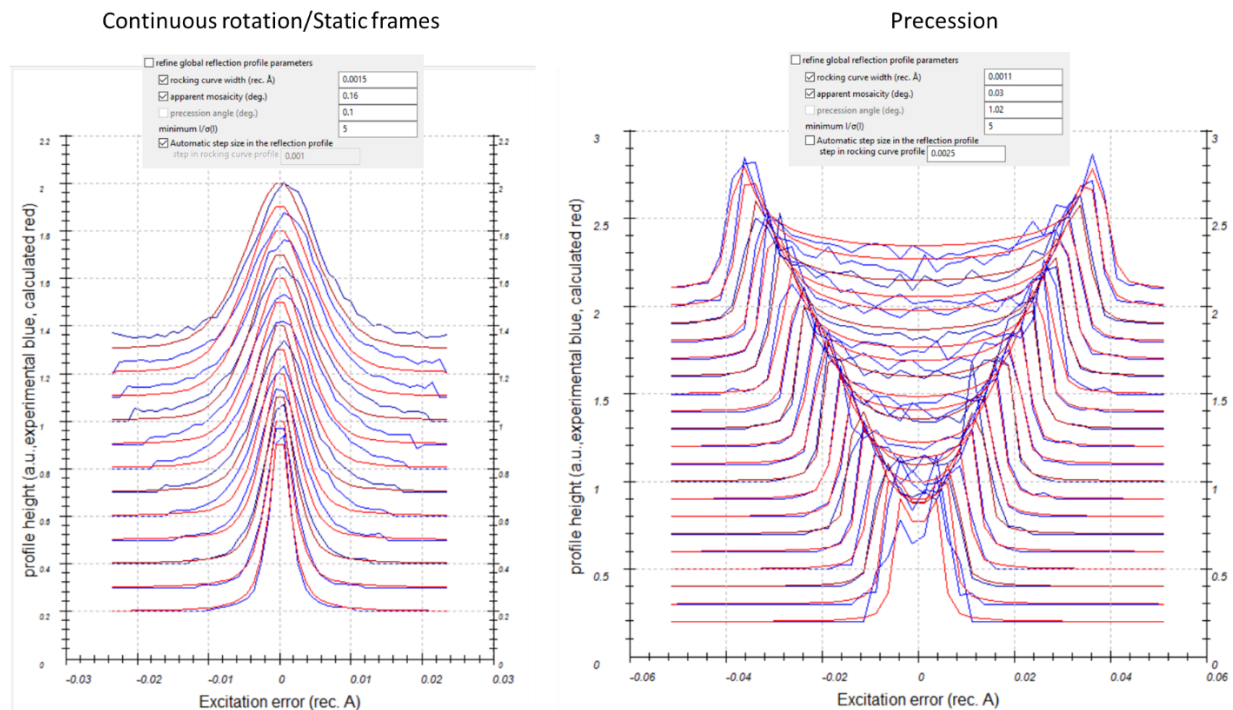


Figure B-54

B.3.3.g. Frame scales

When the integration is “Finalized”, a scaling can be applied for the kinematical hkl files. The graph represents the scale applied for each frame and will appear only when the checkbox “frame scaling” is selected in the section “Finalize integration” (Figure B-55).

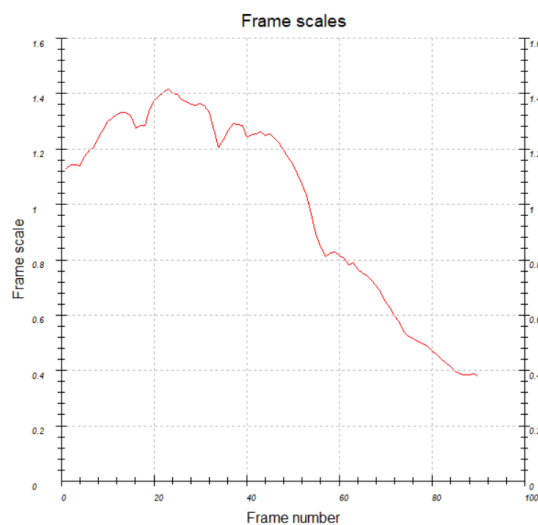


Figure B-55

B.3.3.h. Tilt corrections and origin corrections

These two graphs are produced during the frame geometry optimization (Figure B-56).



In Figure B-56, on the top is the frame-by-frame corrections in degree (Δ angle) applied to the three orientation angles: Δ alpha (red), Δ beta (blue) and Δ omega (green).

A smoothing of the curve can be applied during the optimization to avoid outliers. In that case, the smoothed curve appears with a brighter color than the initial calculated one.

The frame-by-frame corrections of the center of the pattern is expressed with its two Δx and Δy coordinates in pixels (Figure B-56, right).

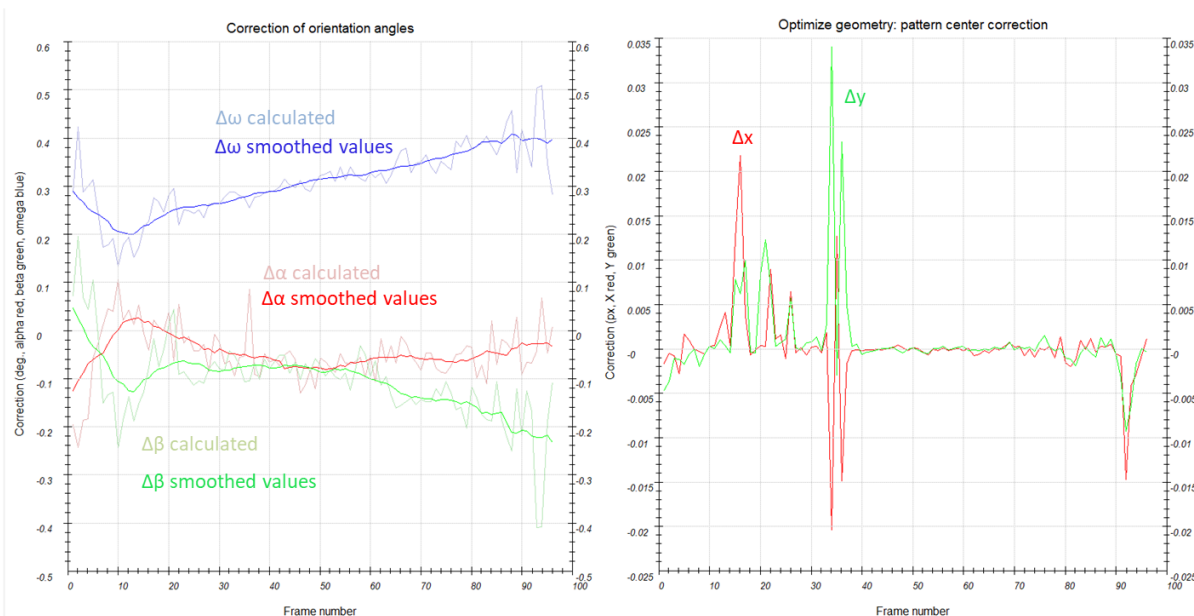


Figure B-56

B.3.3.i. Frame-by-frame distortions

The distortions that are refined frame-by-frame are summarized in a graph where the x-axis is the frame number and the ordinate will depend on the type of distortion (see Figure B-57, left).

- The red curve indicated as “scale” in percent is called “magnification” in the standard mode of the distortion.
- The green curve is the amplitude of the elliptical distortion in percent (elliptical amplitude in the standard mode)
- The blue curve corresponds to the phase of the elliptical distortion expressed in degrees and divided by 100 to match the graph scale of other distortions.
- The magenta curve is the amplitude of the parabolic distortion in percent.
- The blue curve corresponds to the phase of the parabolic distortion expressed in degrees and divided by 100 to match the graph scale of other distortions.

Note that for each frame, the exact value of the distortions refined frame-by-frame can be found in the Image option tab for the corresponding frame number. The other types of distortions are not displayed in a graph as they are not refined frame-by-frame but only globally (see the “Refine” menu of “Find unit cell and orientation matrix”, section B.2.5).



To enable the frame-by-frame distortions refinement: check individual boxes corresponding to the distortions that need to be refined. The last parabolic ones (amplitude and phase) should be selected only for very good data sets (Figure B-58).

When “Replace global distortions” is selected, the average values obtained from the frame-by-frame refinement will replace the global ones determined previously when the unit cell is refined. It is especially useful when the global magnification is off which is visible when the red curve does not cross zero (Figure B-57).

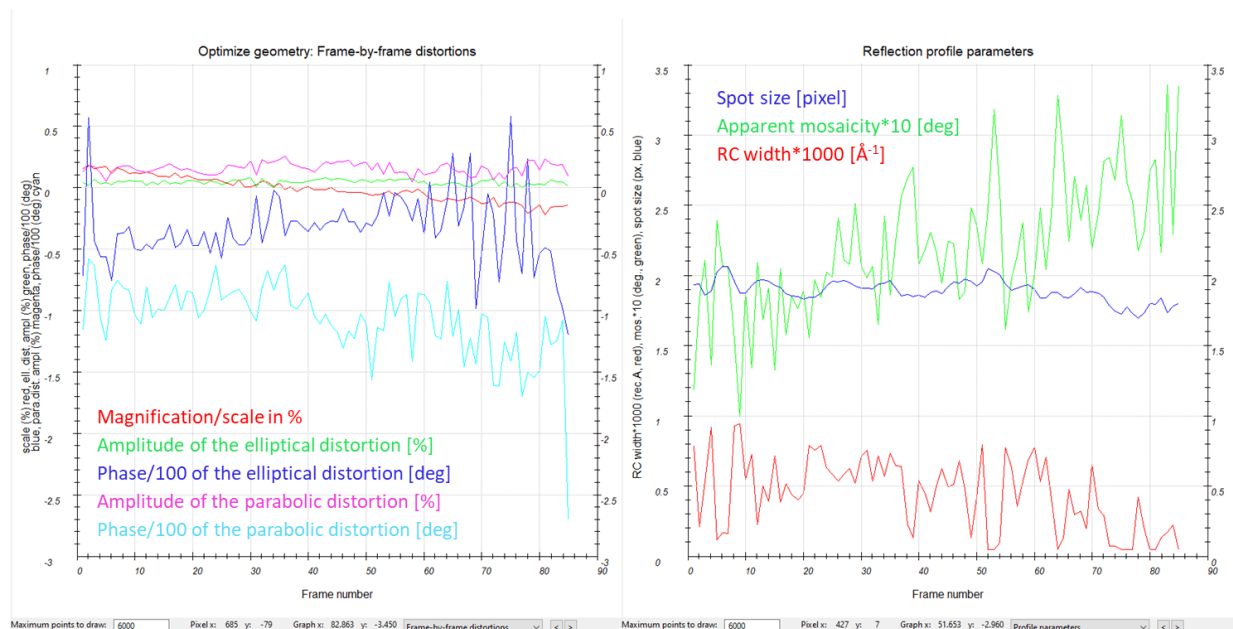


Figure B-57

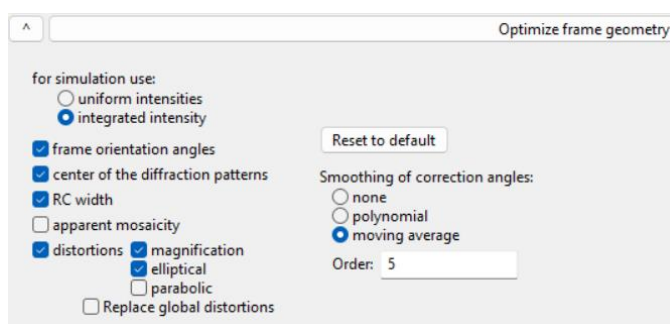


Figure B-58

B.3.3.j. Profile parameters

The rocking curve profile parameters and the average spot size refined frame-by-frame are given in the graph below (Figure B-57, right).

B.3.3.k. Normal probability plot

This graph is produced during the “finalize integration” step. It shows the distribution of $\sigma(I)$ with a histogram and a normal probability plot. On the histogram and the plot, the pink Gaussian and the red line represent the perfect Gaussian distribution. The blue histogram and the green dots are the $\sigma(I)$



distribution observed in data (Figure B-59). Dark red dots in the normal probability plot indicate points labeled as outliers by the outlier rejection algorithm.

