

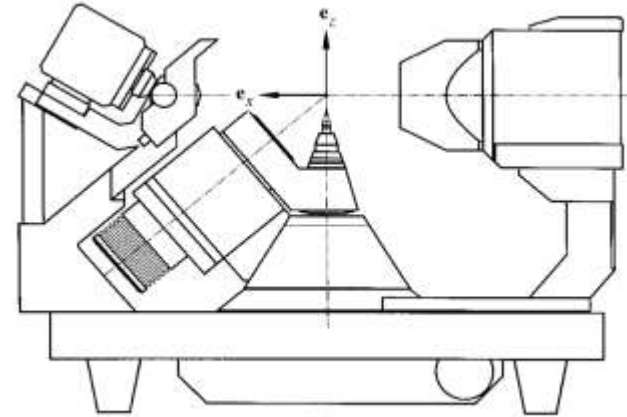
CrysAlis^{Pro}: Data reduction different image formats

Mathias Meyer

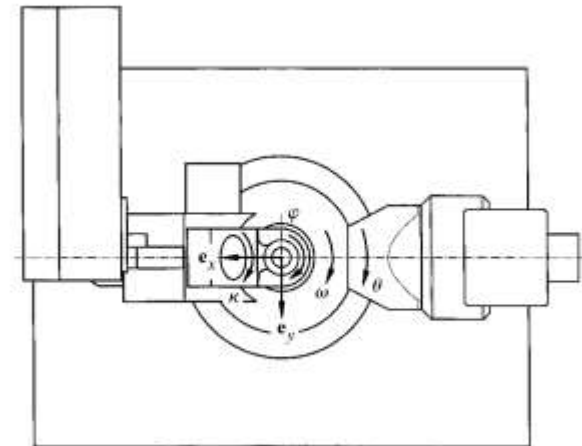
X-ray Group Software Manager

Area detector diffraction experiments

- Understand the experiment
 - Goniometer description
 - Sense of rotation
 - Area detector 'perspective'
 - Zero points
-
- Kappa vs. Euler geometry



(a)



(b)

W. A. Paciorek, M. Meyer and G. Chapuis: 'On the geometry of a modern imaging diffractometer'; *Acta Cryst.* (1999). **A55**, 543-557

Workflow on in-house instruments

- Describe instrument
- Run fully automatic calibration experiment describing fully the instrument at any distance
- Run test data collection on standard sample
- Run new experiment.

Workflow on in-house instruments

Run fully automatic calibration experiment describing fully the instrument at any distance

Full calibration experiment dialog (2.0.4)

Path
Name: C:\XcaliburData
 Experiment in folder C:\XcaliburData\calib_HyPix6000_81016_Sat-Oct-08-23-07-18-2016

Basic system parameters
Dd zero(Cu)=-4.00000, Dd zero(Mo)=-4.00000, Overflow threshold=1048000, Beam stop support orientation=gemini(mkII), HyPix 1x1 binning, Flood correction: off

Options
Crystal Lattice type Lattice min max

User mode parameters
(Parameters: No constraints, Number of reflections to find=2000 (2000 for flood calibration))

Generator at end of experiment
 No change
 Turn down
 Turn off

Calibration mode
 Optimal
 Manual
 User
 Constraint

Cu

Near Collect extra data for better structure refinement
kV mA Exposure time the same for all theta positions: 1.0s/deg, Detector distance=39.00, Scan range=20.0, Scan width=0.1,

Far Collect extra data for better structure refinement
kV mA Exposure time the same for all theta positions: 1.0s/deg, Detector distance=74.00, Scan range=20.0, Scan width=0.1,

Automatic flood field correction calibration
 Run flood calibration File:

Mo

Near Collect extra data for better structure refinement
kV mA Exposure time the same for all theta positions: 5.0s/deg, Detector distance=39.00, Scan range=10.0, Scan width=0.1,

Far Collect extra data for better structure refinement
kV mA Exposure time the same for all theta positions: 5.0s/deg, Detector distance=74.00, Scan range=10.0, Scan width=0.1,

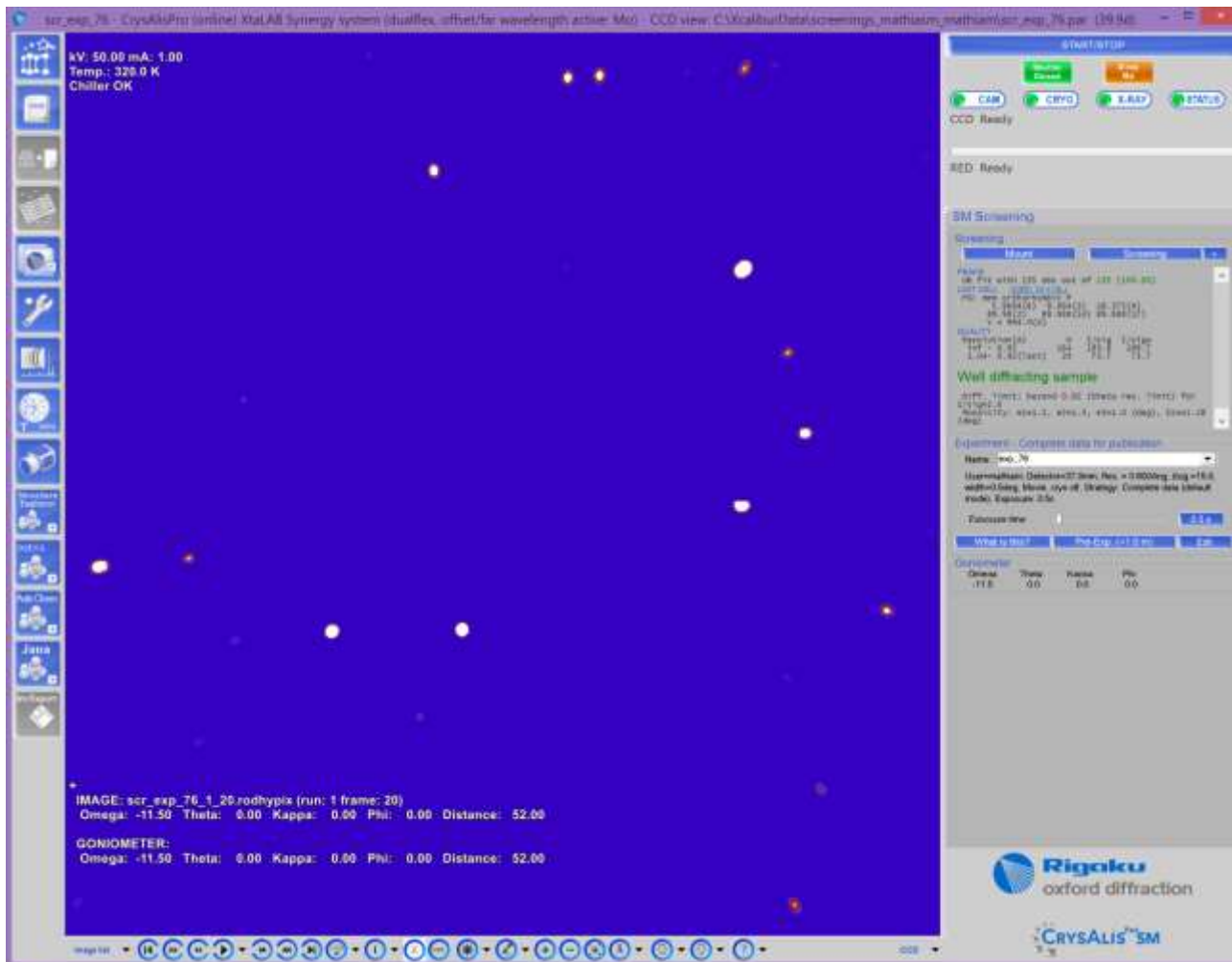
Automatic flood field correction calibration
 Run flood calibration File:

User message
Cytidine cell: a=5.120, b=14.000, c=14.800, alpha=90.000, beta=90.000, gamma=90.000
You have changed cell type parameters, you must regenerate calibration run lists, please click 'Find experiments' button

End of calibration: Sat Oct 08 23:52:17 2016 (44min)

Workflow on in-house instruments

Run test data collection on standard sample



Workflow on in-house instruments

Run new experiment

Experiment Strategy (1.2.0, automatic suggests exposure time 0.32.0sec, scan width 0.50 deg)

Links self for Strategy Calculation: [CCP4 \(1.16\)](#)

Cell: 7.433(12) 14.948(18) 17.481(13) 95.963(13) 95.963(14) 98.271(13) 104.60(1) °P

Strategy parameters

- Resolution: Free Fixed: 0.20
- Auto-merge: Other:
- Final states are equivalent (check for high quality absolute configuration data)

Detector Distance: 37.50

Strategy mode

Complete data (default mode)

Start: 140.0 Calculate New 90.25 %

Automatic experiment settings

Time position based on data to 0.20 Ang	exp time	calculated exposure	merged exposure
30 lines	11.00	03.00	02.84
70 (Empire)			
The same time for all three positions	00.00	00.00	00.00
Different time for each three positions			

Estimated resolution: 2.00

Scan width: 1.0

Repeat the experiment with target exposure time as current time, resolution can be calculated.

Calculate New Strategy

Current Strategy

No. Files/frames: 4/348

Total experiment time: 36.57m

Expected experiment finish from Scan Start 69 (20:27:19 2016)

Completed/Coverage curves

Completed/Coverage tables

Completed/Predicted resolution

IMAGE: jms_exp_76_1_19.res
Omega: -17.00 Theta: 7.12

GONDIOMETER:
Omega: -17.00 Theta: 7.12

Rigaku oxford diffraction

CRYSTALIS™

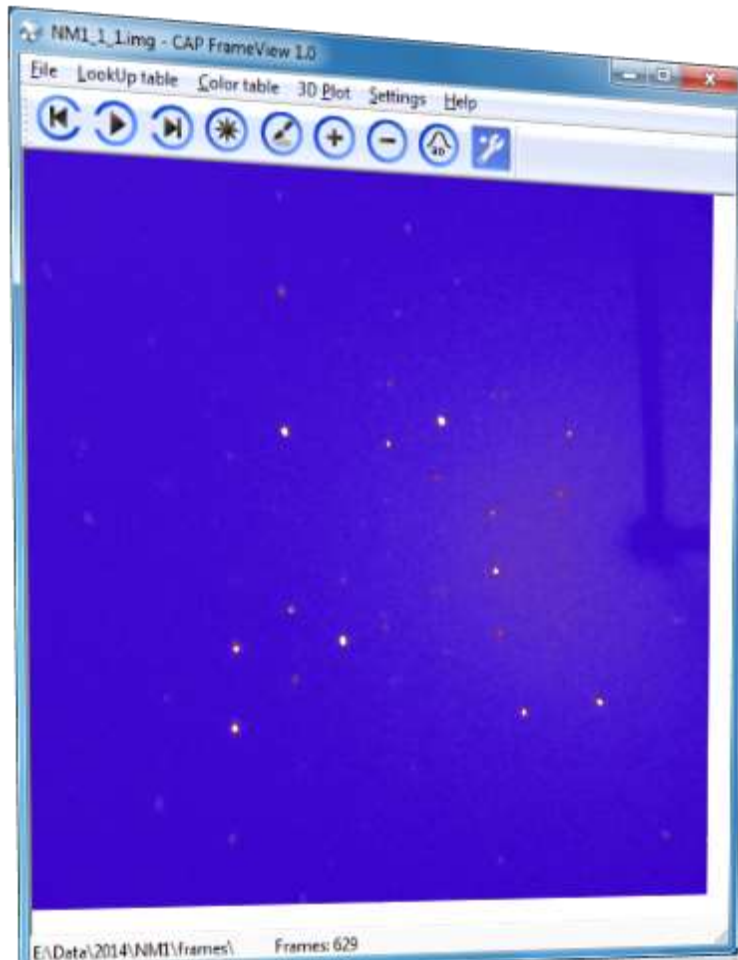
Import: Worse situation

- Depending on the format the instrument model is only known so-so.
- Rather than on a ‚Standard sample‘ the import is tried on something difficult.
- ‚Easy‘: Import of known formats
- ‚Complex‘: Esperanto import

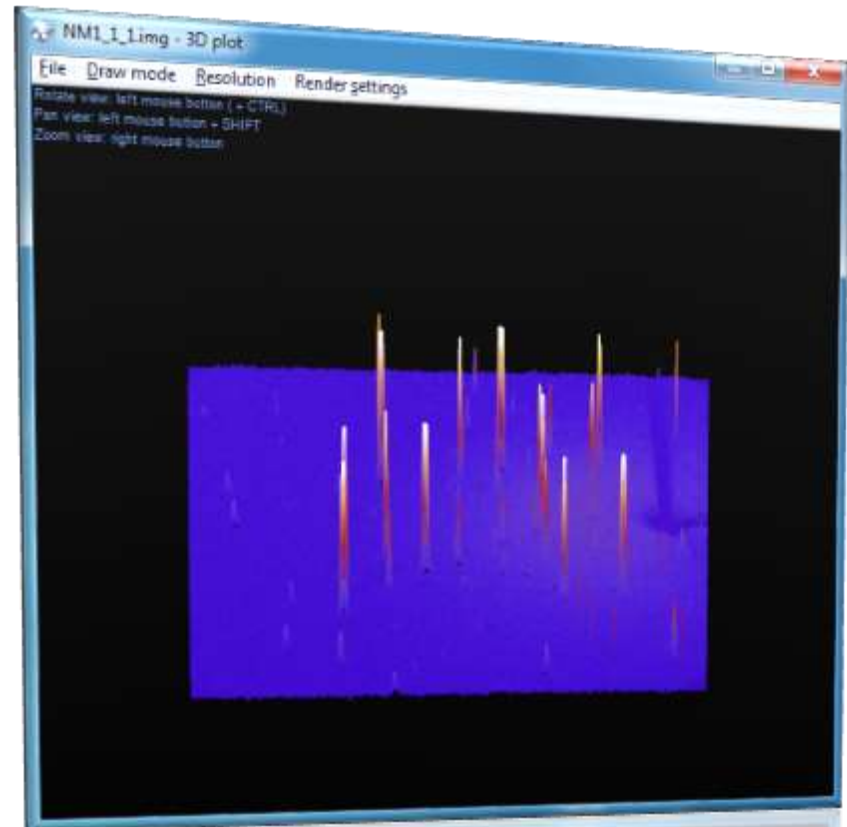
First meeting with the data set

- Install CrysAlisPro: this will install a tool called 'CAPFrameView'. You can inspect all known image formats.
- Use of a file inspection program: 'Norton commander'
- A rename tool.

First meeting with the data set



Main window



3D Plot window

First meeting with the data set

The screenshot displays the Total Commander file manager interface. It features two side-by-side file explorer windows. The left window is titled 'DCE WinMerge dhoI27_binned review_08 Rigaku include DK_ML7-66_MM res' and shows a directory tree for 'dhoI27_binned'. The right window is titled '2016 some_files totalcmd 01_Prolegomena dhoI27_binned ACA_Albuquerque' and shows a directory tree for 'mm3838'. Both windows list files with their names, extensions, and sizes. The status bar at the bottom indicates '0 k / 48'390 k in 0 / 132 Datei(en), 0 / 5 Verzeichnis(sen)'.

Name	Erw.	Größe	Name	Erw.	Größe
[.]	<DIR		[.]	<DIR	
[frames]	<DIR		[frames]	<DIR	
[log]	<DIR		[log]	<DIR	
[sg_dhoI27_binned]	<DIR		[sg_dhoI27_binned]	<DIR	
[struct]	<DIR		[struct]	<DIR	
[tmp]	<DIR		[tmp]	<DIR	
dhoI27_binned			s_57_111007	geo	1'710'
s_57_021007	ccd	1'	s_57_021007	ccd	1'
1713714t	cif	4'	pre_dhoI27_binned_auto	ini	8'
dhoI27_binned	cif	4'	mm3838_rp	ini_report	
mm3838	cif	4'	mm3838_rint	dat	6'
1713714t	cif_od	4'	mm3838_resolutionstats	dat	1'
dhoI27_binned	cif_od	4'	mm3838_refinedsubmodels	dat	13'
mms3838	cif_od	4'	mm3838_red	sum	65'
1713714t_absscale	dat	5'	mm3838_profiles	dat	6'
1713714t_chi2am	dat	3'	mm3838_profilecorres	dat	1'
1713714t_chi2bm	dat	3'	mm3838_profilecorrint	dat	1'
1713714t_lattice	dat	13'	mm3838_profilecorrframe	dat	3'
1713714t_latticeperrun	dat		mm3838_predictaccuracystheta	dat	2'
1713714t_predictaccuracyvframe	dat	7'	mm3838_predictaccuracyvframecycle1	dat	7'
1713714t_predictaccuracyvframecycle1	dat	7'	mm3838_predictaccuracyvframe	dat	7'
1713714t_predictaccuracyvstheta	dat	2'	mm3838_latticeperrun	dat	
1713714t_profilecorrframe	dat	3'	mm3838_lattice	dat	13'
1713714t_profilecorrint	dat	1'	mm3838_hkl_skipregion	txt	1'
1713714t_profilecorres	dat	1'	mm3838_hkl_overflow	txt	
1713714t_profiles	dat	6'	mm3838_hkl_filtered	txt	
1713714t_refinedsubmodels	dat	13'	mm3838_hkl_edgeskip	txt	10'
1713714t_resolutionstats	dat	1'	mm3838_hkl_badprofile	txt	
1713714t_rint	dat	6'	mm3838_dated	ini_re...	12'
dhoI27_binned_absscale	dat	5'	mm3838_crystal	ini_rep...	6'
dhoI27_binned_bfactor	dat	5'	mm3838_coverage	ini_rep...	1'
dhoI27_binned_chi2am	dat	3'	mm3838_chi2bm	dat	3'
dhoI27_binned_chi2bm	dat	3'	mm3838_chi2am	dat	3'
dhoI27_binned_latticeperrun	dat		mm3838_absscale	dat	5'
dhoI27_binned_maxres	dat	8'	mm3838	rrpprof	904'
dhoI27_binned_predictaccuracyvframe	dat	7'	mm3838	p-p	
dhoI27_binned_profilecorrframe	dat	3'	mm3838	ins	

First meeting with the data set rename

File Name Ext Size Date

slip_1_1	img	271,744	02/12/2013 12:27:06
slip_1_2	img	271,744	02/12/2013 12:27:10
slip_1_3	img	271,744	02/12/2013 12:27:14
slip_1_4	img	271,744	02/12/2013 12:27:18
slip_1_5	img	271,744	02/12/2013 12:27:22
slip_1_6	img	271,744	02/12/2013 12:27:26
slip_1_7	img	271,744	02/12/2013 12:27:30
slip_1_8	img	271,744	02/12/2013 12:27:33
slip_1_9	img	271,744	02/12/2013 12:27:37
slip_1_10	img	271,744	02/12/2013 12:27:41
slip_1_11	img	271,744	02/12/2013 12:27:45
slip_1_12	img	271,744	02/12/2013 12:27:49
slip_1_13	img	271,744	02/12/2013 12:27:53
slip_1_14	img	271,744	02/12/2013 12:27:57
slip_1_15	img	271,744	02/12/2013 12:28:01
slip_1_16	img	271,744	02/12/2013 12:28:05
slip_1_17	img	271,744	02/12/2013 12:28:09
slip_1_18	img	271,744	02/12/2013 12:28:13
slip_1_19	img	271,744	02/12/2013 12:28:17
slip_1_20	img	271,744	02/12/2013 12:28:21
slip_1_21	img	271,744	02/12/2013 12:28:25
slip_1_22	img	271,744	02/12/2013 12:28:29
slip_1_23	img	271,744	02/12/2013 12:28:33
slip_1_24	img	271,744	02/12/2013 12:28:37
slip_1_25	img	271,744	02/12/2013 12:28:41
slip_1_26	img	271,744	02/12/2013 12:28:45
slip_1_27	img	271,744	02/12/2013 12:28:49
slip_1_28	img	271,744	02/12/2013 12:28:53
slip_1_29	img	271,744	02/12/2013 12:28:57
slip_1_30	img	271,744	02/12/2013 12:29:01
slip_1_31	img	271,744	02/12/2013 12:29:05
slip_1_32	img	271,744	02/12/2013 12:29:09
slip_1_33	img	271,744	02/12/2013 12:29:13
slip_1_34	img	271,744	02/12/2013 12:29:17

File Name Ext Size Date

slip_1_01	img	271,744	02/12/2013 12:27:06
slip_1_02	img	271,744	02/12/2013 12:27:10
slip_1_03	img	271,744	02/12/2013 12:27:14
slip_1_04	img	271,744	02/12/2013 12:27:18
slip_1_05	img	271,744	02/12/2013 12:27:22
slip_1_06	img	271,744	02/12/2013 12:27:26
slip_1_07	img	271,744	02/12/2013 12:27:30
slip_1_08	img	271,744	02/12/2013 12:27:33
slip_1_09	img	271,744	02/12/2013 12:27:37

Multi-Rename Tool

Rename mask: file name
slip_1_0[C]

Extension: [E]

Search & Replace
Search for: []
Replace with: []
 Upper/lowercase

Define counter [C]
Start at: 1
Step by: 1
Digits: 1

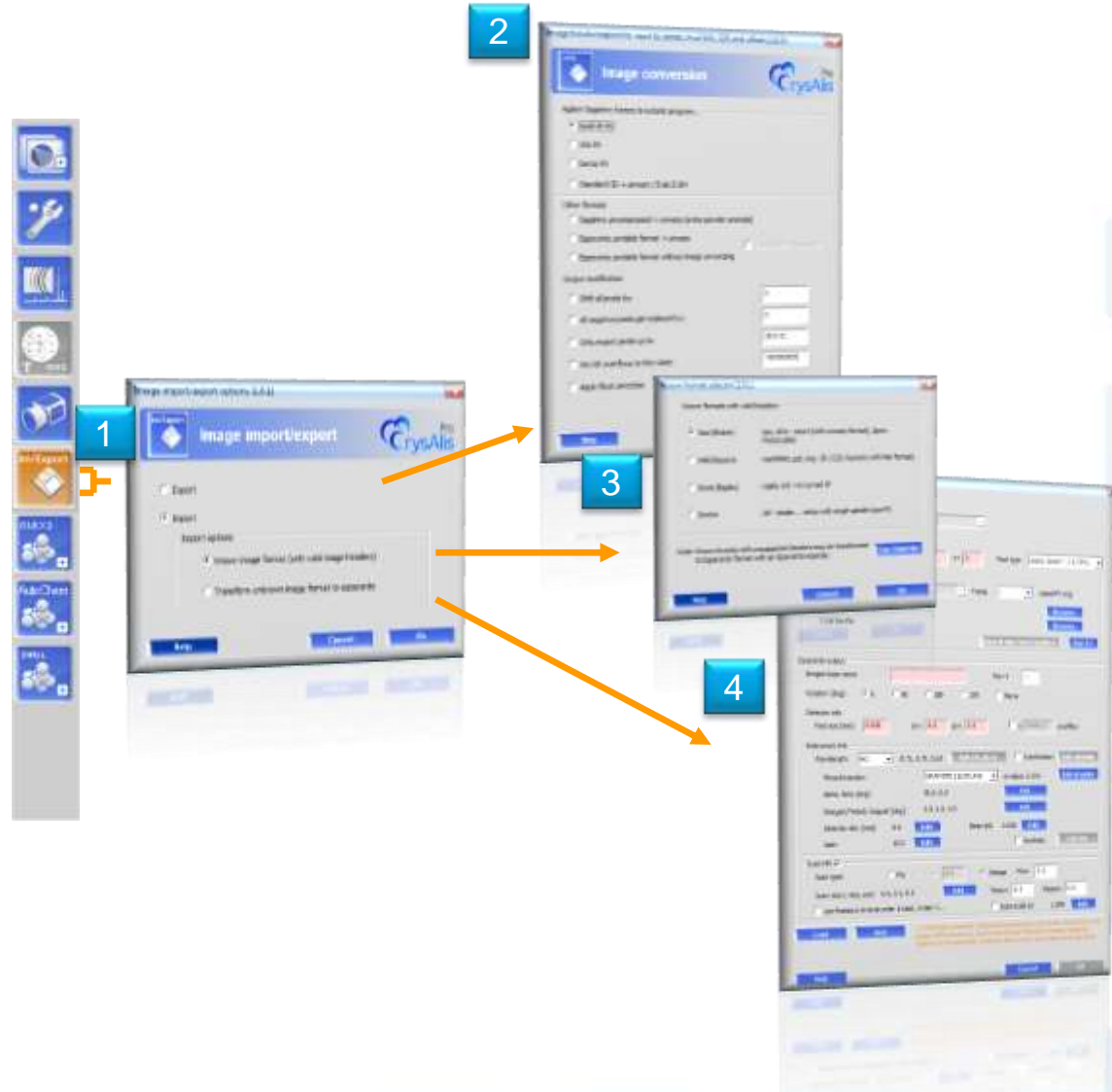
Old name	Ext.	New name	Size	Date	Location
slip_1_1.img		slip_1_01.img	271,744	02/12/2013 12:27:06	F:\Data\2013\Fraser_jump\frames\
slip_1_2.img		slip_1_02.img	271,744	02/12/2013 12:27:10	F:\Data\2013\Fraser_jump\frames\
slip_1_3.img		slip_1_03.img	271,744	02/12/2013 12:27:14	F:\Data\2013\Fraser_jump\frames\
slip_1_4.img		slip_1_04.img	271,744	02/12/2013 12:27:18	F:\Data\2013\Fraser_jump\frames\
slip_1_5.img		slip_1_05.img	271,744	02/12/2013 12:27:22	F:\Data\2013\Fraser_jump\frames\
slip_1_6.img		slip_1_06.img	271,744	02/12/2013 12:27:26	F:\Data\2013\Fraser_jump\frames\
slip_1_7.img		slip_1_07.img	271,744	02/12/2013 12:27:30	F:\Data\2013\Fraser_jump\frames\
slip_1_8.img		slip_1_08.img	271,744	02/12/2013 12:27:33	F:\Data\2013\Fraser_jump\frames\
slip_1_9.img		slip_1_09.img	271,744	02/12/2013 12:27:37	F:\Data\2013\Fraser_jump\frames\

Please press 'Start!' to start renaming!

Start! Undo Result list Close

Import tools

1. Easier access to import/export options (on power toolbar).
2. Organized export options.
3. Importing external images on one clique (instead of typing commands).
4. Esperanto importer for non standard image types.



External Frame & File Formats

Rigaku – dtrek format



Run list and aliases file generator for DTREK data collections

This dialog allows you to quickly generate a *.run file and aliases file for the data reduction of a DTREK data set!

1. Select an image, by clicking 'Browse' button in group box First dc DTREK dc file, e.g. name1001.img
2. Choose whether instrument model will be loaded from selected image header or selected par file
3. Terminator format is automatically set, but you can change it if necessary
4. Also the last image will be automatically found, but you can change it if necessary (if it is not automatically found) Note: It is assumed that all frames between these two are available
5. Save the file
 - You will be prompted for entering some critical parameters (usually default values are OK, as they are taken from image headers)
 - Finally a new CrysAlisPro instance will be launched with the DTREK data set added to the experiment list

NOTE: Using CrysAlisPro you can process only DTREK images from selected Rigaku detectors! R-AXIS format is not supported!

1. First dc DTREK dc file (*.img)

Browse

E:\data\2015\04\Alaska Images_2\MM007Cu\140304_screen0001.img

Image information: detector distance=35.00, wavelength=1.541870, centerx=244.4, centery=206.2, Si thickness=1.000mm

2. Instrument model

Use par file information instead of image header

Browse

E:\data\2015\04\Alaska Images_2\MM007Cu\140304.par

Par file information: detector distance=34.71, wavelength=1.540562, centerx=243.1, centery=204.4, beamstop type: DEF, b1=-0.019; d1=-0.052; d2=0.420; o0=90.205; t0=0.216; al=90.000; be=0.000

3. Terminator format

Run digits

0

Separator

None

Frame digits

4

140304_screenFFFF.img

4. Last dc DTREK dc file

Browse

E:\data\2015\04\Alaska Images_2\MM007Cu\140304_screen0018.img

Help

Run TC

Cancel

Save run file

Example: Apex data from ECM-Basel

- Handling of twin data...
- Dr. Daniel Kratzert (Freiburg, Germany) reduced a Bruker Apex2 twin with CAP and Saint.
- This presentation gives the workflow for importing and reducing Bruker data and handling twinning
- For the evaluation the forum version 38.43 was used.

