

Introduction to Integration – SAINT

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Location on the Computer

The most important file is:

saint.ini

- all parameters (concerning hardware + software) are stored in this file
- this file is **system specific**
 - ↗ same file can't be used on different systems

Location on the computer

SMART Suite: C:\SAXI\SAINT32

APEX2 Suite: C:\bn\src\plugins\saint; C:\bn\SAINT



SAINT.INI

[SAINT]

Version of used saint executable (newest: SAINT V7.56A)

[CONFIGURE]

Parametrisation of hardware
to be adjusted for every single instrument !

[INTEGRATE]

Integration settings
Can be used as general starting default values for every measurement
protein ↔ small molecule

[STAT]

Calculation of statistics based on user-specified Laue group

[SORT]

Sorting of integrated intensities based on the HKL indices according to the user-specified Laue group

[GLOBAL]

Refinement of cell parameter and orientation matrix based on strong reflections of the complete measurement and given/not given constraints



Processing Steps during Integration (1)

- Determination of 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 of the orientation matrix and computation of spatial correction tables
- 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 variation in the path length through the detector faceplate
(unsorted temporary intensity file is written: unsorted.raw)
- Elimination of spots whose shapes correlate poorly with model profile shapes, relative to other spots of similar I/σ

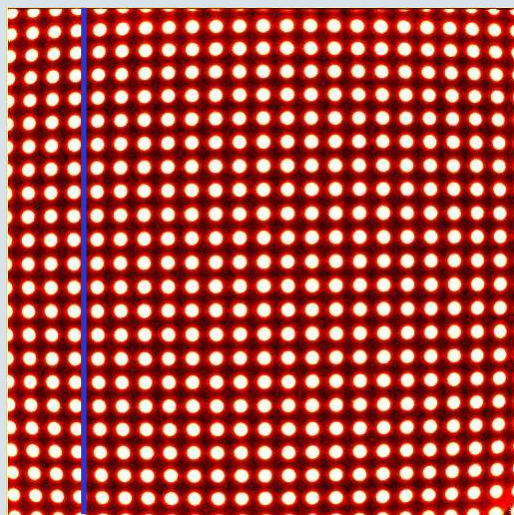
Processing Steps during Integration (2)



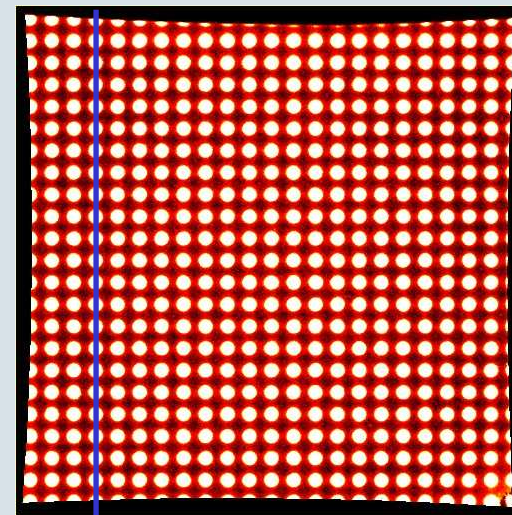
- Sorting of reflections into Laue group equivalent order
- Accumulation and reporting of statistics for the reflections in the output file
- Unit cell parameter refinement with the use of a large number of strong reflection of the entire data set
- Time-decay correction based on multiple measurements from „check“ images
- Accumulation and reporting of statistics for the reflections in the time-decay-corrected output file

Input Files

- Continuous series of images
 - more than 16 runs are possible in the same integration process if version SAINT V7.12A or higher is used
 - length of input string in saint.ini is restricted to 1024 chars
- One or more *.spin (Proteum) or *.p4p (SMART/APEX2) containing the refined orientation matrix, detector position corrections and the spatial correction tables



brass plate (distorted)



spatial correction (unwarping)



Output Files

- Listing files: *_01._ls, *_02._ls, *_03._ls,, *_0m._ls, *_0t._ls
- Parameter files: *_01.spin, *_02.spin, *_03.spin,, *_0u.spin, *_0m.spin, *_0t.spin
- Intensity files:
 - single crystal: *_01.raw, *_02.raw, *_03.raw,, *_0 m*.raw, *_0t*.raw
 - twin: *_01.mul, *_02.mul, *_03.mul,, *_0 m*.mul, *_0t*.mul
- Matrix file: *_01._ma
(binary file, containing strong reflection for global cell refinement)