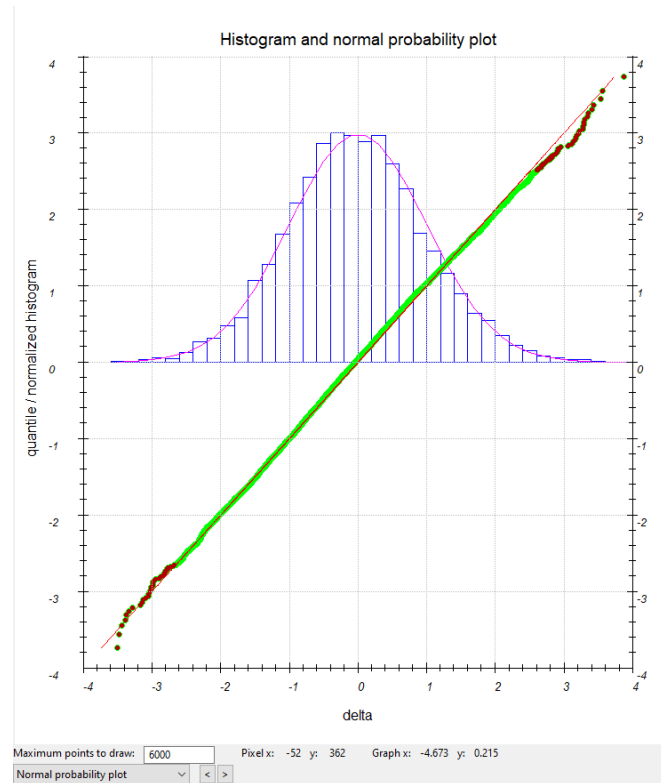


Figure B-59

B.3.4 Cylindrical projection

This tab of the main panel shows only the cylindrical projection that should be the sharpest for the right tilt axis position or omega angle (degree) (Figure B-60). The value of the omega angle can be changed and the cylindrical projection replot in the “Tilt axis” section of the command menu. Below are two examples of such plots. The first one is made with the refined omega and the second with an omega off by 10 deg.

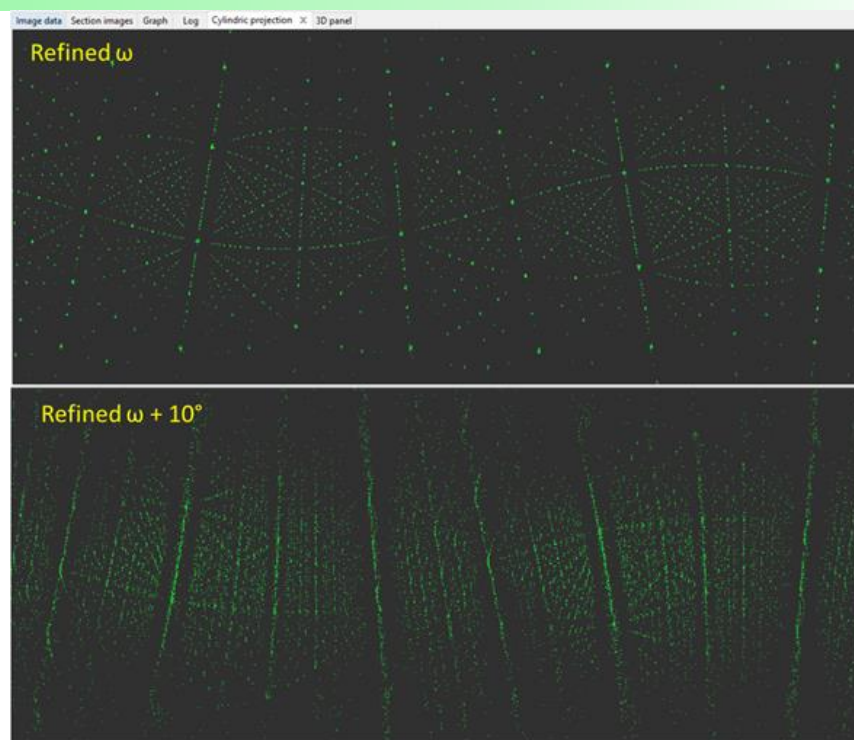


Figure B-60

B.3.5 Log files

Several report files are produced in the html format and can be shown and selected in the log tab of the main panel (Figure B-61). They usually merge information given in the console with the related graphs and used settings. A drop-down menu and the arrows < and > are used to select the log. They are stored in the subdirectory `jobname_petsdata/logs`. Two versions of each file are saved. Pure text file, and a html version with embedded images. The graphs used in the logs are also saved in subfolder `jobname_petsdata/plots`. The table below contains a brief description of each log file.

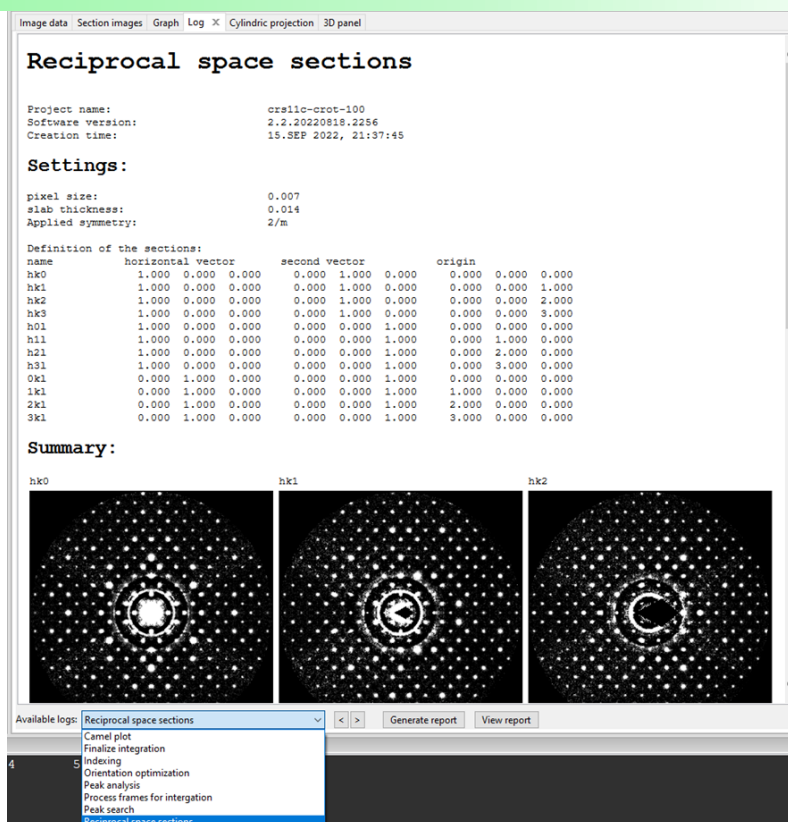


Figure B-61

Log file extension	description
logcml	Camel plot profile + relevant parameters
logfi	Process frames for integration's report: -settings with the cell dimensions, Rocking curve profile parameters, intensity determination method, -a summary with the number of frames used, the min/mean/max resolution etc., number of integrated spot and how many could be fitted with the method. -list of the frames with the number of peaks and the max resolution.
logoo	Frame orientation optimization -settings list -Four graphs related to the geometry optimization of the frame: tilt angles, pattern center, frame-by-frame distortions, and frame-by-frame profile parameters. -Details for each frame with the values of all refined parameters
logpa	Repot for the Peak analysis -Mostly the two graphs and values obtained during the clustering procedure.
logpfi	Report of the Finalize integration step: -the settings used -Graphs for frame scales and histogram and normal probability plot. -the statistics for each Laue class (<i>Rint(obs)</i> and <i>Rint(all)</i> , <i>Rmeas(obs)</i> and <i>Rmeas(all)</i> , <i>Nobs/Nall</i> and redundancy).



	-the statistic for the selected Laue class by resolution range (d^* and d -ranges, $Nobs/Nall/Nthr$, completeness, redundancy, $I/\sigma(I)$, $Rint(obs)$, $Rint(all)$ and $CC1/2$) -the frame scaling frame-by-frame (graph and list).
logps	Peak search report: -settings used and summary -graphs: pattern center from the peak search and maximum resolution graph -list frame-by-frame of the peak search results.
logrss	It corresponds to the report for the reciprocal sections with: -parameters used to build sections -list of the sections with their vectoral definition -pictures
logindex	Indexing report -settings -Details for the active unit cell -Global distortion values

B.3.6 3D panel

The 3D panel displays the 3D reconstructions of the reciprocal space (cor, xyz, clust, or diff files). It is activated with the “Find unit cell and orientation matrix” menu together with the “Indexation display options” tab of the Option panel (see description in the next section B.4).

- The type of reconstruction displayed (the cloud) is selected from the header of the Indexing panel (clust in the example of Figure B-62). On the bottom and the left side of the 3D panel are the intensity histograms (blue in Figure B-62) that can help to set a specific direction.
- To do an in-plane rotation of the cloud, put the cursor out of the cloud area and click + rotate (with the cursor out of the area defined with the green circle in Figure B-62).
- To rotate in the 3 dimensions, click with the cursor inside the cloud area (red cursor, inside the circle in Figure B-62).
- The axis-base at the bottom left of the 3D panel can be changed using the Options panel (laboratory axes, reciprocal axes, or direct axes).
- To zoom in/out, use the mouse wheel in the 3D panel or use the +/- buttons at the bottom left of the 3D panel tab.
- To change the color settings, go to Edit\Settings in the main toolbar.

All other possible actions influencing the 3D reconstruction are presented either in the section related to indexing or the section about the Option panel\Indexation display options.

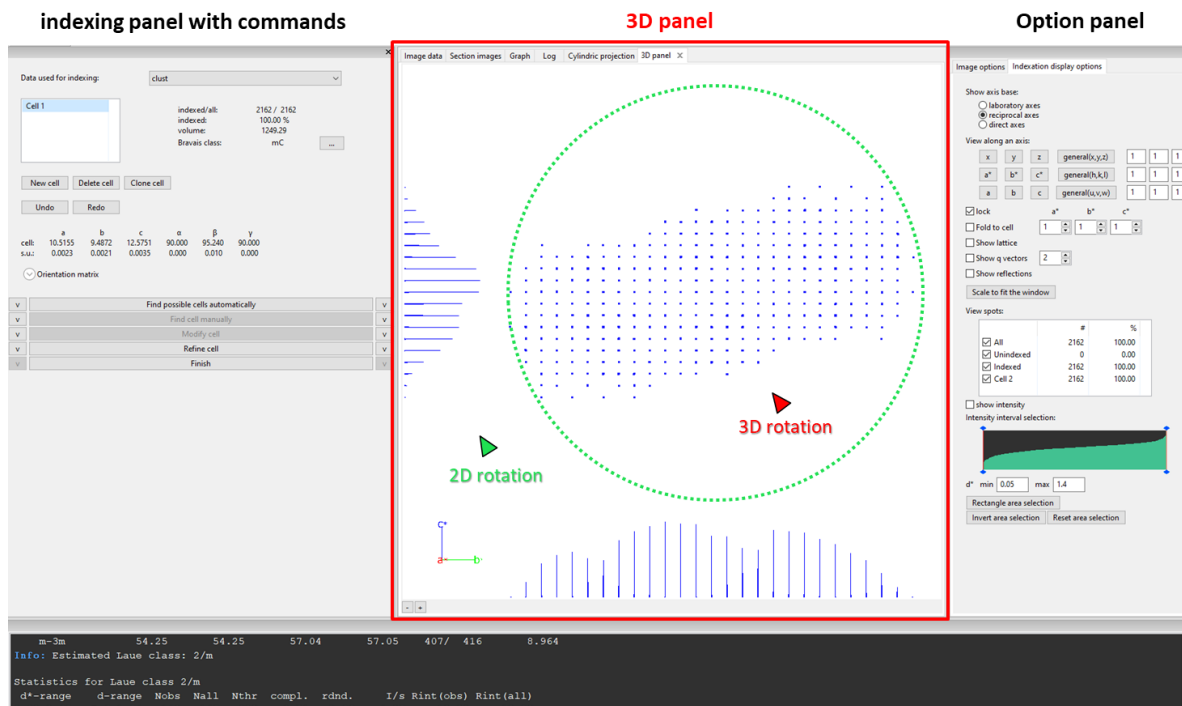


Figure B-62

B.4. Options panels

With two tabs: Image options and Indexation display options.

B.4.1 Indexing display options tab

The “Indexation display options” tab is activated when the menu “Find unit cell and orientation matrix” is opened and it influences the display of the 3D reconstruction of the 3D panel (Figure B-62).

B.4.1.a. Axis bases

Select one of the options to display the axis bases (laboratory axes **xyz**, reciprocal axes **$a^*b^*c^*$** , or direct axes **abc**) at the bottom left of the 3D panel (Figure B-63).