Data set import

The image shows a file explorer window on the left displaying a directory of files named DK_ML766_01_0001 through DK_ML766_01_0035. The files are listed with their extensions (sfrm), sizes, and dates. Overlaid on the file explorer are two dialog boxes. The first is the 'Image import/export options (1.0.1)' dialog, which has a 'CRYSTALIS Pro' logo and a 'Im/Export' icon. It features radio buttons for 'Export' and 'Import', with 'Import' selected. Under 'Import options', there are two radio buttons: 'Known image format (with valid image headers)' (selected) and 'Transform unknown image format to esperanto'. The second dialog is the 'Known format selector (1.0.1)' dialog, which lists 'Known formats with valid headers': 'Dtrek (Rigaku)' (rigaku - CCD/Pilatus, no curved IP), 'MAR/Rayonix' (marNNNN, pck, img - IP, CCD, Rayonix with Mar formats), 'Saxi (Bruker)' (sax, sfrm - smart (with unwarp format), Apex, Photon50/100), and 'Dectris' (cbf - simple ... setup with single spindle type PX). A note at the bottom states: 'Note: Known formats with unsupported headers may be transformed to Esperanto format with an Esperanto importer.' Both dialog boxes have 'Help', 'Cancel', and 'Ok' buttons.

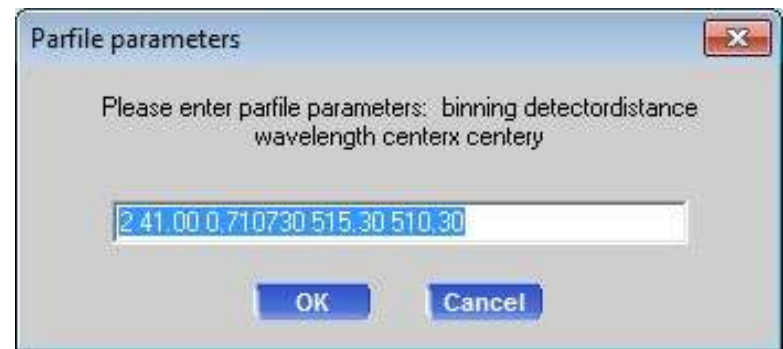
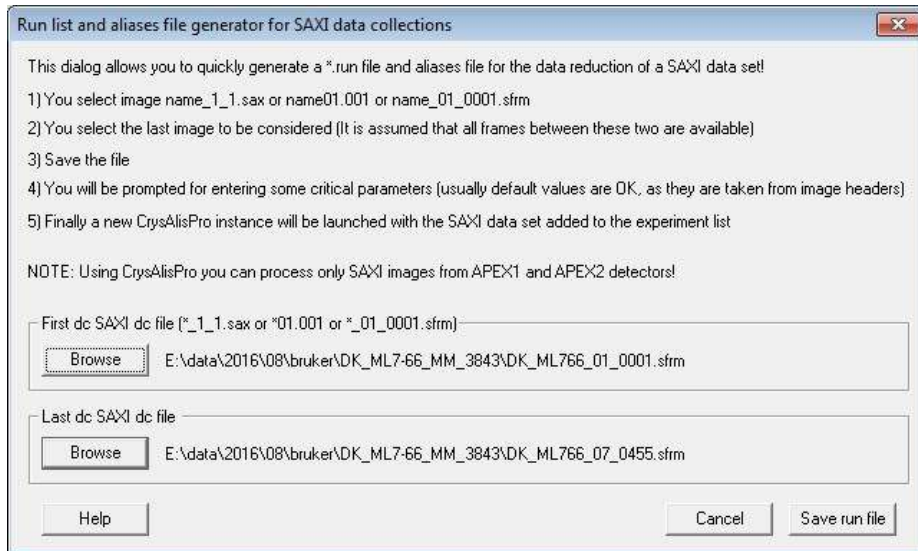
File Explorer: e:\[data] 1.125,870,680 k of 3,906,885,628 k free
e:\data\2016\08\bruker\DK_ML7-66_MM_3843*

Name	Ext	Size	Da
[.]	<DIR>	06	
DK_ML766_01_0001	sfrm	270,080	07
DK_ML766_01_0002	sfrm	270,000	07
DK_ML766_01_0003	sfrm	269,936	07
DK_ML766_01_0004	sfrm	269,952	07
DK_ML766_01_0005	sfrm	269,888	07
DK_ML766_01_0006	sfrm	269,936	07
DK_ML766_01_0007	sfrm	269,984	07
DK_ML766_01_0008	sfrm	270,016	07
DK_ML766_01_0009	sfrm	270,048	07
DK_ML766_01_0010	sfrm	270,016	07
DK_ML766_01_0011	sfrm	269,936	07
DK_ML766_01_0012	sfrm	269,888	07
DK_ML766_01_0013	sfrm	269,904	07
DK_ML766_01_0014	sfrm	270,080	07
DK_ML766_01_0015	sfrm	270,112	07
DK_ML766_01_0016	sfrm	270,016	07
DK_ML766_01_0017	sfrm	270,000	07
DK_ML766_01_0018	sfrm	270,016	07
DK_ML766_01_0019	sfrm	269,936	07
DK_ML766_01_0020	sfrm	269,920	07
DK_ML766_01_0021	sfrm	269,952	07
DK_ML766_01_0022	sfrm	269,952	07
DK_ML766_01_0023	sfrm	269,952	07-10-2011 10:40 -a
DK_ML766_01_0024	sfrm	270,048	07-10-2011 10:41 -a
DK_ML766_01_0025	sfrm	270,000	07-10-2011 10:41 -a
DK_ML766_01_0026	sfrm	269,952	07-10-2011 10:41 -a
DK_ML766_01_0027	sfrm	269,872	07-10-2011 10:41 -a
DK_ML766_01_0028	sfrm	269,856	07-10-2011 10:41 -a
DK_ML766_01_0029	sfrm	269,920	07-10-2011 10:41 -a
DK_ML766_01_0030	sfrm	269,952	07-10-2011 10:41 -a
DK_ML766_01_0031	sfrm	270,016	07-10-2011 10:41 -a
DK_ML766_01_0032	sfrm	269,920	07-10-2011 10:41 -a
DK_ML766_01_0033	sfrm	269,920	07-10-2011 10:41 -a
DK_ML766_01_0034	sfrm	269,984	07-10-2011 10:42 -a
DK_ML766_01_0035	sfrm	269,984	07-10-2011 10:42 -a

0 k / 763.252 k in 0 / 2895 file(s)

- Open any existing experiment
- Import button

Data set import



- Open any existing experiment
- Import button

Data set facts

- Mo, $I_{\mu\text{s}}$, no Si filter showing 3λ effect
- Frame width: 0.4, correlated ? Frames

CrysAlisPro run list data

Data collection mode: correlated

Total number of frames:2889 (scan: 2889, reference: 0)

Disk space: 763.79Mb

Approximate data collection time (h:min): 10:55

#	t	start	end	width	exposure	speed-rat	omega	theta	kappa	phi	# to do	# done	
1	o	1.386	184.186	0.400	5.000+	5.000	0.000	-	30.000	73.926	-0.814	456	456
2	o	-11.114	171.686	0.400	3.000+	3.000	0.000	-	17.500	73.926	4.186	456	456
3	o	21.376	163.775	0.400	3.000+	3.000	0.000	-	10.000	73.926	86.686	356	356
4	o	21.786	174.186	0.400	3.000+	3.000	0.000	-	20.000	73.926	-35.816	380	380
5	o	-28.114	126.686	0.400	5.000+	5.000	0.000	-	-27.500	73.926	11.685	386	386
6	o	18.386	179.186	0.400	4.000+	4.000	0.000	-	25.000	73.926	9.184	401	401
7	o	-7.815	174.186	0.400	3.000+	3.000	0.000	-	20.000	73.926	-60.814	454	454

First opening of the data set

- Select SM/PX nature

Open CrysAlis experiment (1.0.39) - 25 experiments available

Select experiment - standard list

Name	Path	Created	Accessed	Chemical
mrp160014	E:\data\2016\04\Newcastle Face Indexing\mrp160014_copy	Fri Feb 26 12:07:29 2016	Wed May 25 17:59:06 2016	C6 H8 O6
exp_66	E:\data\2016\04\warrick_movie_issue\exp_66_copy	Wed Apr 13 06:32:20 2016	Tue Jun 14 14:10:08 2016	???
jw2new	E:\data\2016\04\warrick_movie_issue\jw2new_copy	Sun Apr 10 08:13:28 2016	Thu Jun 16 18:40:29 2016	C20 H20 N
exp_48	C:\XcaliburData\Mathias_PX_screens\exp_48	Thu May 19 13:09:32 2016	Mon May 23 08:34:47 2016	???
150716_CudppaO2dppm	E:\data\2016\05\saturn_fixedch\FixedChi-Saturn	Mon May 30 11:07:06 2016	Mon May 30 11:07:09 2016	???
150716_CudppaO2dppm	E:\data\2016\05\saturn_fixedch\full	Mon May 30 11:20:22 2016	Mon May 30 11:20:26 2016	C300 H256
Cu_Near48mm	E:\data\2016\05\biberach\calib_XtaLAB_Mon-May-30-18-10-13-...	Mon May 30 16:11:22 2016	Tue May 31 09:57:45 2016	???
13ICR_L35_260x_2p25...	E:\data\2016\05\20160510_p300k_fr\unpack	Tue Jul 21 11:28:37 2015	Tue May 31 10:43:43 2016	C616 H965
pre_exp_5	E:\data\2016\05\biberach\email1\exp_5	Mon May 30 16:03:24 2016	Tue May 31 11:51:33 2016	???
test	E:\data\2016\05\biberach\Pierre	Tue May 31 08:51:38 2016	Tue May 31 13:33:58 2016	???
test2	E:\data\2016\05\biberach\BL_SecondDataCollection	Tue May 31 10:51:16 2016	Tue May 31 13:51:08 2016	???
data	E:\data\2016\06\Japan_Bruker_data\data	Fri Dec 18 05:03:58 2015	Fri Jul 15 10:38:45 2016	C27 H39
pre_exp_49	C:\XcaliburData\Mathias_PX_screens\exp_49	Thu Jun 16 09:12:03 2016	running	???
pre_exp_50	C:\XcaliburData\Mathias_PX_screens\exp_50	Thu Jun 16 09:16:36 2016	Wed Jul 13 17:59:30 2016	???
pre_exp_51	C:\XcaliburData\Mathias_PX_screens\exp_51	Thu Jun 16 16:06:51 2016	Thu Jun 16 16:06:51 2016	???
pre_exp_52	C:\XcaliburData\Mathias_PX_screens\exp_52	Thu Jun 16 17:49:31 2016	Mon Sep 05 12:48:04 2016	???
IBR-co-PHO A-0193-07...	E:\data\2016\07\dusek_twin\IBR-co-PHO A-0193-0721_6	Wed Jun 29 19:01:46 2016	Fri Jul 15 16:42:02 2016	C2 H2 N2
Cy_20160713_2_PAF0...	E:\data\2016\07\hypix3000\XLM_ILMages	Thu Jul 14 14:40:07 2016	Fri Jul 15 17:29:02 2016	C36 H52
MJR1918_cystiene_30...	E:\data\2016\08\george_white\MJR1918_cystiene_300_2	Thu Aug 18 14:32:15 2016	Fri Aug 19 17:47:47 2016	C11 H10 N
DK_ML766	E:\data\2016\08\bruker\DK_ML7-66_MM_3843	Tue Sep 06 17:23:54 2016	Tue Sep 06 17:23:54 2016	???

Hide pre experiments
Hide screenings

Displaying information
 Standard Volume, laue, wavelength, Rint, redundancy Protein screening Custom columns [Change columns](#)

List: Standard [>>](#) [Delete](#) [Rename](#)

[Help](#) [Multiple addition](#) [Browse experiment](#) [Delete experiment\(s\)](#) [Open selected](#)

CrysAlis RED program options (1.1.4)

SM/PX Small Molecule Protein

Lattice finding / Data reduction
Min lattice size: 2, max lattice size: 125
Use pre-emptive SM indexing [400 ref., 5.0s]
Used options: completeness after data red., 2nd cycle in 3D peak analysis, BG determination (GRL) after data red., concurrent data red. used, min frames for do red < 25

Data collection / Strategy
Max automate exposure time (sec): 450, default completeness: 100.0%, 1 sig for max. res. prediction: 2.0
Used options: overlap computation type: complex

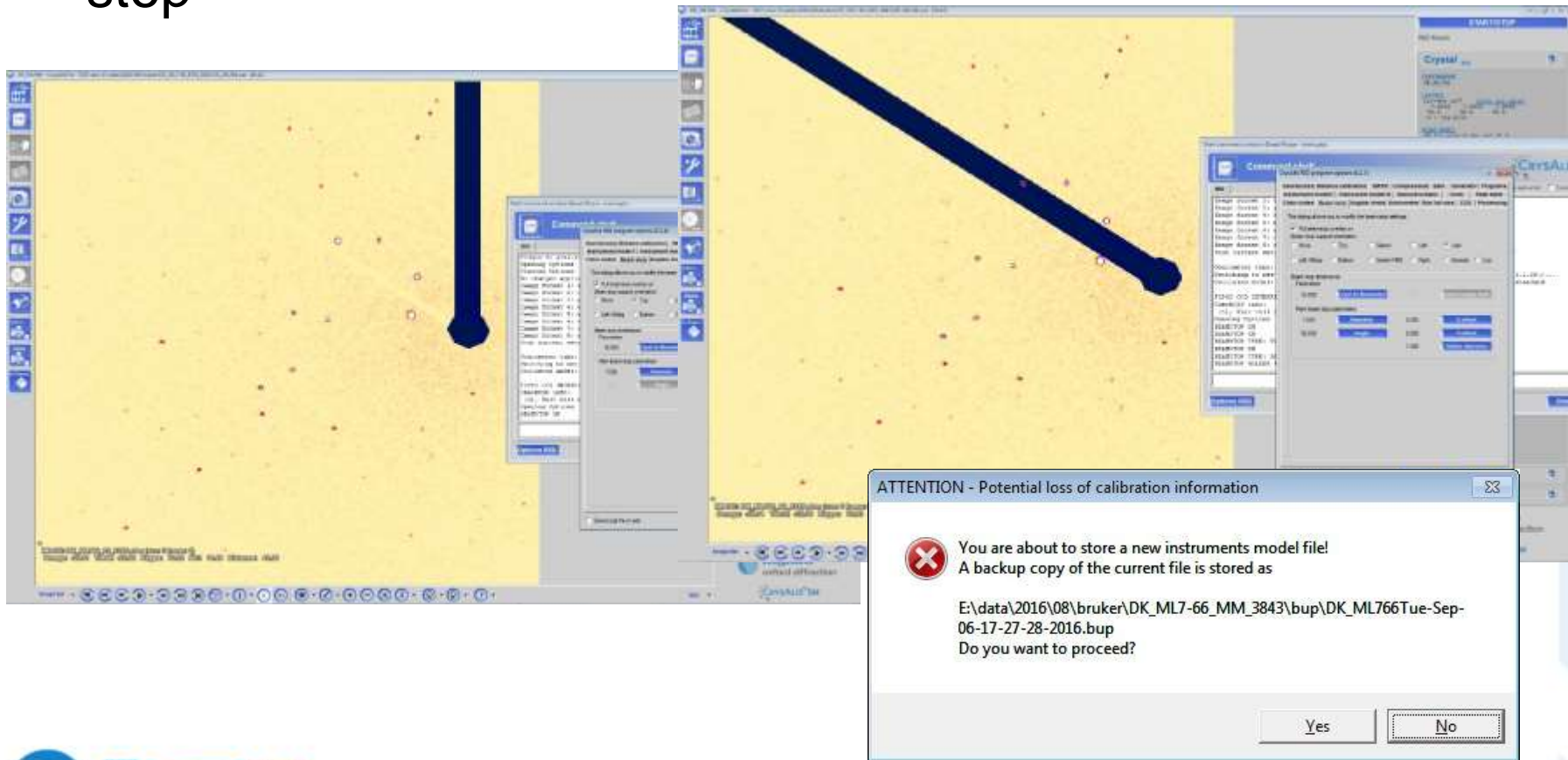
DC JETSHADOW (to realize beforehand use beamstop mask)
DC JETSHADOW not used

[Edit options](#)

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

Set the beam stop

- Apex system sometimes use a user angle for the beam stop



First peak hunting

- Use default

The screenshot displays the 'Lattice wizard' software interface. The main window shows a diffraction pattern with a central spot and surrounding spots. A blue arrow points to the 'Peak hunting' button in the toolbar. The interface includes several panels:

- LATTICE**: Current cell (a, b, c, alpha, beta, gamma) and Lattice reduction status.
- PEAK TABLE**: User-loaded table and 0 obs out of 0 (total: 0, skipped: 0).
- INSTRUMENT MODEL**: Goniometer, Detector, and Wavelength Mo (Ang) parameters.
- Toolbars**: Peak hunting, Unit cell finding, Ewald explorer - reciprocal space, Refine instrument model, Twinning - multi-crystals, Load information, Unwarping - Precession images, and Log window.
- Right Panel**: Crystal information, Data Collection, and Data Reduction options.

Automatic unit cell finding

- Use default, 66% indexed, in spite of slightly off model

Lattice wizard (1.0.33)

Lattice wizard

LATTICE

Current cell (CSD: not done)
8.1341(7) 9.4250(10) 11.6001(13) 79.290(9) 82.878(8) 79.555(8) 855.58(15)

Lattice reduction
selected cell
8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 aP 31
reduced cell
8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 855.4

PEAK TABLE

Peak hunting table
UB fit with 8408 obs out of 12728 (total:12728,skipped:0) (66.06%)

INSTRUMENT MODEL

Goniometer
beam: -0.01932 alpha: 50.05613 beta: 0.00000
om zero: 0.04303 th zero: -0.32229 ka zero: 0.00000
Detector
x-rot: 0.48390 y-rot: 0.13904
x-cen: 515.30000 y-cen: 510.30000 distance: 41.00000
Wavelength Mo (Ang): A1 0.70930 A2 0.71359 B1 0.63229

CRYALIS^{Pro}

Peak hunting
Unit cell finding
Ewald explorer - reciprocal space
Reindexation with current cell
Refine instrument model
Lattice transformation

Compare data with CSD (1.1.0)

Check CSD and local database

Current cell (#1) (aP: 9= 858.5; 8.15 9.43 11.62; 79.4 82.8 79.6; 1 hrd)

Current cell (#1)
Lattice centering: aP
8.1479 9.4331 11.6046 79.4332 82.7719 79.5403 858.5259

Data sent to CSD
Lattice centering: aP
8.1479 9.4331 11.6046 79.4332 82.7719 79.5403 858.5259

CSD v. 2015-03-20 02:43

No.	Cell no.	Volume	a	b	c	alpha	beta	gamma	Formula	Symm	Origin name	Dist. Y	More info	
<input checked="" type="checkbox"/>	1	100.0%	898.7	8.15	9.43	11.62	79.4	82.7	79.6	C23H21N3O1	P-1	CSD: VAWXK	858.7	CCDC0959Cell

Information
Searching completed.

CSD tools
Select all | Deselect all | Show in Memory | Go To WebCIS (license required) | Close

First instrument model refinement

- The header info is not precise. Refine on full data.
- Use default

Lattice wizard (1.0.33)

Lattice wizard

LATTICE
Current cell (CSD: not done)
8.1341(7) 9.4250(10) 11.6001(13) 79.290(9) 82.878(8) 79.555(8) 855.58(15)
Lattice reduction
selected cell
8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 aP 31
reduced cell
8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 855.4

PEAK TABLE
Peak hunting table
UB fit with 8408 obs out of 12728 (total:12728,skipped:0) (66.06%)

INSTRUMENT MODEL
Goniometer
beam: -0.01932 alpha: 50.05613 beta: 0.00000
om zero: 0.04303 th zero: -0.32229 ka zero: 0.00000
Detector
x-rot: 0.48390 y-rot: 0.13904
x-cen: 515.30000 y-cen: 510.30000 distance: 41.00000
Wavelength Mo (Ang): A1 0.70930 A2 0.71359 B1 0.63229

Lattice wizard (1.0.33)

Lattice wizard

LATTICE
Current cell (CSD: not done)
8.1480(3) 9.4339(6) 11.6071(4) 79.434(4) 82.776(3) 79.625(4) 858.76(7)
Lattice reduction
selected cell
8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 aP 31
reduced cell
8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 855.4

PEAK TABLE
Peak hunting table
UB fit with 8602 obs out of 12728 (total:12728,skipped:0) (67.58%)

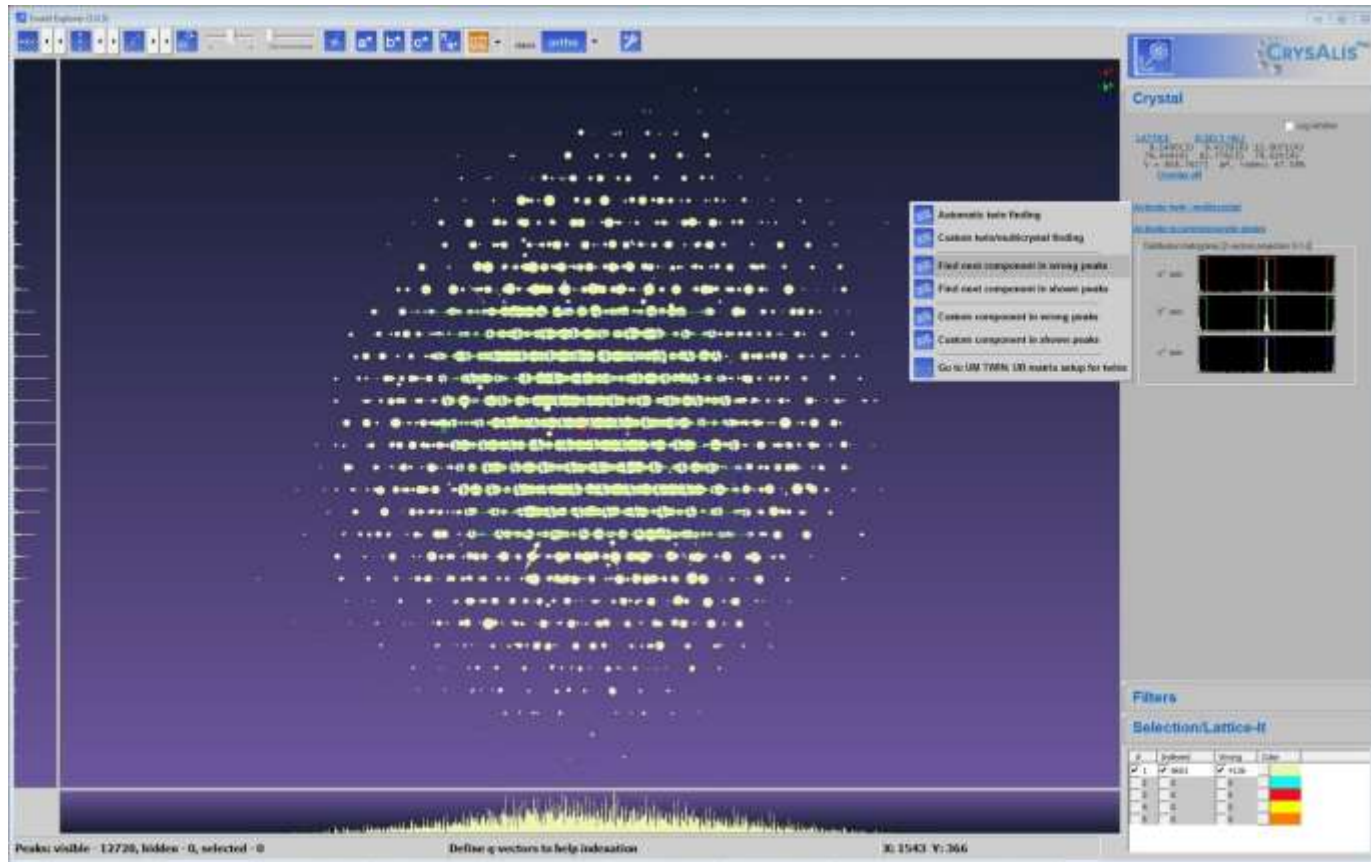
INSTRUMENT MODEL
Goniometer
beam: 0.12847 alpha: 50.05613 beta: 0.00000
om zero: -0.01105 th zero: 0.10058 ka zero: 0.00000
Detector
x-rot: 0.05131 y-rot: 0.24013
x-cen: 520.21123 y-cen: 507.31092 distance: 41.12325
Wavelength Mo (Ang): A1 0.70930 A2 0.71359 B1 0.63229
Refinement
res: 0.010877, ds=0.006531, sx=0.002067, sy=0.002304
h=0.003394, k=0.006851, l=0.002762
#ref: 8565 (skipped: 34)

CRYALIS™

Peak hunting
Unit cell finding
Ewald explorer - reciprocal space
Reindexation with current cell
Refine instrument model
Lattice transformation
Twinning - multi-crystals
Incommensurates / Quasi-crystals
Load information
Save information
Unwrapping - Precession images
Log window
Close

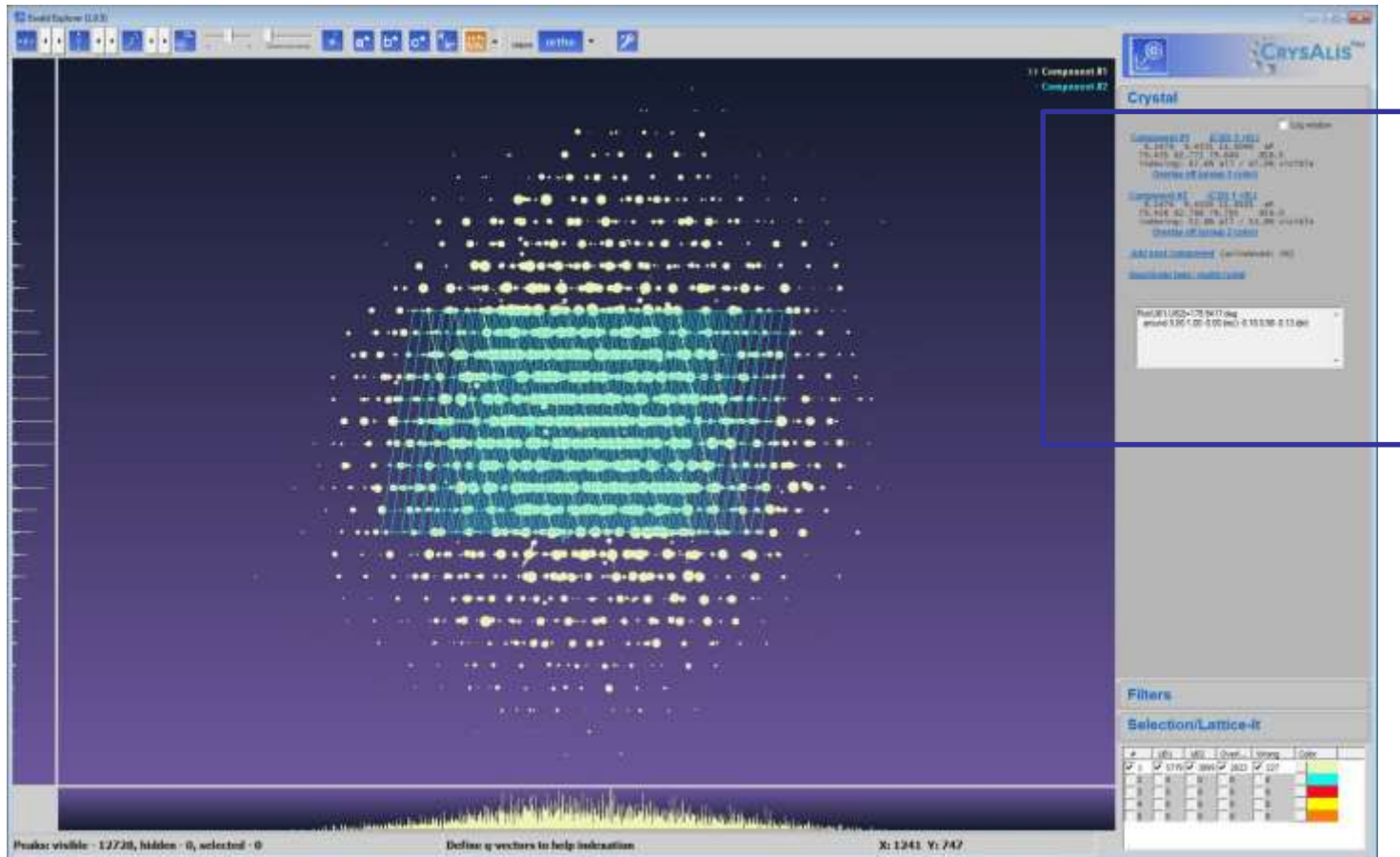
Use EwaldPro to find the twin

- Find next component in wrong peaks



Use EwaldPro to find the twin

- Easy: 180 deg rotation twin



Use EwaldPro to find the twin

- Back to lattice wizard...

