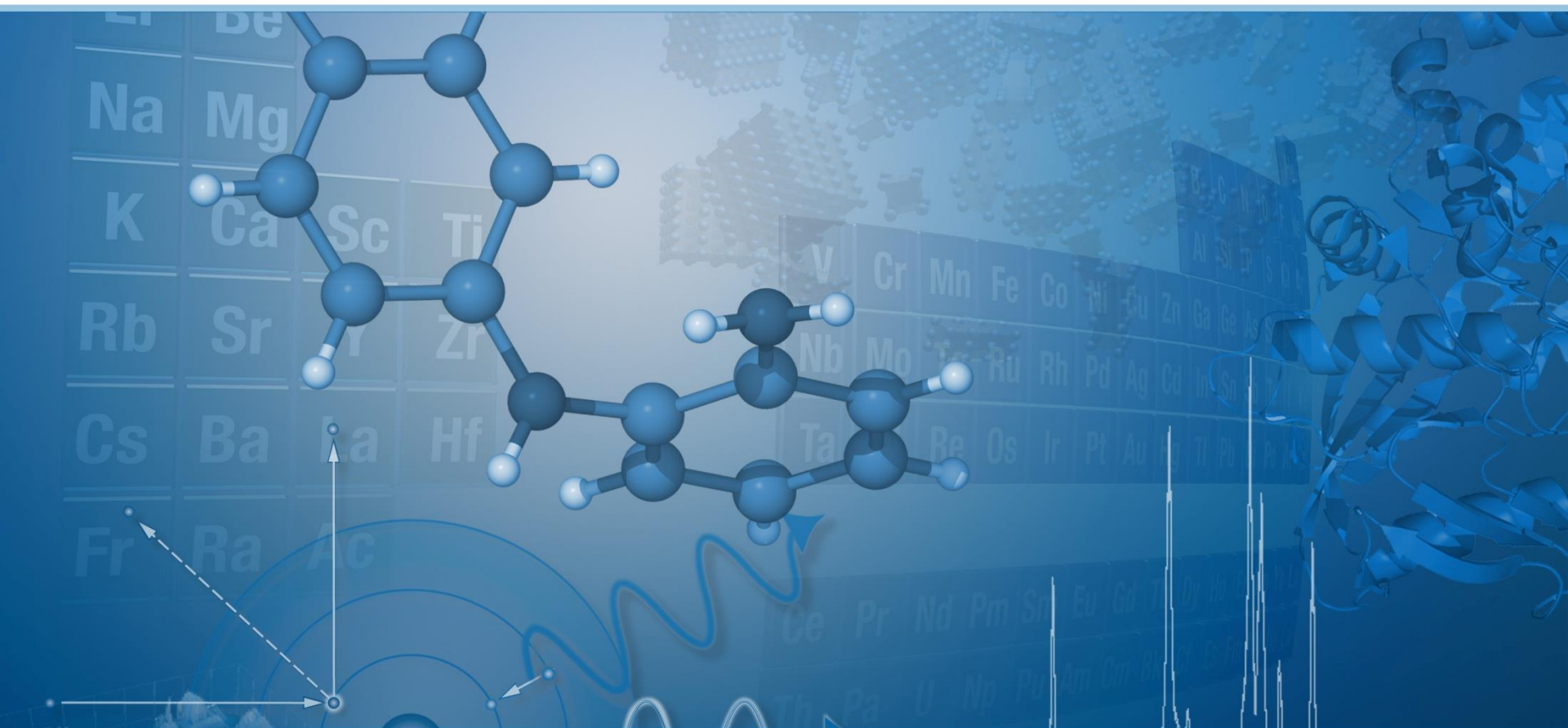


Data Reduction and Evaluation with PROTEUM3



PROTEUM2 Suite

The PROTEUM2 suite has a completely new approach on how a user interacts with a crystallographic experiment. The Graphical User Interface guides the user through the complete experiment with minimal user input and maximal graphical feedback. PROTEUM2 is easy to use for the novice but has all the features required by expert crystallographers.

Some of the software's included in PROTEUM2 suite are:

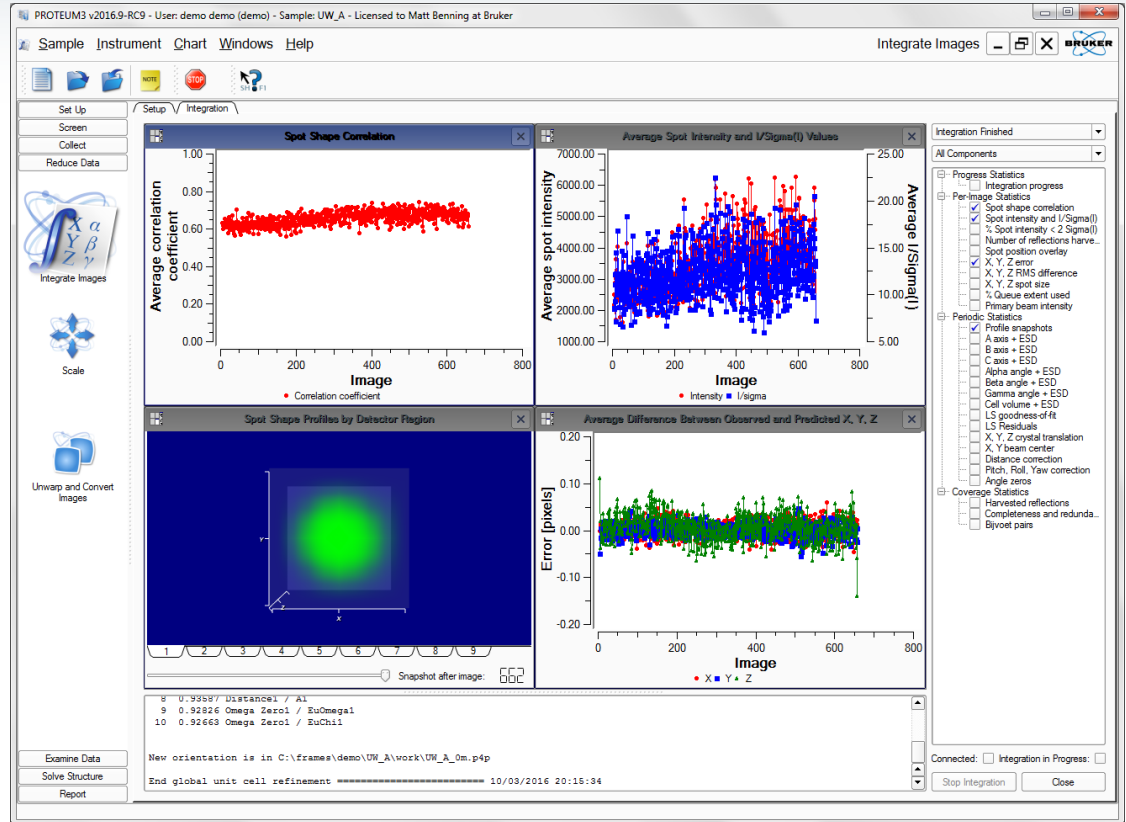
- SAINT – 3D profile integration
- SADABS – data scaling with absorption correction
- XPREP - space group determination and data analysis
- Pointless/Aimless – data analysis and create MTZ

SAINT Integration



Determine the raw intensities of the reflections

- True 3D profile fitting
 - Creates reflection profiles
 - No partial reflections
- Extended Graphical feedback
 - 3D profile display
 - Spot overlays
- Automatic, manual modes
- Easily handles fine sliced data
- Handles twinned data



SAINT

Integration



Steps during integration:

- Determination of an initial background
- Determination of active pixel mask (for marking reflections which are outside the detector active area, behind the beam stop or the shadow of the low temp device)
- Read-in the orientation matrix
- Determination of initial spot shape profiles, with concurrent refinement of the starting orientation matrix and initial background
- Integration of each defined run; output intensities are corrected for Lorentz factor, polarisation, air absorption and absorption due to the variation of the path length through the detector faceplate
- Elimination of spots whose shapes correlate poorly with model profile shapes, relative to other spots of similar $I/\sigma(I)$

SAINT Integration



PROTEUM3 v2016.9-0 - User: demo demo (demo) - Sample: Neil1 - Licensed to Matt Benning at Bruker

Sample Instrument Chart Windows Help

Integrate Images

Set Up / Setup

Starting Image Filename	Images	Output Filename
1 C:\frames\demo\Neil1\S207E3_01_0001.afm	800	C:\frames\demo\Neil1\work\S207E3_01.raw
2		
3		
4		
5		
6		
7		
8		
9		
10		
11		
12		
13		
14		
15		
16		
17		
18		
19		
20		
21		
22		
23		
24		
25		
26		
27		
28		
29		
30		
31		
32		
33		
34		
35		
36		
37		
38		
39		
40		
41		
42		
43		
44		

Resolution Limit (Å): 2.000

Unit Cells:
 a=132.14Å, α= 90.00°, V=769001Å³
b=132.14Å, β= 90.00°, Rhombohedral R
c= 50.86Å, γ=120.00°

Refinement Options...
Integration Options...
Find Runs...
Import Runs from Experiment...
Start Integration...

→ Check resolution limit and unit cell constants

a=132.14Å, α= 90.00°, V=769001Å³
b=132.14Å, β= 90.00°, Rhombohedral R
c= 50.86Å, γ=120.00°

→ Refinement, integration options

Start integration

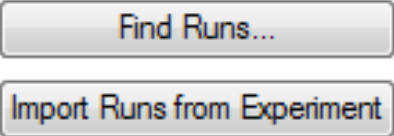
→ Importing runs

SAINT

Importing runs

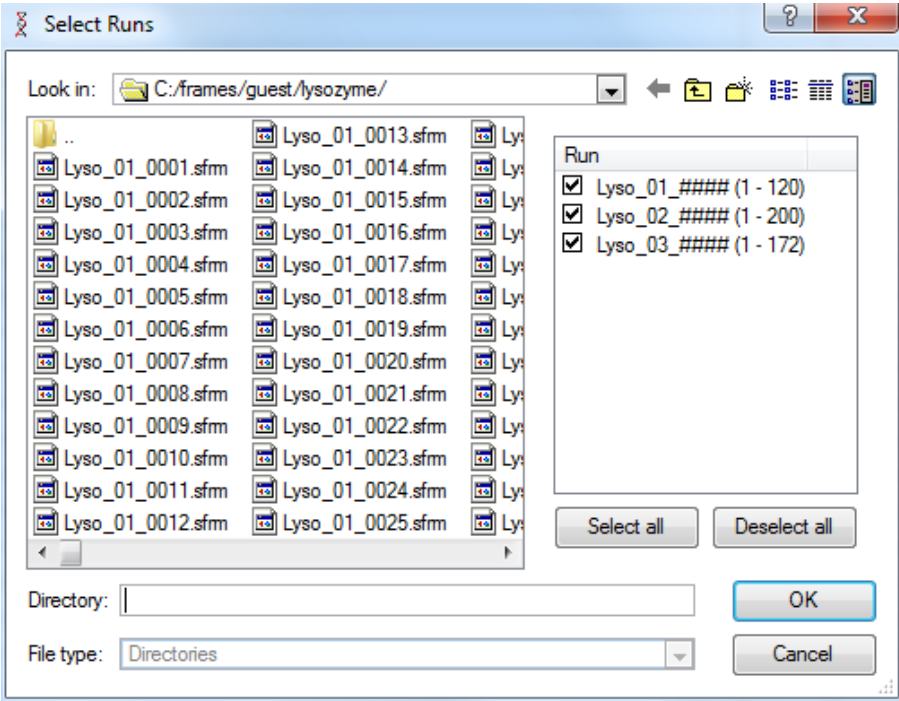
Find Runs

- Looks in the entry folder for the number of runs and images
- You can select all or just the runs you want and click "OK"