1, 2, 3, ... = run number, u = unconstrained, m = combined, t = decay time corrected

Diagnostic output files

- initial background: *_01._ib, *_02._ib, *_03._ib,
- active pixel mask: *_01._am, *_02._am, *_03._am,
- background snapshots: bg_snap_01_0001.sfrm

SAINT Basics

Minimum input information:

- starting frame filename: name of first frame including path
- orientation matrix file name: *.spin, *.p4p (APEX2: info in database)
- output file name: *.raw or *.mul

Setup

	Starting Image Filename	Images	Output Filename
1	D:\frames\guest\SAINT\KHE_test_01_0001.sfrm	416	D:\frames\guest\SAINT\work\KHE_test_01.raw
2	D:\frames\guest\SAINT\KHE_test_02_0001.sfrm	416	D:\frames\guest\SAINT\work\KHE_test_02.raw
3	D:\frames\guest\SAINT\KHE_test_03_0001.sfrm	416	D:\frames\guest\SAINT\work\KHE_test_03.raw
4	D:\frames\guest\SAINT\KHE_test_04_0001.sfrm	416	D:\frames\guest\SAINT\work\KHE_test_04.raw
5			
6			

Resolution Limit [Å]:

Unit Cells:

a= 5.96Å, α=90.00°, V=990Å³
 b= 9.04Å, β=90.00°, Orthorhombic P
 c=18.38Å, γ=90.00°



SAINT Parameter File .P4P

CELL 77.6944 77.6944 77.6944 90.000 90.000 90.000 469168.500

Cell parameter

CELLSD 0.0022 0.0022 0.0022 0.000 0.000 0.000 60.979

Standard deviations of cell parameter

ORT1 1.2806546e-002 -1.1723973e-003 5.6204386e-004

ORT2 6.1861449e-004 5.8652740e-004 -1.2845224e-002

ORT3 1.1471785e-003 1.2795272e-002 6.3422305e-004

3 x 3 Orientation matrix

ZEROS 0.0000000 -0.0249640 -0.0666662 0.0562 0.1121 -0.0226

Goniometer zeros: omega zero [°]; chi zero [°]; crys tal translation X, Y, Z direction [pixel]