Lattice wizard (1.0.33)

Lattice wizard

LATTICE

Current cell (CSDP: 1, 0, 0)

8.1480(3) 9.4341(6) 11.6071(4) 79.433(4) 82.776(3) 79.626(4) 858.78(7)

Lattice reduction

selected cell

8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 ap 31

reduced cell

8.1340 9.4225 11.6005 79.2946 82.9556 79.5359 855.4

Twin information

1: 8.1479 9.4331 11.6046 79.435 82.772 79.640 858.5

2: 8.1474 9.4324 11.6101 79.426 82.788 79.705 859.0

1: Total: 8602(67.6%) Separate: 5779(45.4%) Overlapped: 2823(22.2%)

2: Total: 6722(52.8%) Separate: 3899(30.6%) Overlapped: 2823(22.2%)

Unindexed: 227 (1.8%)

PEAK TABLE

Peak hunting table

UB fit with 8603 obs out of 12728 (total:12728,skipped:0) (67.59%)

INSTRUMENT MODEL

Goniometer

beam: 0.12847 alpha: 50.05613 beta: 0.00000

om zero: -0.01105 th zero: 0.10058 ka zero: 0.00000

Detector

x-rot: 0.05131 y-rot: 0.24013

x-cen: 520.21123 y-cen: 507.31092 distance: 41.12325

Wavelength Mo (Ang): A1 0.70930 A2 0.71359 B1 0.63229

Refinement

res: 0.010877, da=0.006531, sx=0.002067, sy=0.002304

h=0.003394, k=0.006851, l=0.002762

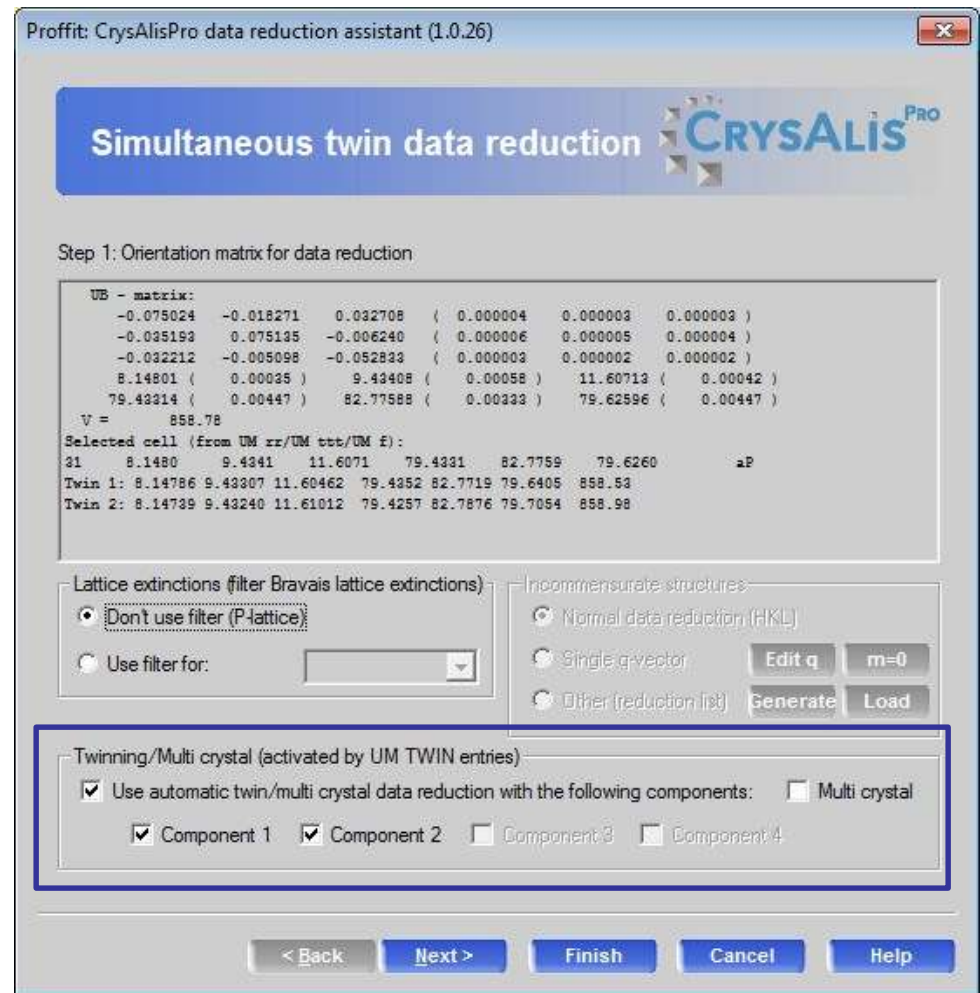
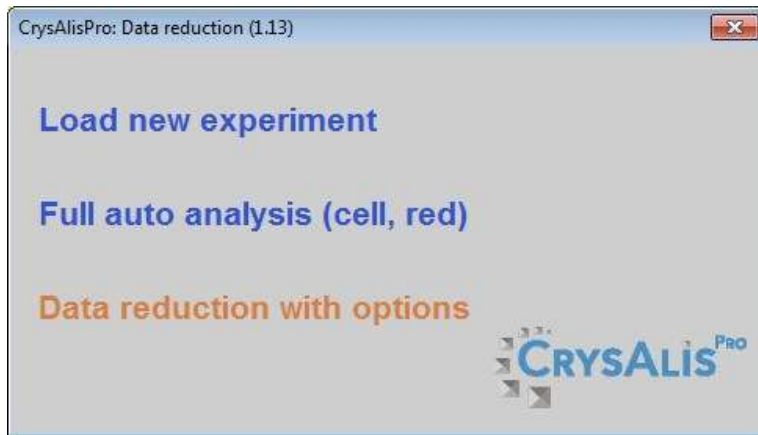
#ref: 8565 (skipped: 34)

CRYSALIS™

- Peak hunting
- Unit cell finding
- Ewald explorer - reciprocal space
- Reindexation with current cell
- Refine instrument model
- Lattice transformation
- Twinning - multi-crystals
- Incommensurates / Quasi-crystals
- Load information
- Save information
- Unwarping - Precession images
- Log window
- Close

Do twin data reduction

- Run the data reduction wizard. Twin reduction auto set...



Do twin data reduction

- Accept the run list

Proffit: CrysAlisPro data reduction assistant (1.0.26)

Simultaneous twin data reduction

CRYALIS^{Pro}

Step 2: Experiment run list for data reduction

Run list: E:\data\2016\08\bruker\DK_ML7-66_MM_3843\DK_ML766

Image dir: E:\data\2016\08\bruker\DK_ML7-66_MM_3843

*.sfm

#	type	start	end	width	exposure	omega	detector	kappa	phi	start	end
1	o	1.39	184.19	0.40	5.00	-	30.00	73.93	-0.81	1,	456
2	o	-11.11	171.69	0.40	3.00	-	17.50	73.93	4.19	1,	456
3	o	21.38	163.78	0.40	3.00	-	10.00	73.93	86.69	1,	356
4	o	21.79	174.19	0.40	3.00	-	20.00	73.93	-39.82	1,	380
5	o	-28.11	126.69	0.40	5.00	-	-27.50	73.93	11.69	1,	386
6	o	18.39	179.19	0.40	4.00	-	25.00	73.93	9.18	1,	401
7	o	-7.81	174.19	0.40	3.00	-	20.00	73.93	-60.81	1,	454

By default the whole experiment will be evaluated. To modify this behaviour edit the run list -->

Edit start num of selected run

Edit end num of selected run

< Back Next > Finish Cancel Help

Do twin data reduction

- Special pars: All default; Limit the data to 0.75Ang (as done in the B set)

The screenshot displays the 'Profit: CrysAlisPro data reduction assistant (1.0.26)' interface. The main window is titled 'Simultaneous twin data reduction' and shows 'Step 3: Basic algorithm parameters'. A 'Resolution limits' dialog box is open, showing the 'd-value (Ang)' parameter set to 'inf' and '0.750'. The 'Edit high limit' button is highlighted. The 'Profit special parameters' dialog box is also open, showing the 'Use resolution limits' checkbox checked and the 'd-value (Ang)' set to 'inf-0.75' and '2theta (deg)' set to '0.00-56.44'. The 'Edit limits' button is highlighted. The 'Resolution limits' dialog box also shows 'Theta (deg)' set to '0.000' and '2 Theta (deg)' set to '0.000'. The 'Edit high limit' button is highlighted. The 'Resolution limits' dialog box also shows 'OK' and 'Cancel' buttons.

Resolution limits

Parameter to enter: d-value (Ang)

Edit low limit Edit high limit

d-value (Ang):	inf	0.750
Theta (deg):	0.000	28.221
2 Theta (deg):	0.000	56.441

OK Cancel

Profit special parameters

3D intensity integration

Reflection positioning and integration

Skip filters

Use resolution limits Edit limits

d-value (Ang): inf-0.75

2theta (deg): 0.00-56.44

Reject reflections with bad profiles (e.g. for HP data)

High > 10 & Profile agreement < 0.8

Extraction rules

DC JETSHADOW (to visualize beforehand use beamstop mask)

Profile fitting

Override integration mask size (generally not recommended, but smaller mask can be useful for strongly overlapping reflections e.g. bins)

Follow profile size changes with incidence angle

Print average profiles to history window

OK Cancel

Step 3: Basic algorithm parameters

Reflection position prediction Skip model refinement

Auto select optimal prediction approach on run

Follow model changes on frame by frame based on model

Follow significant sample wobbling (2-cycle 3D profile)

Follow sudden (discontinuous) changes of sample

Orientation search range (max 1.0 deg) 2.00

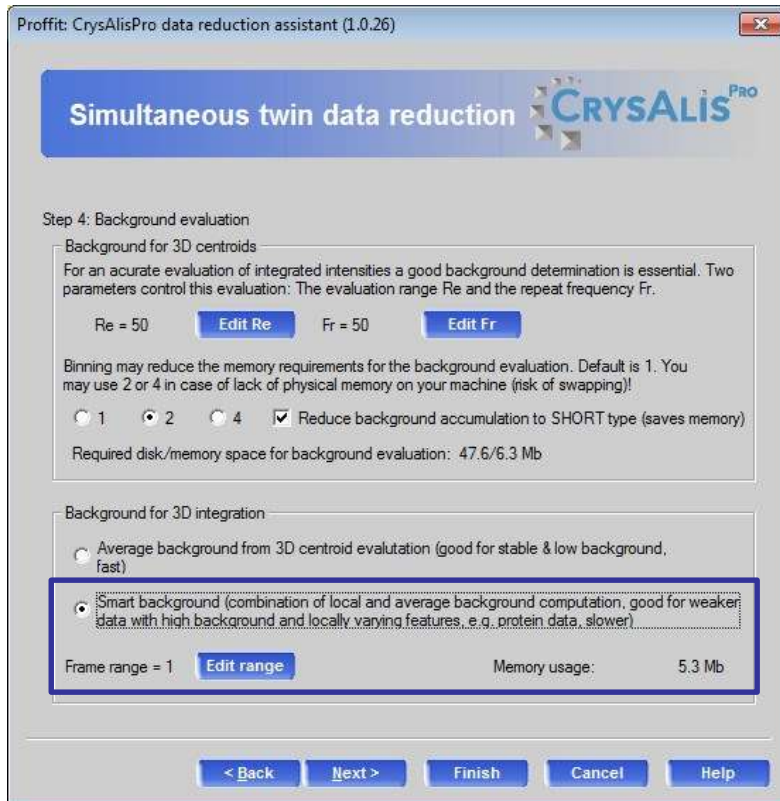
Edit special pars

Clear data from previous run

< Back Next > Finish Cancel Help

Do twin data reduction

- Background: Smart background



This is the most critical for the data set: It seems that the Apex detector has unstable background, thus introducing a bias on the average background method. Such behavior is also seen with other detectors where CAP uses by default Smart background.

Do twin data reduction

- Automatic outlier rejection: default

Proffit: CrysAlisPro data reduction assistant (1.0.26)

Simultaneous twin data reduction 

Step 5: Outlier rejection

CCD data sets usually contain more than the unique data required for the structure determination. This redundant data can be used to check for measurement outliers.
The rejection is based on R. Blessing (1997), J. Appl. Cryst. and additional CCD specific criteria.

Outlier rejection:

Don't use outlier rejection

Use outlier rejection

1

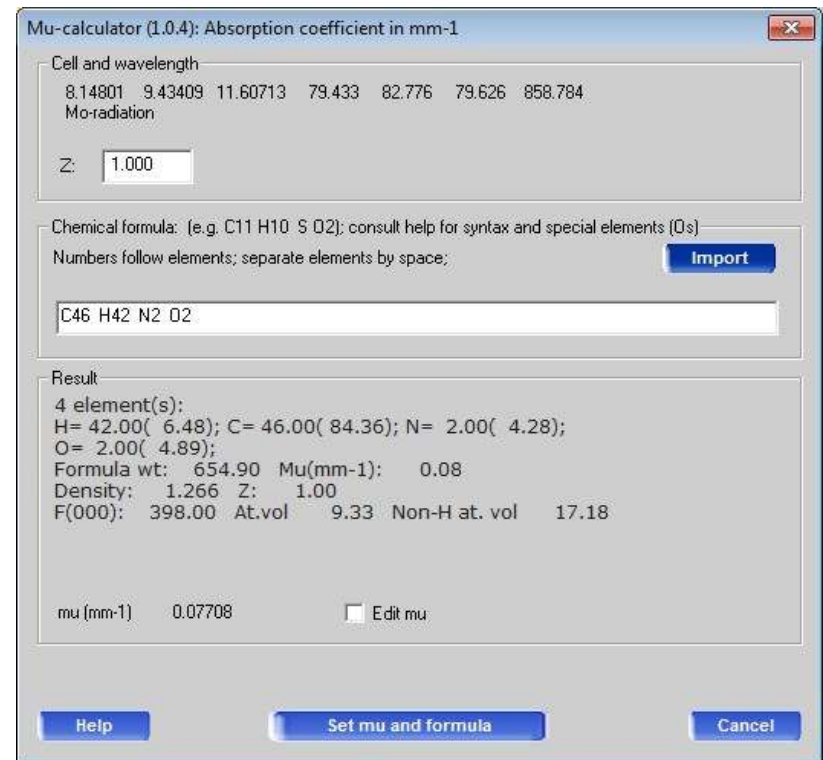
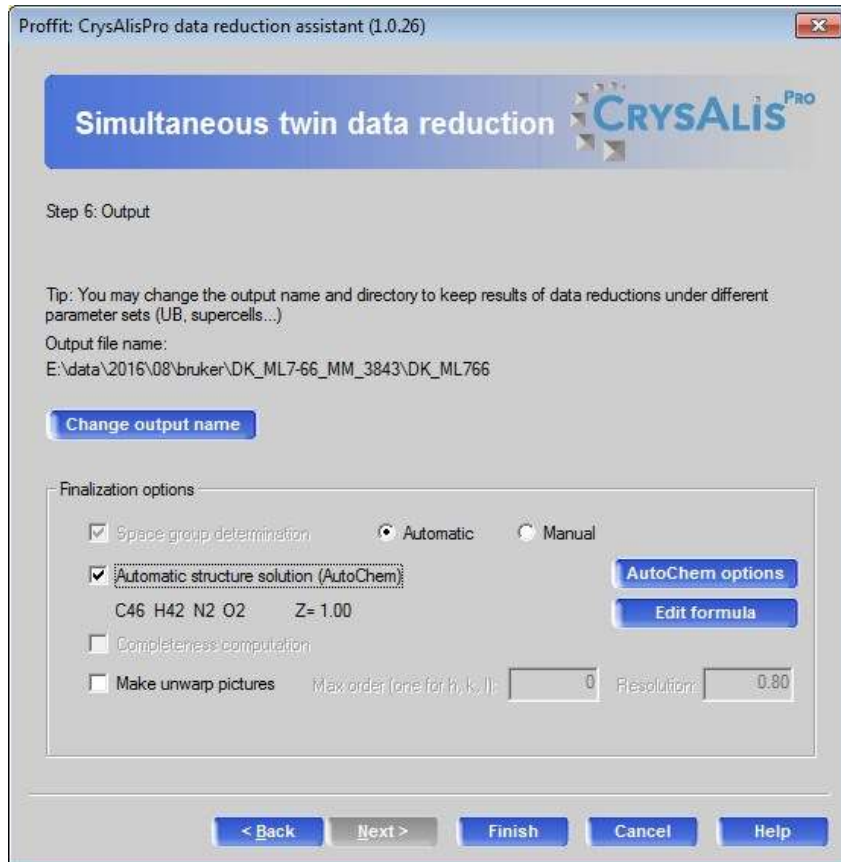
aP 8.14801 9.43408 11.60713 79.43314 82.77588 79.62596

Use Friedel mates as equivalent

< Back Next > Finish Cancel Help

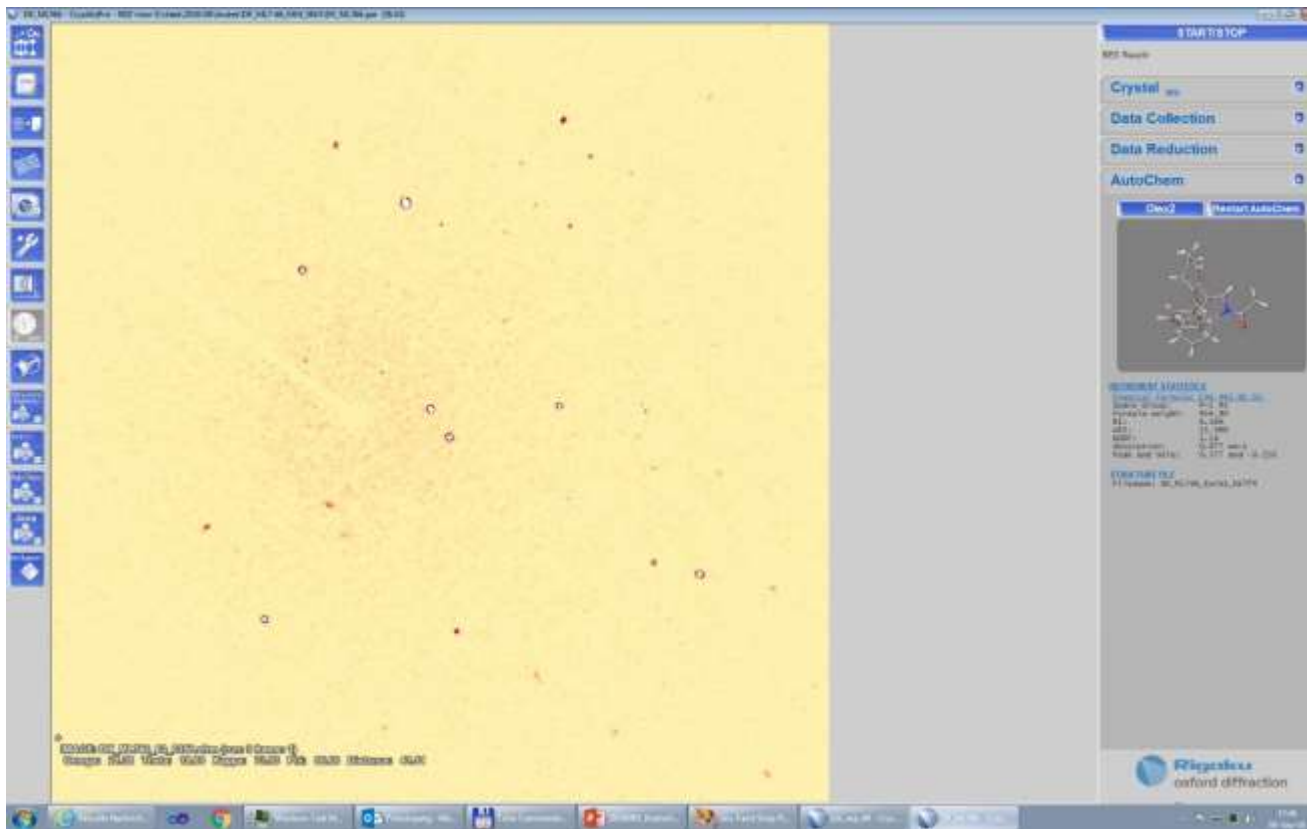
Do twin data reduction

- Chem. formula imported for AutoChem



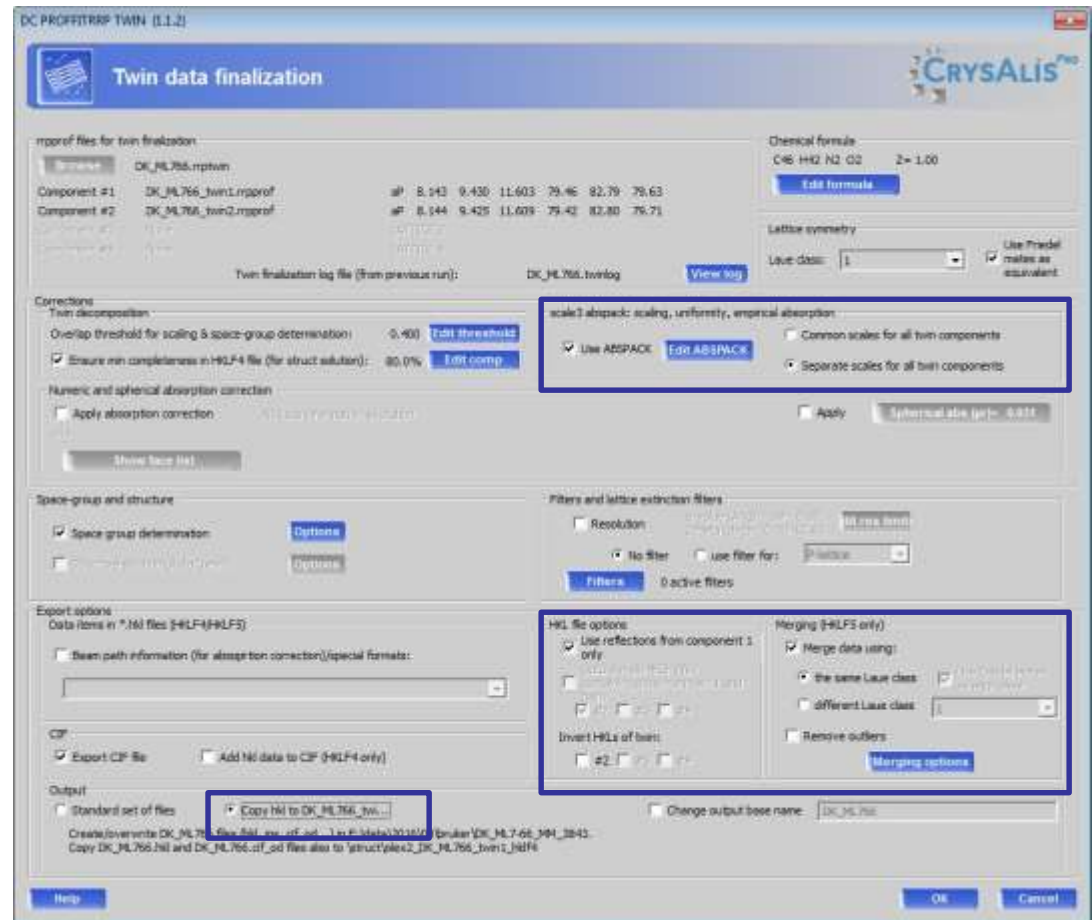
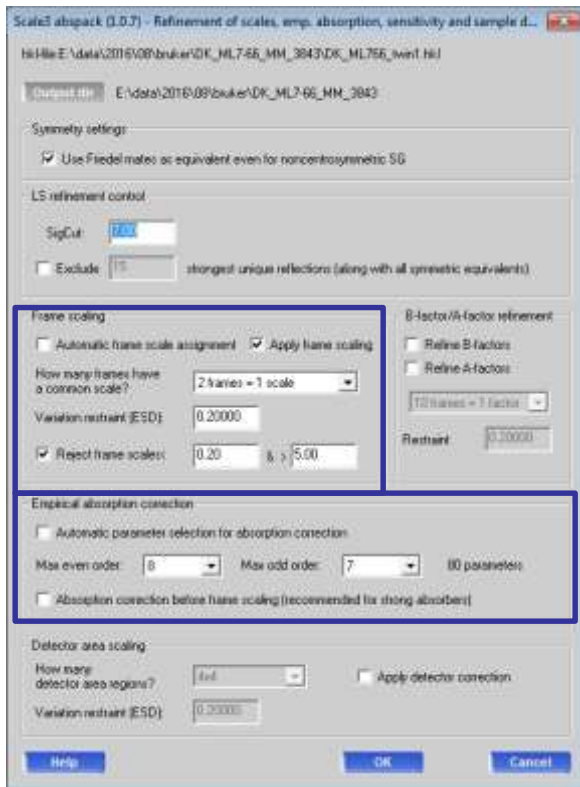
Automatic result

- Auto: based on all hklf4 data.



Tuning your result

- Tuning means what kind of scaling is used and what reflection classes are in the final hklf4 and 5 files



HKLF5 result

The image shows a screenshot of a crystallographic software interface. In the foreground, a 3D ball-and-stick model of a complex organic molecule is displayed, featuring a central blue nitrogen atom and several yellow sulfur atoms. A dialog box titled "Twin refinement options" is open on the left side of the screen. The dialog box contains the following information:

Twin refinement options

Twin refinement method

- Refine structure on whole data set (HKLF5)
- Refine structure on first component only (HKLF4)
- Refine structure on second component only (HKLF4)
- Refine structure on third component only (HKLF4)
- Refine structure on fourth component only (HKLF4)

Information

INS file: ...plex2_DK_ML766_twin1_hklf4\DK_ML766_twin1_hklf4.ins,
HKL file: ...plex2_DK_ML766_twin1_hklf4\DK_ML766_twin1_hklf5.hkl
INS file will be modified with BASF and HKLF 5 instructions.

Refine on exit

Buttons: OK, Cancel

The background interface shows a sidebar with various tool icons and a panel on the right displaying crystallographic data:

STAR T18 TOP

RED Allocation: Finished

Assign Crystal ...

Data Collection

Data Reduction

Structure Explorer

SG: P-1
R1: 5.18%

Peak and hole: 0.47, 0.2

lvs: 0.000, 1.154
Hklwidth: 1.85, 7

$C_{22}H_{21}N_4O_4$

Atom update weights: ON
Weights: 0.027, 0.007
Scale factor: 0.000
Tune ratio: 0.302
Absorption: 0.077 mm⁻¹

Cell and Z
a, b, c (Å): 8.408(4), 8.408(4), 22.829(7)
α, β, γ (°): 90.000(1), 90.000(1), 90.000(1)
Z: 4

Structure solved (see file):
-DK_ML766_twin1_hklf4.ins
-DK_ML766_twin1_hklf5.hkl

Buttons: OK, H, H+, H-, Q to C, O, C, H, H+, H-, Q to C, O, C

Buttons: Refine, Complete, AutoAssign (ATA), History, Ins, Grid, Task

Generic image format 'Esperanto' generator

- Use of Esperanto format for unknown image formats with no compression or known formats with strange instrument configs
- Esperanto fully supports 4 circle instruments.
- Command 'dc rit' rit = raw image transform.
- But it also supports the known formats to handle 'unusual', obstinate images.
- Pixel detectors have an automatic dead zone detection based on the special value -1.
- The Esperanto generator uses a proprietary Agilent bit field format. To get back the uncompressed Esperanto version, please use the export function.