Import Runs from Experiment

- Gets scan information directly from BIS
- Need to be connected to the instrument to import from BIS



SAINT

Refinement options



SAINT Refinement Options

Per-Image Refinement

Enable Orientation Refinement

Enable Box Size Refinement

Damping Factor: 1.000

Initial XYZ Box Size [°]: 0.633 0.633 0.752

Periodic Refinement

Enable Periodic Refinement

Enable Initial Passes

Frequency [Images]: 50

Constrain Metric Symmetry of Unit Cell to:

Tetragonal

Crystal System: Tetragonal

Refinement Parameters

- Detector
 - Horizontal Beam Center
 - Vertical Beam Center
 - Distance
 - Pitch
 - Roll
 - Yaw
- Unit Cell
 - Axes
 - Angles

Global Refinement

Enable Global Refinement

Max. Number of Reflections: 9999

Constrain Metric Symmetry of Unit Cell to:

Tetragonal

Crystal System: Tetragonal

Refinement Parameters

- Detector
 - Horizontal Beam Center
 - Vertical Beam Center
 - Distance
 - Pitch
 - Roll
 - Yaw
- Unit Cell
 - Axes
 - Angles

OK Cancel

← Initial box size

- Determined automatically by the program and refined during integration.
- If the mosaic spread is very high ($> 1.5^\circ$), you may want to turn off the refinement and set the box size based on the initial profiles.

SAINT

Refinement options



The screenshot shows the SAINT Refinement Options dialog box. It is divided into several sections:

- Per-Image Refinement:** Includes checkboxes for "Enable Orientation Refinement" and "Enable Box Size Refinement". It also has a "Damping Factor" field set to 1.000 and "Initial XYZ Box Size" fields set to 0.633, 0.633, and 0.752.
- Periodic Refinement:** Includes checkboxes for "Enable Periodic Refinement" and "Enable Initial Passes". It has a "Frequency [Images]" dropdown set to 50. Under "Constrain Metric Symmetry of Unit Cell to:", the "Tetragonal" radio button is selected, and the "Crystal System" dropdown is set to Tetragonal.
- Global Refinement:** Includes a checkbox for "Enable Global Refinement". It has a "Max. Number of Reflections" dropdown set to 9999. Under "Constrain Metric Symmetry of Unit Cell to:", the "Tetragonal" radio button is selected, and the "Crystal System" dropdown is set to Tetragonal.
- Refinement Parameters:** Two lists are shown, one for Periodic and one for Global refinement. Both lists have "Detector" and "Unit Cell" sections. Under "Detector", parameters include Horizontal Beam Center, Vertical Beam Center, Distance, Pitch, Roll, and Yaw. Under "Unit Cell", parameters include Axes and Angles. All these parameters have checkboxes that are checked.

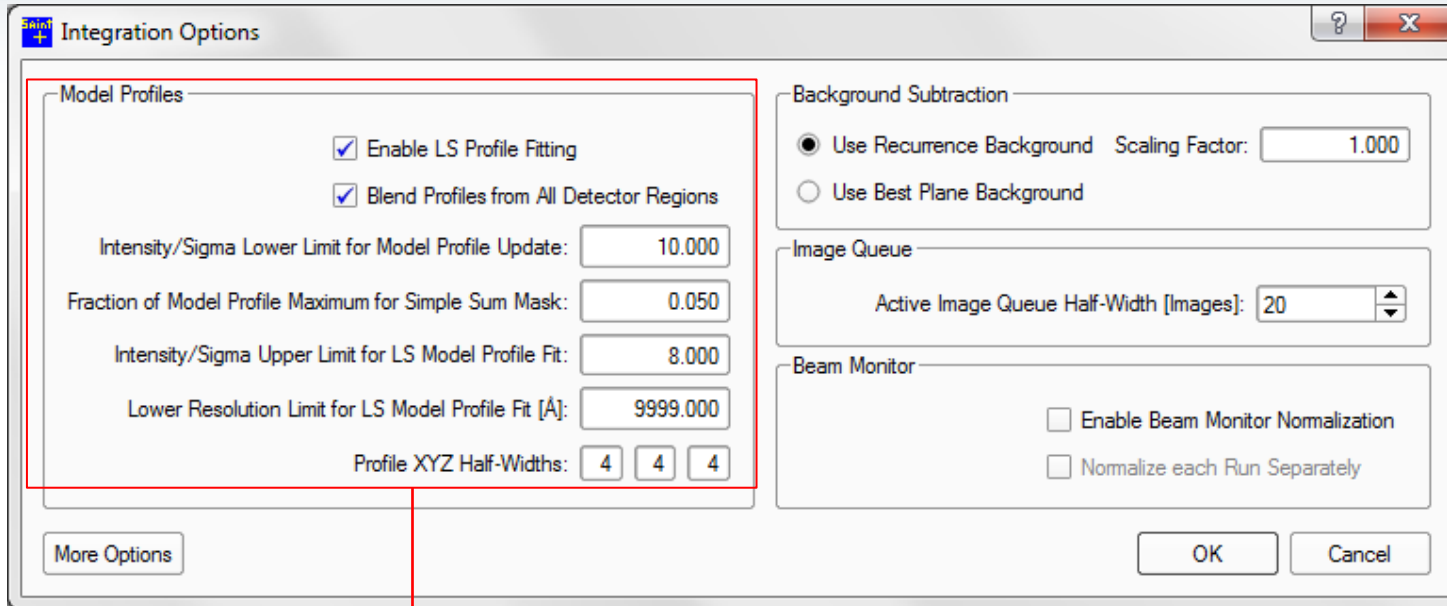
At the bottom of the dialog are "OK" and "Cancel" buttons.

← Cell refinement

- **Periodic LS** refinement during integration after a set of images.
- **Global LS** refinement takes reflections from the whole data set and produces the final unit cell constants
- **Refinement Parameters** assigns the offsets updated during refinement. To add or subtract parameters, click the box next to the offset.

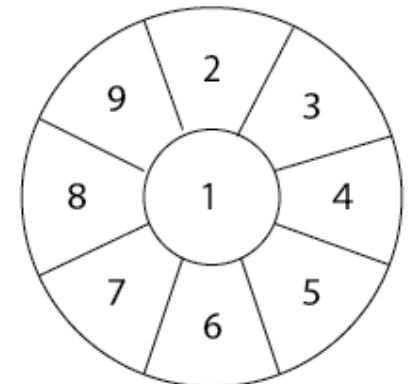
SAINT

Integration options



Model profile determination

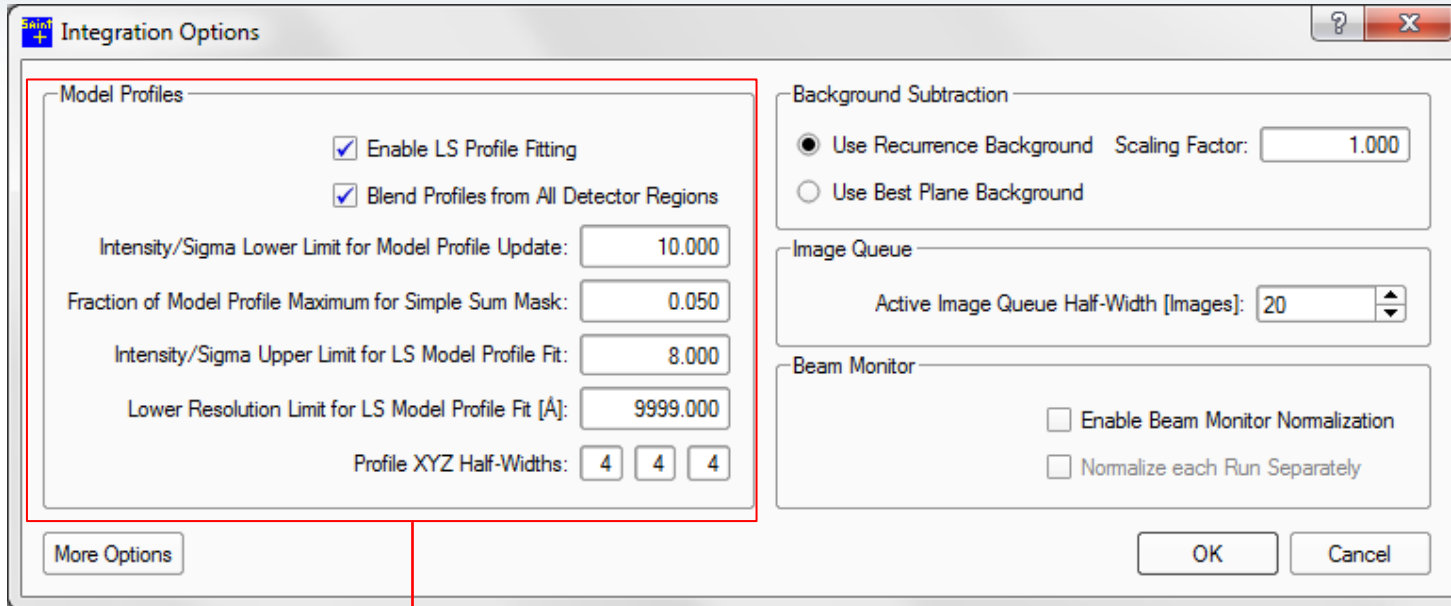
- Use either one profile for the entire detector (Blend) or split the detector into 9 different regions.
- If the detector has enough strong reflections in each region then using nine profiles will probably improve things.
- If the data is weaker, blend the profiles into one global model