SOURCE Cu 1.54184 1.54056 1.54439 2.00000 45.00 90.00

Radiation type

LIMITS -80.00 81.00 0.00 0.00 0.00 0.00 0.00 0.00 -182.20 2.20

Current loaded limit settings

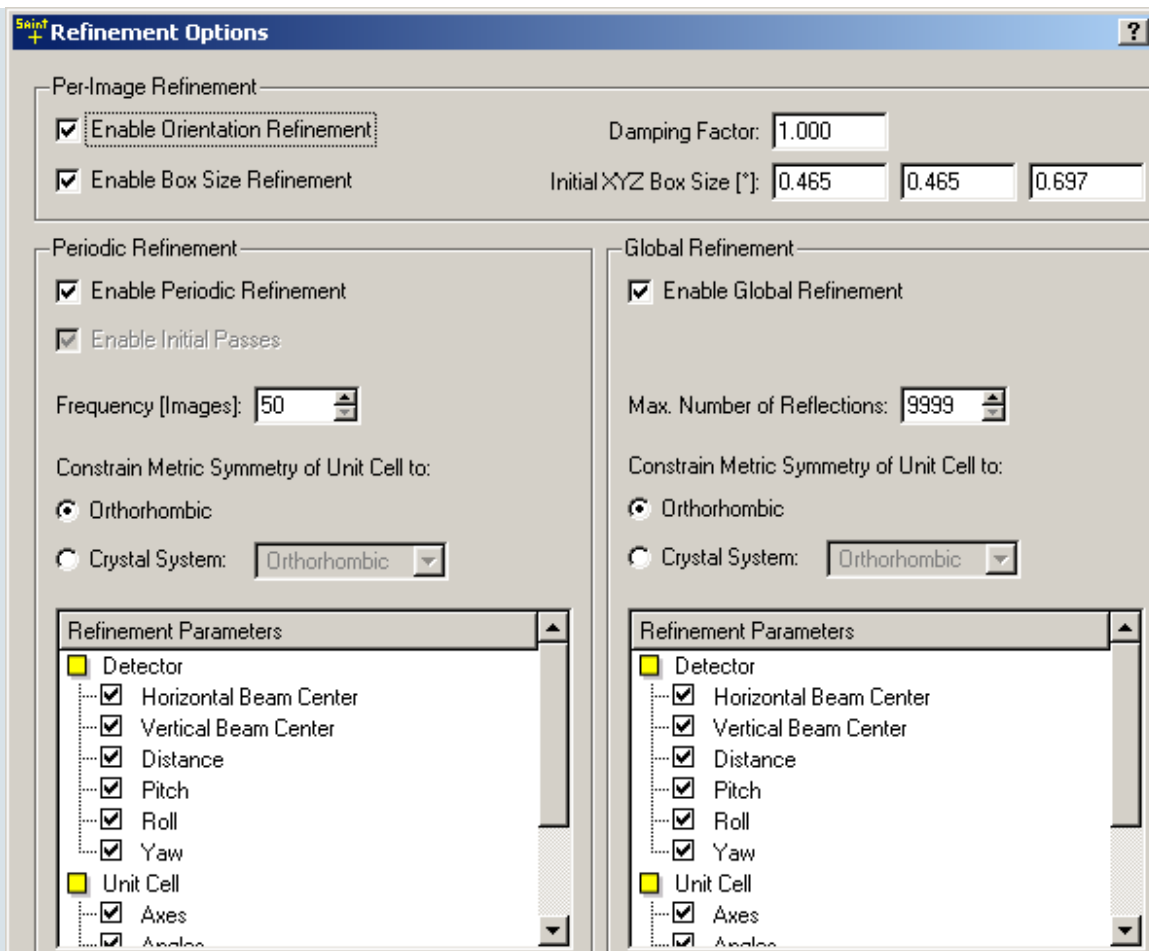
ADPAR 503.0000 511.0000 4.0000 1024

Area detector parameter: beam center X and Y [pixel]; distance [cm]; chip binning

ADCOR -0.2947 -0.0098 -0.0169 0.3182 0.0792 0.1049

Area detector corrections: beam center X and Y [pixel]; distance [cm]; pitch, roll and yaw [°]