Esperanto with bit field compression and pixel detector support

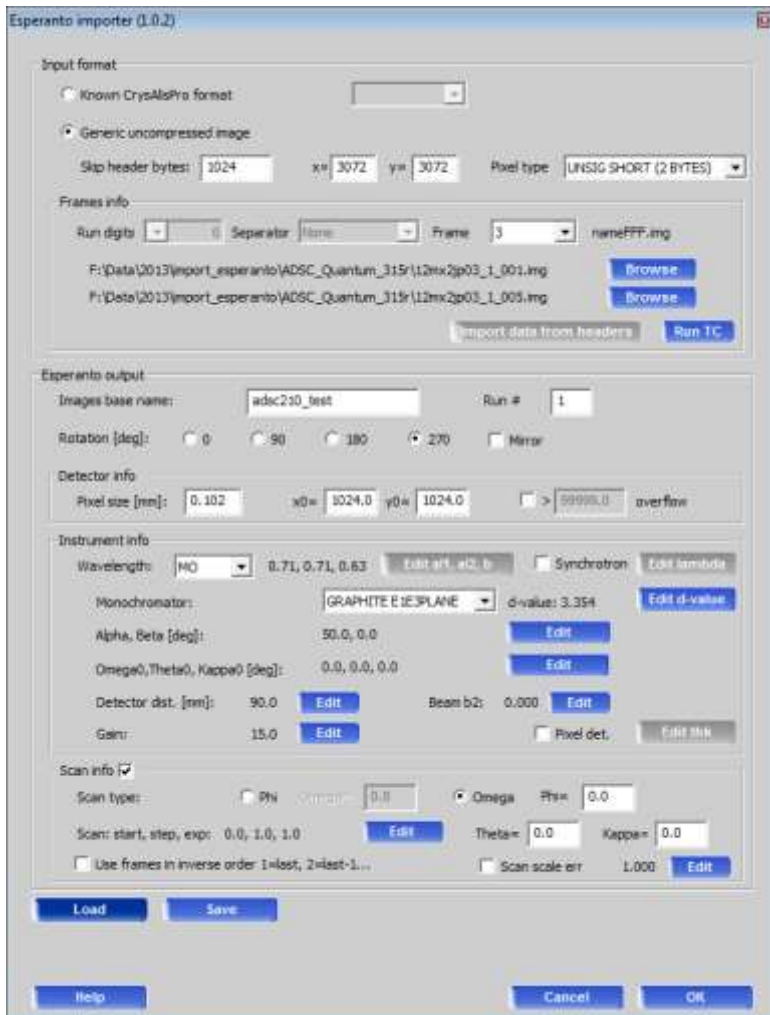
- For our Esperanto importer we now can use Agilent bitfield compression for Esperanto files. The format is not documented yet.
- There was also a pixel detector flag added to support the implemented pixel detector corrections (`[dsithicknessmmmforpixeldetector]` - thickness of Si for pixel detectors; the presence of this number signals a pixel detector. Pixel detector gap zones are marked with `-1`).
- Publication describes the Esperanto format

Single-crystal diffraction at the Extreme Conditions beamline P02.2: procedure for collecting and analyzing high-pressure single-crystal data

André Rothkirch, G. Diego Gatta, Mathias Meyer, Sébastien Merkel, Marco Merlini and Hanns-Peter Liermann

J. Synchrotron Rad. (2013). **20**, 711–720

Dc rit: ADSC 315



- Command dc rit
- Header bytes 1024, x 3072 y 3072 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

Dc rit: ADSC 210

Esperanto importer (1.0.2)

Input format

Known OryxAsPro format

Generic uncompressed image

Skip header bytes: 1024 x= 2048 y= 2048 Pixel type: UNSIG SHORT (2 BYTES)

Frames info

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

F:\Data\2013\import_esperanto\ADSC_Quantum_210\12mx1p05_1_001.img [Browse](#)

F:\Data\2013\import_esperanto\ADSC_Quantum_210\12mx1p05_1_005.img [Browse](#)

[Import data from headers](#) [Run TC](#)

Esperanto output

Images base name: adsc210_test Run #: 1

Rotation [deg]: 0 90 180 270 Mirror

Detector info

Pixel size [nm]: 0.102 x0= 1024.0 y0= 1024.0 > 99999.0 overflow

Instrument info

Wavelength: MO 0.71, 0.71, 0.63 [Edit all, all, n](#) Synchrotron [Edit lambda](#)

Monochromator: GRAPHITE EIE3PLANE d-value: 3.354 [Edit d-value](#)

Alpha, Beta [deg]: 50.0, 0.0 [Edit](#)

Omega0, Theta0, Kappa0 [deg]: 0.0, 0.0, 0.0 [Edit](#)

Detector dist. [mm]: 72.0 [Edit](#) Beam b2: 0.000 [Edit](#)

Gain: 15.0 [Edit](#) Pixel det. [Edit this](#)

Scan info

Scan type: Phi Omega Phi= 0.0

Scans start, step, exp: 0.0, 1.0, 1.0 [Edit](#) Theta= 0.0 Kappa= 0.0

Use frames in inverse order 1=last, 2=last-1... Scan scale err: 1.000 [Edit](#)

[Load](#) [Save](#)

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

- Command dc rit
- Header bytes 1024, x 2048 y 20482 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

Dc rit: MAR165ccd

- Command dc rit
- Known format MAR (mccd)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

Esperanto importer (1.0.2)

Input format

Known CrysAlisPro format MAR marNNNN, pck, img

Generic uncompressed image

Skip header bytes: 0 x= 2048 y= 2048 Pixel type: UNSIG SHORT (2 BYTES)

Frames info

Run digits: 0 Separator: None Frame: 3 nameFFF.img

F:\Data\2013\import_esperanto\MarCCD165\data_01_001.mccd Browse

F:\Data\2013\import_esperanto\MarCCD165\data_01_010.mccd Browse

Import data from headers Run TC

Esperanto output

Images base name: data_01_ Run #: 1

Rotation [deg]: 0 90 180 270 Mirror

Detector info

Pixel size [mm]: 0.079 x0= 1035.0 y0= 1031.0 > 99999.0 overflow

Instrument info

Wavelength: CU 1.54, 1.54, 1.39 Edit a1, a2, b Synchrotron Edit lambda

Monochromator: GRAPHITE E1E3PLANE d-value: 3.354 Edit d-value

Alpha, Beta [deg]: 50.0, 0.0 Edit

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

Detector dist. [mm]: 90.0 Edit Beam b2: 0.000 Edit

Gain: 1.0 Edit Pixel det. Edit thk

Scan info

Scan type: Phi Omega= 57.0 Omega Phi= 75.0

Scan start, step, exp: 75.0, 1.0, 20.0 Edit Theta= 0.0 Kappa= -134.0

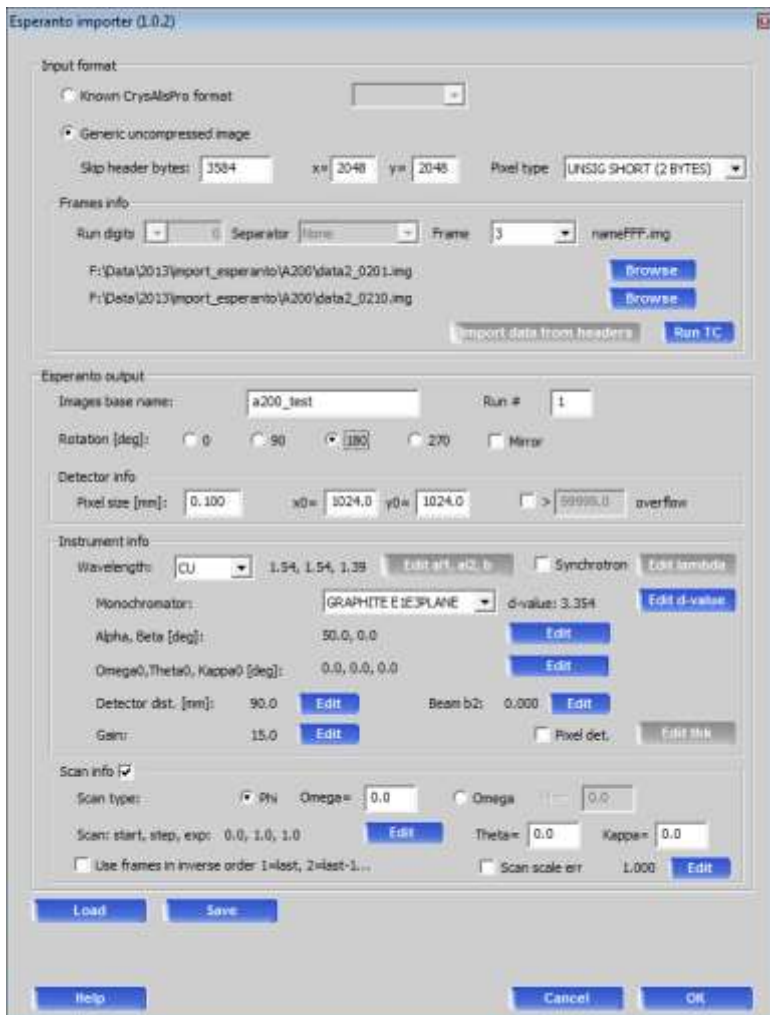
Use frames in inverse order 1=last, 2=last-1,...

Scan scale err 1.000 Edit

Load Save

Help Cancel OK

Dc rit: A200 detector



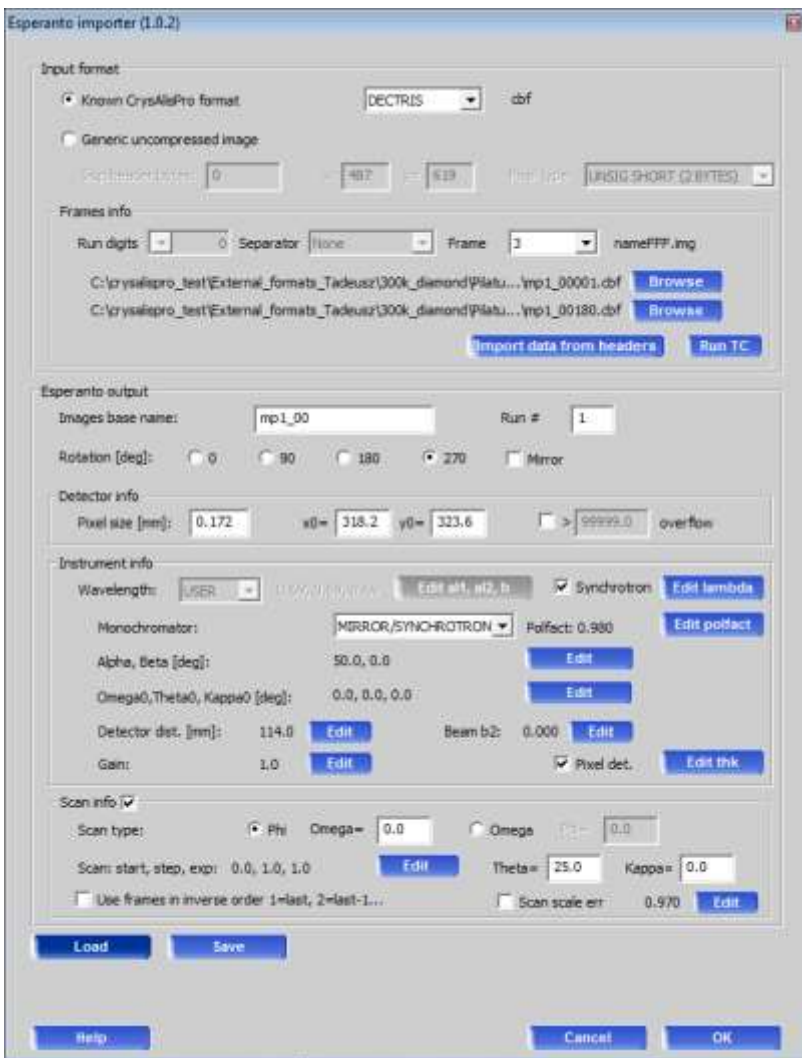
- Command dc rit
- Header bytes 3584, x 2048 y 20482 and other info from text header (f.ex with total commander)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.

Dc rit: Diamond ID 19 Dectris turned



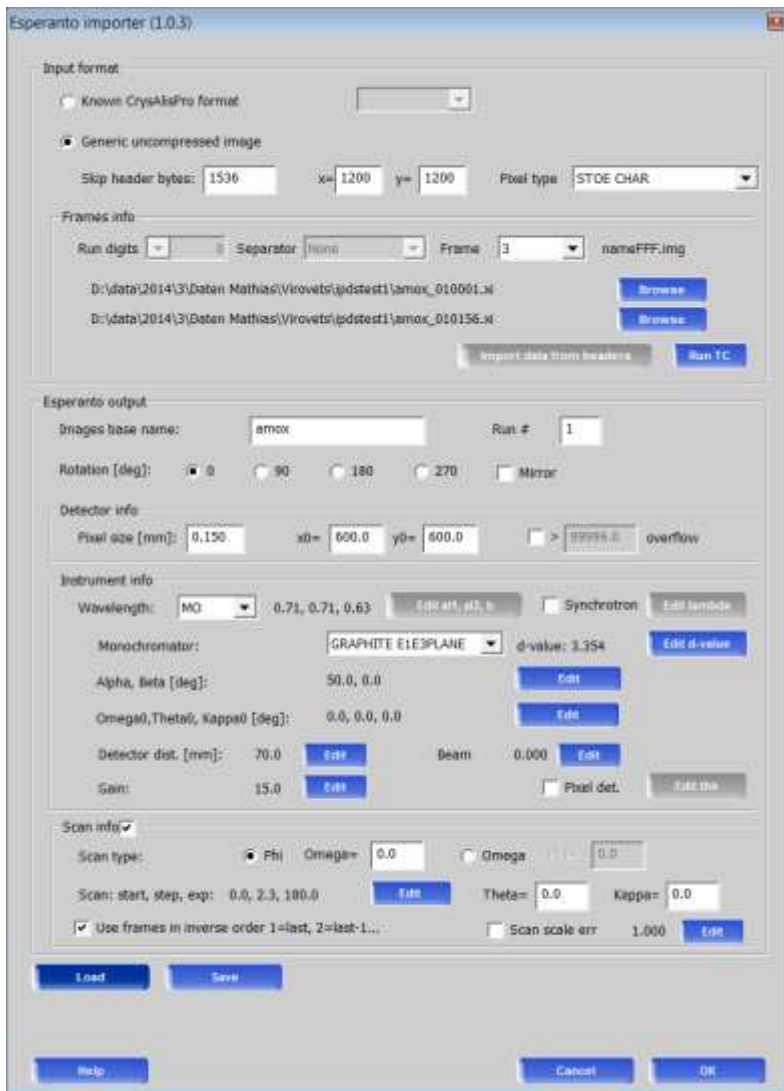
- Command dc rit
- Use of known format dectris. Header values are read.
- Camera turned 270deg. Non-square detector is padded by zeros.
- The header scan values are wrong by 3% (Scan scale err 0.97)
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.
- The several cycles to refine instrument model.

Dc rit: Diamond ID 19 Dectris turned II



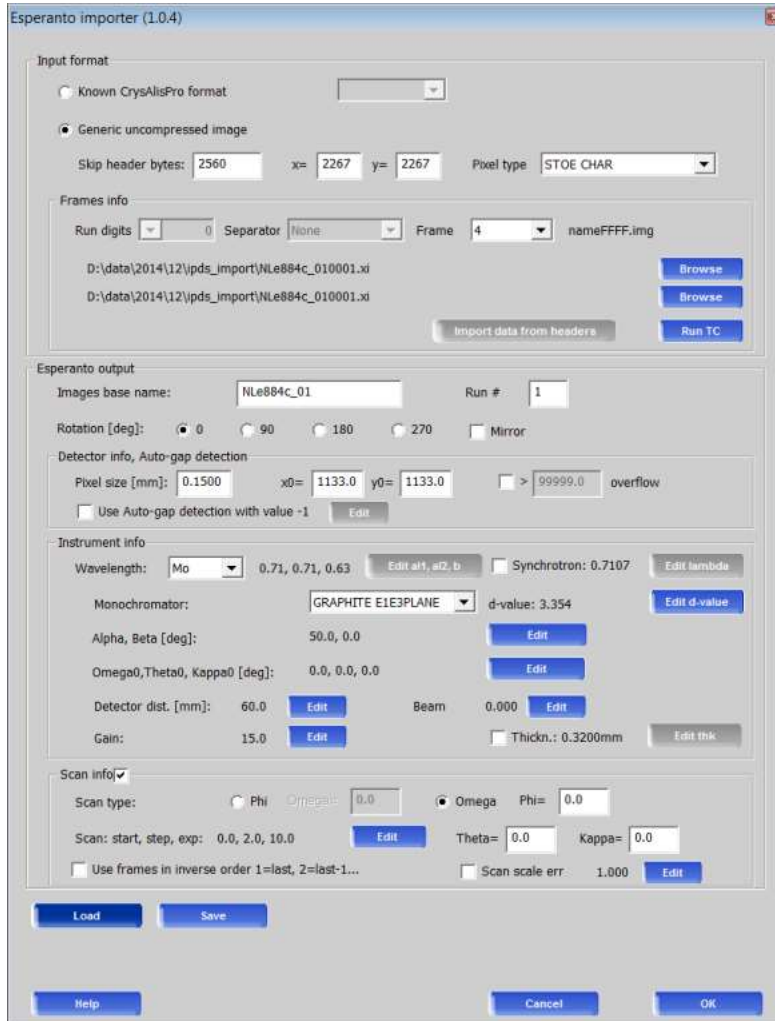
- Command dc rit
- Use of known format dectris. Header values are read.
- Camera turned 270deg. Non-square detector is padded by zeros.
- This data had NO scan scale error!
- Then esperanto createrunlist
- Slight play in EwaldPro to get the center right.
- The several cycles to refine instrument model.

Dc rit: IPDS



- Command dc rit/Import button on power toolbar
- Read detector information from the sum file of IPDS (0.15mm pix, cen x=600, y=600)
- Stoe char as pixel type; .xi files (this is OD compression...)
- Make sure to use resolution limit due to round IP image (Mo typical 0.809Ang)

Dc rit: IPDS 2



- Command dc rit/Import button on power toolbar
- Read detector information from the sum file of IPDS (0.15mm pix, cen x=1133, y=1133)
- Stoe char as pixel type; .xi files (this is OD compression...)
- Make sure to use resolution limit due to round IP image (Mo typical 0.809Ang)

Dc rit: dtrek frame from Japanese synchrotron



- Command dc rit/Import button on power toolbar
- The issue was here that the dtrek image was turn 90deg relative to the inhouse image. The dtrek createrunlist would not work on this.
- Thus the 'dc rit' command can be used to handy obstinate known images...

Dc rit: xpad detector



- Command dc rit/Import button on power toolbar
- The xpad detector is developed in France
- One of it's raw format can be channelled through the Esperanto importer
- As the header info is unknown, it has to be given in the scan info section.
- Provide the raw data file contains the -1 marker for pixel detectors the esperanto createrunlist command will automatically create a ccd file with dead zones.
- Such formats have to be transformed run by run as there is only one field for scan info.

Data finalization – optimal data

- Problems with...
- Experiment
- Unit cell
- Data reduction
- Finalization
- Pseudo symmetry, twinning, incommensurate

Experiment

- Problems with...
- Exposure time too low – diffraction limit
- De-ice
- Movie missing
- Centering – sample mount
- Choice of wavelength

Approach a data set...

- Inspect executive tab

- Warning signs:

- Run list incomplete
- High mosaicity
- Scaling unusual
- I/sig low; low redundancy
- SG issues

```
Data Reduction
FRAMES / RUNS
In run list: 402/7, used: 340/6

3D PROFILE ANALYSIS
Frames done: 340
Reflections tested: 2178, used: 1568
Avg mosaicity (in degrees) - 6 run(s)
  e1=1.10, e2=1.11, e3=1.31
Max incidence angle profile change(e3): 11%

3D INTEGRATION & FITTING
Frames done: 340
Fitted: 2231, overflow: 0, hidden: 15
Outliers rejected: 1

FINALIZATION INPUT FILE
Filename: mm

FINALIZATION OUTPUT HKL FILE
Filename: mm

SCALING / NUMERICAL ABSORPTION
Empirical abs (e=2 o=0): min=0.99,max=1.01
Frame scales ( 1/scale): min=0.97,max=1.05
Friedel pairs treated as equivalent

RESULTS (340 frames) - SYM: Pmmm
Resolution(A) Redundancy F2/sig(F2) Rint
inf - 0.80      1.9      26.7  0.030
inf - 0.84      2.0      27.9  0.030
Completeness: 95.8% (0.84 ANG)
Anom compl.: 83.6% (P222)

SPACE GROUP DESCRIPTOR
P2(1)2(1)2(1) Group #: 19 (3 SG found)
no data coverage: h00, 0k0,

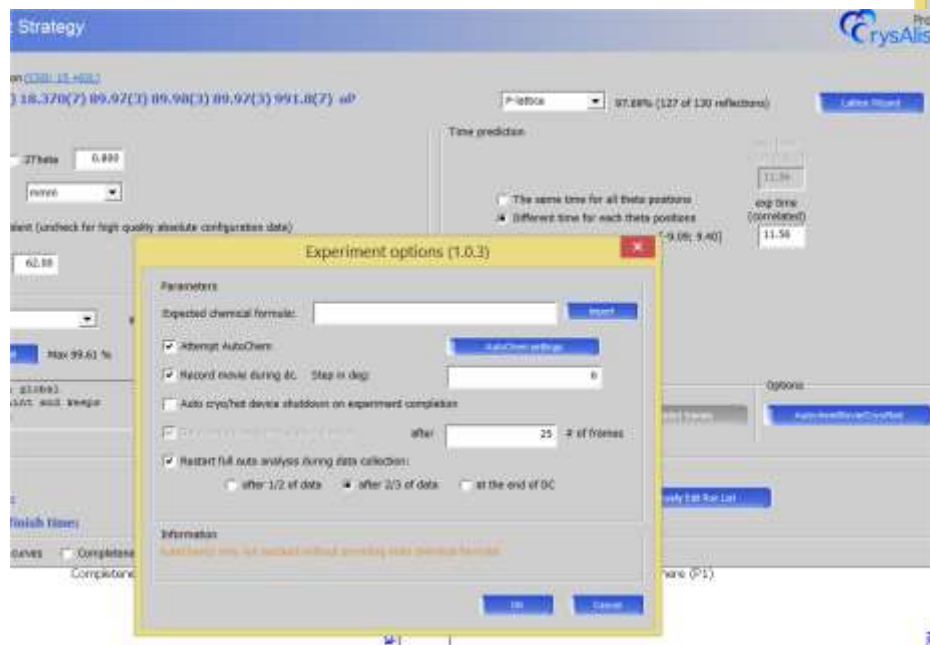

DATA REDUCTION OPTIONS
Per-frame model refinement used
2-cycle 3D peak analysis used
3D profile fitting used
```

Approach a data set...

- Run 'Full auto analysis' on all data
- Concurrent may get stuck

CrysAlisPro: Data reduction (1.13)

- Load new experiment
- Full auto analysis (cell, red)
- Automatic data reduction
- Data reduction with options

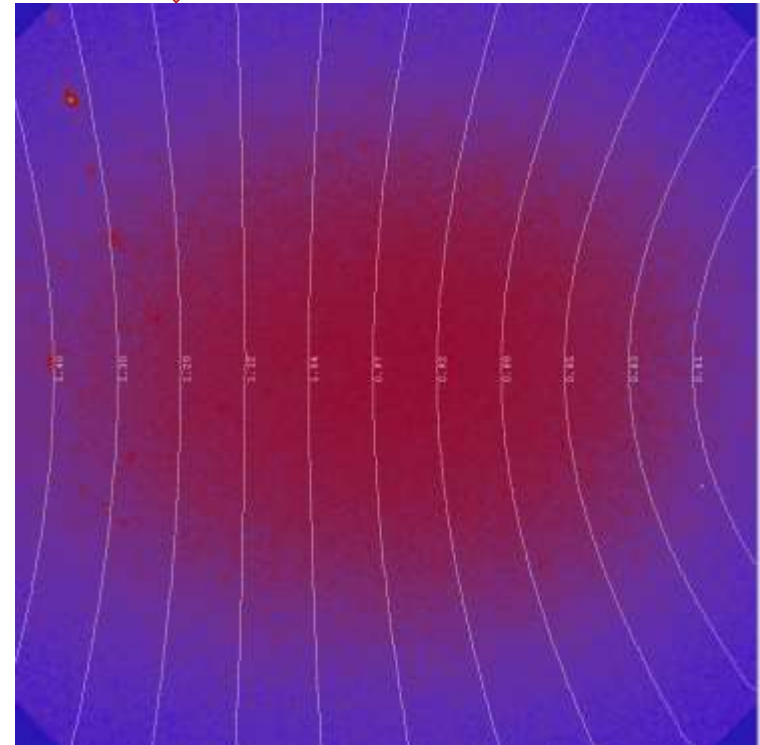
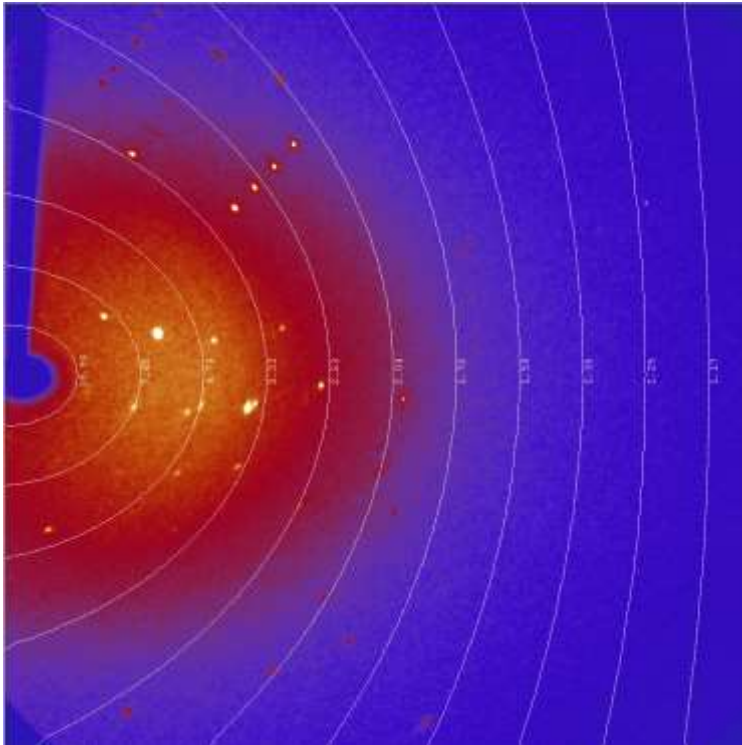


The screenshot shows the 'Strategy' window in CrysAlisPro. The 'Experiment options (1.0.3)' dialog is open, displaying various settings for data collection and analysis. The 'Parameters' section includes fields for 'Expected chemical formula', 'AutoChem settings', and 'Record movie during DC'. The 'Options' section has checkboxes for 'Auto cryostat device shutdown on experiment completion' and 'Restart full auto analysis during data collection'. The 'Information' section contains a warning message: 'AutoChem may not be started without providing valid chemical formulae'.

Approach a data set...

- Inspect frames
 - No diffraction at high angle \rightarrow cut the data to that resolution

Diffraction limit!

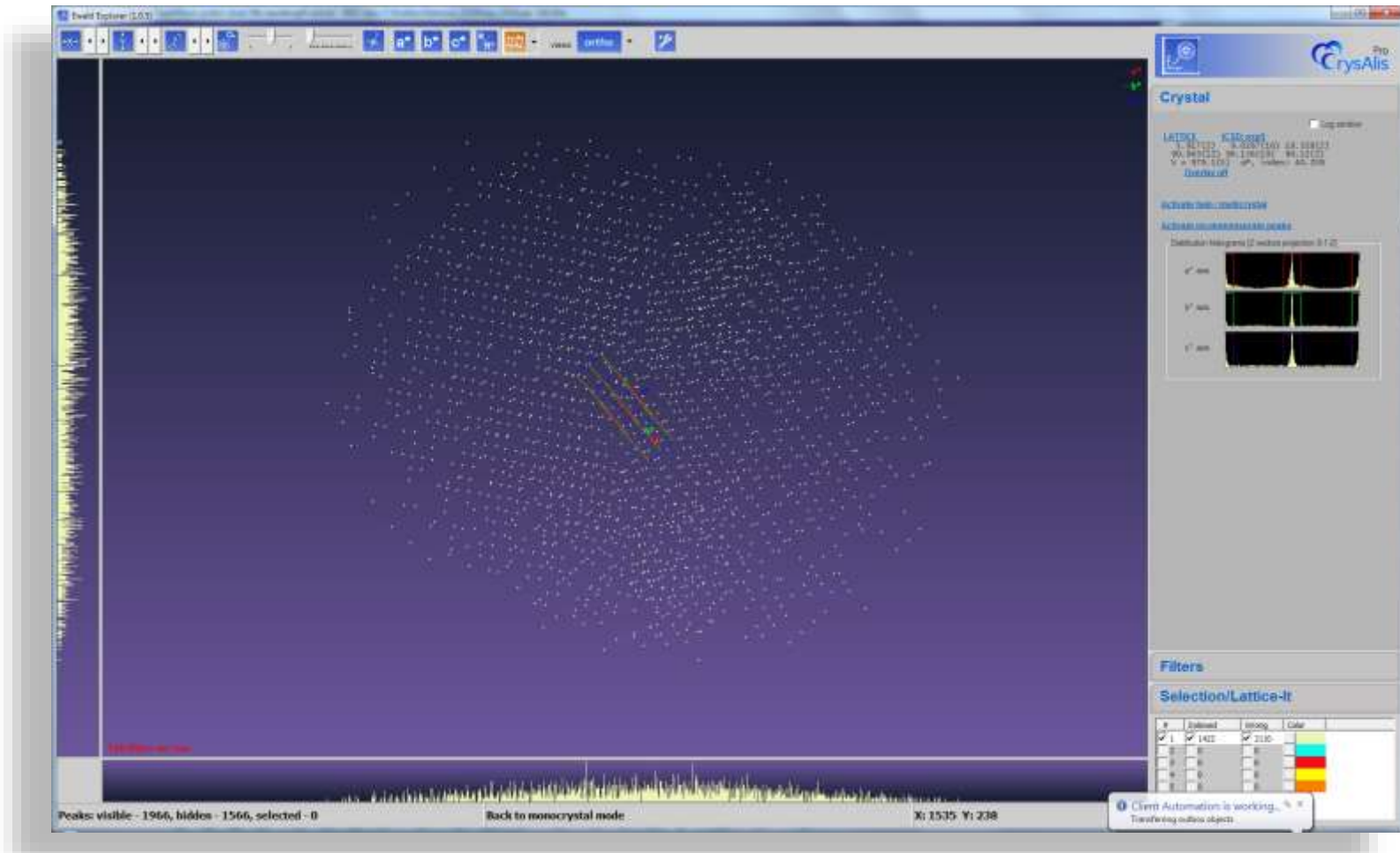


Approach a data set...