Regions for unblended profiles

SAINT

Integration options

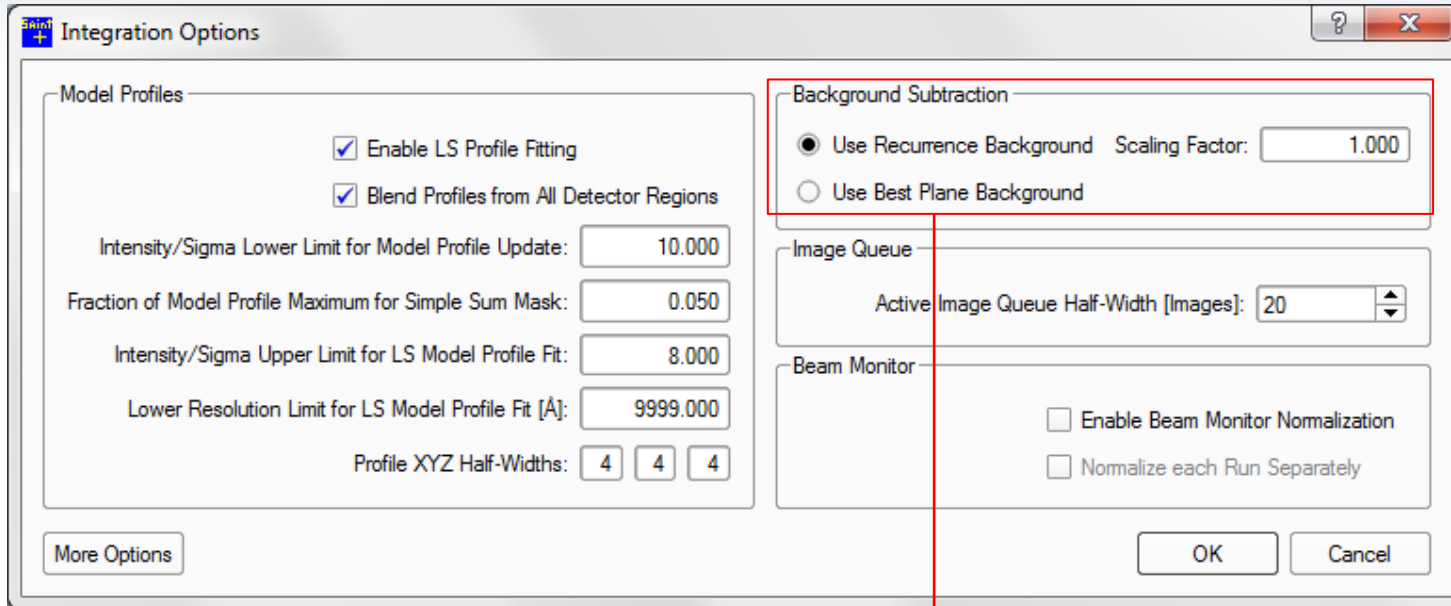


Model profile determination

- Enable LS profile fitting to help model the weak data better.
- Intensity/Sigma Lower Limit is the signal to noise cutoff for reflections used in the model profile determination.
- Profile XYZ Half-Widths – if using very fine slicing (ex 0.1 – 0.2°), try increasing the profile widths. The widths in each direction are $2N + 1$, for 0.2° try 8, 8, 8.

SAINT

Integration options

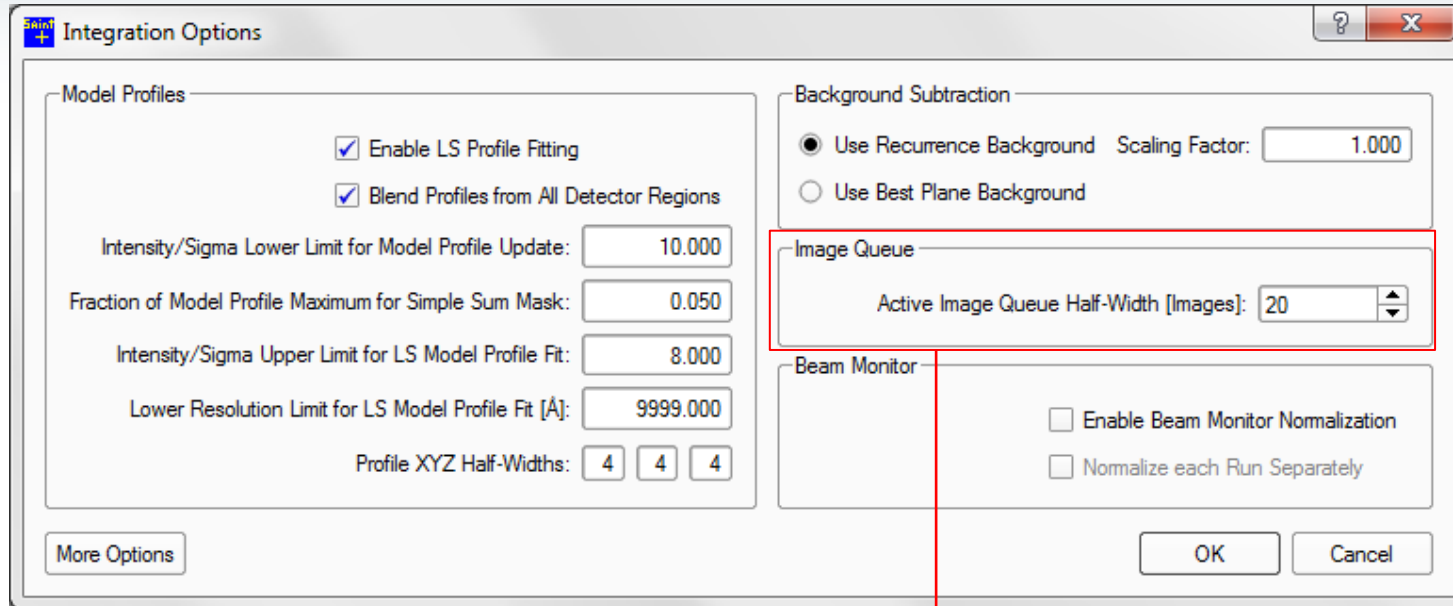


The background scatter is subtracted to increase the signal noise of the reflection

- Recurrence method – Calculates average local background over several frames
- Best Plans method – Determines local background by pixels around the reflection on the current frame only (like HKL, denzo)
- Try both to see which gives the better result

SAINT

Integration options



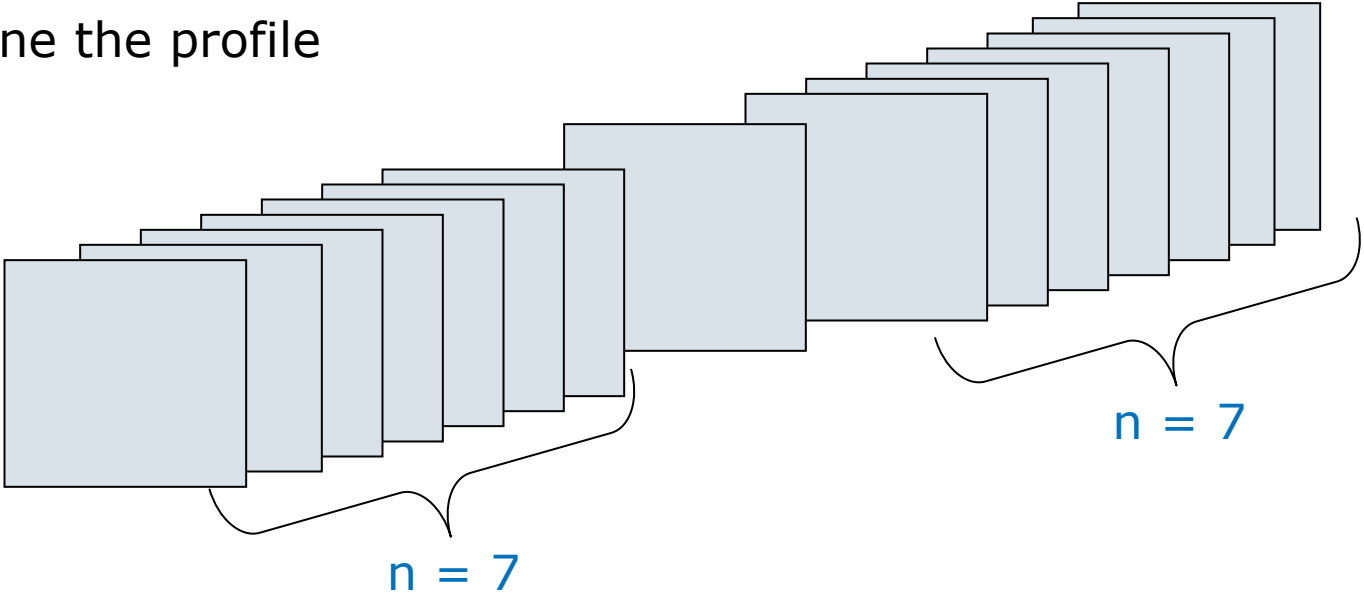
The image queue defines the angular range over which a spot is integrated. Spots that are very wide, like those in the Lorentz region, can be rejected.

- Defines the queue half-width ($2N+1$). For example, if you are collecting 0.2° rotations and have set the image queue to 7, the angular range is: $0.2^\circ \times 2(15) = 6^\circ$.
- Decrease the queue to allow more reflections to be rejected, increase it to integrate more of the data.

SAINT

Image queue

Image queue = set the number of frames used for determine the profile



$$\text{Image queue} = 2n + 1 = 15$$

SAINT

Integration options



Selecting the More Options button shows more parameters

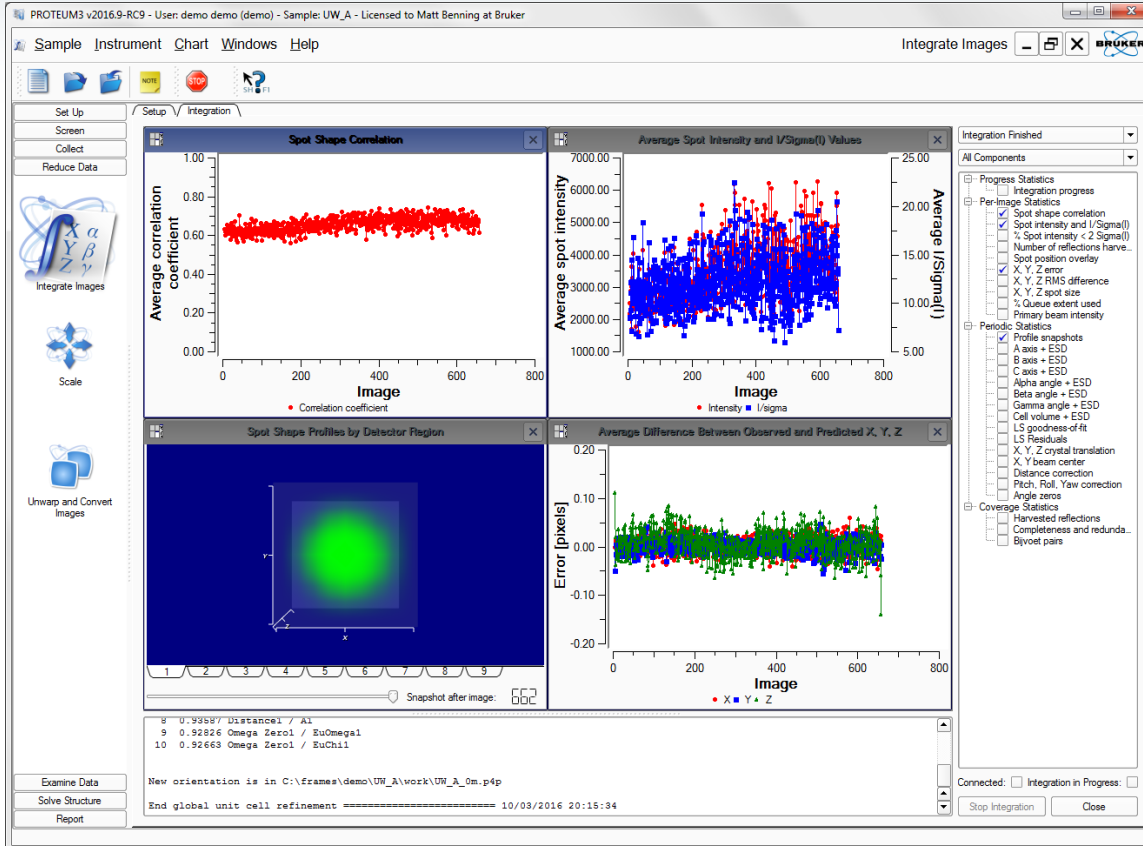
Active Pixel

- Creates a mask for the beamstop shadow
- Program automatically creates a mask if fractional lower limit is set to 0
- Can also read in a predefined mask (Synchrotron detectors)

Algorithm

- Narrow frame for rotation angle $< 1^\circ$
- Try Wide frame for images $> 1^\circ$

SAINT Integration



Spot Shape Correlation

- Agreement between the model profile and reflections.
- Typically > 0.5 , if too low (0.2) then the space group is not correct.
- Integrating at an incorrect resolution limit will also cause the correlation to be low.