SAINT – Refinement Options



Default Refinement Parameter

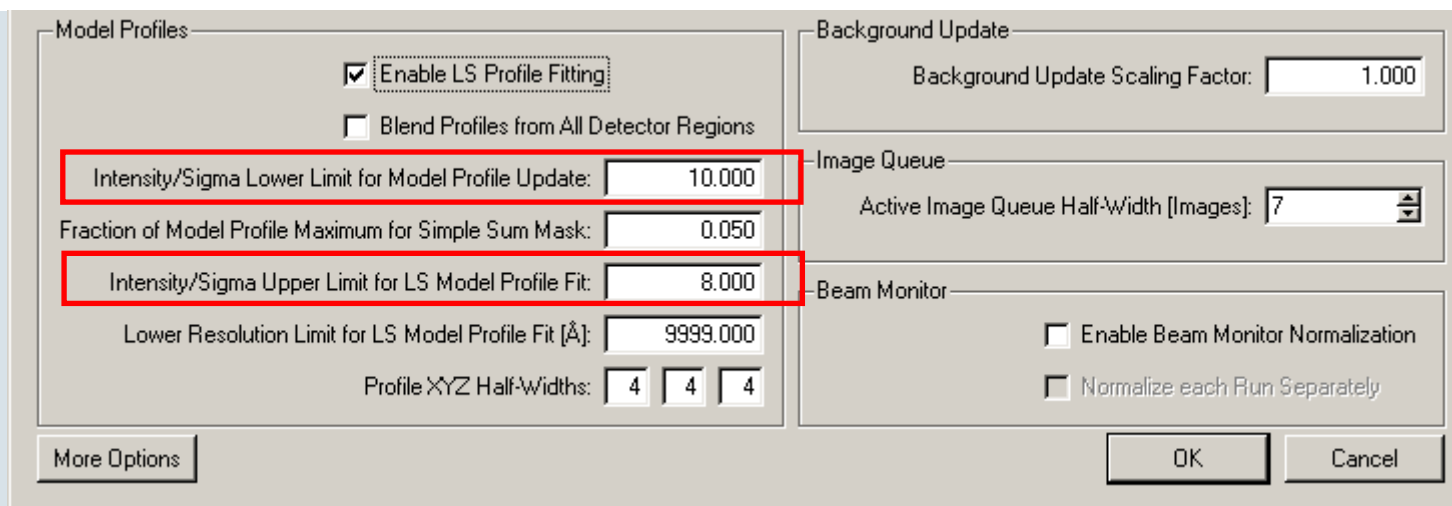
Local Refinement

- All Parameter are refined except 'Crystal Translation'

Global Refinement

- All Parameter are refined

SAINT – Integration Options



The screenshot shows the SAINT Integration Options dialog box. The 'Model Profiles' section contains several settings: 'Enable LS Profile Fitting' is checked, 'Blend Profiles from All Detector Regions' is unchecked, 'Intensity/Sigma Lower Limit for Model Profile Update' is set to 10.000, 'Fraction of Model Profile Maximum for Simple Sum Mask' is 0.050, 'Intensity/Sigma Upper Limit for LS Model Profile Fit' is 8.000, 'Lower Resolution Limit for LS Model Profile Fit (Å)' is 9999.000, and 'Profile XYZ Half-Widths' are all set to 4. The 'Background Update' section has 'Background Update Scaling Factor' set to 1.000. The 'Image Queue' section has 'Active Image Queue Half-Width (Images)' set to 7. The 'Beam Monitor' section has 'Enable Beam Monitor Normalization' and 'Normalize each Run Separately' both unchecked. There are 'More Options', 'OK', and 'Cancel' buttons at the bottom.

Model Profiles

Intensity/Sigma Lower Limit for Model Profile Update

This value is a threshold for reflections that are candidates for updating the model profiles and orientation matrix.

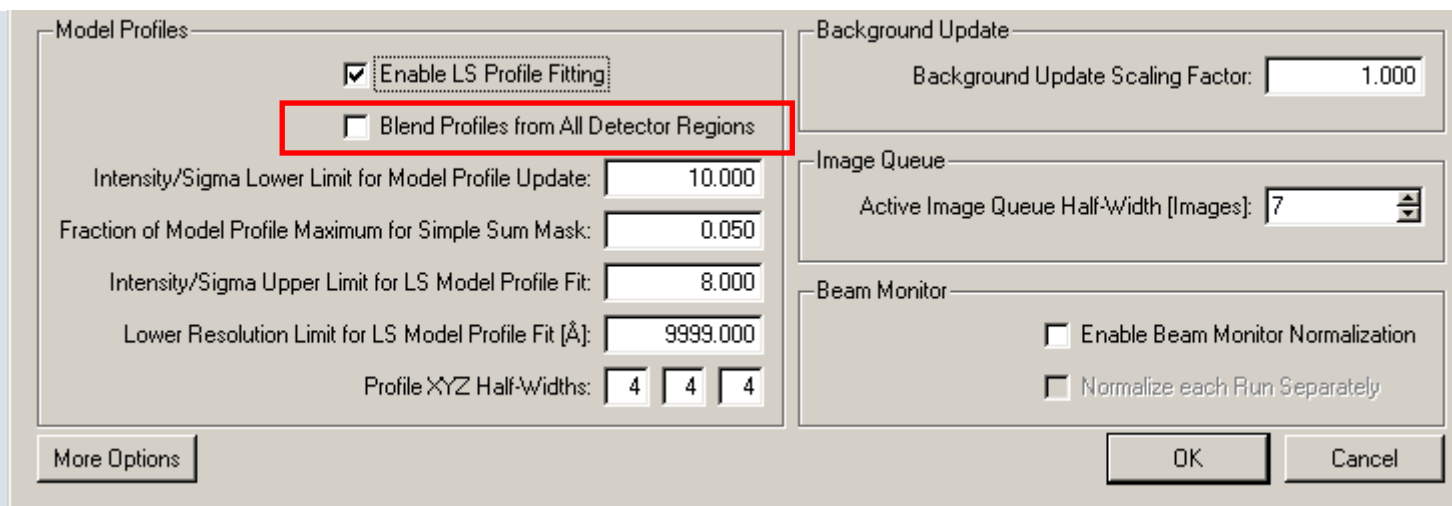
It should be decreased if for weak scatterer following information is shown:

Too few reflections for orientation refinement.