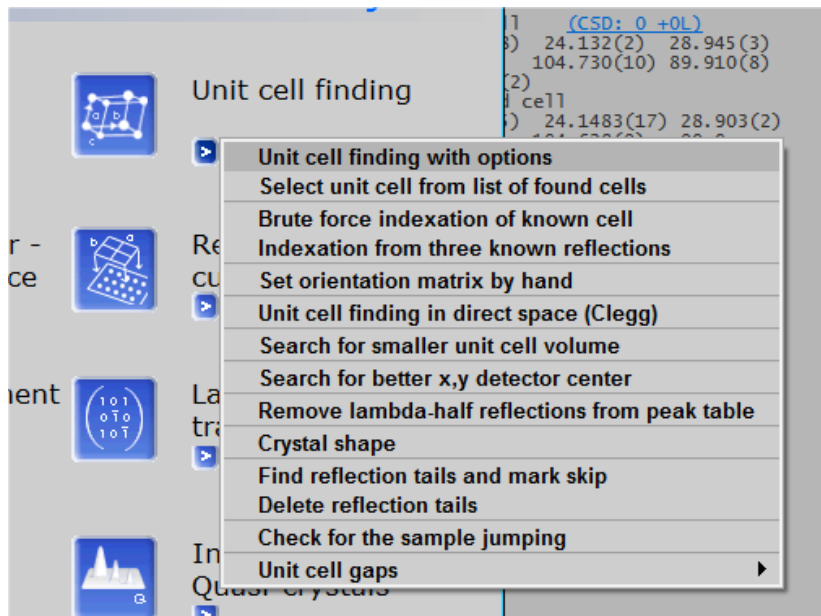
- Inspect frames:
 - Low/high background
 - Diffuse scattering, split reflections, twin
 - Empty frames, strange frames
- Inspect the sample movie (if you have it...):
 - Sample mounting

Unit cell...

- Ewald Explorer

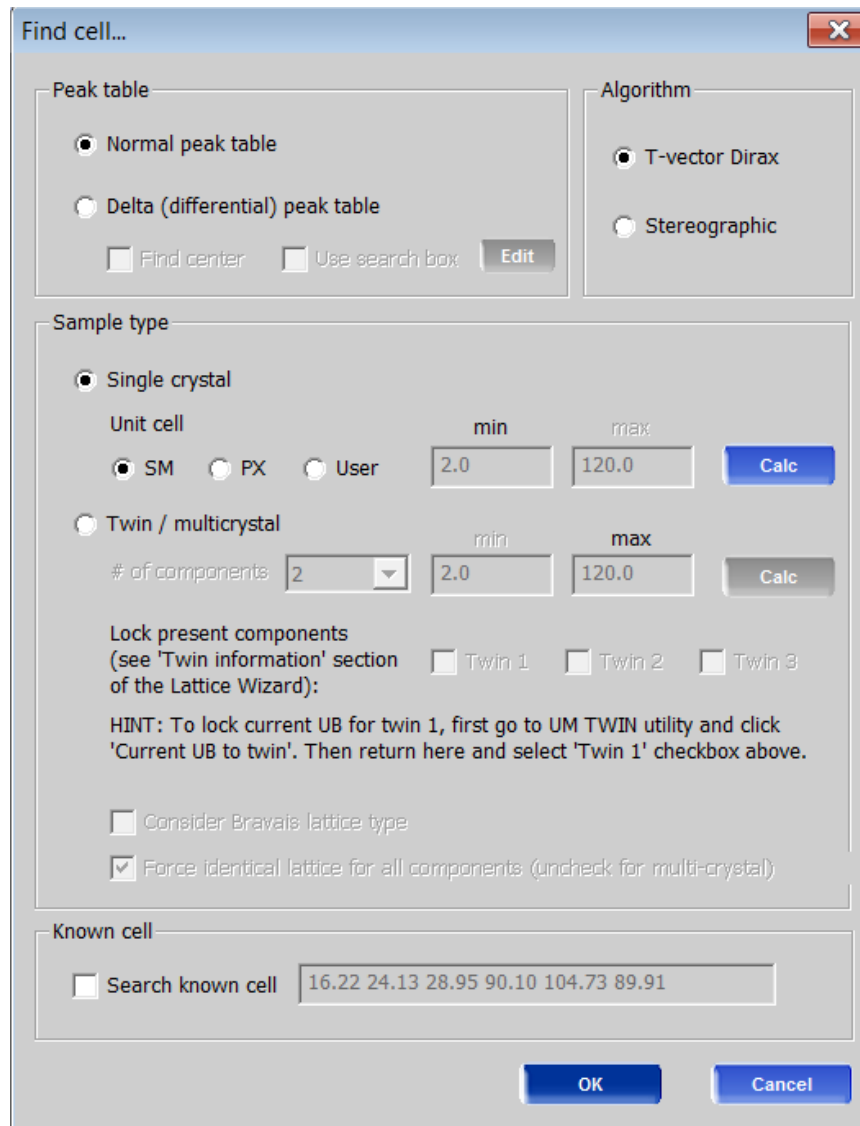


Unit cell finding – Automatic unit cell finding



The screenshot shows the 'Unit cell finding' menu in a software application. The menu is open, displaying several options. The first option is 'Unit cell finding with options', which is expanded to show a list of sub-options: 'Select unit cell from list of found cells', 'Brute force indexation of known cell', 'Indexation from three known reflections', 'Set orientation matrix by hand', 'Unit cell finding in direct space (Clegg)', 'Search for smaller unit cell volume', 'Search for better x,y detector center', 'Remove lambda-half reflections from peak table', 'Crystal shape', 'Find reflection tails and mark skip', 'Delete reflection tails', 'Check for the sample jumping', and 'Unit cell gaps'. The background shows a window titled 'Unit cell finding' with a table of data and a 3D unit cell model.

	(CSD: 0 +0L)
1	24.132(2) 28.945(3)
2	104.730(10) 89.910(8)
3	24.1483(17) 28.903(2)

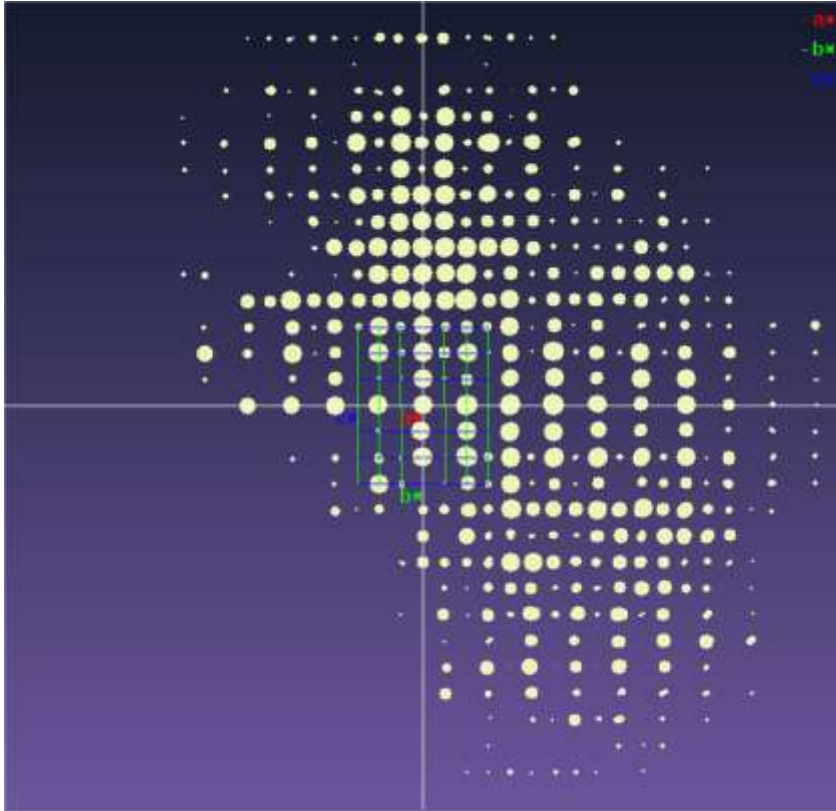


The screenshot shows the 'Find cell...' dialog box. It has a title bar with a close button. The dialog is divided into several sections:

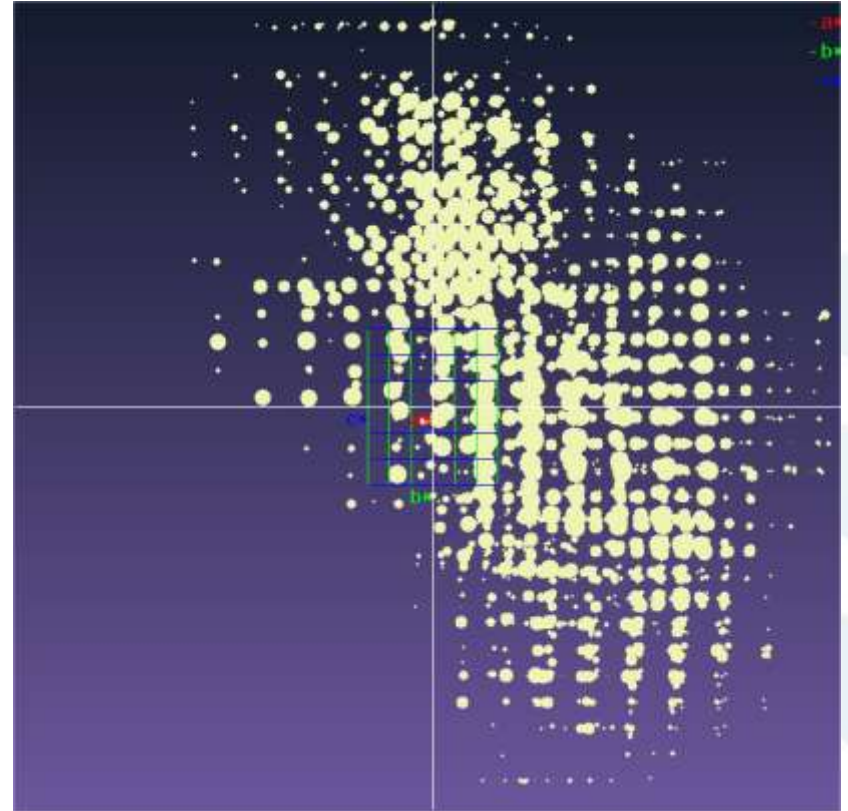
- Peak table:** Contains radio buttons for 'Normal peak table' (selected), 'Delta (differential) peak table', and 'Stereographic'. There are also checkboxes for 'Find center' and 'Use search box', and an 'Edit' button.
- Algorithm:** Contains radio buttons for 'T-vector Dirax' (selected) and 'Stereographic'.
- Sample type:** Contains radio buttons for 'Single crystal' (selected) and 'Twin / multicrystal'.
 - Single crystal:** Includes 'Unit cell' with 'min' (2.0) and 'max' (120.0) input fields, and radio buttons for 'SM', 'PX', and 'User'. A 'Calc' button is present.
 - Twin / multicrystal:** Includes '# of components' (2) in a dropdown, 'min' (2.0) and 'max' (120.0) input fields, and a 'Calc' button.
- Lock present components:** Includes a note: '(see 'Twin information' section of the Lattice Wizard):' and three checkboxes for 'Twin 1', 'Twin 2', and 'Twin 3'.
- HINT:** A text box providing instructions: 'To lock current UB for twin 1, first go to UM TWIN utility and click 'Current UB to twin'. Then return here and select 'Twin 1' checkbox above.'
- Consider Bravais lattice type:** A checkbox that is unchecked.
- Force identical lattice for all components (uncheck for multi-crystal):** A checkbox that is checked.
- Known cell:** Includes a checkbox for 'Search known cell' and a text input field containing '16.22 24.13 28.95 90.10 104.73 89.91'.

At the bottom of the dialog are 'OK' and 'Cancel' buttons.

Unit cell finding – Influence of bad instrument model

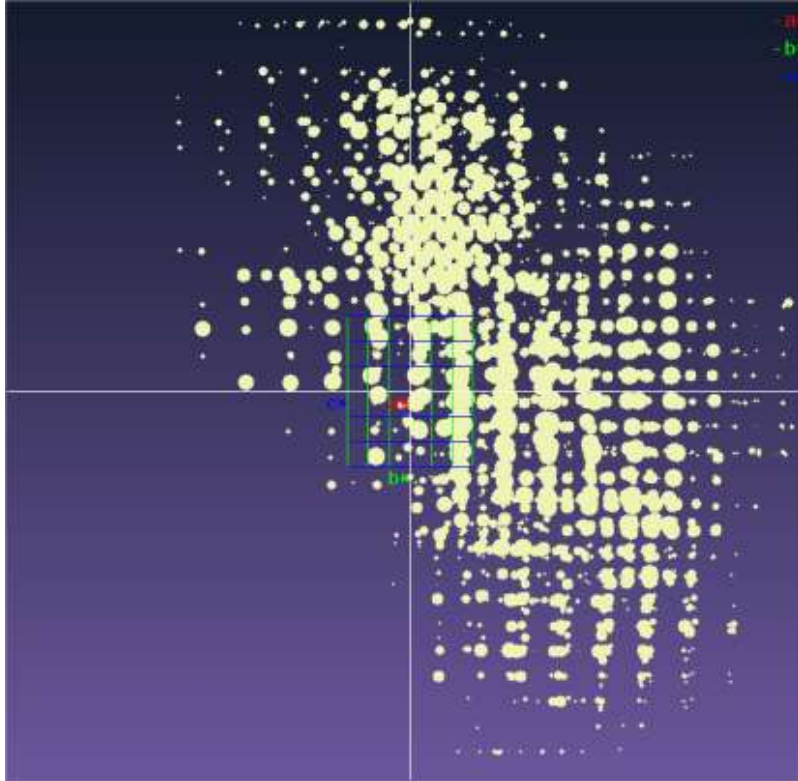


Good instrument model

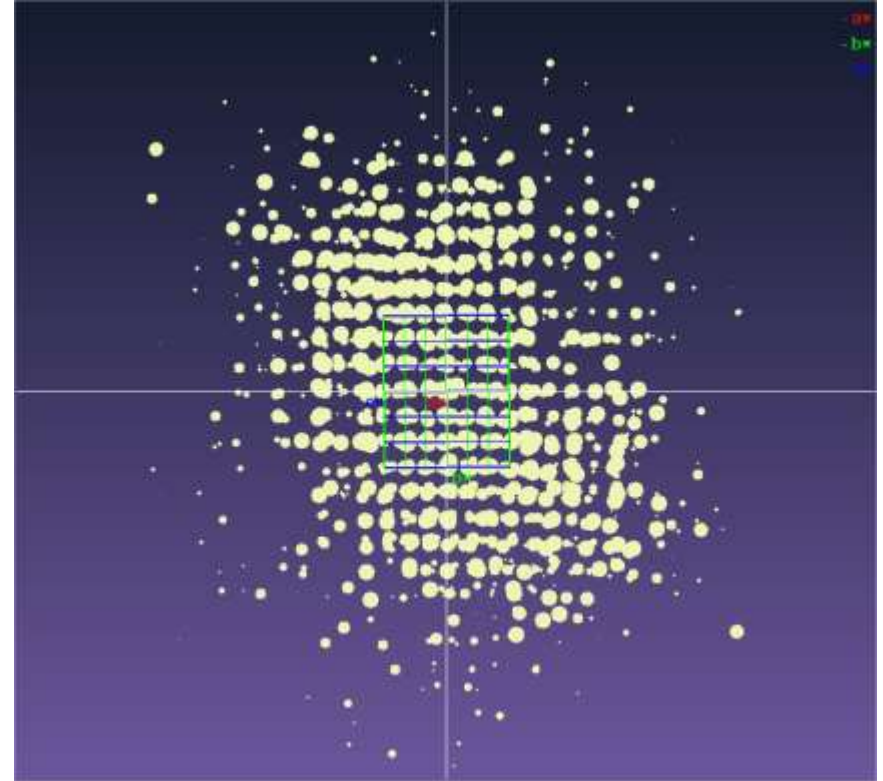


Bad instrument model:
Beam center deviation 40 pix

Unit cell finding – Influence of bad instrument model

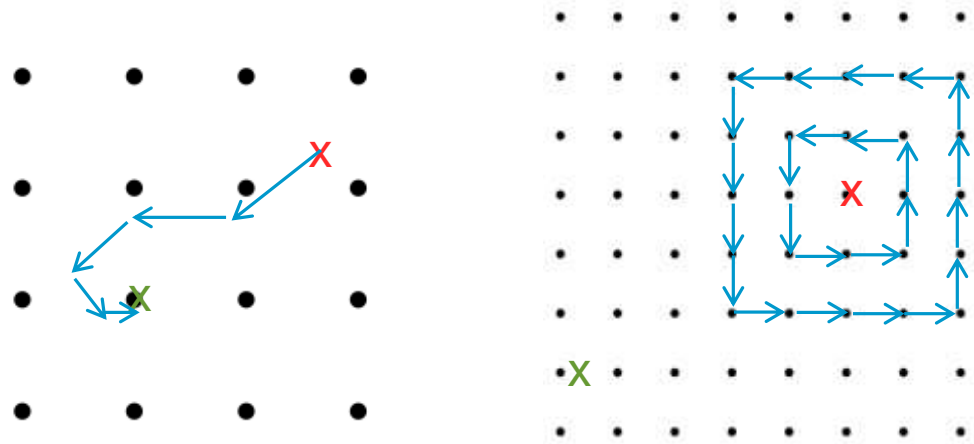
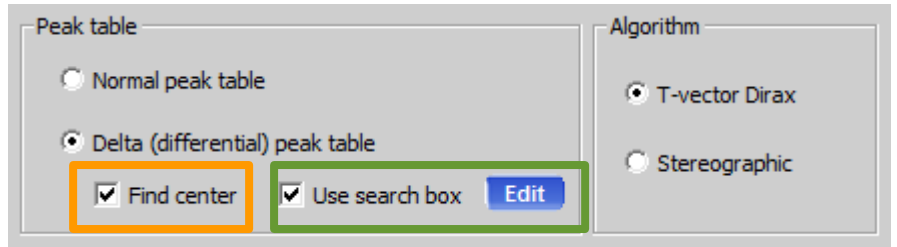
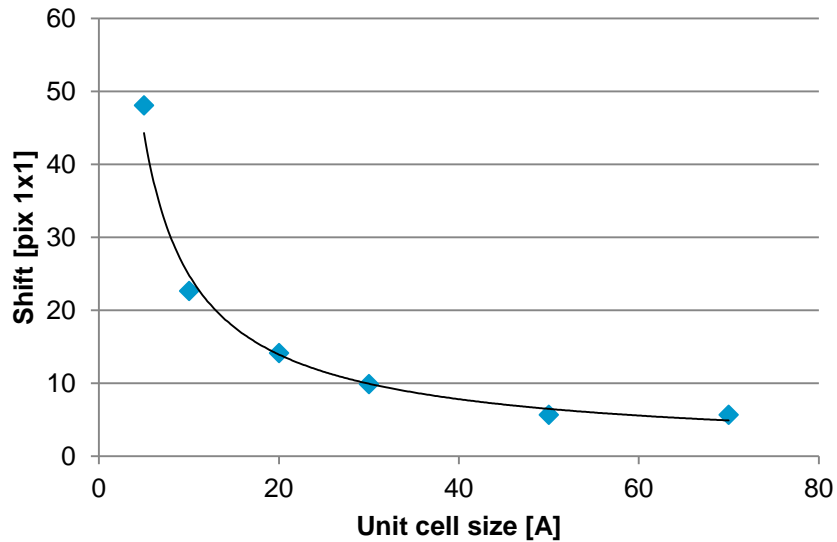


Bad instrument model:
Beam center deviation 40 pix

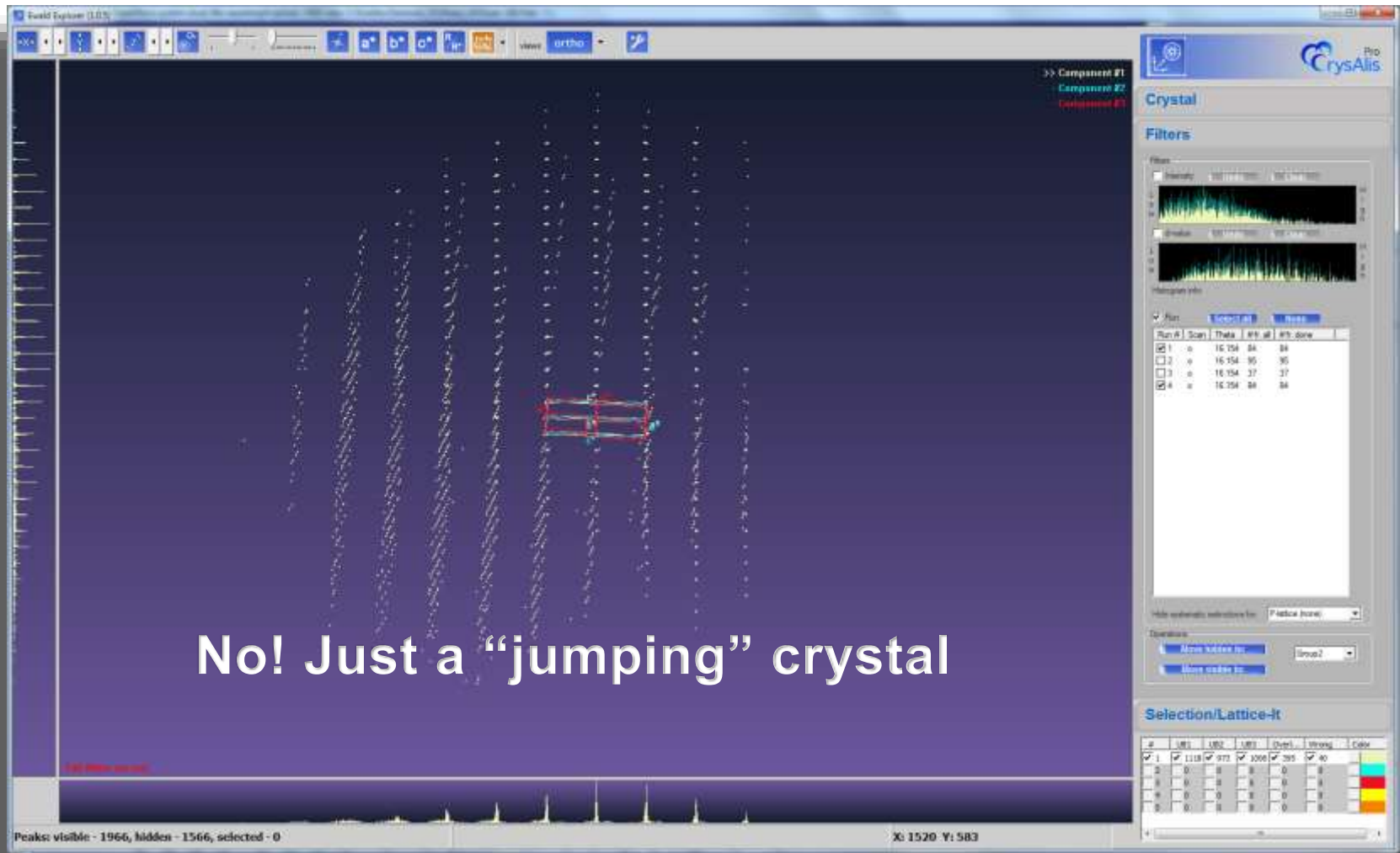


Bad instrument model:
Delta-peak table

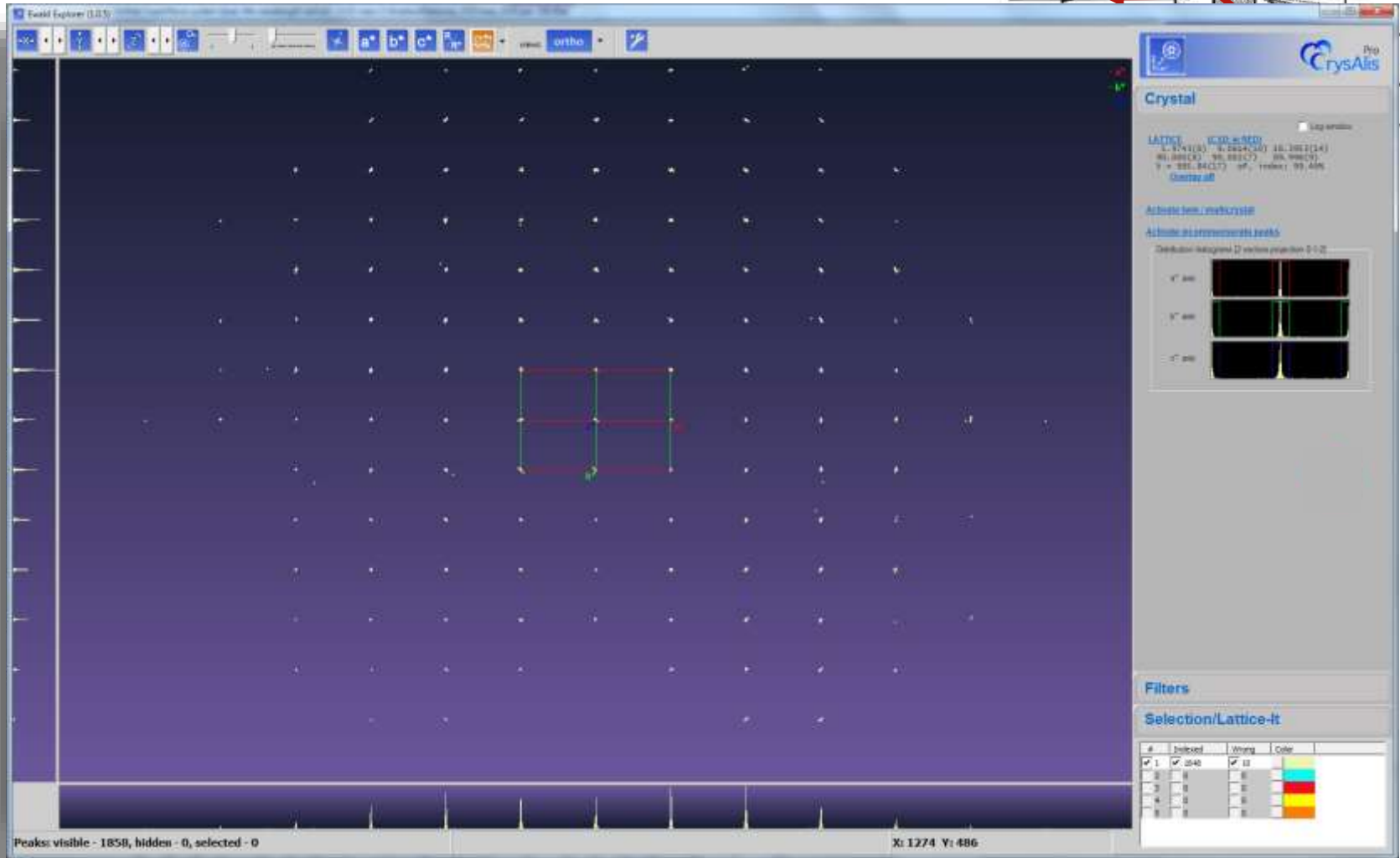
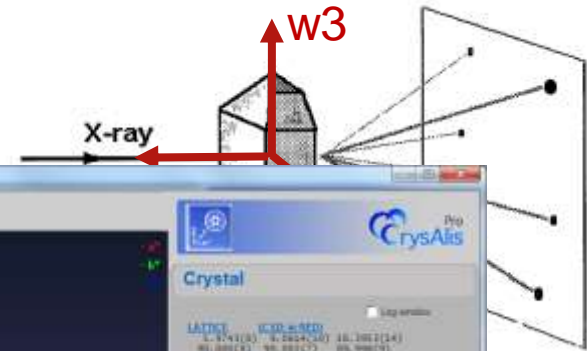
Unit cell finding – Influence of bad instrument model



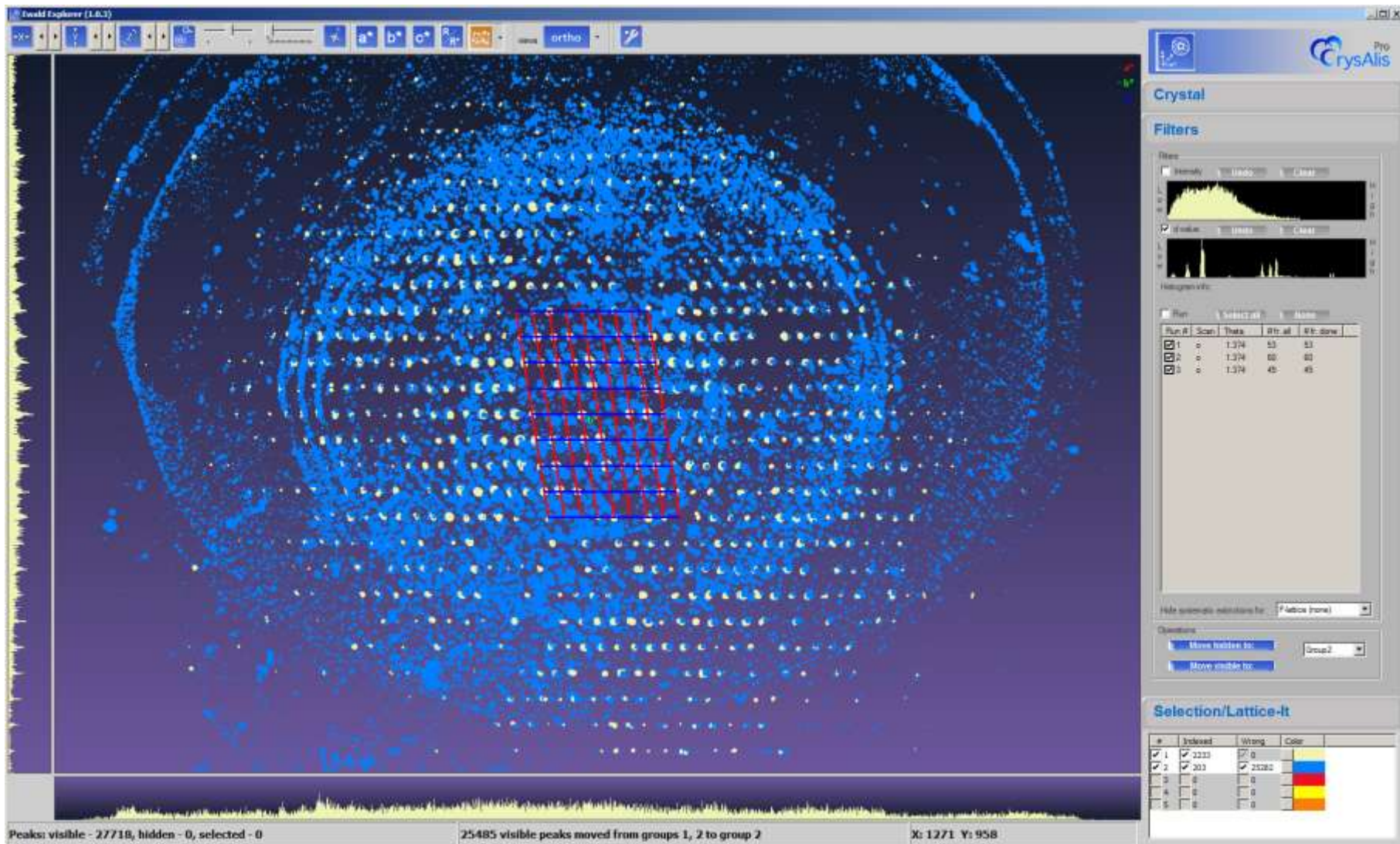
Unit cell (twin vs. Jump)...