Average Spot intensity

- Spot intensity and $I/\sigma I$ values per image

Average Difference: X,Y,Z

- Positional errors between observed and predicted reflections. Values consistently over 0.3 suggest problems

Spot Profiles

- 3-D display of the model spot profiles based on strong reflections

SAINT Integration



PROTEUM3 v2016.9-RC9 - User: demo demo (demo) - Sample: UW_A - Licensed to Matt Benning at Bruker

Sample Instrument Chart Windows Help Integrate Images

Set Up Screen Collect Reduce Data

Starting Image Filename	Images	Output Filename
C:\frames\demo\UW_A\UW_A_01_0001.stm	662	C:\frames\demo\UW_A\work\UW_A_01.raw

Resolution Limit [Å]: 1.903

Unit Cells:
 a=119.14Å, alpha=90.00°, V=340912Å³
b=44.97Å, beta=120.95°, Monoclinic C
c=74.19Å, gamma=90.00°

```
...1.1(1): component 1 in sample 1 (component 1 in UW_A_01.raw)
Centric # Pairs Uniq Meq h<ls <I> <R>Sig <B> Rayn dI/I dI/s R+ Ranom Canon ExK ExY ExZ RmX RmY RmZ
0.000 1966 958 1008 1916 31.6 8897.938 21.74 123.27 0.063 0.000 1.8 0.000 0.120 0.00 0.00 0.00 0.18 .13 .27
2.000

Coverage Statistics
Integration of SW_A
...1.1(1): component 1 in sample 1 (component 1 in UW_A_01.raw)
.....Shell.....
Angstroms #Obs Theory #Comp Redund Rayn Pairs #Pairs Data11 #Sigma #Q2s
to 4.094 2318 2800 82.79 2.72 0.037 2279 81.58 0.037 62.18 3.3
to 3.280 4668 5611 82.86 2.74 0.044 4412 79.51 0.038 29.23 4.4
to 2.859 6788 8236 82.62 2.76 0.048 6886 78.75 0.070 14.07 14.1
to 2.579 8972 10926 82.12 2.77 0.051 8484 77.65 0.082 9.38 21.8
to 2.395 11157 13628 81.87 2.78 0.054 10447 76.66 0.102 6.65 31.4
to 2.283 13287 16280 81.62 2.78 0.057 12310 75.61 0.134 4.86 37.0
to 2.141 15488 18986 81.42 2.78 0.061 14179 74.69 0.154 4.12 39.6
to 2.047 17659 21665 81.19 2.78 0.064 16006 73.88 0.170 3.22 47.7
to 1.969 19793 24354 81.03 2.79 0.067 17815 73.15 0.222 2.08 61.8
to 1.901 21741 27055 80.86 2.78 0.069 19494 71.83 0.290 1.56 70.5

Local IS refinement averages ===== 10/03/2016 20:15:33
Component numbers S.C(I) below: S=sample, C=component in sample, P=component in file
Local averages for component 1.1(1) (component 1 in sample 1, 1 in file)
Number of local refinements averaged: 13
Averaged orientation ('OB') matrix:
0.0012369 0.0093003 -0.0106114
```

Refinement Options...
Integration Options...
Find Runs...
Import Runs from Experiment
Start Integration...

Double clicking on the Output filename activates the buttons.

- The folder button allows you to search for and update the filename.
- The "Is" button opens the log file.

SAINT Integration



Output files in the *work* subdirectory

Integrate Images (SAINT)

Output Files	Extension	Description
Raw intensity	*.raw	Contains the raw unscaled, unmerged intensities. A separate file is created for each scan which has the filename prefix plus the scan number (<i>prefix_#.raw</i>). A merged file is also created containing all the reflections from each scan (<i>prefix_0m.raw</i>).
Log	*._ls	Contains the output from integration. A separate file is created for each scan which has the filename prefix plus the scan number (<i>prefix_#._ls</i>). A merged file is also created containing all the reflections from each scan (<i>prefix_0m._ls</i>).
Matrix	*.p4p	This file contains unit cell information. When the integration is finished, a file called <i>prefix_0m.p4p</i> is created which contains the updated cell information. There is also a file written, <i>prefix_0u.p4p</i> which contains the unconstrained cell constants. This file can be manually created in PROTEUM by selecting "export>p4p" file from the "Sample" menu in the upper right corner. The p4p file also contains the table for the detector spatial correction. If you're creating a new database entry to work with old data, be sure to read in a p4p file before continuing after opening the entry by selecting "Import>p4p" from the "Sample" menu.
Active Mask	*.sfrm	This is an image file which contains the mask for the beamstop shadow. The filename contains the frame prefix, run number and frame number (0001). For example, <i>prefix_am_01_0001.sfrm</i> . You can view this file in PROTEUM as you would any image file to verify that SAINT is properly masking out the shadow.
Charting	*.cht	This file contains all the charts that were displayed in PROTEUM during the integration. The file can be re-opened in PROTEUM by clicking on the "Integrate Images" plugin and selecting "Open Chart File" from the Chart menu in the upper right corner of the GUI.

SADABS

Data scaling

Steps during scaling:

- Scaling: determination of scaling and absorption parameters that assure the data is internally consistent
- Error model: the standard deviations of the intensities are modelled so that they are consistent with the deviation of the individual intensities from the mean intensity of group of equivalents.

Systematic errors:

- Absorption of the primary beam by the crystal (and support)
- Crystal decomposition
- Intensity variation of the primary beam (e.g. synchrotron)
- Changes in the effective volume irradiated.
- Beam inhomogeneity.

SADABS

Inputting Raw files



The screenshot shows the PROTEUM3 software interface. An 'Open File' dialog is open, displaying a list of files in the 'C:\frames\demo\Neil1\work' directory. The file 'S207E3_01.raw' is selected. Below the dialog, the 'File name' field contains 'S207E3_01.raw' and the 'Files of type' dropdown is set to 'Reflection files(*raw *.ram *.mul *.sam)'. To the right, the 'Setup' window is visible, showing the 'Input Folder' as 'C:\frames\demo\Neil1\work' and the 'Input File(s)' list containing 'S207E3_01.raw'. Below the file list, there are 'Select All' and 'Deselect All' buttons. Further down, the 'Lave Group' and 'Point Group' dropdown menus are set to '-3'. A red arrow points to the 'Point Group' dropdown. Below these, there is a checkbox for 'Additional Spherical Absorption Correction' and a text field for 'Mu of Equivalent Sphere' set to '0.20'. At the bottom, there are radio buttons for 'Absorption Correction' with 'Multi Scan' selected. At the very bottom of the 'Setup' window, there are 'Start Over', 'Start', and 'Finish' buttons.

Name	Size	Type	Date Modified
S207E3_01.raw	20.9 MB	raw File	1/6/2017 8:51:04 AM

Unchecking "Merged Batches" allows you to deselect runs

Clicking the browser button for the base name opens the selection window.

- Select any filename to input a single raw file

Point Group

- The point group will be set based on the assignment during indexing but you can change it by clicking the arrow
- To keep the Friedel mates separate uncheck the "Use only centrosymmetry point groups" box. All possible point groups will then be available.

SADABS

Advanced setup



Setup	
Advanced Setup	
Output File Type	Unmerged .hkl file
Output Base Name	S207E3
Output HKL File Name	S207E3_0m.hkl
Output HKLF5 File Name	
Diagnostic Plots File Name	S207E3.eps
Title of Diagnostic Plots	S207E3
Log File Name	S207E3.abs
Fast Scan Resolution Cutoff [Å]	1.5
Allow for crystal decomposition by B-value refinement	None
Extra Linear Correction to be Applied to Each Reflection:	None
Spatial display of $(I-\langle I \rangle)/su$ greater than	3.0
<input type="checkbox"/> Apply angle of incidence correction	
Phosphor Efficiency	Auto
Apply lambda correction	None
Lambda Correction Factor	0.0015

Output filenames are suggested based on the entry name. These can be changed by editing the box.

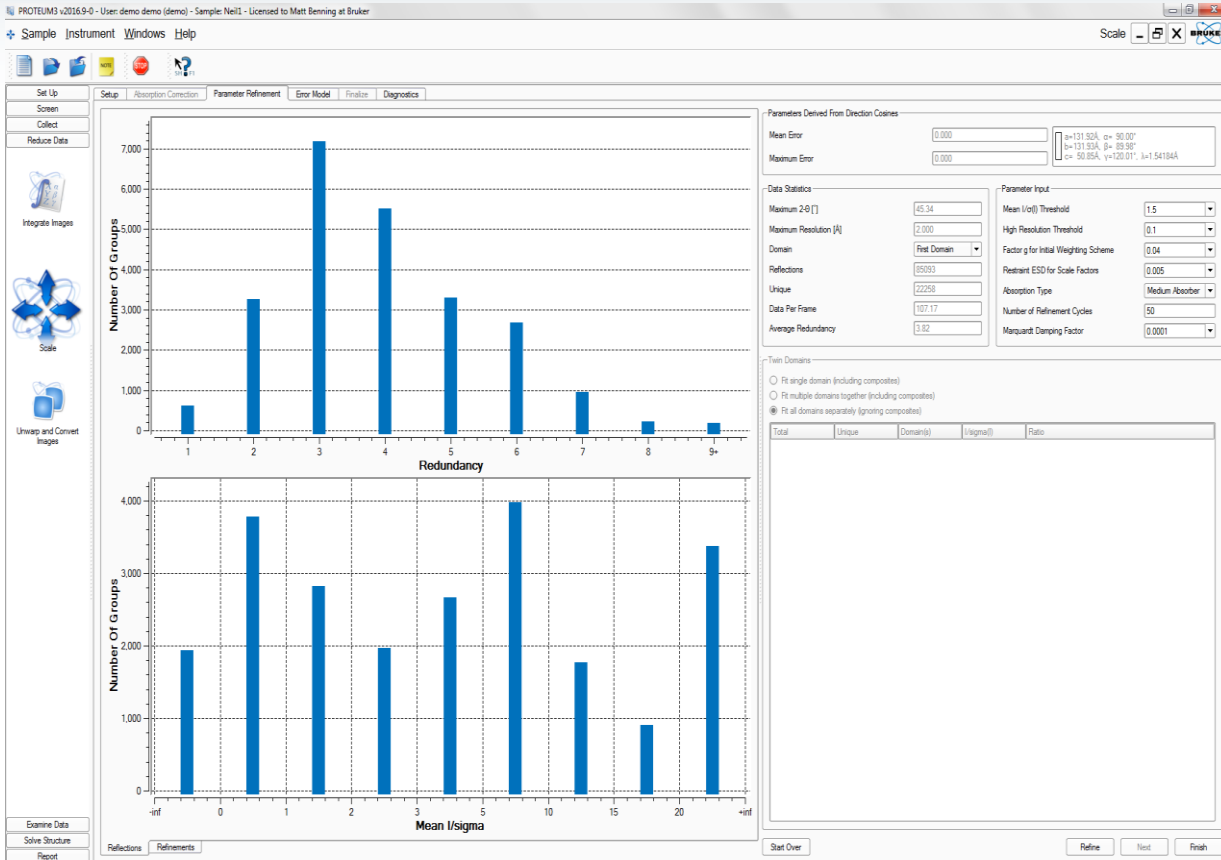
Zero-dose correction

Compare the same reflection collected as a function of time to model radiation decay