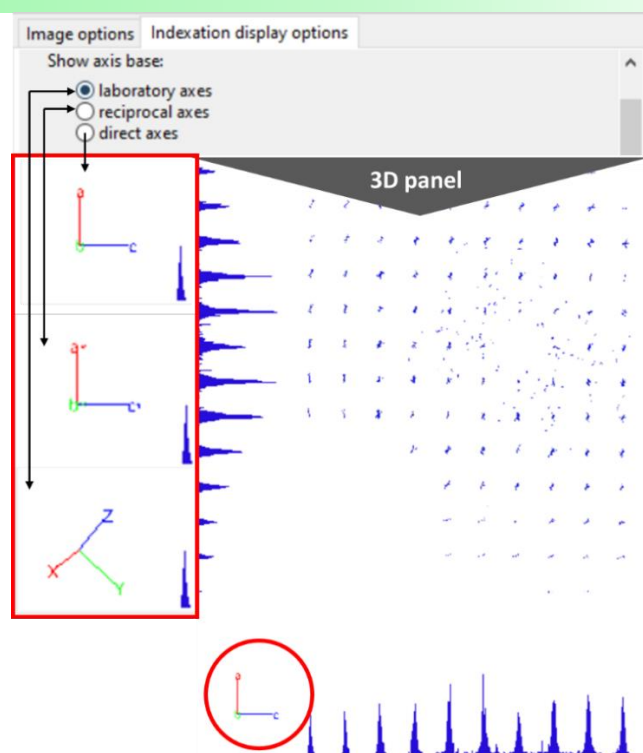


Figure B-63

B.4.1.b. View along an axis

To change the direction of the 3D reconstruction (in the 3D panel), use the buttons of the Options panel as shown below in Figure B-64. You can select the main directions or define a general one.

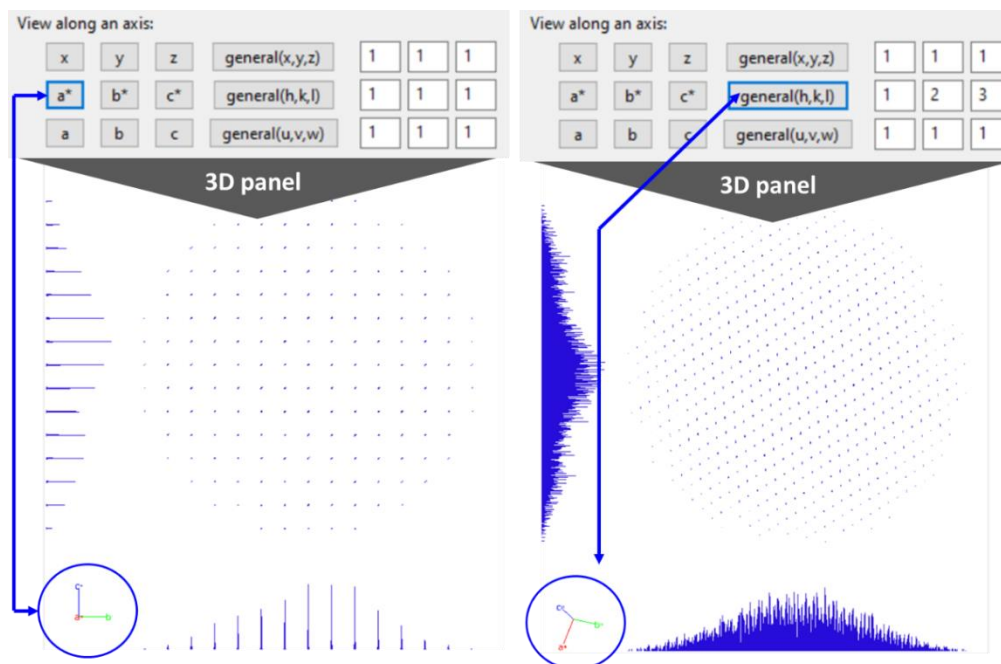


Figure B-64



B.4.1.c. Unit cell display options

- Show lattice: check the “Show lattice” to display the lattice as an overlay on the reconstruction. The unit cell overlay can be manually extended along a^* , b^* and c^* by changing the value as shown in Figure B-65 (right).
- Fold to cell: check the option “Fold to cell” to project all the 3D reconstruction into a certain number of unit cell units. The number of unit cells in which the 3D reconstruction is folded along a^* , b^* and c^* can be changed manually by changing the value as shown in Figure B-65 (right).
- Lock: Check the lock box to apply the same parameters to fold the cell and display the lattice overlay (see Figure B-65, left).

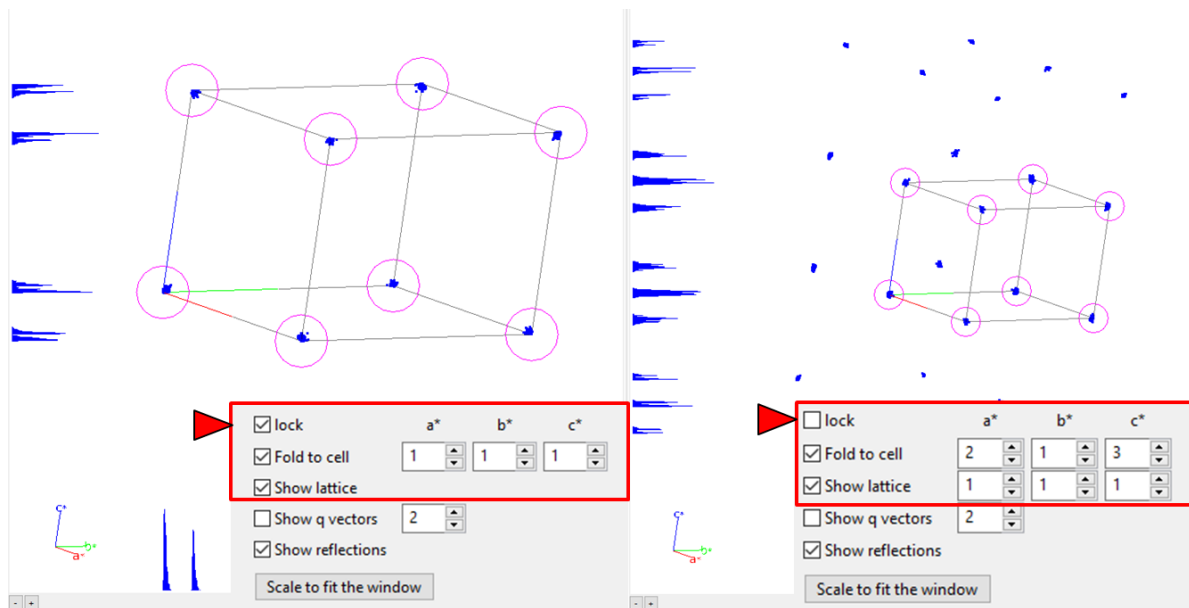


Figure B-65

- Show reflections: main and satellite reflections:
 - Check the option “show reflections” to display circles (purple in Figure B-65) on the main reflections. The diameter of the circles depends on the value of the maximal d^* difference for indexing (\AA^{-1}).
 - For modulated structures (Figure B-66), once one or more modulation vectors are defined, the satellite reflections can be displayed up to a given order (order = value next to the option) by checking the option “Show q vectors”. For more than one defined modulation wave vector, the combined q wave vectors will also be displayed (q_1+q_2 , q_1-q_2 , etc..).

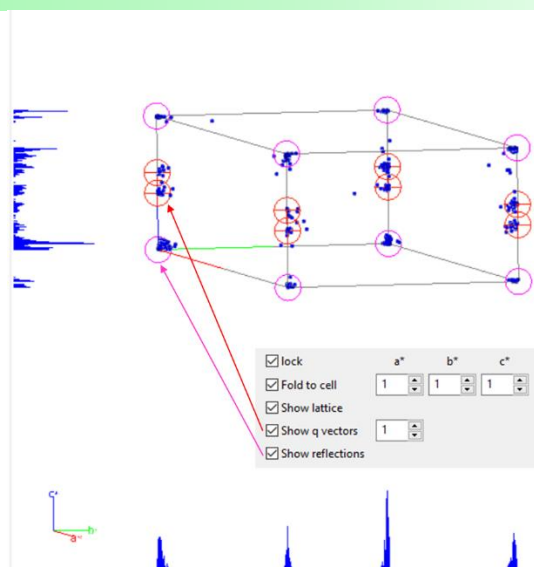


Figure B-66

- Scale to fit the window: rescale the view to match the window size (Figure B-67).

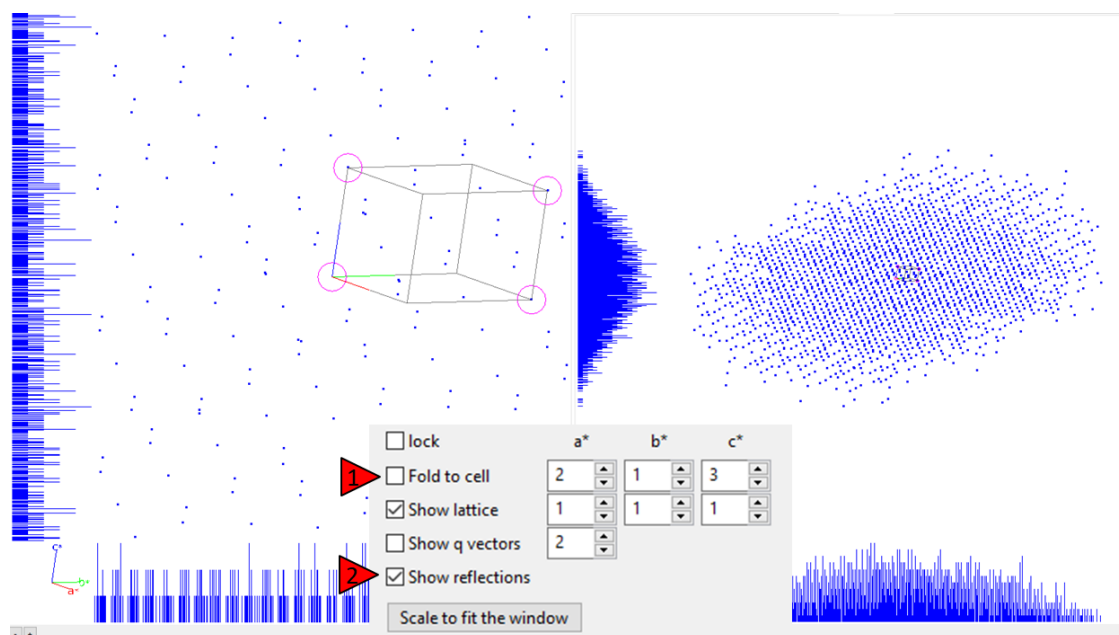


Figure B-67

B.4.1.d. Cloud display options

- View spots: Selection of the visible spots

By default, all the checkboxes in the section “View spots” are checked (see the middle of Figure B-68), meaning that all the reflections for a specific 3D reconstruction are displayed. To apply a selection to the reflections depending on their indexing, use the checkboxes as shown below (Figure B-68). In that example, only one cell (Cell1) is present because only one cell was defined. The list will contain as many cells as the user specifies.

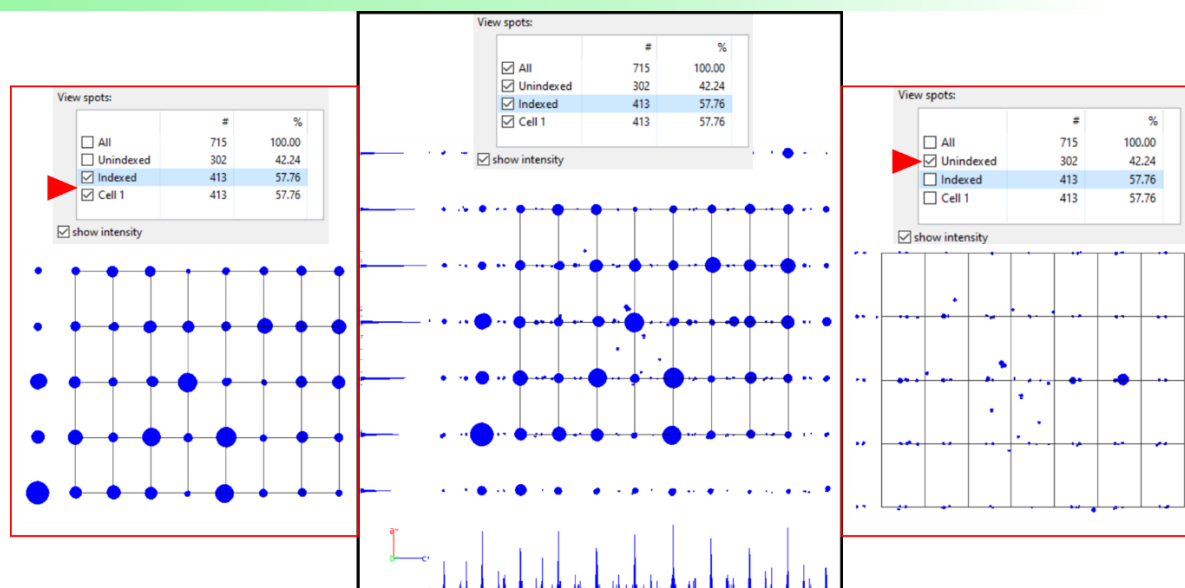


Figure B-68

➤ Show intensity of the reflections

Check the box “show intensity” to display the reflection with variable radius corresponding to their intensity (Figure B-69).