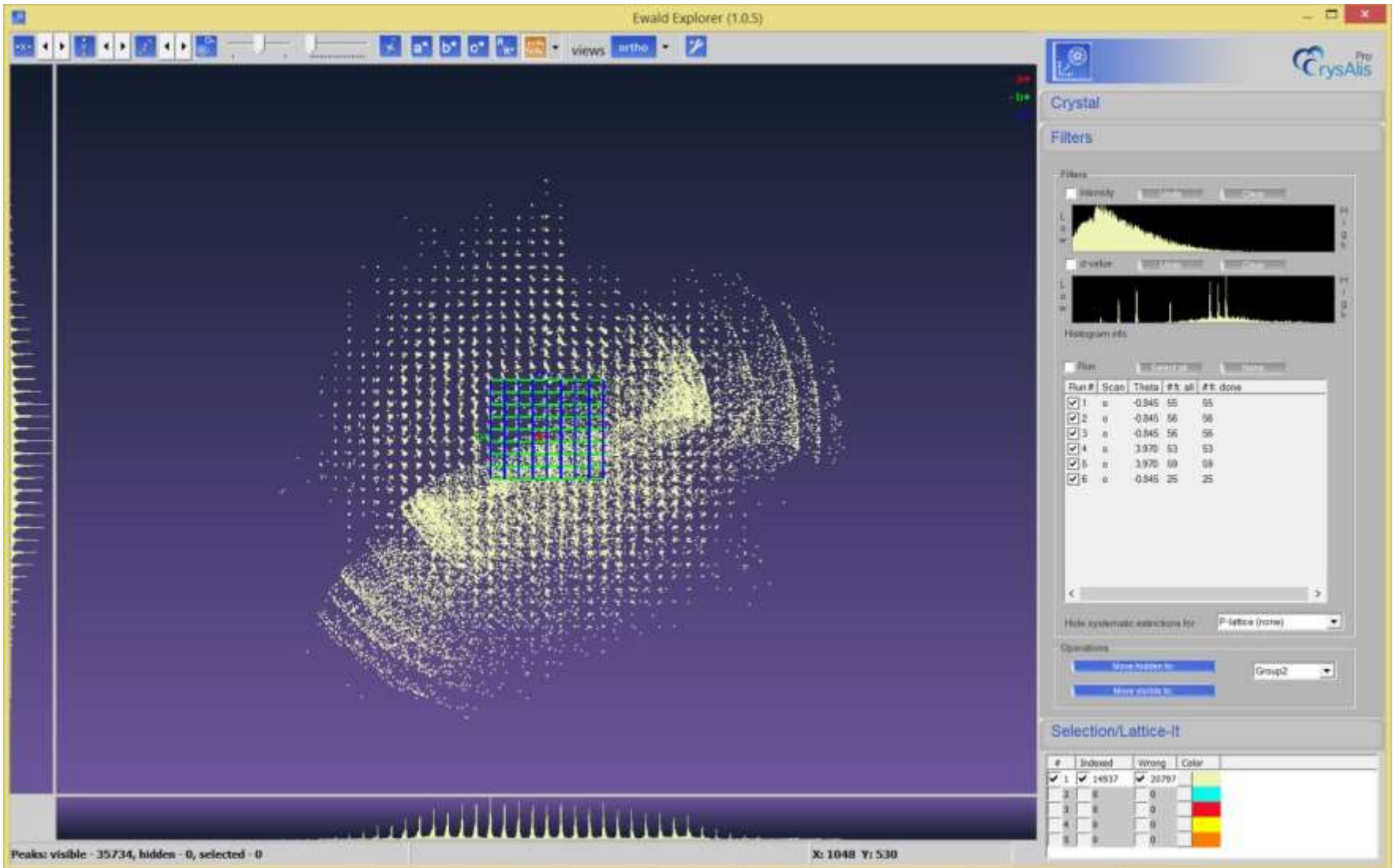
Unit cell (wobble).



Unit cell (ice ring)...



Unit cell (filters)...



Unit cell (filters)...

The screenshot displays the Ewald Explorer (1.0.5) software interface. The main window shows a diffraction pattern with a grid overlay. An 'Ewald Explorer options 1.1.1' dialog box is open, showing various settings for appearance, user interface, and scan parameters. On the right, there are panels for 'Crystal', 'Filters', and 'Selection/Lattice-It'.

Ewald Explorer options 1.1.1

Appearance

Size of peaks: 1 2 3 4 5 6 7 8 9 10
 Lattice size: 4

Lattice overlay and gnomonic vectors thickness: 1 2 3

Background color (top): [button] Set default colors [button]
 Background color (bottom): [button]
 Lattice color: [button]

Number of groups: 5 [button] Default group colors [button]

User interface settings

Show legend
 Always hide EwaldPro (viewer) (small screen)
 Toolbar position: up down

Compatibility

Save hidden peaks with slip flag (in end)

Scan parameters

ω = 1072.42 [button] [button] Show screen center
 ϕ = 1007.67 [button] [button]
 θ = 85.38 [button] [button]

Help [button] Update [button] OK [button] Cancel [button]

Crystal

Filters

Intensity [button] [button] [button]
 [Graph]
 [button] [button] [button]
 [Graph]
 Histogram info

Run [button] [button] [button]

Run #	Scan	Theta	#h all	#h done
<input checked="" type="checkbox"/>	1	h	-0.845 55	55
<input checked="" type="checkbox"/>	2	h	-0.845 56	56
<input checked="" type="checkbox"/>	3	h	-0.845 56	56
<input checked="" type="checkbox"/>	4	h	3.970 53	53
<input checked="" type="checkbox"/>	5	h	3.970 59	59
<input checked="" type="checkbox"/>	6	h	-0.845 25	25

Hide systematic absences for: P-100 (none)

Operators

Show lattice to: [button] Group2 [button]
 Show axes to: [button]

Selection/Lattice-It

#	Indexed	Wrong	Color
<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	<input checked="" type="checkbox"/>	20797
2	0	0	
3	0	0	
4	0	0	
5	0	0	

Peaks: visible - 35734, hidden - 0, selected - 0
 X: 483 Y: 359

Unit cell (filters)...

Ewald Explorer (1.0.5)

Crystal

Filters

Intensity

Visibility

Drag to skip intensity
Current position: 1170

Run #	Scan	Theta	#h	#k	#l	d/aoe
<input checked="" type="checkbox"/>	1	-18.170	76	76		
<input checked="" type="checkbox"/>	2	-18.170	142	142		
<input checked="" type="checkbox"/>	3	-18.170	87	87		
<input checked="" type="checkbox"/>	4	-18.170	93	93		
<input checked="" type="checkbox"/>	5	-18.170	47	47		
<input checked="" type="checkbox"/>	6	-18.170	87	87		
<input checked="" type="checkbox"/>	7	-18.170	47	47		
<input checked="" type="checkbox"/>	8	-18.170	76	76		
<input checked="" type="checkbox"/>	9	-18.170	87	87		
<input checked="" type="checkbox"/>	10	-18.170	76	76		
<input checked="" type="checkbox"/>	11	16.217	56	56		
<input checked="" type="checkbox"/>	12	16.217	87	87		
<input checked="" type="checkbox"/>	13	16.217	87	87		

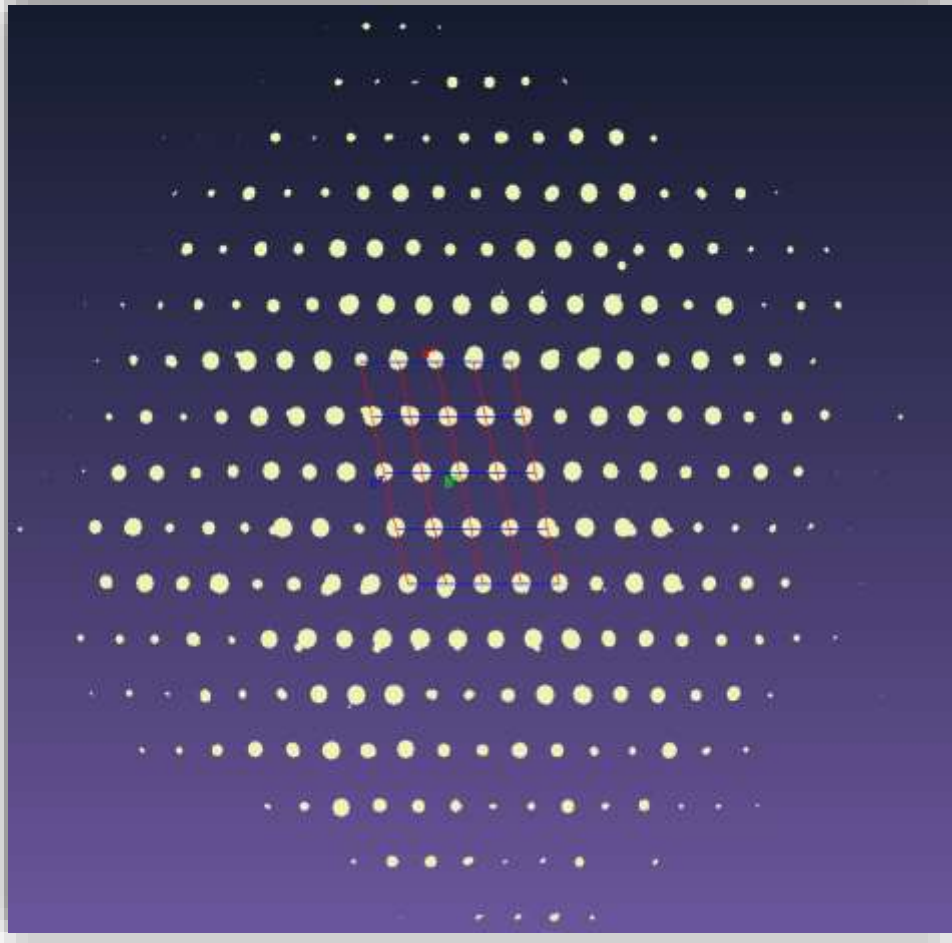
Hide systematic extinctions for: I-lattice

Operations

Peaks: visible - 2516, hidden - 0, selected - 0

Ewald^{Pro} Collapse view

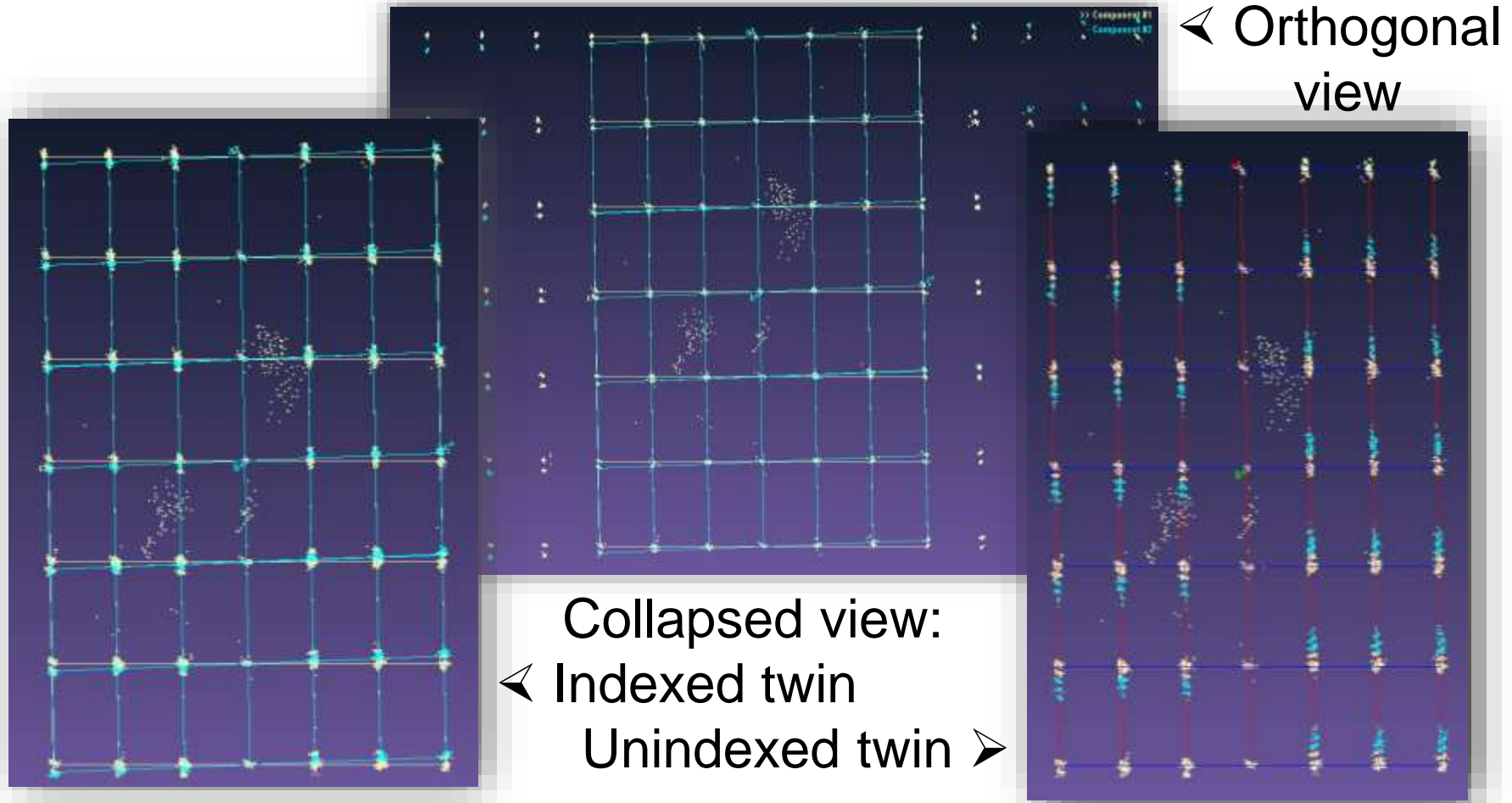
Collapse peak view – construction



1. Lattice vectors are multiplied by lattice overlay size
2. Subtract lattice vectors until given peak hits range

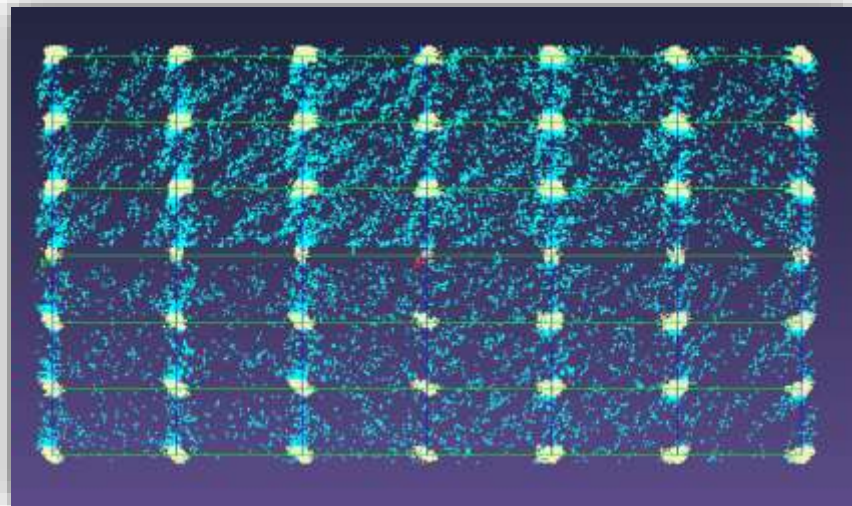
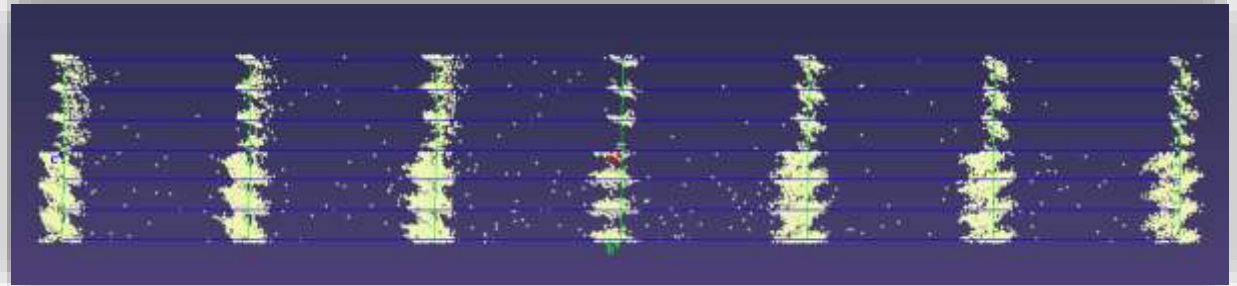
Ewald^{Pro} Collapse view

Collapse peak view – twin example



Ewald^{Pro} Collapse view

Collapse peak view – other examples



▲ moving crystal

◀ multicrystal



incommensurate

Data reduction

During experiment - concurrent data processing

- In most cases provides good, close to optimal results
- Features improving data quality:
 - Robust prediction model refinement
 - Selection of background evaluation mode



START/STOP

Shutter Open X-ray Cu 2 x 2

CCD Cryo Xray IO

CCD Collecting... (116,464,end:Wed Mar 18 14:26:58 2015)

RED Processing image 52 of run 1 (52/92)

Crystal RED

Data Collection

Data Reduction

FRAMES / RUNS
In run list: 464/10, used: 92/2

3D PROFILE ANALYSIS
Frames done: 92
Reflections tested: 315, used: 255
Avg mosaicity (in degrees) - 2 run(s)
e1=1.53, e2=1.53, e3=1.21
Max incidence angle profile change(e3): 57%

3D INTEGRATION & FITTING
Frames done: 52
Fitted: 0, overflow: 0, hidden: 8
Outliers rejected: 0

RESULTS (32 frames) - SYM: Pmmm
Resolution(A) Redundancy F2/sig(F2) Rint
inf - 1.26 1.2 32.9 0.041
Completeness: 8.7% (0.84 ANG)
Anom compl.: 6.2% (P222)

SPACE GROUP DESCRIPTOR
P2(1)2(1)2(1) Group #: 19 (8 SG found)
no data coverage: 0k1, h01, h01, h00, 0k0, 0

DATA REDUCTION OPTIONS
Per-frame model refinement used
3D profile fitting used

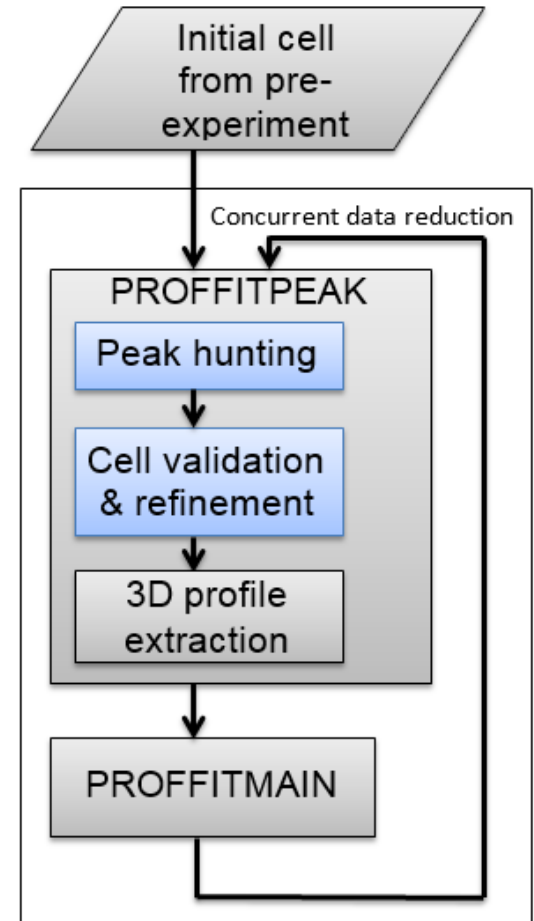
Data reduction

Concurrent data processing - Robust cell / model refinement

- The key problem:
 - Inaccurate initial cell from pre-exp
 - Cell/Model can't predict well low/high theta
 - Misaligned/jumping sample

- Solution:

PROFFITPEAK module does standard peak-hunting and cell/orientation refinement before profile learning / analysis phase



Data reduction

Concurrent processing - Automatic selection of background

Average background level > threshold

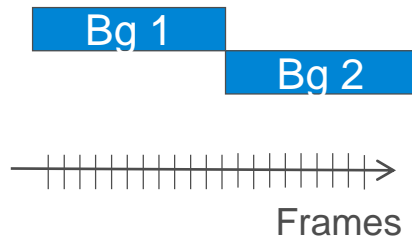
No



- Average background (Re > 10 frames)

- Background image estimated once per specified frame range

Re = Fr (default, >10 frames)



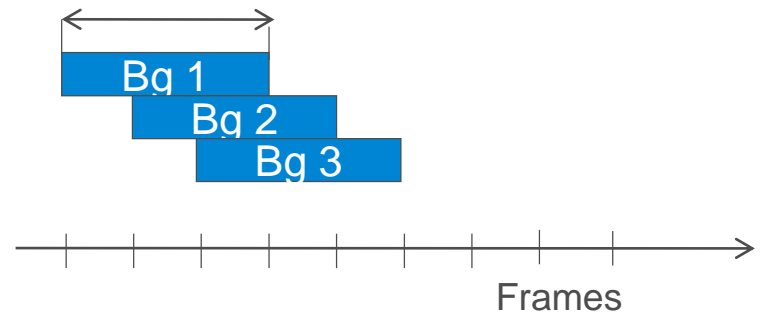
Yes



- Smart background

- Local background recomputed on every frame and fitted individually for every spot


Frame range: 1 (default), 3 or more available through the wizard



Data reduction

Use of lattice filters

Proffit: CrysAlisPro data reduction assistant (1.0.26) ✕



Profile fitting data reduction

Step 1: Orientation matrix for data reduction

```
UB - matrix:
-0.016259  0.026962  0.037017  ( 0.000003  0.000004  0.000006 )
-0.018898 -0.024647  0.038739  ( 0.000003  0.000004  0.000007 )
 0.027229 -0.000954  0.049096  ( 0.000003  0.000003  0.000006 )
19.21287 ( 0.00171 ) 19.41060 ( 0.00194 ) 9.76017 ( 0.00089 )
89.92280 ( 0.00771 ) 90.06198 ( 0.00728 ) 90.06002 ( 0.00764 )
V = 3639.89
Selected cell (from UM rr/UM ttt/UM f):
18 19.2129 19.4106 9.7602 89.9228 90.0620 90.0600 tI
Twin 1: 19.20994 19.41533 9.76215 89.9473 89.9374 89.9540 3640.96
```

Lattice extinctions (filter Bravais lattice extinctions)

Don't use filter (P-lattice)

Use filter for: Lattice

Incommensurate structures

Normal data reduction (HKL)

Single q-vector

Other (reduction list)

Twinning/Multi crystal (activated by UM TWIN entries)

Use automatic twin/multi crystal data reduction with the following components: Multi crystal