- Linear
- Quadratic

SADABS

Scale factors



Check function

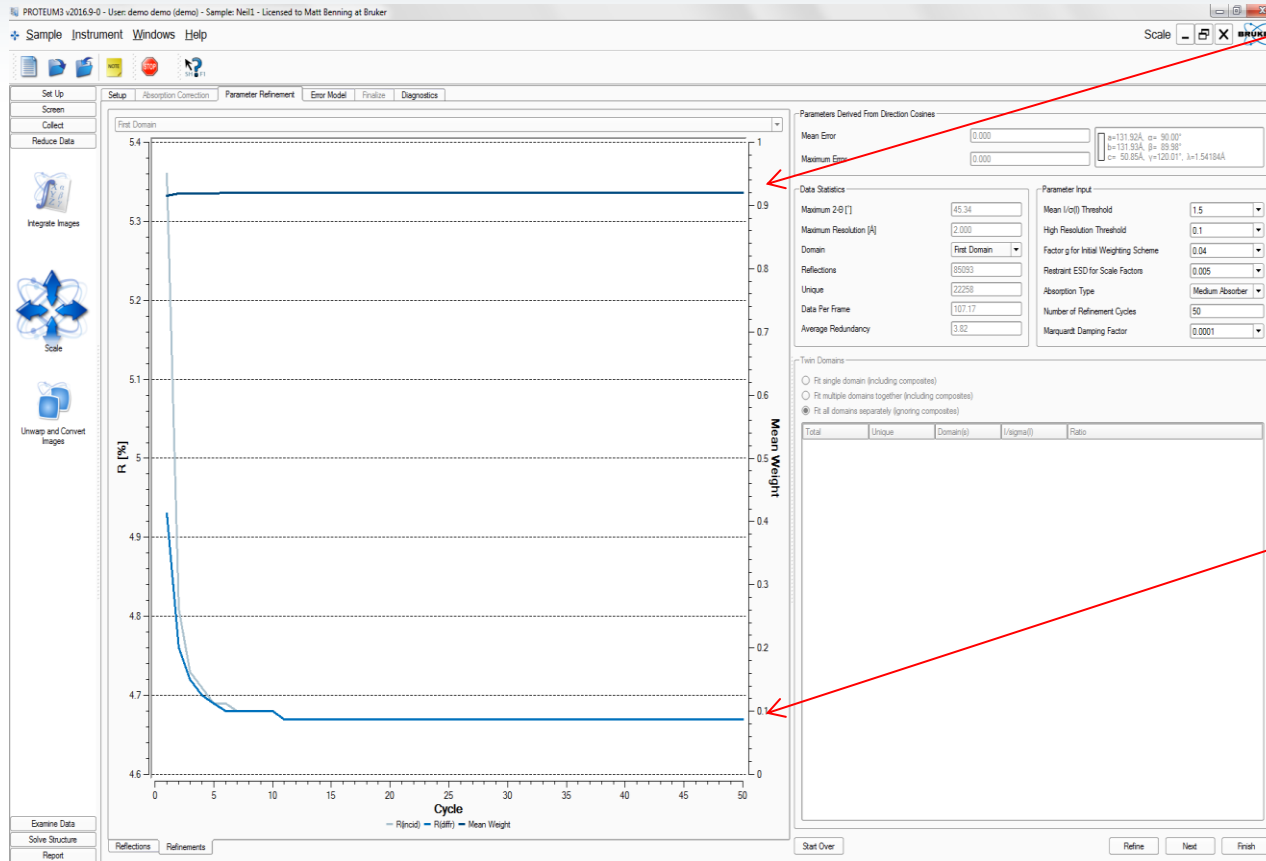
- Unconstrained cell constants and instrument error. Mean error should be >0.005 .

Parameters refinement

- Scale factor restraint prevents overfitting data. Can loosen a bit, 0.01
- Absorption type, medium works well for most but if there are heavy atoms and enough data can try strong absorber

SADABS

Scale factor

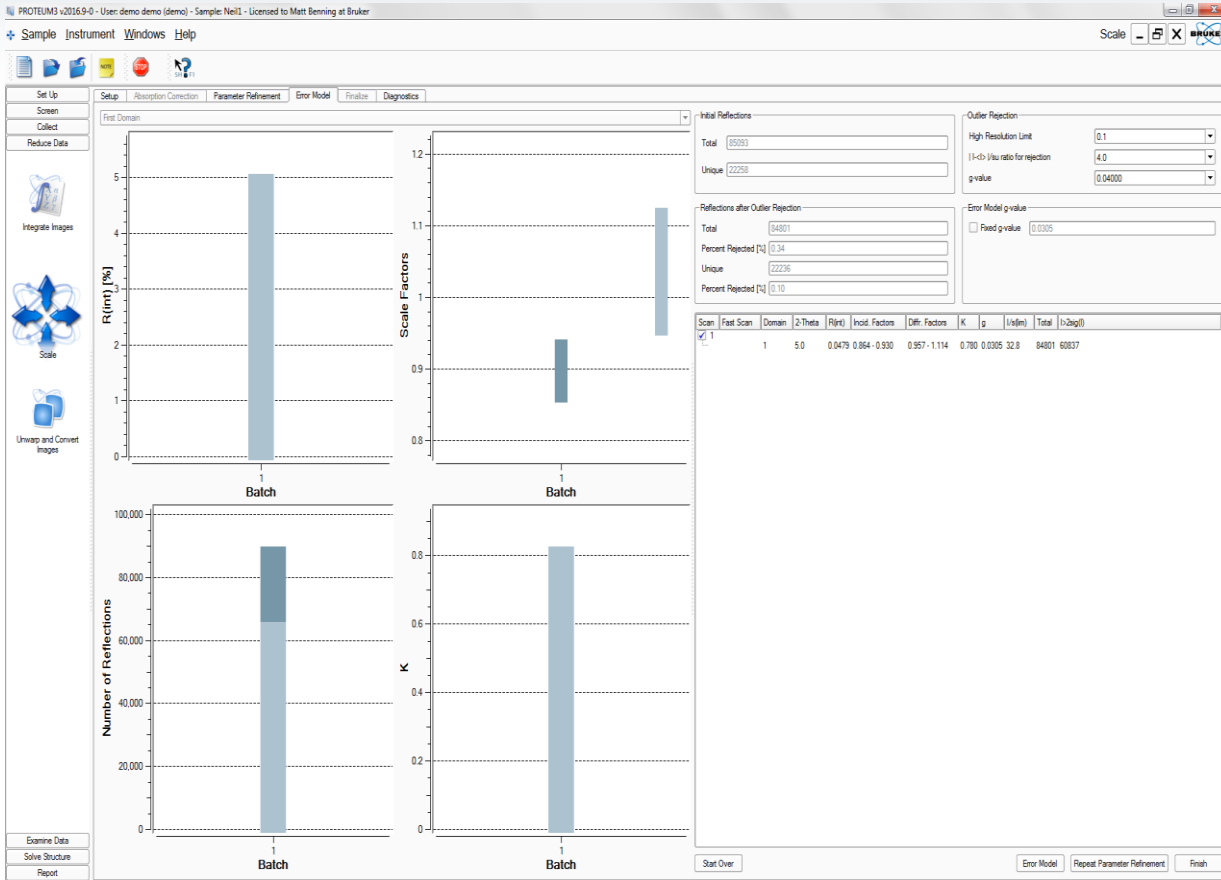


- Blue line shows the mean weight of the observations for all the reflections. As the observations get farther from the mean, they are down weighted. If the Mean Weight falls below 0.75, the data agreement is not good.

- Light blue line represents the Rfactor with scale factors only, the dark blue line is the Rfactor adjusted for adsorption. Most of the time they will converge but when there is a significant absorption affect, the blue line may exhibit a lower Rfactor.

SADABS

Error model



- Determination of an error model for errors that cause equivalent reflections to disagree.
- It deletes a small number of reflections that are completely incompatible with their equivalents, for example reflections blocked by the beam stop etc.
- Then determines an error model for the remaining reflections by fitting χ^2 to unity to put $\sigma(I)$ onto an absolute scale.