A smaller strong-reflection threshold might help

If you do it you also have to decrease *Intensity/Sigma Upper Limit for LS Model Profile Fit*

SAINT – Integration Options



The screenshot shows the SAINT Integration Options dialog box. The 'Model Profiles' section contains the following options:

- Enable LS Profile Fitting
- Blend Profiles from All Detector Regions (highlighted with a red box)
- Intensity/Sigma Lower Limit for Model Profile Update: 10.000
- Fraction of Model Profile Maximum for Simple Sum Mask: 0.050
- Intensity/Sigma Upper Limit for LS Model Profile Fit: 8.000
- Lower Resolution Limit for LS Model Profile Fit (Å): 9999.000
- Profile XYZ Half-Widths: 4 4 4

The 'Background Update' section contains:

- Background Update Scaling Factor: 1.000

The 'Image Queue' section contains:

- Active Image Queue Half-Width (Images): 7

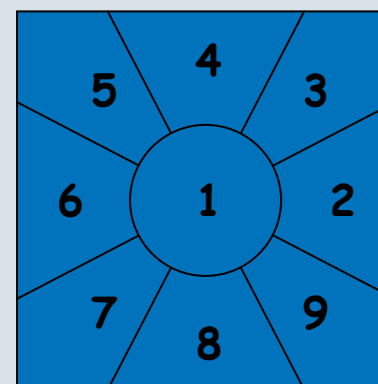
The 'Beam Monitor' section contains:

- Enable Beam Monitor Normalization
- Normalize each Run Separately

Buttons at the bottom include 'More Options', 'OK', and 'Cancel'.

Blend Profiles

SAINT determines reflection spot shapes for nine regions on the detector of roughly equal areas. The model profile shapes are also used to calculate correlation coefficients for purpose of data rejection and for profile fitting of weak reflections.