Component 1 Component 2 Component 3 Component 4

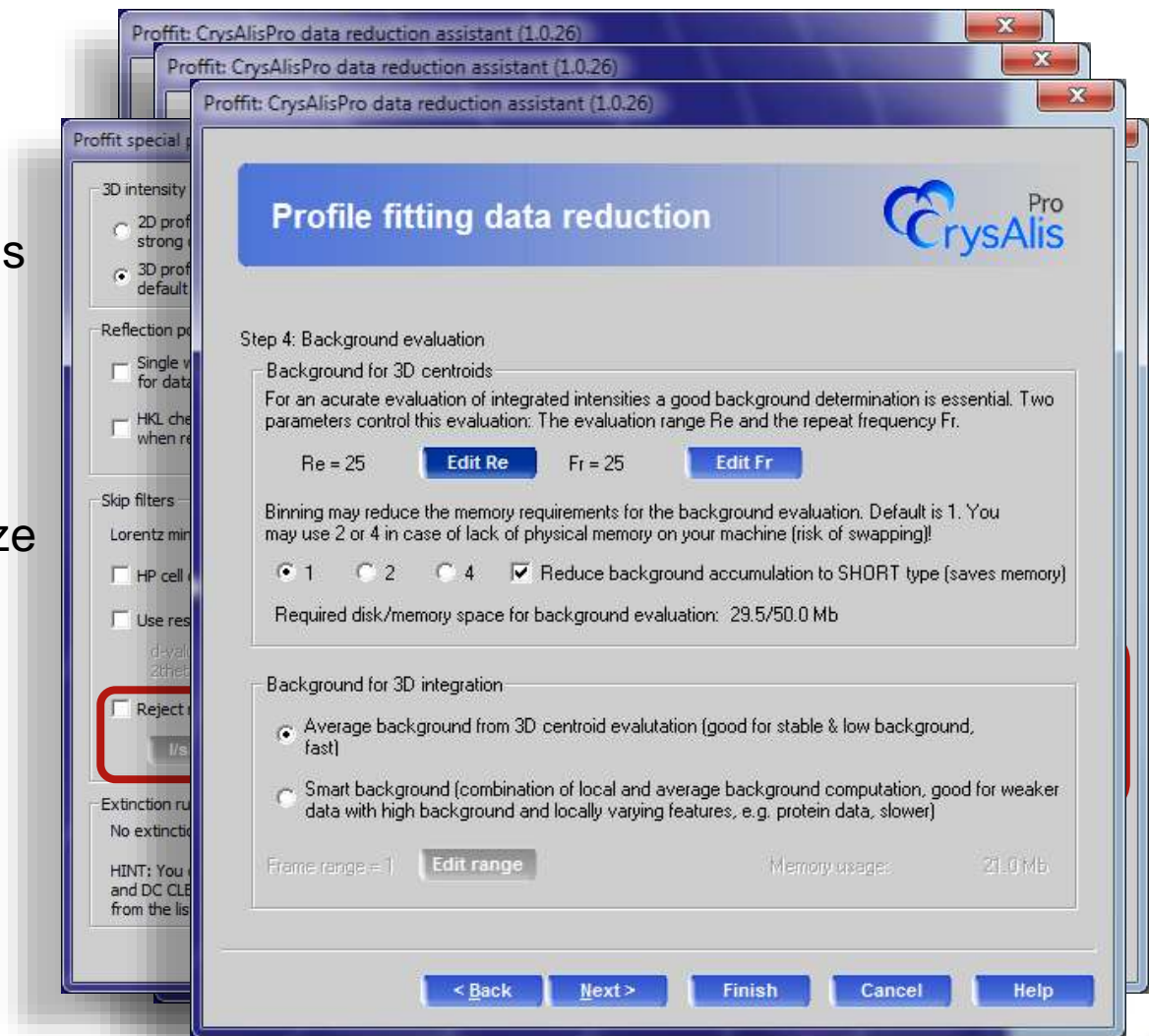
< Zurück Weiter > Fertig stellen Abbrechen Hilfe

Data reduction

Data reduction wizard

Settings worth attention:

- Model refinement options
- Special parameters:
 - Integration mask size
 - Bad profile filter
- Background options



Data reduction

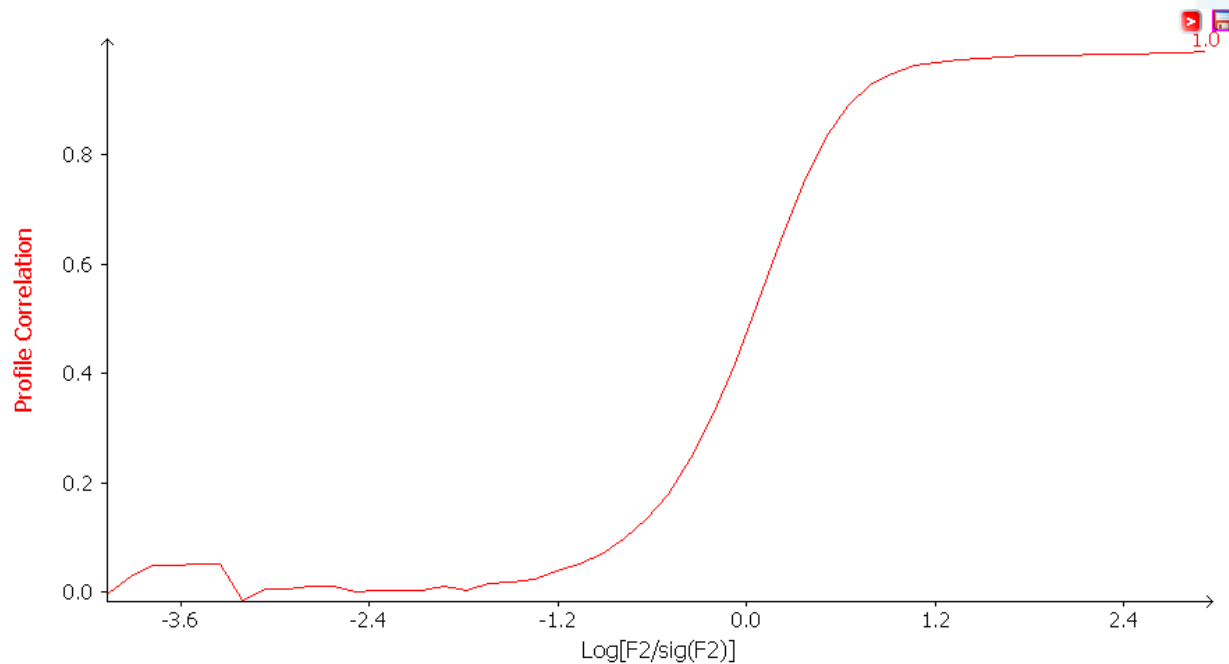
3D profile fitting

- **Distorted rotation method data is mapped to 'Kabsch-space'.** Similar like XDS, but more complex
- Strong reflection data serve as reference profile. No shape assumption is made!
- **All data is profile fitted to the 'nearby' reference profile.** For strong data this means summation, for weak filtering
- You may choose to take less/more than 4sig of reference profile

Data reduction

Special pars- outliers

- Filter intruders by correlation coefficient.
- All strong reflections are self similar.



Data reduction

Special pars - incidence

Profile fitting

Override integration mask size (generally not recommended, but smaller mask can be useful for strongly overlapping reflections e.g. twins) 1.00 of original size

Follow profile size changes with incidence angle

Adjust masks according to prediction uncertainty (for high angle data)

Print average profiles to history window

Profile size analysis (per incidence angle)

Average profile size - assuming Gaussian shape (in degrees)					
Incidence angle (deg)	# of peaks	sig_e1 (stddev)	sig_e2 (stddev)	sig_e3 (stddev)	
0-12.6	769	1.639 (0.304)	1.430 (0.233)	1.757 (0.880)	
12.7-18.1	769	1.624 (0.354)	1.430 (0.242)	1.649 (0.875)	
18.1-22.5	769	1.624 (0.357)	1.431 (0.258)	1.572 (0.828)	
22.5-26.2	769	1.594 (0.369)	1.414 (0.258)	1.542 (0.839)	
26.2-29.9	769	1.627 (0.372)	1.410 (0.282)	1.440 (0.736)	
29.9-32.8	769	1.630 (0.364)	1.382 (0.255)	1.391 (0.719)	
32.8-35.8	769	1.594 (0.341)	1.341 (0.267)	1.392 (0.708)	
35.8-38.9	769	1.632 (0.349)	1.337 (0.266)	1.315 (0.594)	
38.9-41.9	769	1.638 (0.330)	1.294 (0.269)	1.303 (0.659)	
41.9-51.6	769	1.618 (0.323)	1.221 (0.270)	1.188 (0.610)	
0-51.6	7690	1.622 (0.347)	1.369 (0.269)	1.455 (0.769)	

Fitted profile normalization line parameters

e1 dimension: a=0.0022 b=0.99

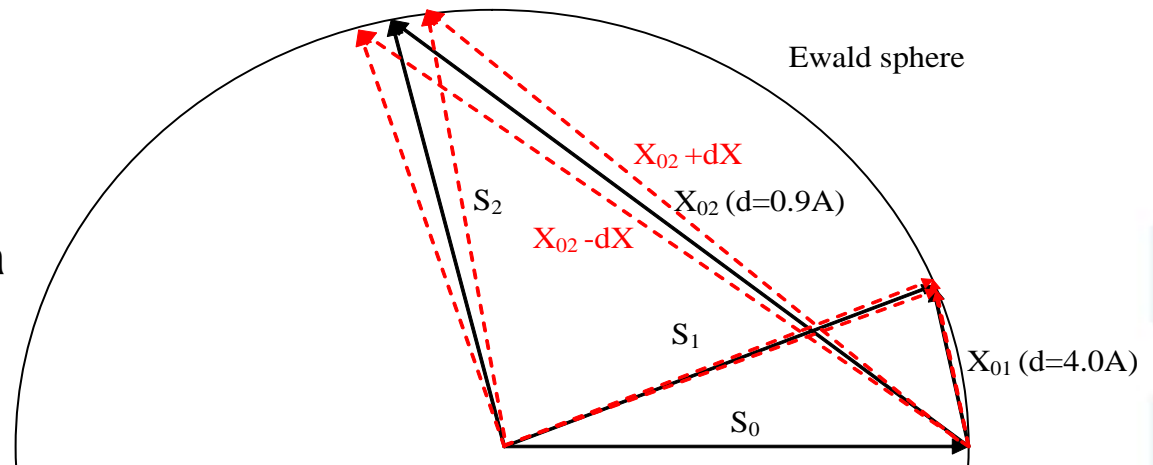
e2 dimension: a=-0.0019 b=1.08

e3 dimension: a=-0.0136 b=1.46

Data reduction

Prediction uncertainty – problem

- Problem lies in spot prediction uncertainty
- Higher inaccuracy at high theta



For profile size of 0.8 deg integration mask size is 8 pixels at incidence angle 0 deg (Atlas detector, 2x2 binning, at 55 mm)

Detector theta (deg)	Std dev of misprediction (deg)	Std dev of misprediction (pix)	Max misprediction (pix)
11	0.014	0.13	0.78
24	0.02	0.2	1.2
40	0.025	0.25	1.5
111	0.04 – 0.08	0.4 – 0.8	2.4 – 4.8

Data reduction

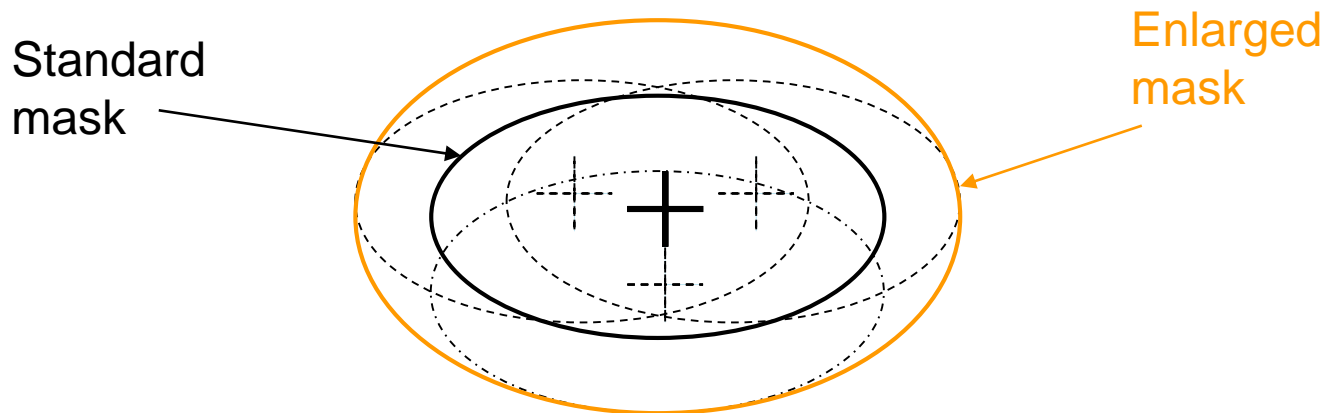
Prediction uncertainty – solution

- Estimate prediction uncertainty at given theta

Prediction accuracy statistics (in degrees)

Resolution	# of peaks	Average prediction error (in degrees)		
		delta_e1 (stddev)	delta_e2 (stddev)	delta_e3 (stddev)
1.35-1.22	82	0.002 (0.020)	0.001 (0.013)	0.003 (0.170)
1.22-1.14	82	-0.002 (0.025)	0.009 (0.016)	0.020 (0.165)
1.14-1.08	82	0.003 (0.024)	0.004 (0.020)	0.020 (0.175)
1.08-1.04	82	-0.012 (0.034)	-0.002 (0.021)	-0.026 (0.153)
1.04-0.99	82	0.001 (0.026)	-0.003 (0.021)	-0.018 (0.153)
0.99-0.95	82	-0.007 (0.033)	-0.005 (0.030)	-0.004 (0.147)
0.95-0.91	82	-0.005 (0.038)	-0.009 (0.029)	-0.001 (0.132)
0.91-0.87	82	-0.008 (0.038)	-0.015 (0.041)	-0.002 (0.127)
0.87-0.84	82	0.006 (0.038)	-0.012 (0.041)	-0.016 (0.106)
0.84-0.80	73	0.005 (0.051)	0.017 (0.087)	0.002 (0.103)
1.35-0.80	811	-0.002 (0.034)	-0.002 (0.038)	-0.002 (0.146)

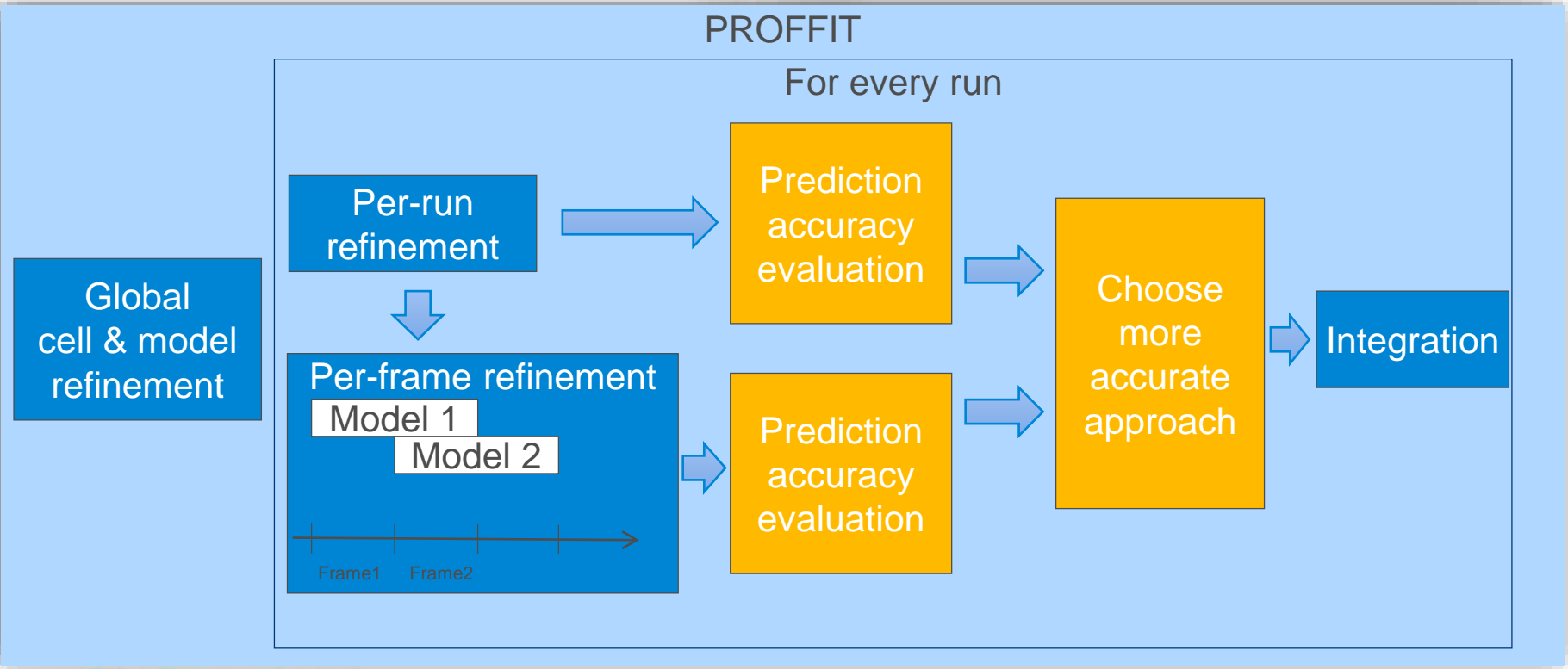
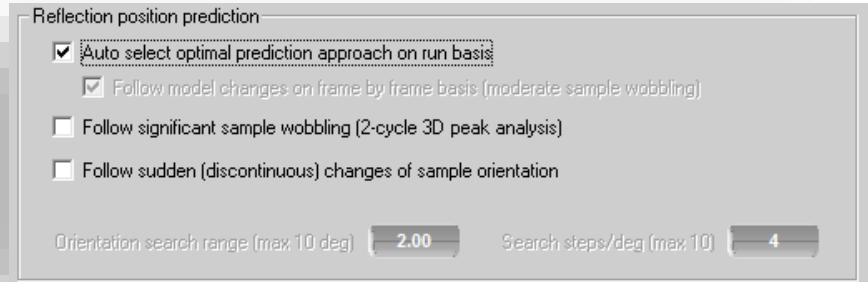
- Enlarge integration mask according to prediction uncertainty



Data reduction

Model refinement options

No need to decide
– program does it for you!



Data reduction

Model refinement options

Reflection position prediction

- Auto select optimal prediction approach on run basis
 - Follow model changes on frame by frame basis (moderate sample wobbling)
 - Follow significant sample wobbling (2-cycle 3D peak analysis)
 - Follow sudden (discontinuous) changes of sample orientation

Orientation search range (max 10 deg)

2.00

Search steps/deg (max 10)

4

- 2-cycle PROFFITPEAK
- Covers more difficult “wobbling” cases

PROFFITPEAK

For every run

Profile analysis

Per-run
refinement

Per-frame
refinement

Choose more accurate
approach

Profile analysis

PROFFITMAIN

Cell/model
refinement

For every run

Per-run
refinement

Per-frame
refinement

Choose more accurate
approach

Integration

Data reduction

Model refinement options

Reflection position prediction

- Auto select optimal prediction approach on run basis
 - Follow model changes on frame by frame basis (moderate sample wobbling)
 - Follow significant sample wobbling (2-cycle 3D peak analysis)
 - Follow sudden (discontinuous) changes of sample orientation

Orientation search range (max 10 deg) Search steps/deg (max 10)

- Model refinement with matrix orientation search
- For discontinuous sample jumps (LT, flexible holder, not fixed properly, etc.)

PROFFITPEAK

For every run

Cell orientation search

Profile analysis

Per-run refinement

Per-frame refinement

Choose more accurate approach

Profile analysis

PROFFITMAIN

Cell/model refinement

For every run

Cell orientation search

Per-run refinement

Per-frame refinement

Choose more accurate approach

Integration

Manual Data Reduction

Sample slippage example

- Superficially gives impression of twin
 - Twin indexing matches 96.8% of reflections

TWIN ANALYSIS

Component	Ratio	Isolated	Overlapped
1	0.37	1676	24
2	0.63	1690	24

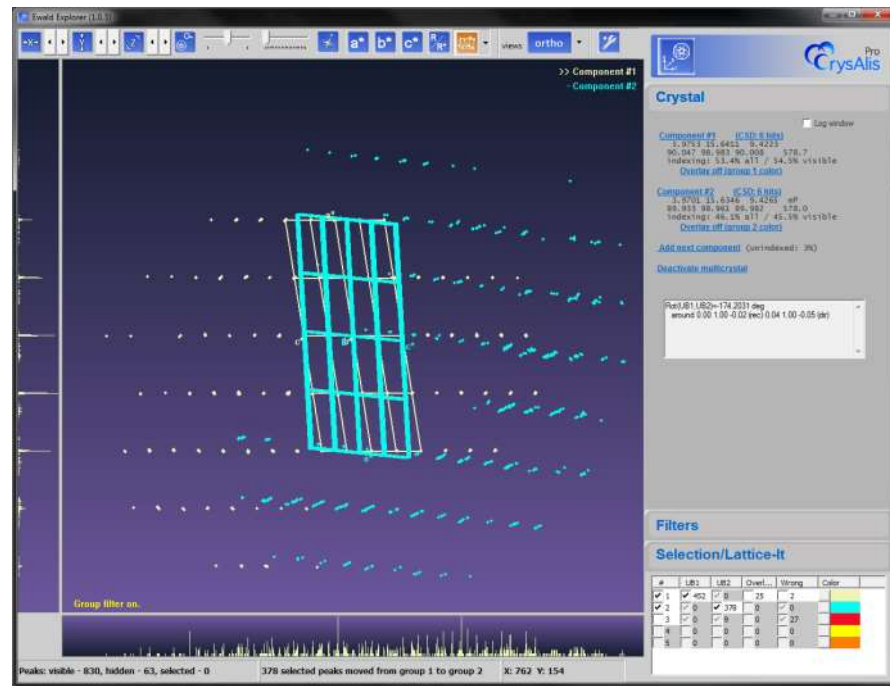
DECOMPOSED TWIN DATA STATISTICS (<0.80 overlap)

Component	Redundancy	F2/sig(F2)	Rint
1	1.5	9.7	0.245
2	1.5	7.0	0.658

Overlap limit for HKLF4 export: 0.80

TWIN HKLF5 STATISTICS FOR OVERLAPPED OBS

Components	Redundancy	F2/sig(F2)	Rint
1,2	1.3	24.8	0.223



... but twin integration doesn't help

Manual Data Reduction

Sample slippage example

Lattice wizard (1.0.32)

Lattice wizard

LATTICE

Current cell (CSD: 6 hits)
3.977(2) 15.622(7) 9.424(12) 90.08(7) 98.83(8) 89.98(4) 578.5(8)

Constrained current cell
No constrained unit cell present!

Lattice reduction
selected cell
3.9790 15.6360 9.4181 90.0060 98.9536 89.9391 mP 34
reduced cell
3.9790 9.4181 15.6360 89.9940 89.9391 81.0464 578.8

PEAK TABLE

Peak hunting table
UB fit with 477 obs out of 893 (total:893,skipped:0) (53.42%)
After per-run orientation adjustment:
UB fit with 860 obs out of 893 (96.30%)

INSTRUMENT MODEL

Goniometer
beam: 0.06483 alpha: 50.06949 beta: -0.06608
om zero: 0.08435 th zero: -0.13584 ka zero: -0.05539

Detector
x-rot: 0.45333 y-rot: -0.14434
x-cen: 1026.96119 y-cen: 1038.70213 distance: 50.00000
Wavelength Cu (Ang): A1 1.54056 A2 1.54439 B1 1.39222

Peak hunting

Ewald explorer - reciprocal space

Refine instrument model

Twinning - multi-crystals

Load information

Unwarping - Precession images

Log window

Unit cell finding

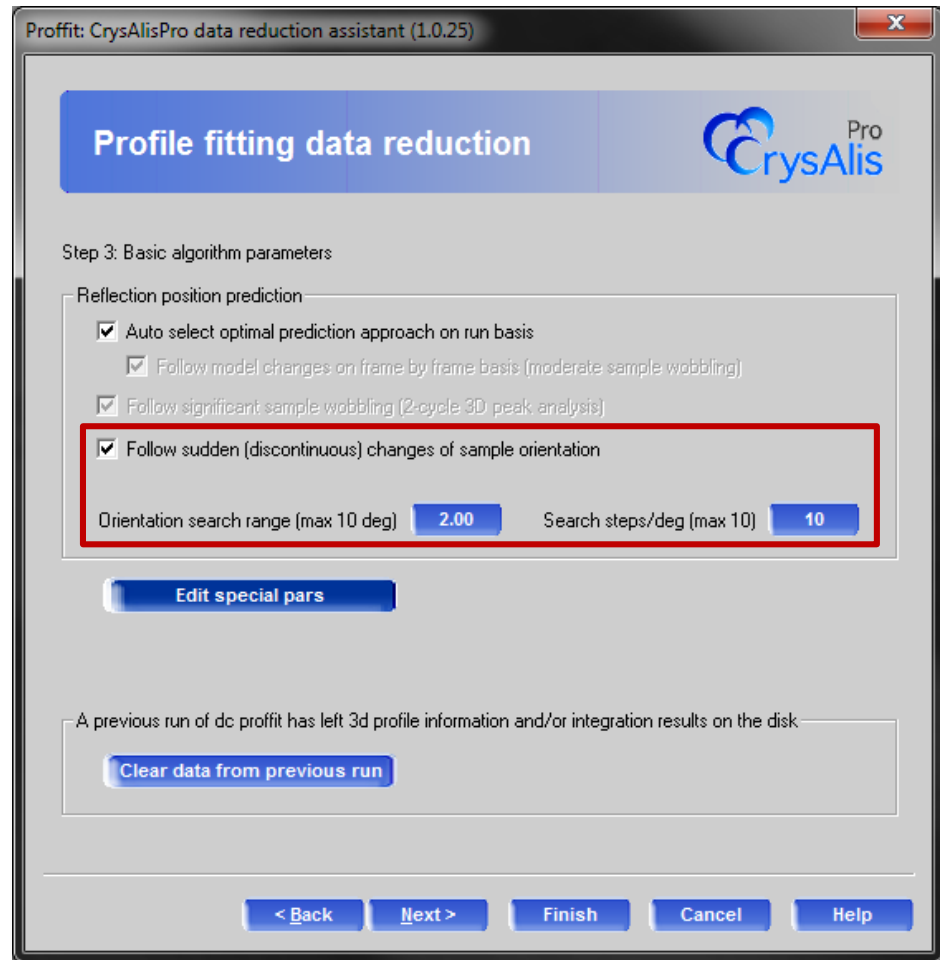
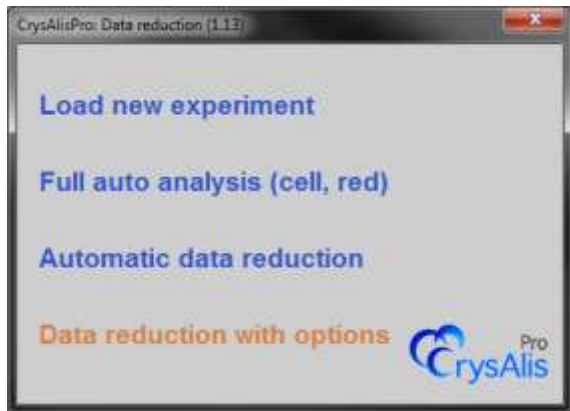
- Unit cell finding with options
- Select unit cell from list of found cells
- Brute force indexation of known cell
- Indexation from three known reflections
- Set orientation matrix by hand
- Unit cell finding in direct space (Clegg)
- Search for smaller unit cell volume
- Search for better x,y detector center
- Remove lambda-half reflections from peak table
- Crystal shape
- Find reflection tails and mark skip
- Delete reflection tails
- Check for the sample jumping
- Unit cell gaps

Save information

Close

Manual Data Reduction

Sample slippage example



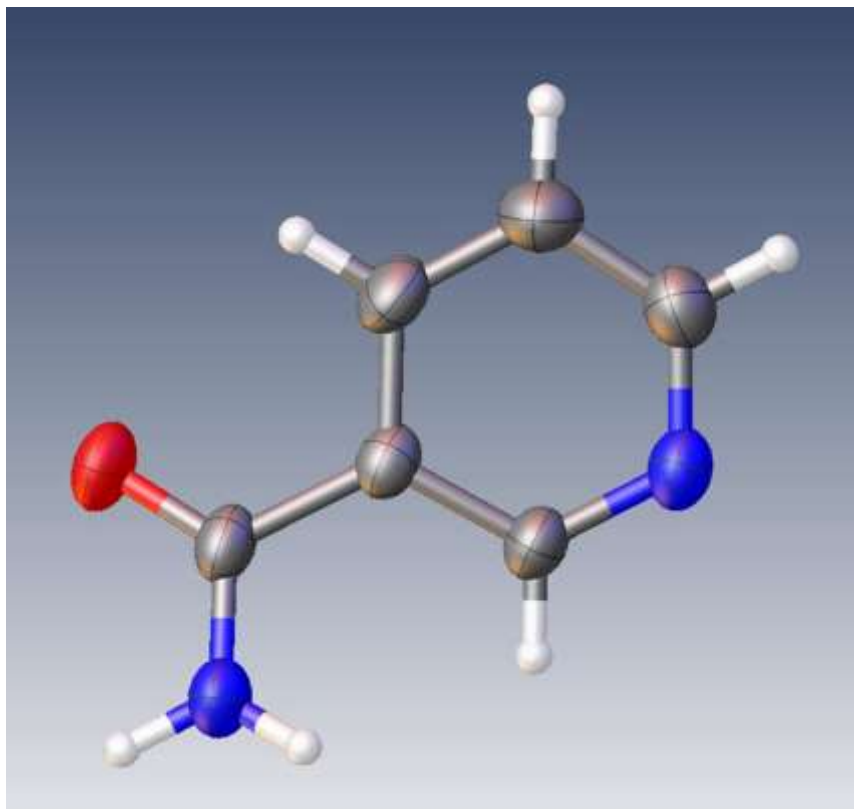
RESULTS (466 frames) - SYM: P2/m (b-unique)

Resolution(A)	Redundancy	F2/sig(F2)	Rint
inf - 0.80	1.5	22.4	0.016
inf - 0.84	1.5	23.2	0.016

Completeness: 98.4% (0.84 ANG)

Manual Data Reduction

Sample slippage example




	No slip	Intentional sample slip	
	Reference data	Slip Data (Pre-Treatment)	Slip Data (Post-Treatment)
R_{int} (%)	1.6	14.7	1.6
I/σ	22.0	5.0	22.9
R_1 (%)	3.32	43.88	3.46
Comp (%)	98.5	95.2%	98.4%

Manual Data Reduction

Background correction

Proffit: CrysAlisPro data reduction assistant (1.0.25)

Profile fitting data reduction 

Step 4: Background evaluation

Background for 3D centroids

For an accurate evaluation of integrated intensities a good background determination is essential. Two parameters control this evaluation: The evaluation range R_e and the repeat frequency F_r .