SADABS Diagnostics



PROTEUM3 v2016.9-0 - User: demo demo (demo) - Sample: Neil1 - Licensed to Matt Benning at Bruker

Sample Instrument Windows Help

Scale

Set Up
Screen
Collect
Reduce Data

Integrate Images

Scale

Unwrap and Convert Images

Statistics Reflection Graphs Refinement Graph Error Model Graphs Scale Variations Intensity Statistics Chi-Squared Spatial Distribution Diederichs Graph

Exit

Setup Absorption Correction Parameter Refinement Error Model Finalize Diagnostics

Parameters Derived From Direction Cosines

Mean Error: 0.0
Maximum Error: 0.0
Wavelength [Å]: 1.54184

Approximate Unit Cell

a	b	c	α	β	γ
131.92	131.93	50.849	90.005	89.979	120.007

Data Statistics

Maximum 2 θ [°]: 45.34
Maximum Resolution [Å]: 2.000
Domain: First Domain
Reflections: 85093
Unique: 22258
Data Per Frame: 107.17
Average Redundancy: 3.82

Initial Reflections

Total: 85093
Unique: 22258

Reflections After Outlier Rejection

Total: 84801
Percent Rejected [%]: 0.34
Unique: 22236
Percent Rejected [%]: 0.10

Numerical Absorption Correction

Absorption Coefficient [μ in-1]:

wR2(int) Parameter Refinement

Initial	Final
refinement	0.0551 0.0467

Error Model σ value

Suggested: 0.0305
Use: 0.0305

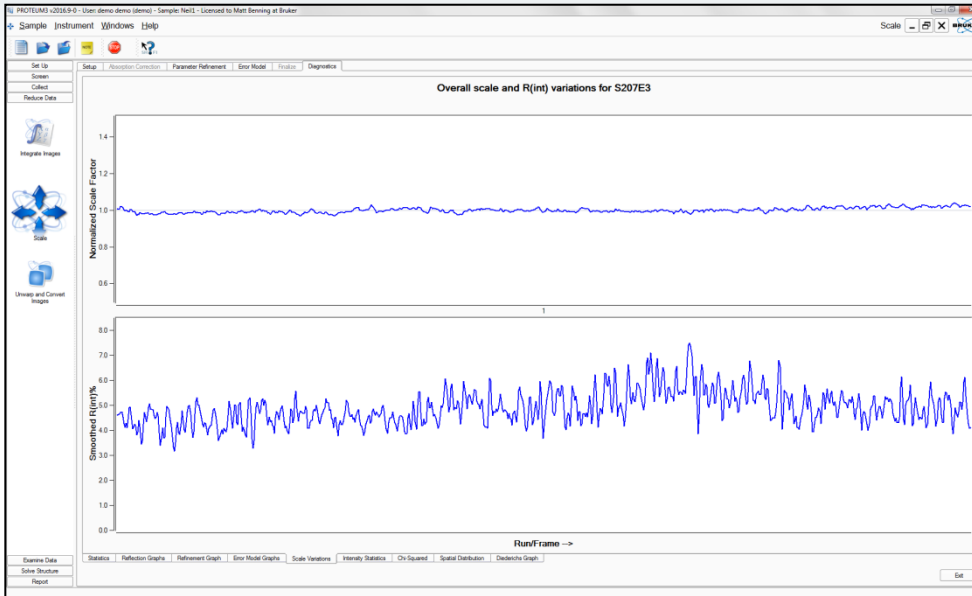
HKL Transmission Data

Corrected Reflections: 84801
Replaced Reflections:
Minimum Transmission: 0.858800
Maximum Transmission: 1.000000
Ratio of Min/Max Transmission: 0.858800

HKLF 5 Transmission Data

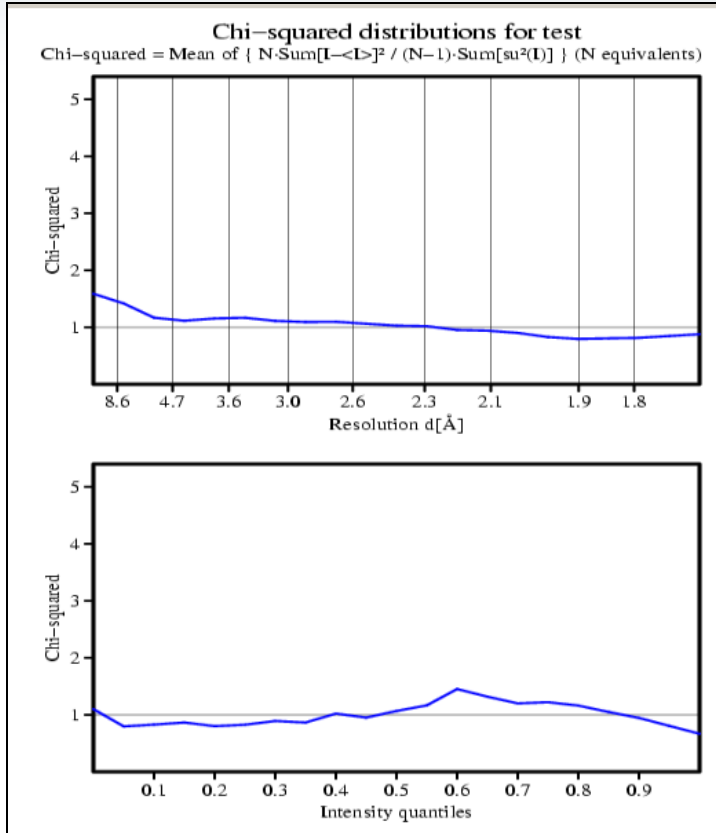
Corrected Reflections:
Minimum Transmission:
Maximum Transmission:
Ratio of Min/Max Transmission:

SADABS Plots

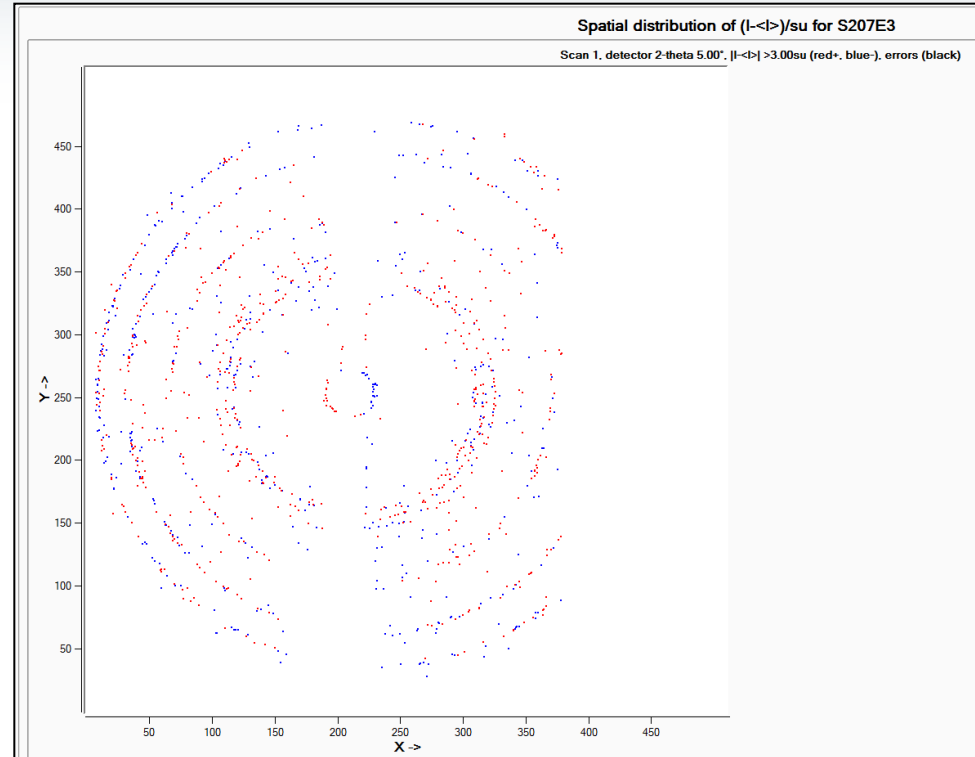


- Upper graph: scale factors *versus* frames and runs. Big variation are due to different illuminated volume.
- Bottom graph: R_{int} *versus* frames and run.

SADABS Plots



χ^2 versus resolution and intensity. It should be closer to 1.



Outliers relative to detector area for each different 2θ angle. Show bad pixels, shadows, ice rings...

SADABS

Output



Output files in the *work* subdirectory

Output Files	Extension	Description
Scaled Intensities	*.hkl	File contains the scaled, unmerged intensities in SHELX HKLF4 format
Log	*.abs	Log file from SADABS

XPREP

- Space group determination and data statistics are carried out with the software XPREP.
- Steps during space group determination:
 - Determine metric symmetry and lattice group
 - Determine Laue symmetry (R_{int})
 - Find systematic absences
- XPREP can also be used to calculate statistics, calculate anomalous signal, merged data, prepare files for ShelxD...

XPREP

Space Groups and Statistics



PROTEUM3 v2016.9-0 - User: demo demo (demo) - Sample: Neil1 - Licensed to Matt Benning at Bruker

Sample Instrument Windows Help Determine Space Group

Set Up
Screen
Collect
Reduce Data
Examine Data

Temp.p4p
*m.hkl
Determine Space Group

Analyze Data

Compare Unit Cells

Synthesize Precession Images

Find a Reflection

Solve Structure
Report

Setup Lattice Exceptions Space Group Determination Statistics Cell Information Diagnostics

Input Files
hkl file: S207E3_0m.hkl
p4p file: S207E3_0m.p4p

Output Files
output hkl file: S207E3_0m.hkl
p4p file: S207E3_0m.p4p
 output sca file: S207E3_0m.sca

Unit Cell

	a	b	c	alpha	beta	gamma
cell	131.911	131.911	50.835	90	90	120
cell esds	0.006	0.000	0.002	0	0	0

Experimental Parameters

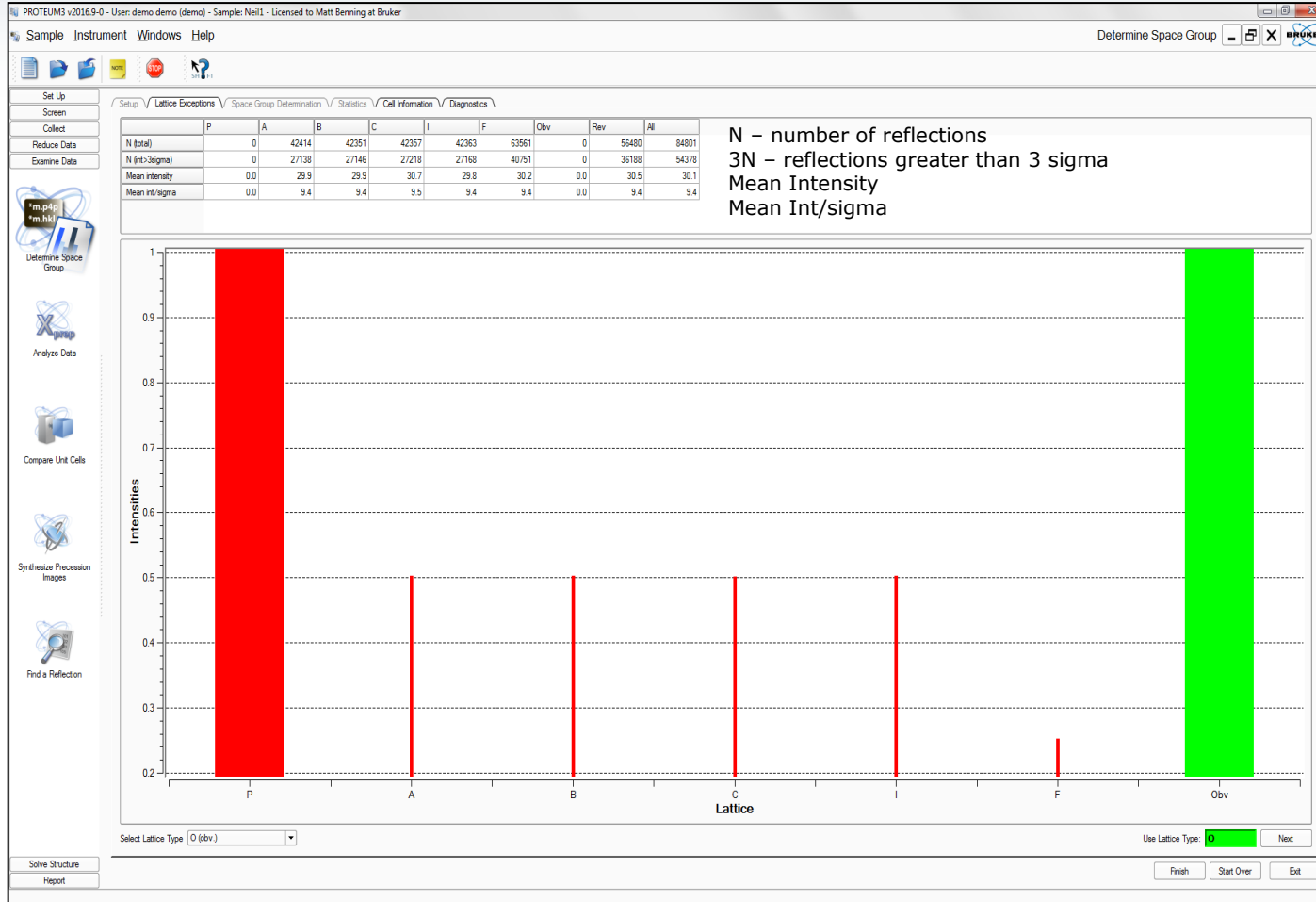
Must be chiral
Radiation Type: Cu

Next
Finish Start Over Exit

- Most of the information comes from the Database
- Can output a scalepack in addition to SHELX HKL