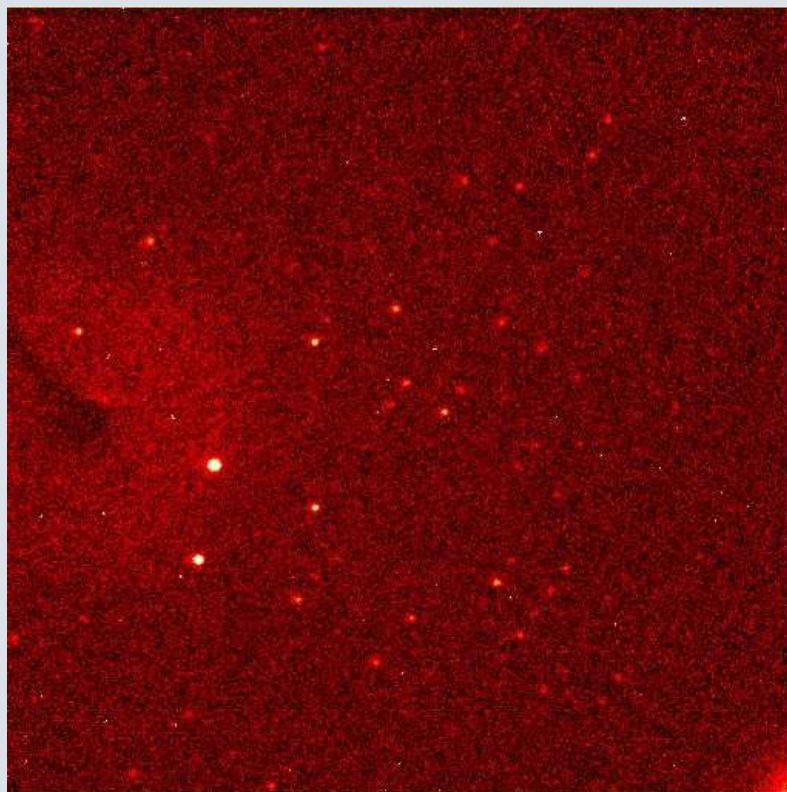


SAINT – Integration Options

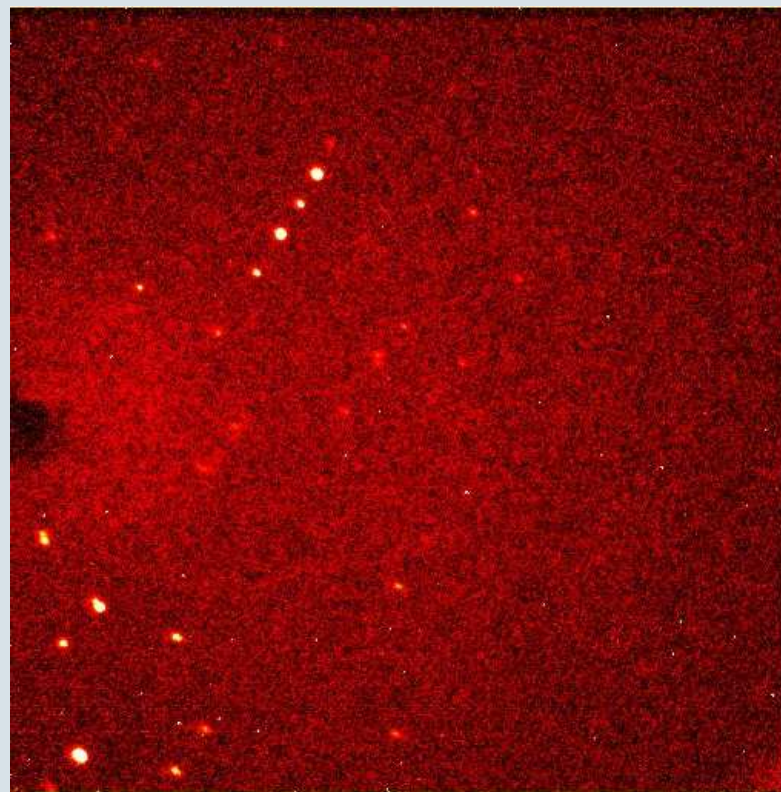


Blend 9 profiles

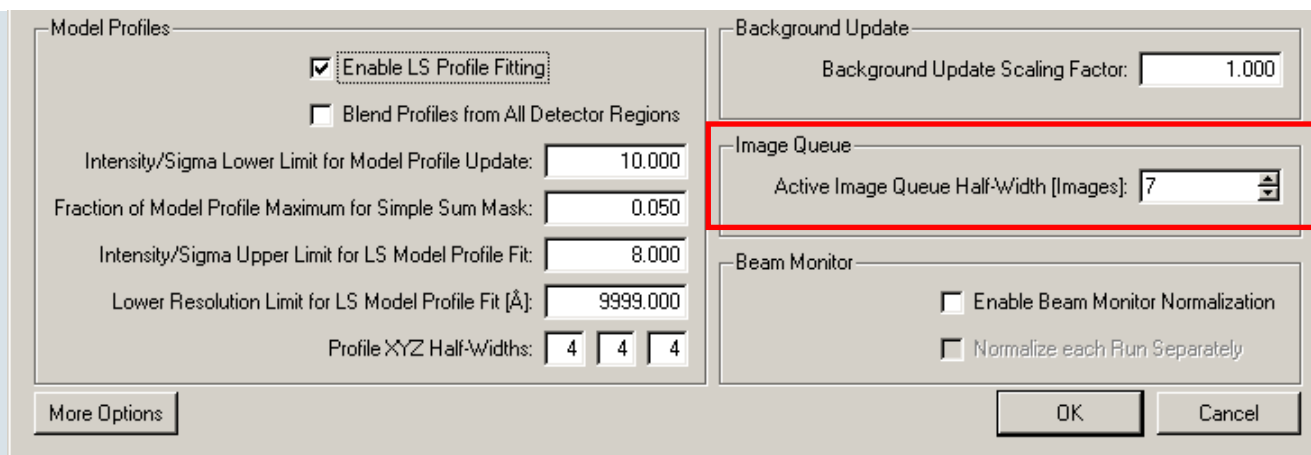
No



Yes



SAINT – Integration Options



The screenshot shows the SAINT Integration Options dialog box. The 'Image Queue' section is highlighted with a red box. The 'Active Image Queue Half-Width [Images]' is set to 7. Other sections include 'Model Profiles', 'Background Update', and 'Beam Monitor'.