The intensity pattern might look different on the cor/xyz 3D reconstruction and the clustered files (clust and diff).

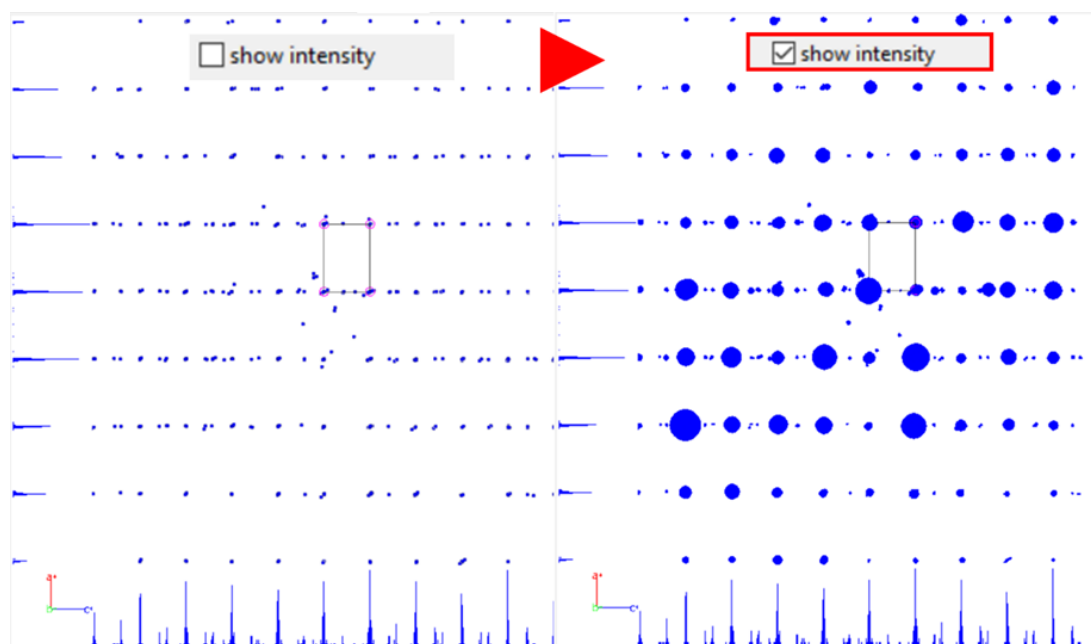


Figure B-69

➤ Intensity interval selection

To skip the weakest/strongest reflections, move the left/right slider on the intensity distribution histogram (see Figure B-70, left).



By default, the resolution range is defined from the d* min and max values used for the peak search in the “Parameters” of the commands panel (by default: from 0.05 to 1.4 Å⁻¹). To remove low-resolution or high-resolution reflections in the 3D cloud, change the values for d*min and d*max as shown in the right panel of Figure B-70.

-Rectangle area selection: to select reflections within a rectangular area of the 3D cloud (e.g., to select only one reciprocal-space layer), hit the button “rectangle area selection” and go to the 3D panel to drag the mouse to define the area (see red area in Figure B-71). The 3D panel will only display the selection (Figure B-71, middle).

-Reset area selection: to go back to the complete 3D cloud.

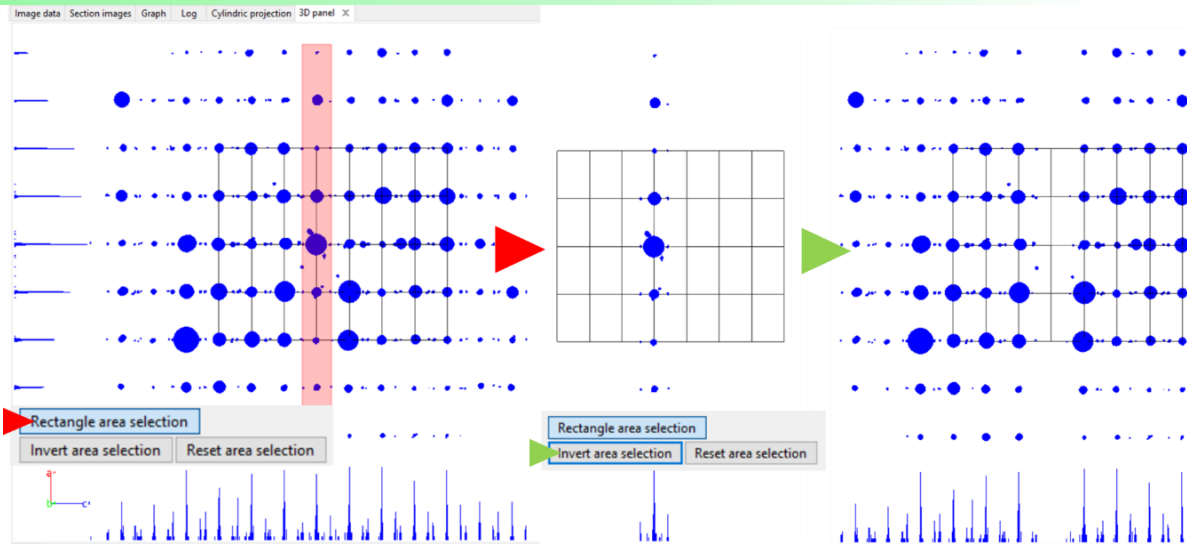


Figure B-71

B.4.2 Image options tab

All the options shown below will affect the Image tab of the Main panel, and some of them are also accessible at the bottom of the Image tab. Most of them were described previously in the “Image tab” section (section B.3.1).

B.4.2.a. General options

The general options are the image number that can be changed by hitting previous or next or changing the value of the frame (orange area in Figure B-72), the display cut-off (yellow), the image type (blue) and the possible overlays (pink) selected with radio buttons. All those options are defined previously in the Image tab section.

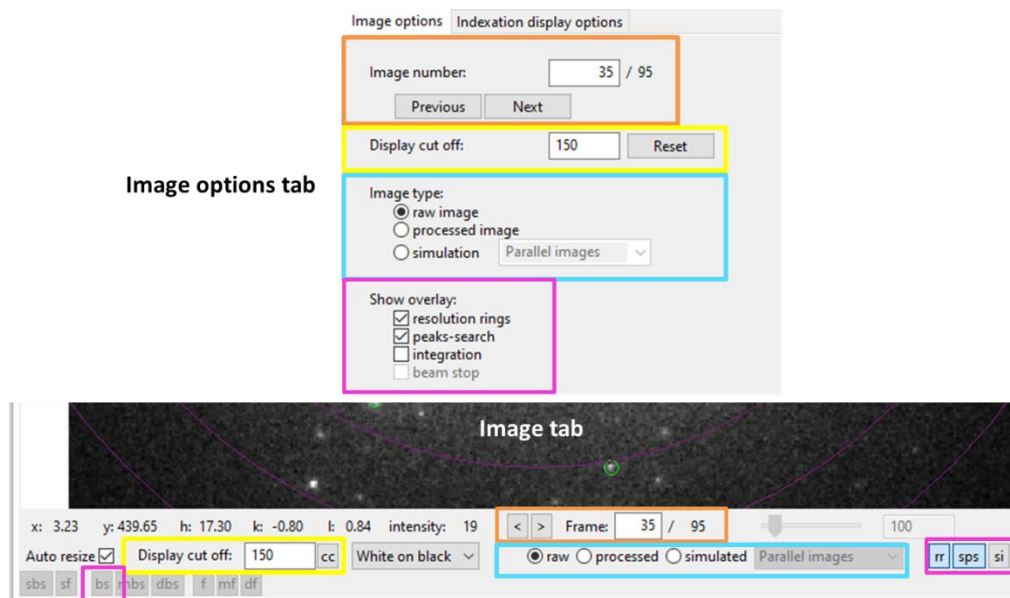


Figure B-72



B.4.2.b. Single frame options

The second part of the Image options tab is frame dependent (Figure B-73).

For each frame (= Image number selected above), the visible options are:

- A checkbox indicates if the selected frame is included in the calculation/data reduction.
- The x and y coordinates of frame's center,
- The tilt-angles (alpha, beta, $\Delta\omega$),
- The intensity scale,
- The distortions that can be refined frame-by-frame.

<input checked="" type="checkbox"/> use for calculation		
Center: x	254.1713	
y	264.4643	
Angles: α	-10.5563	
β	-0.0787	
$\Delta\omega$	0.0015	
intensity scale	1.2898	
<input type="button" value="Frame dialog"/>		
^ Distortions (in %)		
magnification:	0.1161	
elliptical amplitude:	0.0377	phase: 40.3139
parabolic amplitude:	0.301	phase: -80.648

Figure B-73

The **frame dialog button** (Figure B-73) opens the menu as shown in Figure B-74. This dialog provides options to edit several frames at once. This window was introduced in Sections A.4.1 and B.1.2.

Reminder: On the left side is a list of the frames with their number, the file name, and its path. For each frame, a check box on the left indicates if the frame is used in the data reduction or not.

To select all the frames of the list, press Ctrl+A in the window.

To select a limited number of frames: select the first frame to select, press SHIFT and select the last frame of the selection. At the bottom of the left window there are 4 buttons to define the alpha tilt from an existing list of frames (Define alpha), to add a frame list from a PTS (Add from PTS) or to add or remove single frames (Add/Remove).

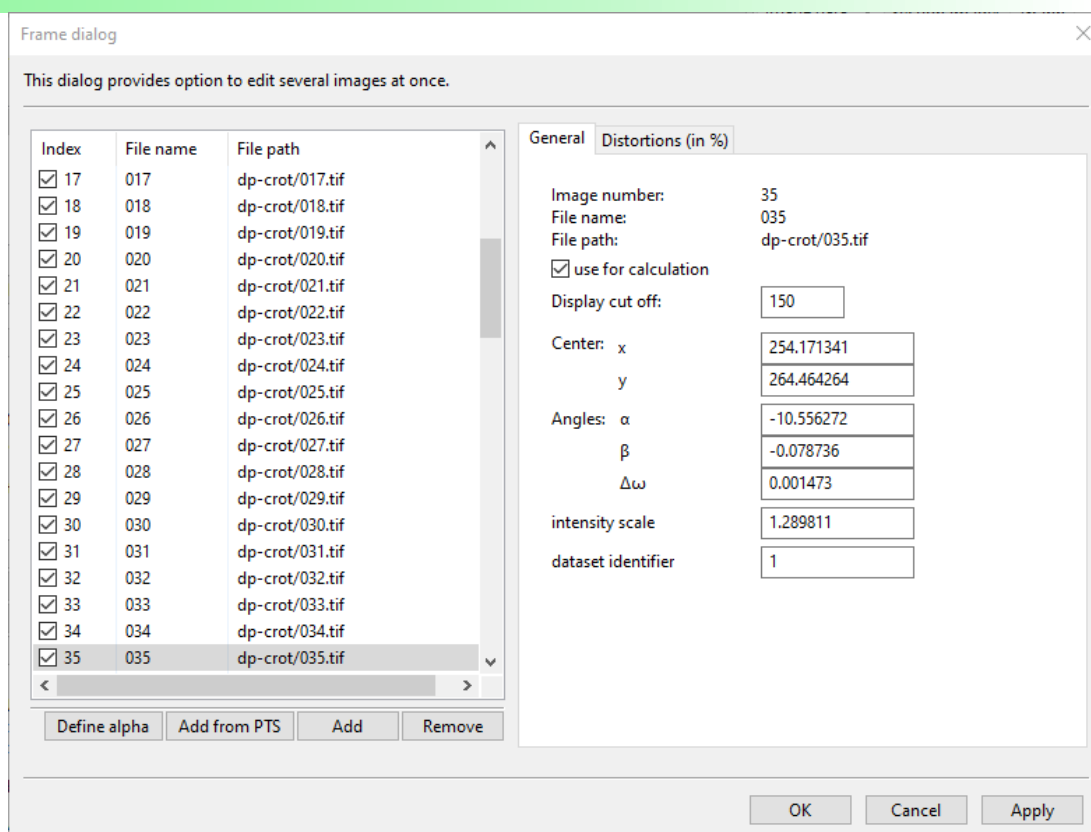


Figure B-74

To define the alpha-tilt for all frames or a selection of frames, hit “Define Alpha”. Then, Indicate the alpha-tilt (in degrees) of the first frame of your data set and the increment between two frames (α step) (Figure B-75). Press OK;

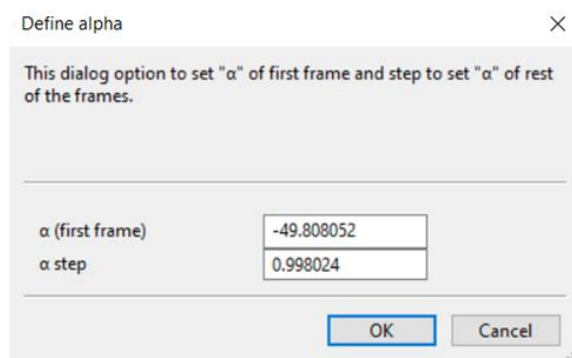


Figure B-75

The right part of the Frame dialog (Figure B-74) displays again what is already visible in the “Image options” tab for every frame (General information and distortions (in %)).