$R_e = 25$ $F_r = 25$

Binning may reduce the memory requirements for the background evaluation. Default is 1. You may use 2 or 4 in case of lack of physical memory on your machine (risk of swapping)!

1 2 4 Reduce background accumulation to SHORT type (saves memory)

Required disk/memory space for background evaluation: 189.8/50.0 Mb

Background for 3D integration

Average background from 3D centroid evaluation (good for stable & low background, fast)

Smart background (combination of local and average background computation, good for weaker data with high background and locally varying features, e.g. protein data, slower)

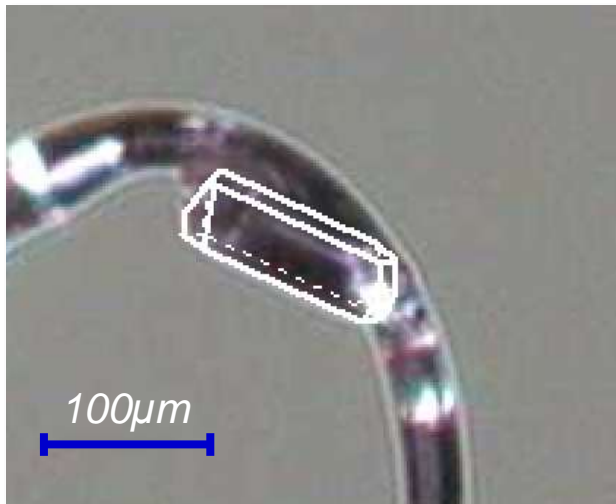
Frame range = 5 Memory usage: 44.0 Mb

Choice of background correction:

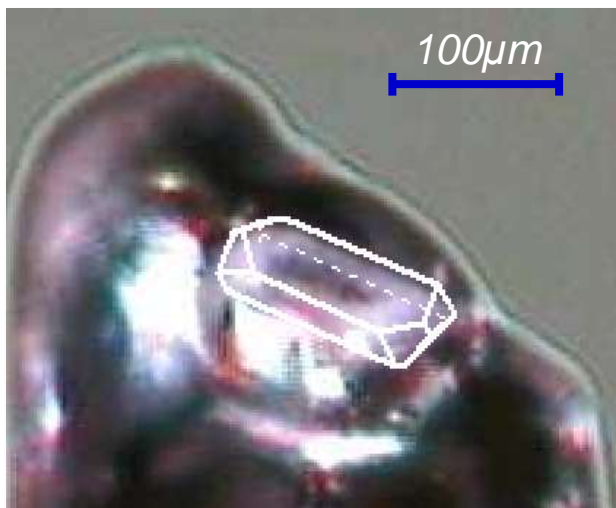
- Average background
 - Define range and frequency
- Smart background
 - Combination of local and average background
 - Improves statistics ($1/\sigma$) for samples with varying background features

Manual Data Reduction

Background correction



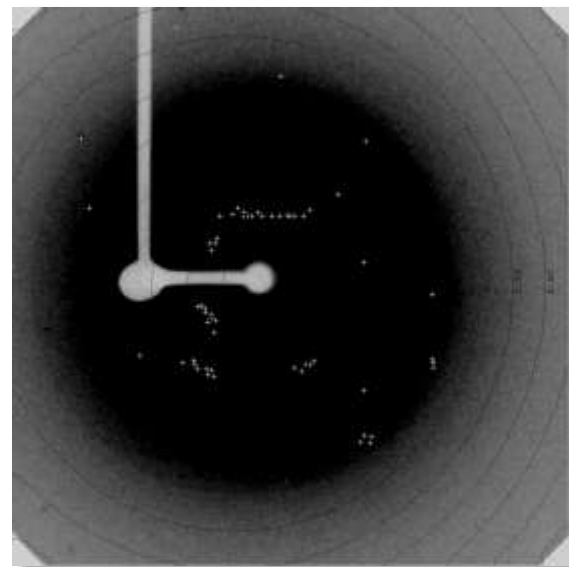
Well-mounted
sample



Intentionally
badly-mounted
sample

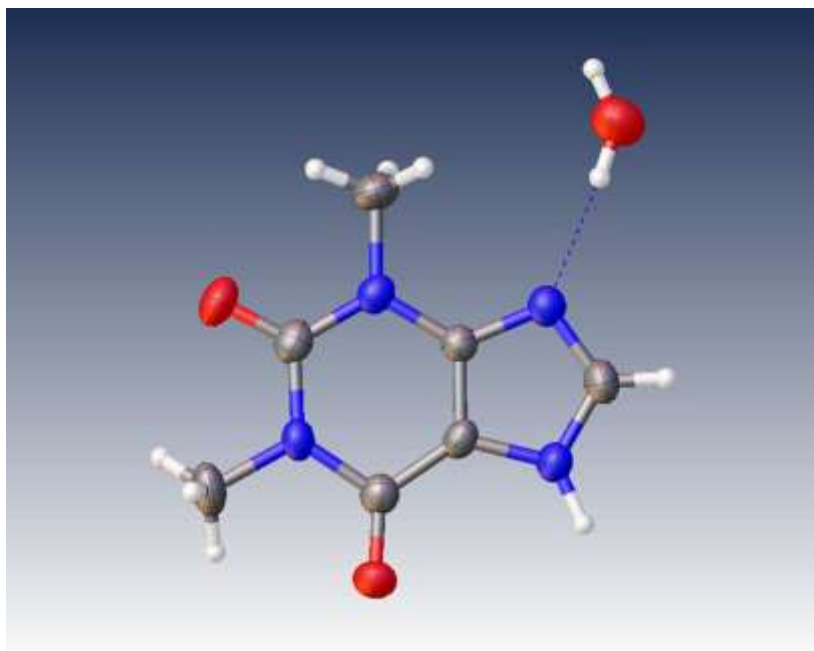


Standard peak-hunting
produces many non-lattice
peaks.



Manual Data Reduction

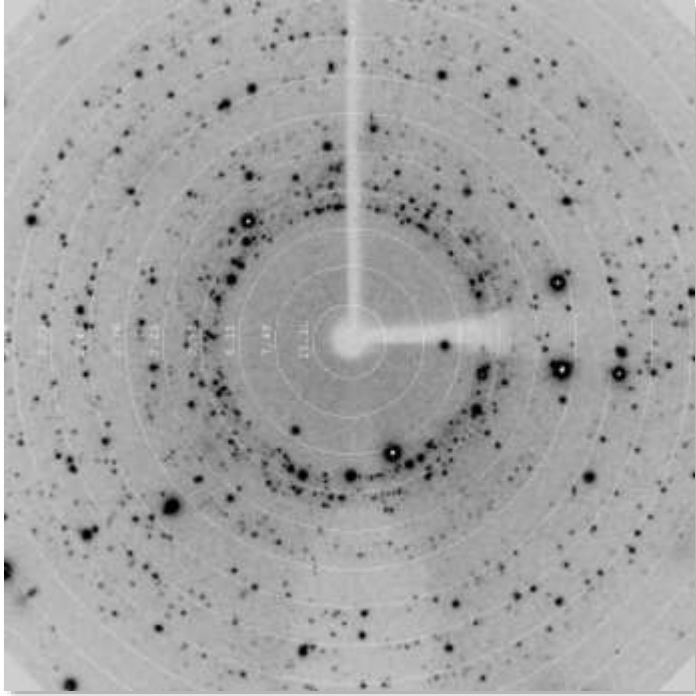
Background correction



	Well-mounted	Badly-mounted	
	Reference Data	Auto analysis	Smart Background
Time	3h 8m	16h 18m	16h 18m
Diff. Limit	0.92	1.41	0.97
R _{int} (%)	3.1	14.4	5.8
I/σ	13.5	3.0	7.8
R ₁ (%)	5.28	-	6.22
Comp (%)	99.5	99.5	99.5

Manual Data Reduction

Bad profile rejection

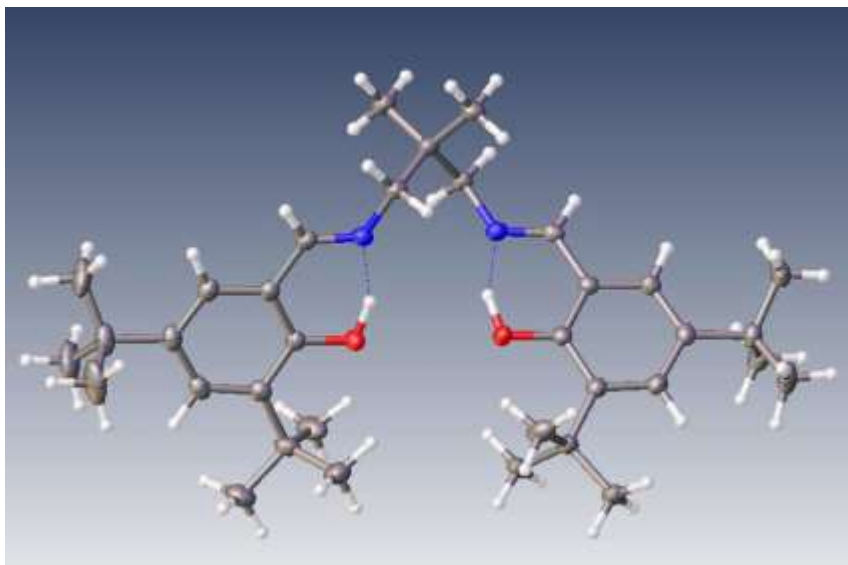


Simulation of cryo-failure
(shield flow turned off)



Manual Data Reduction

Bad profile rejection



No ice

Large ice build-up

	Reference Data	Auto analysis	d range and run Filtering	Bad profile filtering
R_{int} (%)	2.6	10.5	3.2	4.0
I/σ	17.7	8.4	14.0	12.7
R_1 (%)	3.83	6.11	4.11	4.50
Comp (%)	99.9	99.9	92.6	98.6

Manual Data Reduction

XX PROFFITLOOP - ultimate tool

- Afterwards browse the results in the finalizer window

The screenshot displays the 'Inspect data collection and reduction results' window. It features a table of data reduction statistics and a summary table below it.

Data reduction file contents	Data reduction output	Red graphs	Data collection output	Devices log
inf-2.04	29	49	26	53.1
2.04-2.32	36	40	26	65.0
2.32-1.99	27	50	26	52.0
1.98-1.82	35	37	26	70.3
1.82-1.69	30	51	26	51.0
1.68-1.56	26	51	26	51.0
1.56-1.47	28	52	26	50.0
1.47-1.41	27	57	26	45.6
1.40-1.34	27	59	27	45.8
1.33-1.26	26	89	26	29.2
inf-1.26	291	537	261	48.6

Statistics vs resolution (taking redundancy into account) - Leue group (anomalous pairs merged): Phase	resolution(Å)	# kept	# theory	# unique	% complete	average redundancy	mean F2	mean F2/sig(F2)	Rint	RsigmaB
inf-2.04	30	42	25	59.5	1.2	2779347.65	94.61	0.004	0.009	
2.03-2.17	46	38	25	65.0	1.8	1451383.82	68.79	0.011	0.011	
2.15-1.90	39	36	25	69.4	1.6	963106.64	44.19	0.014	0.016	
1.89-1.73	36	35	25	71.4	1.4	542996.56	25.45	0.040	0.031	
1.72-1.56	35	41	25	61.0	1.4	701577.69	29.48	0.030	0.028	
1.55-1.46	32	41	25	61.0	1.9	539831.23	21.38	0.028	0.032	
1.45-1.36	35	45	25	55.6	1.4	402046.47	17.89	0.018	0.036	
1.35-1.26	38	68	32	47.1	1.2	340238.39	15.65	0.027	0.041	
inf-1.26	291	351	207	59.0	1.4	948740.98	39.79	0.015	0.017	

Data reduction ended at Wed Mar 18 12:21:33 2015

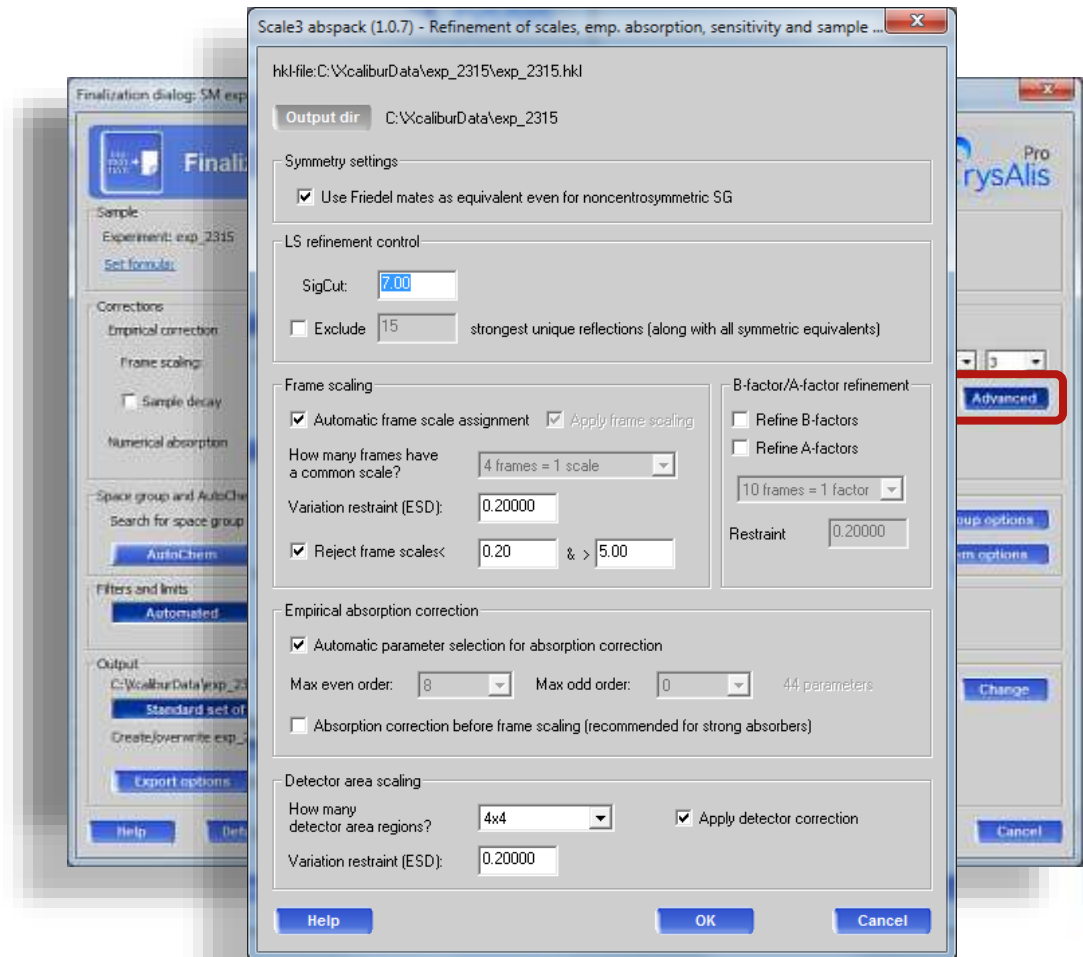
Buttons: Refinalize, Crystal movie, OK

Dropdown menu (selected):
 exp_2315_of_mask
 exp_2315_of_mask_on_75_bkg1
 exp_2315_of_mask
 exp_2315_of_mask_bkg1
 exp_2315_of_mask_on_75
 exp_2315_of_mask_on_75_bkg1

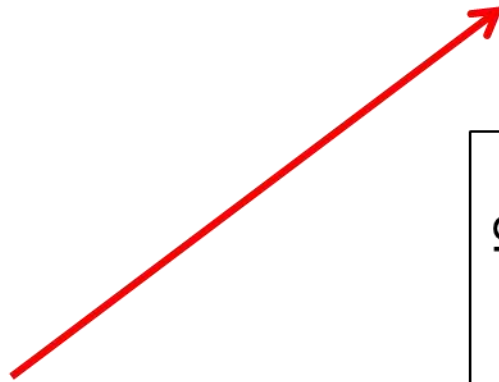
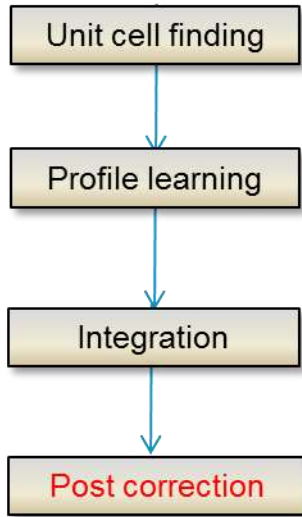
Post-integration empirical corrections

- Scaling
- Empirical absorption based on spherical harmonics
- Decay
- Detector sensitivity

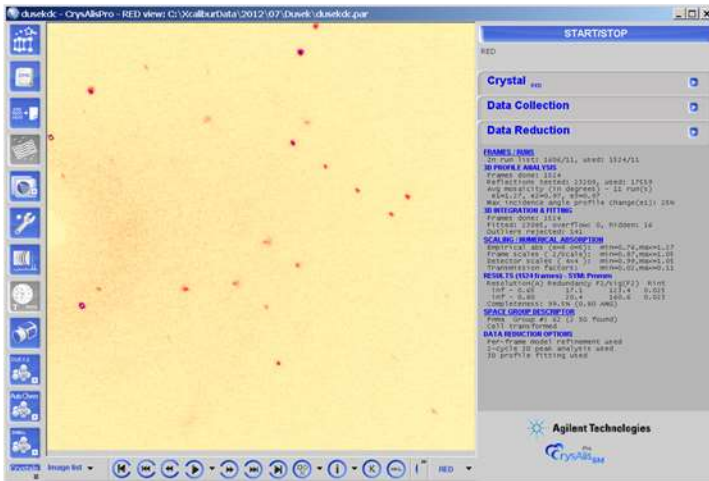
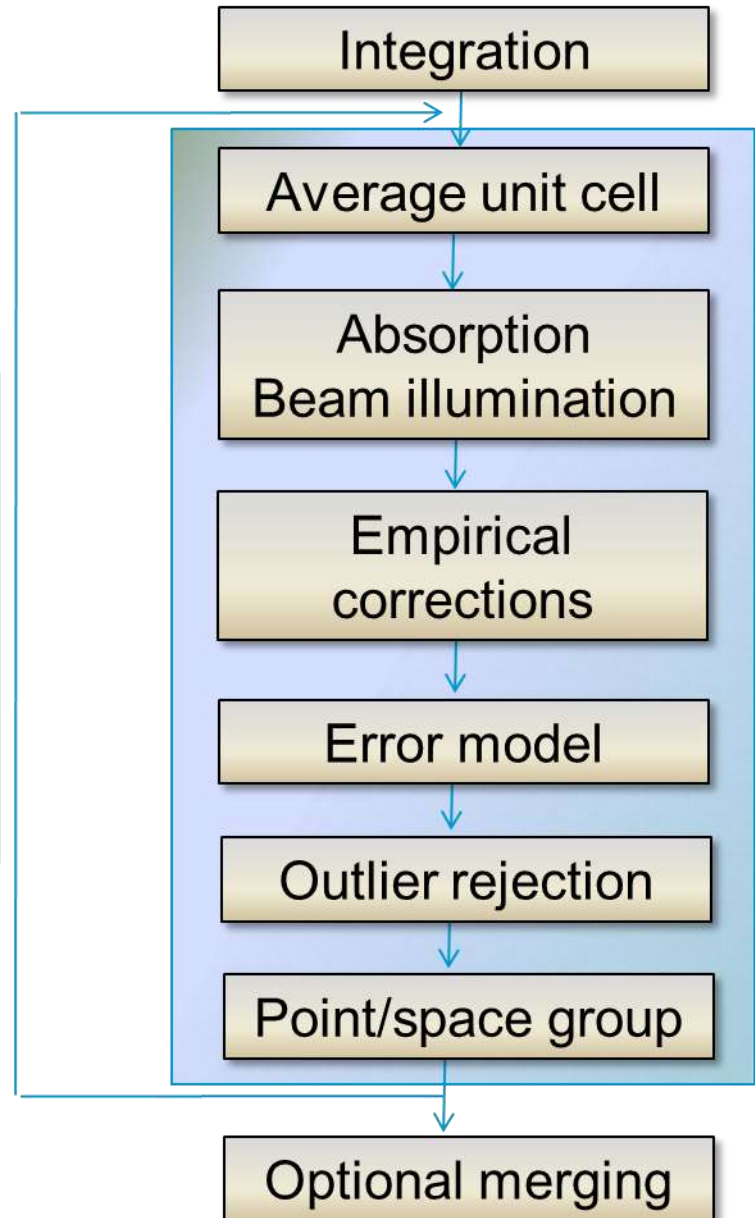
Try manual settings!



Remark on scaling of non-centro data

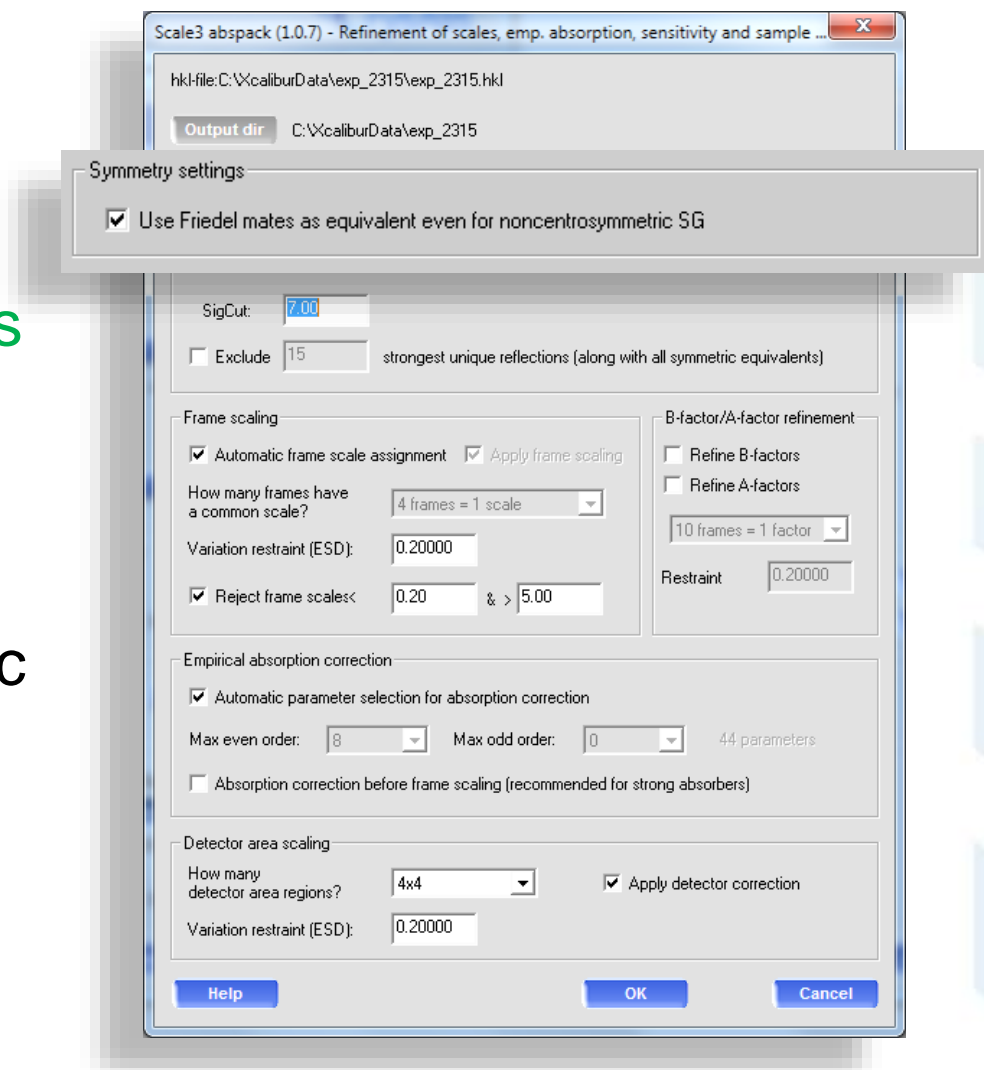


PG changed?



Remark on scaling of non-centro data

- Organic samples – Friedel pairs equivalent
- Samples with heavier atoms – scaling with Friedel pairs merged may destroy anomalous signal info
- Version 38 makes automatic decision based on provided formula (“heavy” means Si for Cu, Sc for Mo)



Optimal data – hints at experiment time

- Centering/Sample choice/holder/amount of oil
- Low T: de-ice runs
- Absorption: make movie 1-6 deg
- Concurrent data red re-start
- Cu – Mo choice
- Collect redundant data
- Rather reduce scan width than increase dd
- Check your diffraction limit

Optimal data – hints at unit cell finding time

- Check for non-indexing reflections
- Garbage (ice rings, powder), twin, sample jump
- Re-run refine model
- Ewald
 - Use filters (intensity, lattice type) and groups
 - Use intensity view
- Check chemical formula unit cell consistency

Optimal data – hints at data reduction time

- Check for experiment artifacts (empty frames, trips)
- Apply Bravais lattice where obvious
- Special pars
 - Use bad reflection filter
 - Use reduced profile size if overlapping
 - Incidence correction, prediction accuracy
- Smart background on high background data
- xx proffitloop

Optimal data – hints at data finalization time

- Hand set empirical parameters
- Use shape based absorption correction
- Apply filters carefully (e.g. Rint)
- Interactively decide space group
- Remove unnecessary data via d-value filter

Software Updates

- **CrysAlis^{Pro}** is frequently updated with fixes for known problems
- New features are introduced in annual major updates
- All updates are **Free** and available from our user forum,
<http://www.rigakuxrayforum.com>
- **Free** multi-user, multi-site license

The screenshot displays the Rigaku Oxford Diffraction forum interface. At the top, the Rigaku logo and navigation links (Portal, Search, Calendar, Help) are visible. A user login bar shows 'Welcome back, mathias meyer' with a 'Log Out' link. Below the navigation, the forum is organized into several sections:

- Announcements:** A table with columns 'Forum', 'Threads', 'Posts', and 'Last Post'. The 'General Updates' forum has 36 threads and 58 posts, with the last post by 'Mrs Gibbs' on 14-06-2015 at 04:07 AM.
- Software:** A section for downloading, getting help with, and discussing software. It includes a link to 'CrysAlisPro Download'. Below it is a table with columns 'Forum', 'Threads', 'Posts', and 'Last Post'.
 - CrysAlisPro:** A sub-forum for the CrysAlisPro software including downloads, manuals, guides and discussion areas. It has 378 threads and 1,395 posts. The last post is 'Experimental setup to rec...' by 'peterbus' on 19-06-2015 at 08:13 AM.
 - CrysAlisEvo:** The most recent version of CrysAlis for the PC. It has 1 thread and 1 post. The last post is 'Demonstration videos' by 'Flaser White' on 20-06-2015 at 02:00 PM.
 - Other third party software:** A place to discuss and get help with non-Rigaku software. It has 0 threads and 0 posts, with the last post being 'Never'.
- General Crystallography:** A non-product specific forum for crystallographic discussion of such things as matters, mineral space or whatever you fancy. It has a table with columns 'Forum', 'Threads', 'Posts', and 'Last Post'. The 'Applications' forum has 120 threads and 893 posts, with the last post 'RPO STRUCTS' by 'kirkball' on 18-06-2015 at 12:13 PM.
- Conferences, Exhibitions, and Presentations:** Which conferences we'll be attending, and presentations we've given. It has a table with columns 'Forum', 'Threads', 'Posts', and 'Last Post'.
 - Literature, Posters and Presentations:** Links & Downloads to application notes, posters and presentations from various conferences. It has 0 threads and 24 posts. The last post is 'European X-ray Crystallog...' by 'Flaser White' on 08-04-2015 at 08:03 AM.
 - Conferences and Exhibitions:** Upcoming events. It has 1 thread and 1 post. The last post is 'Upcoming Events' by 'Flaser White' on 27-06-2015 at 11:03 AM.

Thank you for listening!

Find out more at

www.rigaku.com