Image Queue

Active frame queue half-width defines the total number of frames ($2N + 1$) stored to monitor reflection overlap (see SAINT output %Ful)

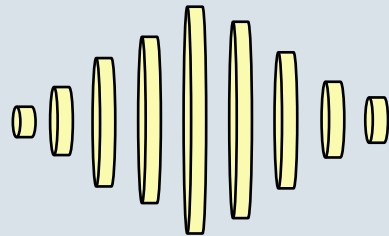
The frame queue serves as a temporary storage area for assembling partial reflections and for tracking reflections close to diffracting condition.

The %Ful item in the SAINT statistics reflects the average spot span in Z (crystal mosaicity) relative to the span of the frame queue. **Spots which are wider than the frame queue are “rejected”** and are not written to the output file.

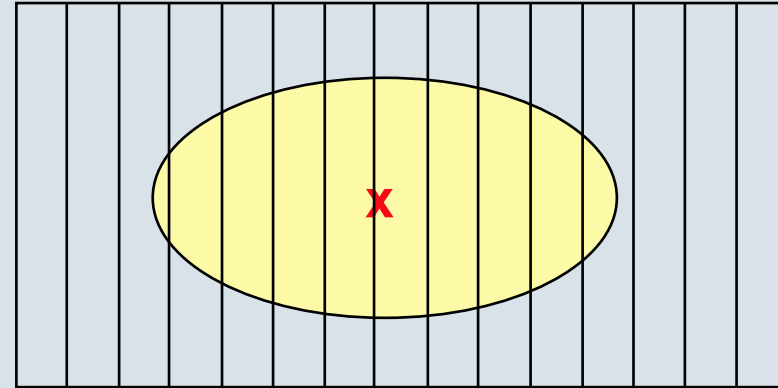
for 0.2° slicing: monitoring over 3.0° ⇒ 😊 for “normal” mosaicity

If %Ful is consistently 80% or more, one should increase the number of frames in the queue from the default of 15 (7-frame "half width").