B.5. Console panel

Text window showing what is currently happening in PETS2 with log messages, info, warnings or errors. Keep an eye on that window every time a command is run.



Most information given in the console panel will be later reported in the log files.

Below is an example of basic information you might get during a data reduction. When an error occurs, the console displays specific error messages. They should help understanding the source of the problem.

► After opening an existing pts, or a pts2 file

```
Reading the input file test.pts.
The input file test.pts was succesfully read.
```

If the pts/pts2 file contains an error, an error message will appear in the console. As an example, here, one frame 097 listed in the pts file was not found in the subdirectory with all frames.

```
Reading the input file test.pts.
Error: File dp-100\097.tif does not exist.
Error: Error reading keyword imagelist.
Error: There were 1 errors in the input file.
```

► Peak search

For each frame, the console gives the beam position and the number of Friedel pairs. The last line is the total number of peaks detected above the $I/\sigma(I)$ set, and within the resolution limit.

```
>>> 96/ 96 Image dp-100/096.tif: primary beam position: 254.03 264.46 from
2 Friedel pairs.

Minimum, average and maximum position of the primary beam: 253.89 254.87
255.33 | 262.81 264.53 265.09

Finished reading 2300 peaks from the file crs11p-100_petsdata/crs11p-
100.rpl.
```

► Tilt axis: GLOBAL SEARCH

The console shows the list of tests performed to optimize the tilt axis. For each value of omega (10 degrees step) a score is evaluated: the higher the better. In the example below, a global search for the tilt axis orientation omega was carried out. The final omega value and the score is given, the rpl file is rebuilt with the new omega value.

```
Looking for the best omega
Value 0.000, score 7.251
Value 10.000, score 1.409
Value 20.000, score 0.916
Value 30.000, score 0.787
Value 40.000, score 0.724
Value 50.000, score 0.685
Value 60.000, score 0.694
Value 70.000, score 0.741
Value 80.000, score 0.746
Value 90.000, score 0.762
Value 100.000, score 0.791
Value 110.000, score 0.740
Value 120.000, score 0.733
Value 130.000, score 0.704
Value 140.000, score 0.615
```



```

Value 150.000, score 0.648
Value 160.000, score 0.758
Value 170.000, score 1.185
Value 180.000, score 4.017
Value 190.000, score 1.099
Value 200.000, score 0.694
Value 210.000, score 0.607
Value 220.000, score 0.569
Value 230.000, score 0.567
Value 240.000, score 0.597
Value 250.000, score 0.659
Value 260.000, score 0.689
Value 270.000, score 0.727
Value 280.000, score 0.770
Value 290.000, score 0.751
Value 300.000, score 0.765
Value 310.000, score 0.771
Value 320.000, score 0.705
Value 330.000, score 0.780
Value 340.000, score 0.926
Value 350.000, score 1.497
Final value of omega:
omega : 0.000 7.251
Finished reading 2300 peaks from the file crs11p-100_petsdata/crs11p-
100.rpl.

```

► Tilt axis: FINE REFINEMENT

For a finer refinement of omega, the $\Delta\omega$ will be smaller. The refinement of omega is done first, the delta tilt axis position (if refined) is done after the omega refinement. The best omega and delta values correspond to the highest score values.

```

Refining the position of the tilt axis:
Refinement of omega:
Value -0.017, score 7.250745
Value 0.003, score 7.251493
Value 0.035, score 7.250298
Value 0.003, score 7.251493
....
Refinement of delta:
Value -0.020, score 7.250822
Value 0.000, score 7.251548
Value 0.032, score 7.250340
Value 0.000, score 7.251548
Value 0.012, score 7.251393
....
Optimized angles: 0.00231 -0.00001 7.25155
Finished reading 2300 peaks from the file crs11p-100_petsdata/crs11p-
100.rpl.

```

► Peak analysis

STEP 1: In-plane distances in pixels (see Graph “in-plane distance plot” associated)

```

Finished reading 2300 peaks from the file crs11p-100_petsdata/crs11p-
100.rpl.
Number of entries in the distance table: 6277

```



```
Estimated threshold: 1.21 pixels.
Info: Press Continue, if you are happy with the result, or enter the new
threshold by clicking in the graph and then press Continue.
```

STEP 2 (Peak analysis (continue)): 3D distances in angstrom (see Graph “3D difference space distance plot” associated)

```
Thresholds for considering two peaks the same: 1.21 pixels, and 4.00 deg.
2300 peaks merged into 796 clusters, 590 with more than one peak.
14988 difference peaks saved to crs11p-100_petsdata/crs11p-100.diff.
Number of entries in the distance table: 760075
Estimated threshold: 0.0068 A-1.
Info: Press Continue, if you are happy with the result, or enter the new
threshold by clicking in the graph and then press Continue.
```

STEP 3 (Peak analysis (continue)): result of the clustering (clust, xyz, diff reconstructions).

```
Thresholds for considering two peaks the same: 0.0068 reciprocal angstroms.
14988 peaks merged into 5666 clusters, 1332 with more than one peak.
Peak analysis successfully finished.
```

► Find unit cell and orientation matrix

FIND CELL AUTOMATICALLY:

```
Current cell was rewritten by the best found cell.
```

CHECK CENTERING:

When no new centering is found

```
Check centering: The centering aP was confirmed.
```

When a new centering is detected (here C centering): a warning message appears to indicate that the initial centering (P) was automatically replaced by the new one (C).

```
Warning: Check centering: New lattice centering found. Centering vectors were
updated.
```

GO TO SUPERCELL:

```
Sorry, no frequent fraction vector was found.
No suitable supercell was found.
```

MODIFY CELL:

The console indicates if the modification could be performed or not and how the unit cell volume is affected.

```
Determinant of transformation matrix is 1.00, volume of cell is multiplied
by 1.00
Error: Determinant of transformation matrix is negative, please try again.
```



REFINE CELL:

The console gives information only when the unit cell is refined with distortions. The console shows the starting and the final lattice parameters with the new orientation matrix. For each cycle, the console displays the Root Mean Square Deviation (RMSD) between predicted and observed reflection positions (in pixels), the maximal parameter shift/e.s.d., and the number of indexed peaks/the total number of peaks. As the distortion parameters change, the rpl file and the cluster files of the 3D representations are recalculated after the refinement, as indicated in the two last lines. In the last line, 14990 peaks are, in fact, 14990 “difference space” peaks.

```

Finished reading      2300 peaks from the file crs11p-100_petsdata/crs11p-
100.rpl.
Starting cell parameters: 10.513   9.485  12.593  90.000  95.294  90.000
Cycle      RMSD  MaxShift  Number of good peaks/all peaks
  0         1.310      ----  2222/  2300
  1         0.832    27.7385  2246/  2300
  2         0.609    22.6593  2248/  2300
  3         0.536    13.3251  2248/  2300
  4         0.507     7.0302  2247/  2300
  5         0.502     3.4346  2247/  2300
  6         0.501     1.7174  2247/  2300
  7         0.501     0.8610  2247/  2300
  8         0.500     0.4349  2247/  2300
  9         0.500     0.2128  2247/  2300
 10         0.500     0.1077  2247/  2300
 11         0.500    -0.0700  2247/  2300
 12         0.500    -0.1498  2247/  2300
 13         0.500     0.1711  2247/  2300
 14         0.500     0.0319  2247/  2300
 15         0.500     0.0884  2247/  2300
 16         0.500    -0.2143  2247/  2300
 17         0.500    -0.0973  2247/  2300
 18         0.500     0.0236  2247/  2300
 19         0.500    -0.0116  2247/  2300
 20         0.500    -0.0943  2247/  2300
 21         0.500     0.0629  2247/  2300
 22         0.500     0.0861  2247/  2300
 23         0.500    -0.1704  2247/  2300
 24         0.500    -0.1188  2247/  2300
 25         0.500     0.1134  2247/  2300
Final orientation matrix:
  0.081640 -0.053859  0.013653
  0.049426  0.087485 -0.013047
  0.003020  0.024184  0.077602
Cell parameters: 10.518   9.475  12.575  90.000  95.298  90.000
Finished reading      2300 peaks from the file crs11p-100_petsdata/crs11p-
100.rpl.
 2300 peaks merged into  796 clusters,   590 with more than one peak.
14990 peaks merged into 5664 clusters, 1328 with more than one peak.

```

- Process frame for integration: the console only displays the frame processed, no specific information here.
- Optimize reflection profile

The combined values of RC width (rec. Å) and apparent mosaicity (in radians) are associated with a reliability factor that is minimized. After the list, the console gives the two optimized values with the RC



width (rec. Å) and apparent mosaicity (in degrees). The number of reflections used to calculate the camel plot depends on the $1/\sigma(I)$ value given in the section “optimize reflection profile”, not the one used for the peak hunting.

The last sentence gives an idea of the real resolution of the data by giving the last resolution shell with more than 3 reflections per one point in the camel plot. In that example, the process frame for integration was carried out with a $d^*(\max)$ value of 1.4 rec. Å. The console indicates that not enough significant data is found above a resolution of 1.3 rec. Å to provide a reliable curve in the camel plot.

```
Rocking curve analysis:
Refinement of reflection profile parameters:
0.001987 0.002517 1.1320
0.001156 0.003865 1.0303
0.000861 0.003950 1.0157
0.000884 0.003910 1.0156
0.000885 0.003910 1.0156

Refined values of relrodsigma and mosaicity: 0.00088 0.22401
Camel plot calculated from 1036 reflections.
Highest resolution shell with more than 3 reflections per non-zero grid
point: 1.30
```

► Optimize frame geometry

For each frame, the console will give the optimized alpha-tilt, beta-tilt, omega-tilt, the new x and y center of the frame, The RC width, mosaicity, sigma of the reflection size (in pixels), scale for the simulated frame, reliability factor (that should be minimized).

The values of the frame-by-frame distortions are not listed in the console. They are visible in the related graph and in the “Image options” tab for individual frames.

At last, the vector of the tilt axis in the microscope coordinates is given. Here 1 0 0 means that our tilt axis is almost perfectly aligned with the x-axis of the microscope. The second line reports the calculated angle that vector forms with the x-axis of the microscope (in-plane deviation) and the xy plane (out-of-plane deviation). Here again, in our example, the in-plane deviation is almost zero, and the out-of-plane deviation is 0.079 degrees.

```
Analysing frame nr. 1
Result: -45.069389 0.332473 0.053814 254.777451 262.473419 0.000810
0.254500 1.257329 1.100700 0.9979
...
...
Analysing frame nr. 96
Result: 50.149651 0.216620 -0.051968 254.171509 264.361267 0.000810
0.254500 1.336086 2.883678 0.9812
Finished reading 2300 peaks from the file crs11p-100_petsdata/crs11p-
100.rpl.
Optimization finished
Average orientation of the tilt axis: 1.00000 0.00002 0.00137
Angles from x-axis and from xy plane: 0.00125 0.07861
```

► Finalize integration

A log file “Finalize integration” with all helpful information is written simultaneously.



-The console gives first all the necessary parameters influencing the integration: $d^*(\max)$, the *RC width*, the *apparent mosaicity*, the integration mode, and the Laue class used for the frame scaling if applied.