XPREP

Space Groups and Statistics



- Find the correct metric symmetry (correct lattice type) by checking systematic absences

XPREP

Space Groups and Statistics



PROTEUMS v2016.9-0 - User: demo demo (demo) - Sample: Neil1 - Licensed to Matt Benning at Bruker

Sample Instrument Windows Help Determine Space Group

Set Up Screen Collect Reduce Data Examine Data

Setup Lattice Exceptions Space Group Determination Statistics Cell Information Diagnostics

Bravais Lattice

Option	A	B	C	Alpha	Beta	Gamma	Volume	R _{lattice}
Bravais Lattice								
RHOMBOHEDRAL Cubic	131.911	131.911	50.035	90.00	90.00	120.00	766946.75	0.045
RHOMBOHEDRAL Rhombo	78.021	78.021	78.021	115.42	115.42	115.42	255340.84	0.046
Retain Original Cell								

Systematic absence exceptions

Systematic absences not required for triclinic systems

	h1/65	h2/31	h3	h<-	h<+
N	7	0	7	1649	338
N I/3 ₂	6	0	6	1124	655
h<+	230.4	0.0	230.4	35.9	35.4
h</h>	23.2	0.0	23.2	11.4	11.7

- Six measured reflections possible for a six-fold screw axis
- Most are strong, $> 3\sigma$ and mean I and $I/\sigma I$ are similar
- No translational symmetry

E-value statistics

Non-centrosymmetric: I 0.736 Mean |E|E|:1 0.805 Centrosymmetric: I 0.968

Identical indices and Friedel opposites combined before calculating R_{lattice}

Space Group	No.	Type	Axes	CSD	R _{lattice}	h<+>	Syst. Abs.	CFOM
Space Groups								
R-3	#148	centro	1	232	0.046	35739	0.0 / 9.4	4.14
R3	#146	chiral	1	85	0.046	35739	0.0 / 9.4	2.70

Choose a different space group: P1

Repeat Next Finish Start Over Exit

- Find translational symmetry by looking at the potential systematic absences
- Will only have Screw axis for protein crystals

XPREP

Space Groups and Statistics



PROTEUMS v2016.9.0 - User: demo demo (demo) - Sample: Neil1 - Licensed to Matt Benning at Bruker

Sample Instrument Windows Help Determine Space Group

Set Up Screen Collect Reduce Data Examine Data

Setup Lattice Exceptions Space Group Determination Statistics Cell Information Diagnostics

Current dataset: Dataset 1 84801 data points S207E3_0m.Hkl

Merge Data in Output Files Merge ALL equivalents (including Friedel opposites)

Change Resolution Limits (Å):
 Low: infinity High: 0.84 Set New Limits Set Limits and Redo Statistics

Resolution	#Data	#Theory	%Complete	Redundancy	Mean I	Mean I/s	Rint	Rsigma	
1	20.84 - 7.97	334	361	92.5	4.27	139.9	58.68	0.0161	0.0160
2	7.97 - 5.40	782	783	99.9	4.68	62.5	47.93	0.0194	0.0183
3	5.40 - 4.29	1119	1119	100.0	4.69	97.2	48.82	0.0188	0.0178
4	4.29 - 3.76	1103	1103	99.9	4.58	90.6	42.93	0.0265	0.0194
5	3.76 - 3.41	1136	1139	99.7	4.50	69.0	36.45	0.0368	0.0226
6	3.41 - 3.17	1100	1101	99.9	4.59	44.1	29.24	0.0386	0.0281
7	3.17 - 2.98	1134	1134	100.0	4.59	29.5	23.46	0.0507	0.0351
8	2.98 - 2.83	1128	1128	100.0	4.51	21.8	18.79	0.0614	0.0435
9	2.83 - 2.71	1097	1097	100.0	4.55	16.1	15.62	0.0727	0.0532
10	2.71 - 2.60	1182	1182	100.0	4.41	11.8	12.55	0.1134	0.0693
11	2.60 - 2.51	1133	1133	100.0	4.30	10.6	11.23	0.1060	0.0778
12	2.51 - 2.44	989	989	100.0	3.81	9.3	9.42	0.1136	0.0930
13	2.44 - 2.37	1146	1146	100.0	3.56	7.5	7.66	0.1364	0.1187
14	2.37 - 2.30	1246	1246	100.0	3.40	7.1	6.99	0.1420	0.1307
15	2.30 - 2.25	990	994	99.6	3.06	6.3	5.76	0.2000	0.1638
16	2.25 - 2.20	1084	1089	99.5	2.92	6.0	5.08	0.2343	0.1869
17	2.20 - 2.15	1208	1208	100.0	3.06	5.2	4.72	0.1916	0.2024
18	2.15 - 2.11	1033	1033	100.0	2.93	4.3	3.87	0.2357	0.2482
19	2.11 - 2.07	1118	1123	99.6	2.79	3.6	3.13	0.3232	0.3151
20	2.07 - 2.03	1197	1204	99.4	2.69	3.1	2.63	0.4075	0.3744
21	2.03 - 2.00	978	1080	89.9	2.14	3.1	2.61	0.2978	0.3946
22									
23	2.10 - 2.00	3023	3145	96.1	2.51	3.20	2.73	0.3570	0.3664
24	20.84 - 2.00	22236	22399	99.3	3.79	26.69	17.18	0.0461	0.0425

Charts Graphs 1 Graphs 2

Overall Weighted R(int): 0.0461 Overall Weighted R(sigma): 0.0425 Anomalous Completeness %: 57.0

Lowest Resolution (Å): 20.84 Write Reflection File

Solve Structure Report Finish Start Over Exit

XPREP Output



Output files in the *work* subdirectory

Output Files	Extension	Description
Log	*.prp	The file is actively updated as you navigate through XPREP or "Space Groups and Statistics" (PROTEUM's GUI interface for XPREP).
Different file formats		The intensity file output from SADABS (*.hkl) can be converted to other file formats using XPREP. Using the "W" option from the "Read, modify or merge DATASETS" ([D]) menu, you can output the intensities in Scalepack, CNS or X-PLOR formats. You can also output a Scalepack HKL file from "Space Groups and Statistics" by checking the "output .sca file" box.



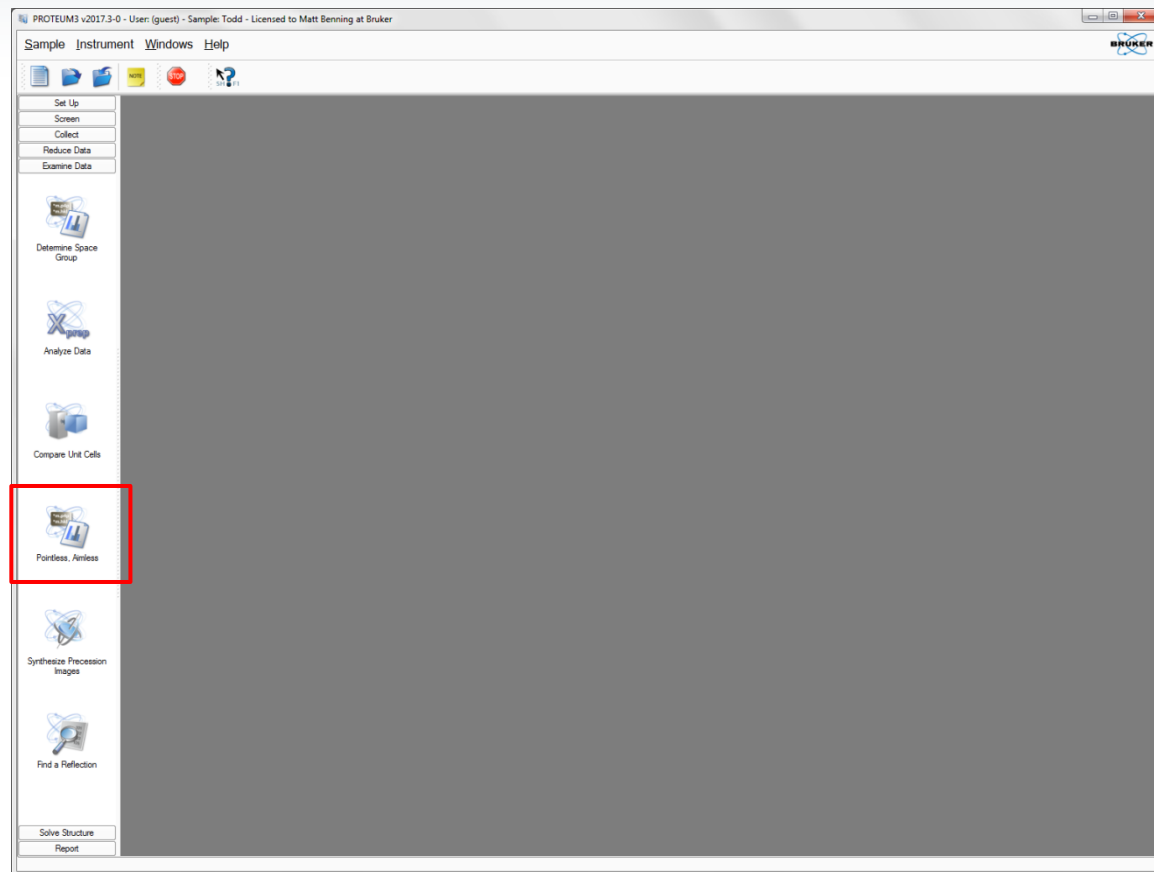
Pointless, Aimless

If you have CCP4 installed, add the following 3 lines to the end of the `bn-config.py` file

- `ccp4 = "C:/CCP4-7/7.0"`
- `ccp4_range = [22.0,1.85]`
- `ccp4_autoprocess = True`