-When the frame scaling is applied, the minimum and the maximum intensities found in the data set are given in the console. The integrated intensities are all rescaled using a factor that is a power of 10. This overall rescaling is a way to keep the accuracy carried by the decimals that can be otherwise lost in the data processing. The factor is set so that the largest intensity of the data set once rescaled, stays below 100 000. As an example, here, the largest intensity is 204.63. The largest factor that can be used to stay below 100 000 is 100 (20463). This rescaling is an overall rescaling, not the frame-by-frame scaling that is displayed in the log files, the graph tab “frame scales”, as well as in the Image option tab for individual frames.

-The three parameters used to correct the $\sigma(I)$ are given in the console (see section B.2.9).

-The following line gives the number of outliers kicked out of the final *hkl*-type files. In that example, 45 out of 3879 reflections are rejected using the parameters outlier detection limit for symmetry averaging = 1.5 (default value) (see section B.2.9).

Intensity statistics:

- Observed/Total number of unmerged integrated reflections.

-Intensity statistics for each Laue class. The table is Laue class/Rint(obs)/Rint(all) /Rmeas(obs)/Rmeas(all)/Number of observed reflections (for $I/\sigma(I) > 3$) /Number of all reflections/ redundancy.

After the list, PETS2 evaluates the most likely Laue class. Note that this estimation and the statistics are influenced by the Laue class used to scale the frames (if used).

-Another table presents the statistic by resolution shell (in d^* and d) as following:

Resolution shell in \AA / Resolution shell in \AA / number of observed reflections/number of all measured reflections/ number of theoretical reflections possible given the symmetry/data completeness for the resolution shell/ redundancy/Intensity/ $\sigma(I)$ /Rint(obs), Rint(all), and CC1/2.

```
*** Kinematical integration ***
Settings:
  dstarmax: 1.400
  RC width: 0.00100
  mosaicity: 0.100
  integration mode: fit profile
  frame scaling: applied, Laue class 2/m

Refinement of frame scales...
Profile-based outlier rejection:
Number of peaks considered: 13719
Number of peaks rejected : 0
Total percentage rejected : 0.00%
Total percentage rejected : 0.00%
... successfully finished.
Minimum and maximum intensity before rescaling: -6.92 204.63
Integrated intensities rescaled by a factor 100.00
Error model refinement...
Refined parameters of the error model: s_fac = 0.7286, s_b = 0.0932, s_add = 0.2524.
Info: 45 out of 3879 reflections identified as outliers at the rejection limit of
1.50 and rejected.

Intensity statistics:
Observed/Total number of integrated reflections: 2297/ 3834
cwl Laue class Rint(obs) Rint(all) Rmeas(obs) Rmeas(all) Nobs/Nall redundancy
* -1 9.36 12.36 13.22 17.45 1172/ 1984 1.932
```




```

* 2/m      13.62    17.29    16.74    21.44    803/ 1371    2.796
  112/m     31.37    33.76    37.06    40.34    760/ 1359    2.821
  2/m11     29.80    32.04    35.30    38.30    756/ 1335    2.872
  mmm      36.17    38.59    40.15    43.19    487/  882    4.347
  4/m      47.68    49.76    52.74    55.39    467/  875    4.382
  4/mmm     51.61    54.09    54.92    57.83    290/  549    6.984
  -3       26.85    29.72    31.96    35.90    985/ 1691    2.267
 -31m     44.64    48.09    50.21    54.39    615/ 1097    3.495
 -3m1     47.65    50.37    53.82    57.25    635/ 1142    3.357
  6/m      45.19    48.22    50.51    54.33    599/ 1106    3.467
  6/mmm     53.76    58.00    58.23    62.90    388/  743    5.160
  m-3      43.56    47.08    46.89    50.84    340/  640    5.991
  m-3m     53.21    56.95    55.96    59.98    209/  418    9.172

```

Info: Estimated Laue class: 2/m

Statistics for Laue class 2/m

d*-range	d-range	Nobs	Nall	Nthr	compl.	rdnd.	I/s	Rint(obs)	Rint(all)	CC1/2
0.00-0.47	Inf-2.14	52	56	79	0.709	2.68	4.74	9.03	9.30	96.93
0.47-0.66	2.14-1.52	78	93	132	0.705	2.80	4.60	10.41	11.25	95.58
0.66-0.81	1.52-1.24	109	127	175	0.726	2.89	4.32	14.16	15.18	96.11
0.81-0.93	1.24-1.07	113	143	193	0.741	2.84	4.04	15.54	16.88	94.85
0.93-1.04	1.07-0.96	121	163	228	0.715	2.80	3.90	15.97	17.87	90.74
1.04-1.14	0.96-0.87	101	167	227	0.736	2.84	3.50	15.16	19.82	90.87
1.14-1.23	0.87-0.81	110	207	283	0.731	2.84	3.15	15.48	22.19	86.93
1.23-1.32	0.81-0.76	76	209	282	0.741	2.81	2.66	19.64	31.68	64.36
1.32-1.40	0.76-0.71	43	206	295	0.698	2.65	2.03	27.10	51.75	50.29

0.00-1.40	Inf.-0.71	803	1371	1894	0.724	2.80	3.84	13.62	17.29	96.23

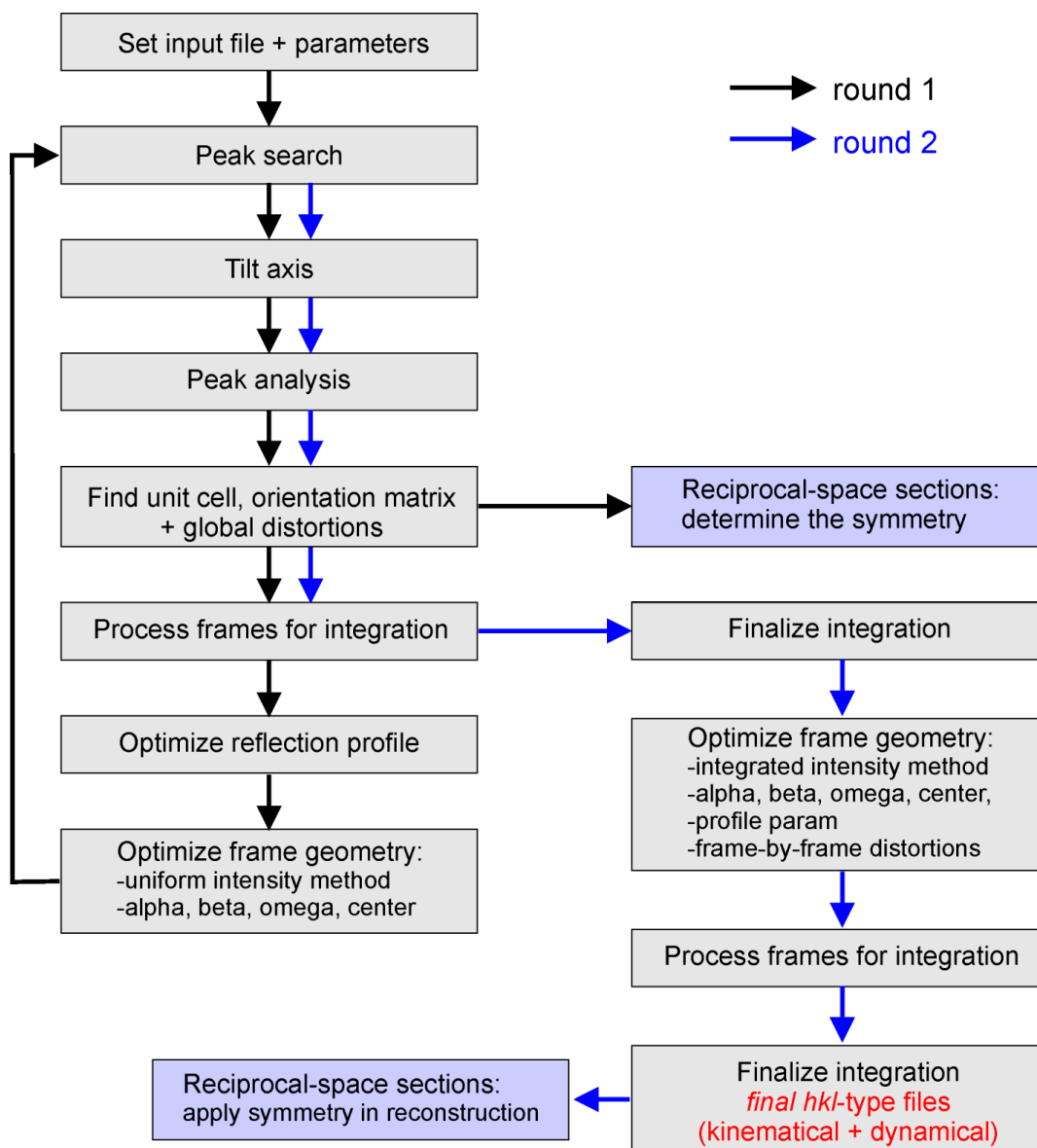
*** Dynamical integration ***

Dynamical integration finished successfully.



C BASIC PROCEDURE

The scheme below represents a standard procedure that should lead to good results for good 3D ED data. For non-standard/difficult data, the procedure may need to be adjusted, but this is still a good start. We recommend for the second round keeping the refined centers for the new peak search.





D KEYWORDS AND OPTIONS AVAILABLE IN THE PTS2 INPUT FILE

List of tasks and options to be automatically performed after the start.

The table summarizes all the keywords/commands in a PTS2 file with their options (red). Although most are accessible from the GUI; some will be changed in the input file (GIU yes/no).

The comments (labeled #) are already in the PTS2 file above the corresponding keyword. A more extended description is given for some keywords (labeled ##).

Note that to start a basic data reduction, a simpler PTS file can be created (as already explained in section A). When the data reduction starts, a pts2 file is generated with all entries, and it needs to be saved.

Command default option/value	#comments/ options present in the input file pts2, ## additional information	GUI
autotask endautotask	# peak search, tilt axis, peak analysis, find cell, refine cell, process frames, optimize geometry, finalize integration, generate 3D map, sections, check files, quit, break, set. ## keyword set can be followed by any valid one-line command. The effect is the same as if this command was read from a pts2 file. E.g., "set reflectionsizes 10" will change the reflection size to 10.	no
lambda value	#wavelength in angstroms ##lambda: relativistic wavelength of the incident electrons in angstroms. For $U_{acc} = 100\text{kV}$, $\lambda_{100} = 0.0370\text{\AA}$, 120kV : $\lambda_{120} = 0.0335\text{\AA}$, 200kV : $\lambda_{200} = 0.0251\text{\AA}$, 300kV : $\lambda_{300} = 0.0197\text{\AA}$.	yes
aperpixel value	#image calibration in reciprocal angstroms/pixel ## calculated as $\text{aperpixel} = (\text{pixel size for one given detector})/(\lambda(\text{in } \text{\AA}) * \text{camera length calibration})$	yes
geometry option	#experimental geometry. Options: continuous rotation , precession , static frames .	yes
detector default	#detector type. Options: default , asi . More to come... ## When default is selected, nothing is done on the frames. With asi, the cross due to the 4 detector blocks is corrected. The correction is fine-tuned for the ASI Cheetah detector. Please contact us if you need a correction for another detector type.	no
badpixels endbadpixels	#list of coordinates of bad pixels. These pixels are ignored and their value is interpolated from the values of the neighboring pixels.	



center AUTO	#center of the diffraction pattern. Options: AUTO = find center automatically; two numbers x y - position of the pattern center on the first frame in pixels. ## For a manual determination of the center, the x and y value (un-binned) can be read in the pets' GUI from the Image data tab below the frame pictures. The entry is written (as an example: center 250 240). The manual option is useful if the automatic procedure fails to determine the center.	yes
centermode friedelpairs 1	#Mode of center determination. centralbeam = use central beam, friedelpairs = use friedel pairs, useold = take whatever was previously set. Optional second argument: always accept center? (0/1). Applied only to Friedel pairs.	yes
beamstop no OR beamstop 8 223 283 210 293 263 81 250 12 236 endbeamstop	#beamstop settings. beamstop no with no beamstop. " beamstop followed by a list of beamstop points, if beamstop is used. ## With no beamstop the entry is beamstop no . With a beamstop the entry becomes beamstop x1 y1 x2 y2 etc. endbeamstop Beamstop defines a polygon that is excluded on each frame. It is a multiline list of coordinates, each line is one point of the polygon, x and y, unbinned pixels. The easiest way to define the beamstop is to use the GUI.	yes
mask -500 -500 500 -500 500 500 -500 500 -500 -500 endmask	#mask defines a polygon that is excluded on each frame. It is a multiline list of coordinates, each line is one point of the polygon, x and y, unbinned pixels	
dstarmax 1.4	#maximum dstar (rec.angstroms) for integration ## The default value is 1.4 rec.angstroms	yes
dstarmaxps 1.400	#maximum dstar (rec.angstroms) for peaksearch	yes
dstarmin 0.050	#minimum dstar (rec.angstroms) for integration and peaksearch ## 0.05 = default value	yes
integrationmode fit 1 5 3 0.800	#Integration settings: first the mode: fit , integrate , bestpattern or maximum . Second value: do framescaling? (0/1).	yes