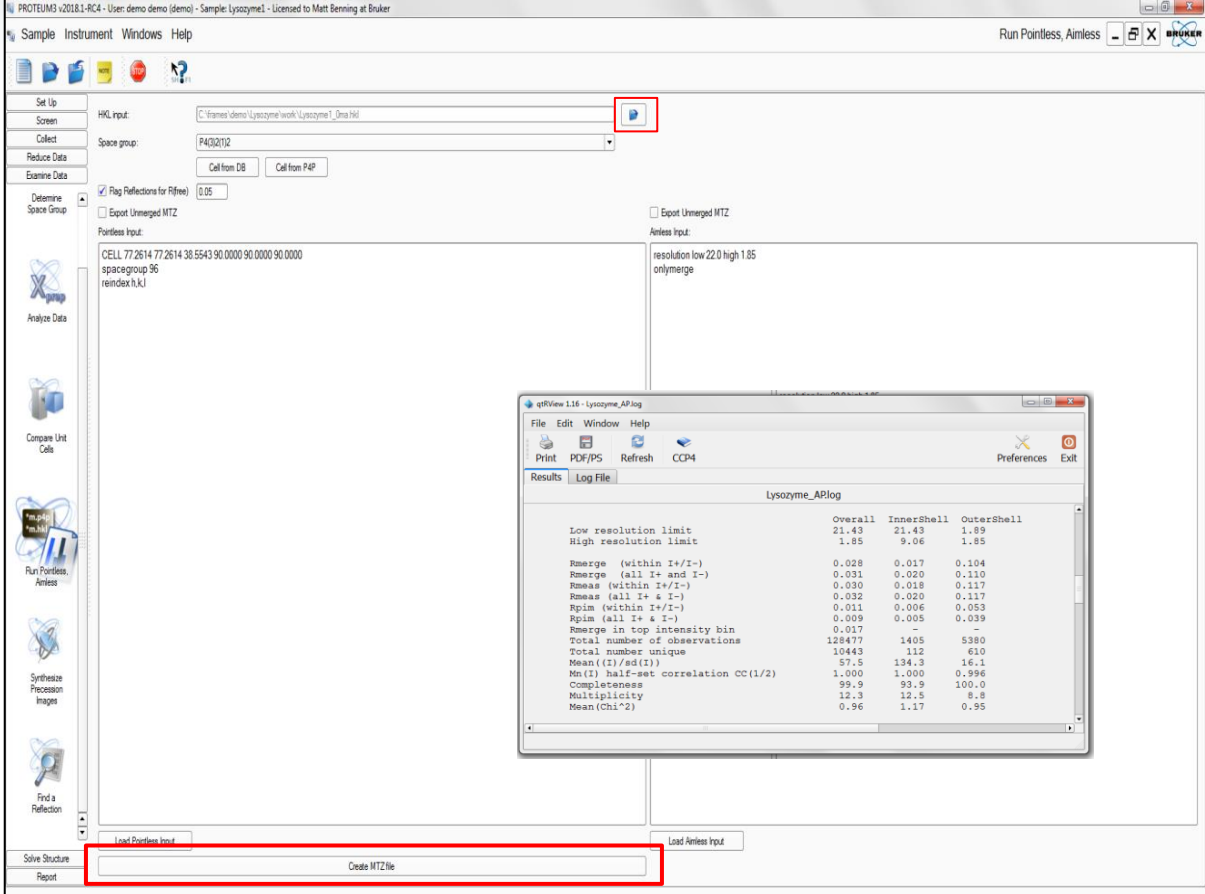
Pointless, Aimless

- Open the "Examine Data" menu
- Select the "Pointless, Aimless" icon



Pointless, Aimless

- If there is no MTZ file in the work folder, PROTEUM will automatically run Pointless and Aimless based on default values and display the aimless output.
- Default resolution 25 – 1.85 Å
- The pointless and aimless fields are editable so you can add keywords, change the defaults and click “create MTZ file” at the bottom left to rerun the programs. The new Aimless log will appear when both programs are finished.
- If the space group is not assigned (default), PROTEUM lets pointless perform a space group search.
- The plugin will search for the [HKL filename_0m.hkl](#) in the work directory but you can also search for a HKL file using the browser button.



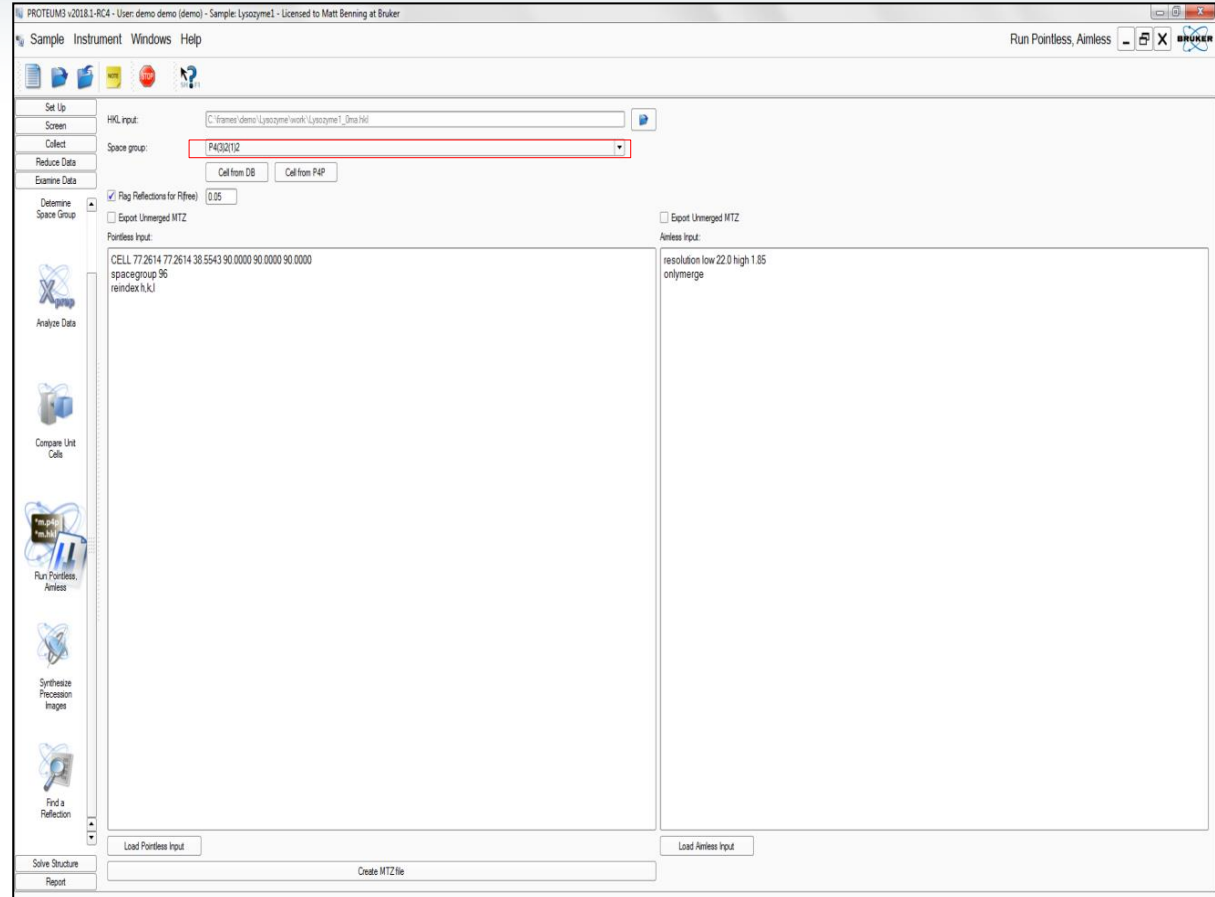
qtReview 1.16 - Lysozyme_AP.log

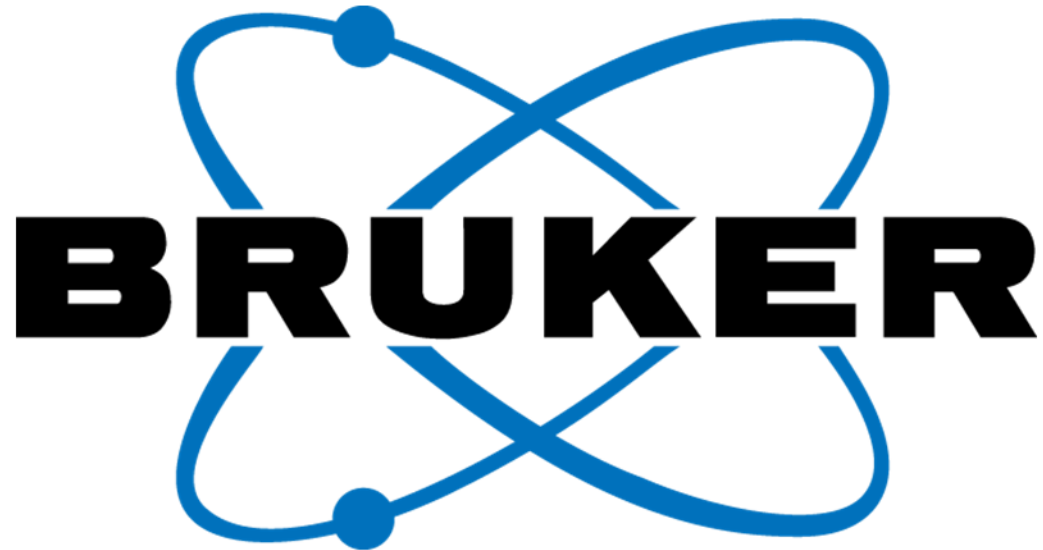
	Overall	InnerShell	OuterShell
Low resolution limit	21.43	21.43	1.89
High resolution limit	1.85	9.06	1.85
Rmerge (within I+/-)	0.028	0.017	0.104
Rmerge (all I+ and I-)	0.031	0.020	0.110
Rmeas (within I+/-)	0.030	0.018	0.117
Rmeas (all I+ & I-)	0.032	0.020	0.117
Rpim (within I+/-)	0.011	0.006	0.053
Rpim (all I+ & I-)	0.009	0.005	0.039
Rmerge in top intensity bin	0.017	-	-
Total number of observations	128477	1405	5380
Total number unique	10443	112	610
Mean(I)/sd(I)	57.5	134.3	16.1
Mn(I) half-set correlation CC(1/2)	1.000	1.000	0.996
Completeness	99.9	93.9	100.0
Multiplicity	12.3	12.5	8.8
Mean(Chi^2)	0.96	1.17	0.95



Pointless, Aimless

- If you want to assign a space group, select the desired group in the box below the input HKL filename. This will fix the space group to the that group assigned.
- A merged MTZ file is written out by Aimless, if you want to write out a unmerged MTZ file as well, check the "Export Unmerged MTZ"
- Output files are written to the work folder.
 - *Entry prefix_AP.log* is the output logfile from Aimless
 - *HKL filename_merged.mtz* is the merged MTZ file output by Aimless
 - *HKL filename_umerged.mtz* is the corresponding unmerged MTZ





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