	<p>Third value: Laue class number for frame scaling.</p> <p>Fourth value: range for frame scale restraints.</p> <p>Fifth value: weight of the frame scale restraint.</p> <p>## The third number is called interframe correlation range and represents how many frames are considered with close scaling, the fourth number = interframe correlation weight and defines how strongly the scales of consecutive frames are forced to be close, higher is the number, stronger is the restriction. By default, those two numbers are set to 0. A good starting point is 3 and 0.8.</p>	
intensitymethod profilesum	<p>#Method for peak intensity determination: profilesum or profilefit</p> <p>##The profilesum option is the older method and the default one. The intensity of reflections is determined by summing the entire signal in the integration mask minus the background. With the fit option, the integration is processed using an average profile of the reflections which is refined. It makes the integration more robust in case of large lattice parameters or smeared reflections to avoid overlaps.</p>	yes
integrationparams 0.0010 0.1000 1 1.00	<p>#parameters of the profile - rocking curve width (rec. angstroms), mosaicity (deg.), minimum number of measurements per reflection, range of integration (as a multiple of the sigma of reflection profile).</p> <p>##The minimum number of measurements per reflection is how many time one reflection has to be found in the frame to be considered in the final integration step. The more one reflection <i>hkl</i> is measured on different frames the better its intensity profile can be described, and its intensity properly evaluated. For 1, all reflections are considered. For structure solution, it is often better to keep all reflections. A more selective approach can be used for the refinement to avoid outliers.</p> <p>The reflection width multiplier is how many times the standard deviation of the reflection width is multiplied to extend the integration of the reflection along <i>Sg</i>. The latest option can be used to compensate for big gaps between frames as it is often the case for static frame experiments.</p>	yes
adjustreflbox yes	<p>#If yes, integration circle will be shifted to maximum intensity during intensity extraction. Useful for distorted data, dangerous for dense patterns.</p> <p>##this option is now rather robust when combined with the profilefit intensitymethod.</p>	yes
intkinematical yes	#If yes, kinematical intensity integration will be performed in Finalize Integration.	yes
intdynamical yes	#If yes, dynamical intensity integration will be performed in Finalize Integration	yes
maxindex 2	<p>#maximum satellite index used in integration. (Applies only to modulated structures.)</p> <p># for 3D periodic structure, this parameter is ignored</p>	yes
phi value	#precession or integration (semi)angle. Must be zero for static geometry.	yes



omega value 0 1	#angle between the positive horizontal axis on the image and the projection of the rotation axis on the image. Two keys define, if global search and local refinement should be performed.	yes
pixelsize 0.0100	#size of the pixel in the 3D map of reciprocal space.	yes
bin value	#binning of the images after reading in. Should be an even number.	yes
i/sigma 5.00 10.00	#Intensity/sigma for peak search and for the calculation of the camel plot	yes
background 0 1.000000	#Constant background to be subtracted from all images after reading in. May be negative if needed. Second optional argument is the factor that multiplies the raw image at reading ##The first number is a linear transformation of the input intensities (background threshold). The second number is a scaling of the background.	no
noiseparameters 1 40	#Parameters allowing to calculate the sigma(count) on every pixel. The first is G*gamma (gain*cascade factor), the second is sigma**2 of the dark image. ##Those two values depend on the detector and need to be adjusted for your camera.	yes
errormodel 1.0000 0.0000 0.0000 1 1.50	#Error model parameters. -The first is s_fac, -the second s_b, -the third s_add. $\sigma^2 = s_{fac}^2 * (\sigma_{macnt}^2 + s_b^2 * int + s_{add}^2 * int^2)$, with int the maximum intensity of symmetry related reflections. Then the refinement flag (1= refine error model). -Last: level for outlier rejection.	yes
reflectionsiz value	#Diameter of integration circle of the reflections (pixels, unbinned)	yes
simulationpower 0.500	#An exponent applied to experimental and simulated counts in orientation refinement. Typically, <1 to suppress overweighting of the strong reflections in the fit. (Applied in the orientation refinement, it fits pixels. If very strong reflections, they tend to dominate the fit. If they are also off, the fit is not successful. We can take all intensities to one power (0.5) to reduce the sensitivity to strong reflections).	no
rcshape pv	#Shape of the reflection profile. gaussian, pv (pseudovoigt: RCwidth Lorentzian, mosaicity Gaussian), lorentzian.	no
refinecamelparams 1 1 0 1 0.0020	#Keys of the camel refinement. -1=apply, 0= don't apply: -refine RC width, -refine mosaicity, -refine precession angle. -Automatic/User defined camel plot step (0/1),	yes

30



	<div> <div> <input checked="" type="radio"/> in % <input type="radio"/> in pixels </div> <div> <div>Standard mode</div> <div>Expert mode</div> </div> <div> Center: x <input type="text" value="0"/> y <input type="text" value="0"/> </div> <div> Diff. center shift: x <input type="text" value="0"/> y <input type="text" value="0"/> </div> <div> <div>radial</div> <div>linear</div> <div>quadratic</div> <div>cubic</div> <div>phase</div> </div> <div> 0 <input type="checkbox"/> 0.015 <input type="checkbox"/> 0 <input checked="" type="checkbox"/> 0.3945 <input type="checkbox"/> 0 </div> <div> 1 <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 0 </div> <div> 2 <input checked="" type="checkbox"/> 0.0299 <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input checked="" type="checkbox"/> 139.5735 </div> <div> sg terms <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 0 </div> <div> <div>tangent.</div> <div>linear</div> <div>quadratic</div> <div>cubic</div> <div>phase</div> </div> <div> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input checked="" type="checkbox"/> 0.7006 <input type="checkbox"/> -90 </div> <div> 1 <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 94.5735 </div> <div> 2 <input type="checkbox"/> 0.0299 <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 0 </div> <div> sg terms <input type="checkbox"/> 0 <input type="checkbox"/> 0 <input type="checkbox"/> 0 </div> <div> <input checked="" type="checkbox"/> tie elliptical distortion <input type="checkbox"/> tie parabolic distortion </div> </div> <div> <div> <input checked="" type="radio"/> in % <input type="radio"/> in pixels </div> <div> <div>Standard mode</div> <div>Expert mode</div> </div> <div> magnification: <input type="text" value="0.015"/> </div> <div> barrel-pincushion: <input checked="" type="checkbox"/> 0.3945 </div> <div> spiral: <input checked="" type="checkbox"/> 0.7006 </div> <div> elliptical amplitude: <input checked="" type="checkbox"/> 0.0299 </div> <div> radial SgPara: <input type="text" value="0"/> </div> <div> phase: <input checked="" type="checkbox"/> 139.5735 </div> <div> Rerefine tilt axis </div> </div>
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h0l 1.000 0.000 0.000 0.000 0.000 1.000 0.000 0.000 0.000 0kl 0.000 1.000 0.000 0.000 0.000 1.000 0.000 0.000 0.00.... Endreconstruction		
reconstructionparams 0.0070 0.0140 1	#Parameters for the sections of rec. space. Pixel size (rec. angstroms) and thickness of the summed region perpendicular to the section. Switch from 0 to 1 to apply symmetry in the reconstruction. # The thickness is in Å, and 1/0 = apply/don't apply the symmetry in the reconstructions.	yes
removebackground yes yes	#If yes, background subtraction is done on reconstructions. If no, raw images are used. -First argument: 2D reconstructions (rec. space sections), -2 nd argument: 3D map reconstruction.	no
globalorisearch no	#Experimental. If yes, a global orientation search is performed on all frames at the very beginning. Three reals: step between templates (deg.), max resolution of templates (rec.A), maximum deviation from the original orientation. Finally, a switch to perform or not fine refinements of the result (0/1). Only for initiated users! (for never...later maybe)	yes
backgroundmethod median	#Method for background subtraction. median = median filter (default, the best), average = average in concentric circles, fft = background by Gaussian smearing. Median should be used in normal circumstances. #3 ways of subtraction of the Bg, median is best and other options might be removed in later versions, fft removes low frequencies from the image. median>fft>average.	no
skipsaturated no	#If yes, reflections containing saturated pixels are not written in the output reflection list. # For structure solution, it is often best to keep all reflections, even saturated. For the refinement, you might consider removing them.	yes
saturationlimit 64000	#Above this number the pixel is considered saturated. ## 13000 is the default value for our CCD camera, 65000 for asi, etc.	yes
minclusterpoints 2	#Minimum number of points in a cluster (used during peak analysis). ##2 is the default value	no
resshellfraction 0.5000	#Limit between inner and outer shell for the calculation of average I/sigma (shown in the plot made during integration + in the file framstats). ## Multiplier of the dstart value used to process frame for integration. The shell below dstart*threshold is considered as the inner shell. It does not influence the integration steps but is a way to visualize some part of the resolution range when needed.	no



indexingmode diffspace	#Algorithm for automatic cell determination. diffspace = new algorithm using difference space clustering, triplets = old "jana-style" algorithm. ##diffspace and triplets are two different algorithms of automatic indexing. diffspace procedure uses the clust reconstruction. Triplets option uses the reconstruction selected in the GUI (clust, xyz, or cor).	yes
indexingparameters 0.0140 0.6000 3.0000 1.0000	#Parameters for cell determination: indexing tolerance (rec. A), relative length tolerance (%), angular tolerance (deg.), maximum Sg for indexing (distortions only). ##The first number = indexing tolerance is used both for indexing and the refinement of the unit cell parameters. 0.6 degree and 3% are the default angular and length tolerances respectively. They are used during the indexing to guess the possible crystal system and centering. The last number is the excitation error Sg considered for the refinement. 1 is almost like infinite.	Yes
cellrefinemode cellanddistort	#Algorithm for cell refinement. cellandub = refinement from 3D peak coordinates (standard), cellfromd = refinement against lengths of the diffraction vectors, cellanddistort = cell from 2D peak positions plus, optionally, distortion parameters. ## The refinement with distortions automatically uses the cor file reconstruction. For the other refinement options, the selected reconstruction is used.	yes
cellrefineparameters 2 1 1	#Parameters for cell refinement: crystal system index , key to refine cell in cellanddistort (0/1), key to refine distortions in cellanddistort (0/1). # crystal system index: 2 = monoclinic, refine cell or not = 1/0, refine distortions/not = 1/0. This part will be filled through the GUI.	yes
referencecell 10.00000 10.00000 10.00000 90.00000 90.00000 90.00000 0 0	#Cell reference to be used in cell refinement (a b c alpha beta gamma). The 7th parameter says if lattice scaling is allowed (0/1). The 8 th parameter specifies if the cell should be used also as a source for orientation matrix in global orientation search. ##When the 7 th number = 1, the lattice scaling is fixed up to a scale factor keeping the a/b, b/c, a/c ratios. If 0, the lattice parameters will be refined to be exactly what is expected. This last option is only accessible for the refinement with UB cell.	yes
peakanalysis 0 0 3.2262 0.0044	#Peak analysis options: estimate cluster limits automatically (0) or use preset values (1), process automatically (1) or wait for confirmation (0), xyz cluster limit (in pixels), 3D cluster limit (in rec. Angstroms).	yes
virtualframes 1 1 -1 1	#Virtual frames -first the number of summed frames, -second the step between frames, -third 1 to sum all intensities, only intensities on the virtual frame, -1 - decide based on geometry. -fourth: determine the first and second number automatically/manually: 1/0 .	yes



avoidicerings yes/no icerings 0.2735 0.4446 endicerings	#list of ice ring diameters. Peaks in the vicinity of these rings are ignored, if avoidicerings is yes.	
imagelistheader imgname alpha beta omega alphaorig betaorig omegaorig xcenter ycenter intscale diffbfac magcorr elliaamp elliph paraamp paraph useforcalc dataset	# Order of items in each line of the image list ## Only the three first columns are needed to start a basic run from a simpler version of the pts input file done manually or generated from in house software. The additional columns will appear when the project will be saved in a pts2 file during the procedure.	no
imagelist "framefolder\name001.tif" alpha beta "framefolder\name002.tif" alpha2 beta2 etc. endimagelist	#List of images ## Only the three first columns are needed to start a basic run from a simpler version of the pts input file done manually or generated from in house software. Additional columns will appear when the project will be saved in a pts2 file during the procedure.	yes

E OUTPUT FILES

List of all output files created during the data reduction and given either in the same directory as the PTS2 file or in subdirectories.

Folder\File	When produced	Description
Jobname.pts2	Whenever a pts/pts2 file is saved	A pts2 file is the main input file with all necessary commands to run the data reduction from a tilt series of frames. See Section C
Jobname_petsdata\ Jobname.rpl	Peak search	rpl stands for raw peak list. 12 columns: Frame-by-frame peak list, 1-3: raw 3d coordinates in the Cartesian reference coordinate system (microscope settings labelled xyz in the GUI). The coordinates in the raw file are not corrected for effects like tilt-axis refinement etc. and should not be used for any other than internal purposes. The corrections are applied to the coordinates in the Jobname.cor file.



		4: integrated intensity, 5: sigma(I) 6-7: x and y positions of the intensity maximum on the frame (integer, unbinned) 8-9: x and y refined positions of the peak when the distribution of the intensity is considered. 10: alpha angle 11: maximum intensity value 12: frame number where the peak is found
Jobname_petsdata\ Jobname.cor	Peak search	12 columns: For each peak detected during the peak search and sorted by their integrated intensity, 1-3: 3d coordinates (corrected with the omega rotation axis) in the Cartesian referential (microscope settings labelled xyz in the GUI) 4: integrated intensity, 5: sigma(I) 6-7: x and y positions of the reflection on the frame (integer, unbinned) 8-9: x and y refined positions of the peak when the distribution of the intensity is considered. 10: alpha angle 11: maximum intensity value intensity 12: frame number where the peak is found <i>Remark: when the box "show intensity" in the indexation display options tab is checked it corresponds to the integrated intensity.</i>
Jobname_petsdata\ Jobname.perspik	Peak search	x and y coordinates of badly behaving pixels that will be ignored in all frames. This list is not frame dependent and is generated for each dataset automatically during the peak search.
Jobname_petsdata\ Jobname.resolution	Peak search	6 columns For each frame: 1: frame path\name 2-6: 5 highest resolution peaks from the highest to the lowest. The resolutions are expressed as the length of diffraction vector in \AA^{-1} . <i>Note: this file gives rough information on the resolution in each frame.</i>
Jobname_petsdata\ Jobname.app	Peak search	the average reflection profile used for the fitting procedure
Jobname_petsdata\ Jobname.xyz	Peak analysis step 2	The xyz file is already a clustered file of the cor file.



		<p>11 columns:</p> <p>1-3: 3d coordinates (corrected with the omega rotation axis) in the Cartesian referential (microscope settings labelled xyz in the GUI)</p> <p>4: integrated intensity,</p> <p>5: $\sigma(I) = 0$ because there is no sigma for a clustered file</p> <p>6-7: x and y positions of the reflection on the frame (integer, unbinned)</p> <p>8-9: x and y refined positions of the peak when the distribution of the intensity is considered.</p> <p>10: peak number in the cor file. There are always a group of peaks in the cor file that are merged together in the xyz file. The column is just the position corresponding to the first peak of the group in the cor.</p> <p>11: number of peaks in the cluster</p>
Jobname_petsdata\ Jobname.diff	Peak analysis step 2	<p>5 columns</p> <p>3d coordinates (xyz), not real intensity, geometric mean of the intensities of the the two peaks that form the difference vector. (the larger this number, the more intense on average are the two peaks), last number is the same as the previous. The file follows the hkl intensity sigma format, but no sigma is assigned, hence, the intensity is repeated.</p>
Jobname_petsdata\ Jobname.clust	Peak analysis step 3	xyz, I, sigma, number of peaks contributing to the cluster.
Jobname_petsdata\ Jobname.sphtest	Find unit cell auto	Output file of the procedure find unit cell automatically with all observed directions, possible cells found by the algorithm, and the selected cell.
Jobname_petsdata\ Jobname.symmlog	Find unit cell auto	<p>This file is the output file from procedure Check centering. In this procedure search of the highest symmetry (centered) cell is provided. Input unit cell must be primitive (not centered) cell.</p> <p>Jobname.symmlog contains at the beginning the reduced cell corresponding to input unit cell. After this cell, information is given about cells found during the search for higher-symmetry centered cells. The cell information contains cell parameters, cell volume, UB matrix and Bravais class, and transformation matrix from the primitive to the centred cell. At the end of Jobname.symmlog, there is final observed cell with the highest symmetry. If cubic symmetry is observed also hexagonal and tetragonal cells are considered. If hexagonal primitive cell is observed also orthorhombic cells are considered.</p>



Jobname_petsdata\ Jobname.distcormat	Ref with distortions	Distortion correlation matrix showing correlations between the parameters refined during the cell and distortion refinement. Name of param, value of param, (standard uncertainty). Number of the param from 1 to... 1; Stars = large correlation (>0.8).
Jobname_petsdata\ Jobname.celllist	When exiting the Indexing panel.	List of indexed unit cells with their parameters, centering, and orientation matrices, cell directions. The unit cell used in the data reduction is labelled "active".
Jobname_petsdata\ Jobname.framestat	Process frame for integration	It contains the numbers shown in the plot average I/sigma, i.e. the average I/sigma in lower and higher resolution shells.
Jobname_petsdata\ Jobname.failedint	Process frame for integration	Contains list of reflections that are not integrated properly: reflections close to an edge or beamstop. They will be filter out in the finalize integration step.
Jobname_petsdata\ Jobname.dyntmp	Process frame for integration	15 columns h k l, Intensity, sigma, integer position of the peak x and y on the image predicted, refined position (if shift integration mask is used), frame number, number of saturated pixels, last four numbers = resolution (length of the dif vector), excitation error, RSg (can be negative), distance of the reflection from the 0 plane (z coordinate of the reflection – not really useful in 3DED data, introduced for special purposes).
Jobname_petsdata\ Jobname.cml	Process frame for integration/ Optimize reflection profile.	Camel file: resolution shell, excitation error, RSg, calculated R curve, experimental RC.
Jobname_petsdata\ Jobname.rprofall	Process frame for integration/ Optimize reflection profile.	Reflection profile for all reflections H k l Resolution, excitation, RSg, Iobs, sigma, Icalc, frame number. Azimuth of the reflection = angle from the horizontal axis in radians. This file was made to be plotted in gnuplot, each block is one reflection, this file is a list of all reflections.
Jobname_petsdata\ Jobname.rprofstr	Process frame for integration/	Reflection profile strong (measure 4 times, and if at least one of the reflections that form the profile as an I more than 20 sigma). Same as the previous one but with strong reflections only.
Jobname_petsdata\ Jobname.ptsoptlist	Optimize frame geometry	Copy of the console after the geometry optimization (will be soon removes and placed in the log file)

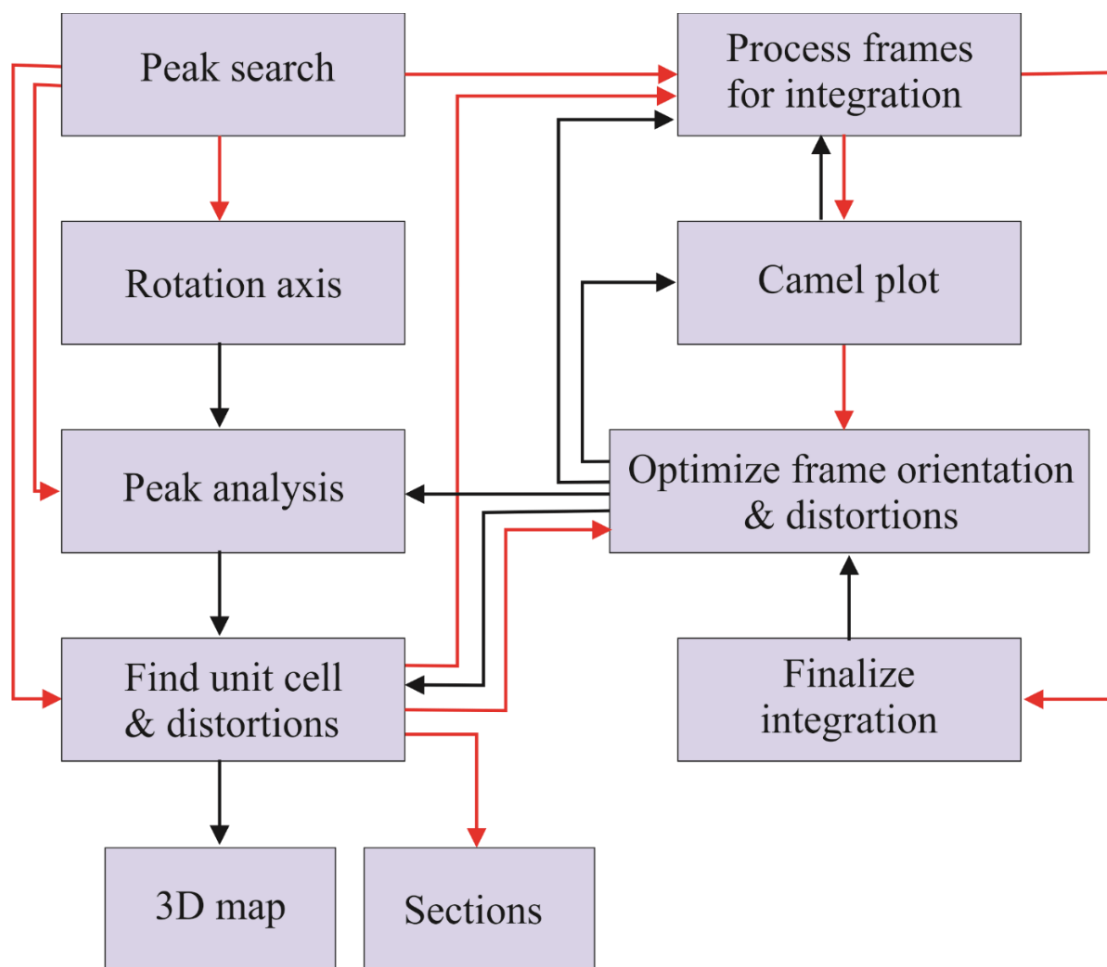


Jobname_petsdata\ Jobname.cif_pets	Finalize int	The basic output file with the CIF format, for structure solution and kinematical refinement. Contains integrated reflection intensities and standard deviations with a header giving the basic unit cell and experimental information
Jobname_dyn.cif_pets	Finalize int	The basic output file with the CIF format, for dynamical refinement. Contains frame-based reflection intensities and standard deviations with a header giving the basic unit cell and experimental information and the information on the (overlapping virtual) frames.
Jobname.hkl	Finalize int	H k l list with I and sigma(I)
Jobname.xyzcheck	Write check files	for diagnostic and development purposes
Jobname.corcheck	Write check files	for diagnostic and development purposes
Jobname_petsdata\processed*.tiff	Peak search	Processed frames in TIFF format
Jobname_petsdata\simulation*.tiff	Optimize frame geometry	Simulated frames in TIFF format
Jobname_petsdata\sections	Reciprocal-space sections	Folder containing the sections (tiff)
Jobname_petsdata\sections\png	Reciprocal-space sections/save sections	Folder containing the sections (png) initially created with the sections. Those sections can be updated using a different cutoff, color themes etc. and can be more conveniently used to display the sections in documents/presentations than the 16bit tiffs. New sections can be produced using the new settings by selecting “save sections” in the toolbar of the “Section images tab”.
Jobname_petsdata\Jobname.xplor /ccp4/hdf5	Generate 3D map	3D map of intensities in the reciprocal-space. Can be viewed by external programs like VESTA or UCSF Chimera
Jobname_petsdata\Jobname.gos	Serial ED	Short listing of the global orientation search /SerialED run. For each frame it lists the orientation angles of a couple of the best matching templates and the associated figures of merit. Only symmetry independent templates are listed.
Jobname_petsdata\ Jobname.gosfull	Serial ED	Like Jobname.gos, but with the complete listing of all best matching templates, including the symmetry-related. Only for checking and development purposes.
Jobname_petsdata\ Jobname.templ	Serial ED	The definition of the templates. The header contains the settings used to generate the templates (orientation matrix, maximum resolution, angular step between templates). The for each template the angular settings of the template is given, followed by the list of coordinates of all peaks with their intensity



F DEPENDENCY SCHEME

This scheme shows how each action relates to other possible actions in PETS2. Performing an action can either be necessary before another action is performed (marked by a red arrow), or it may change some parameters/settings that may influence the result of the other action (black arrow).



- Prerequisite to carry out the next action
- Only influences the next action



REFERENCES

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