SAINT – Integration Options



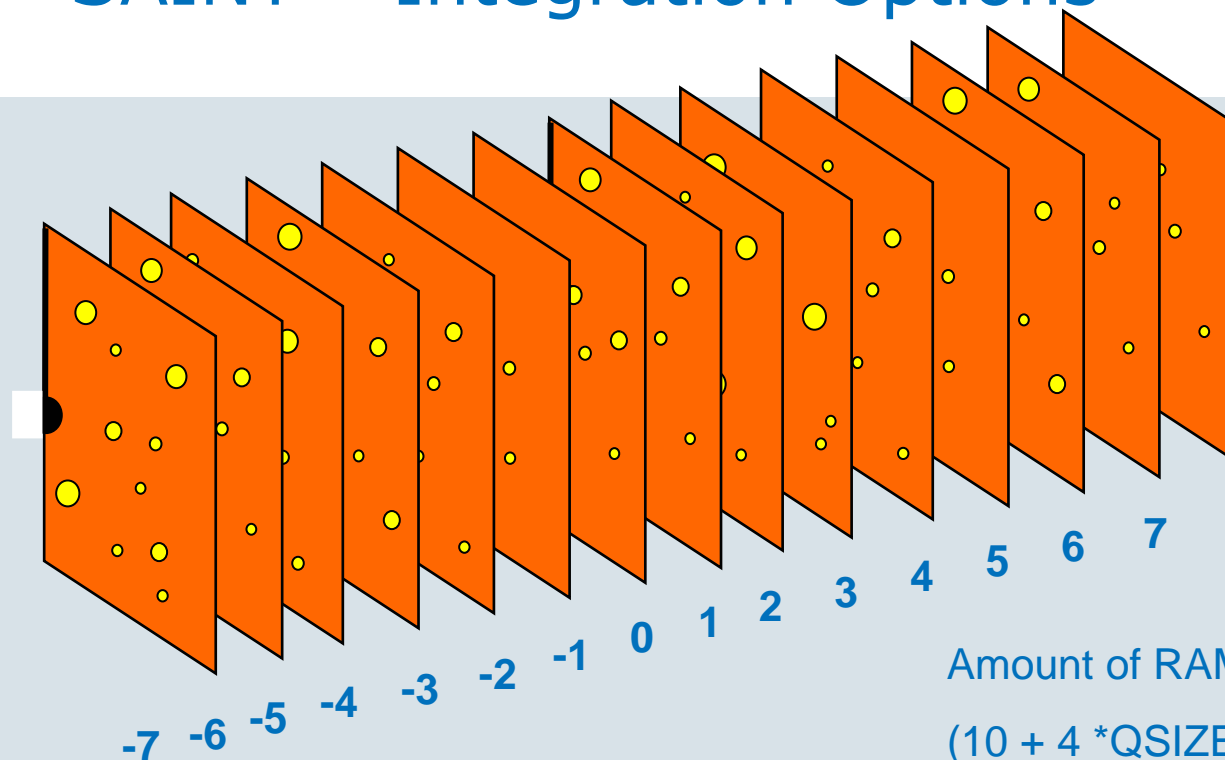
frame 1 2 3 4 5 6 7 8 9



x center of reflection [x, y, z]

$\int V = \text{intensity}$

SAINT – Integration Options



Frame queue $2N + 1$

Half-width = 7

Amount of RAM recommended

$$(10 + 4 * QSIZE) * NQS$$

QSIZE = total number of frames in queue
 NQS = square of linear frame dimension
 (e.g. number of pixels per frame)

frame size	total SAINT memory	physically resident (for QSIZE = 15)
512	$24 + 18 = 42$ Mb	18 Mb
1024	$24 + 70 = 94$ Mb	70 Mb
2048	$24 + 294 = 318$ Mb	294 Mb

SAINT – Integration Options

Active Mask

Generate Mask:
Fractional Lower Limit of Average Intensity:

Use Pre-Existing Static Mask:
Active Mask File:

Use Pre-Existing Dynamic Masks

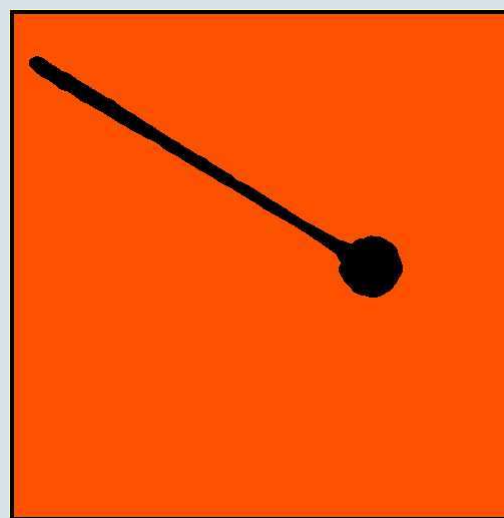
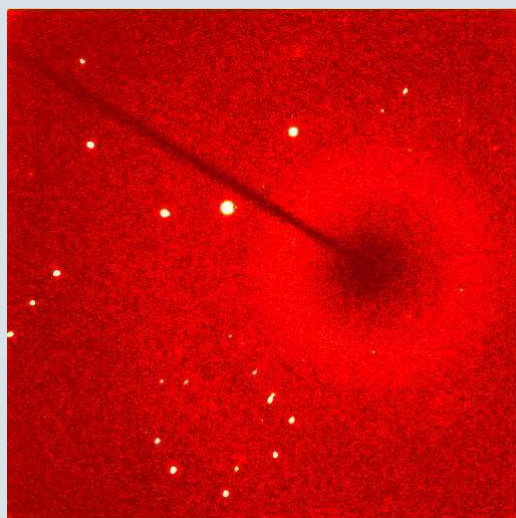
Algorithm

Use Narrow Frame Algorithm Use Wide Frame Algorithm

Active Mask

The active pixel mask is an image containing a small nonzero value for each pixel which is fully capable of receiving x-ray events, or zero for those pixel which are outside the active area or behind the beam stop.

The input is the fraction of mean I to qualify as active pixel. If the default 0 is used nothing is done.





SAINT – Listing (Log) File (for each run)

Background pixels updated = 90.83%

Port, connections: 51408, 1

# File	#Ref	ErrX	ErrY	ErrZ	RmsX	RmsY	RmsZ
0.sfrm	0	0.00	0.00	0.00	0.00	0.00	0.00
1.sfrm	0	0.00	0.00	0.00	0.00	0.00	0.00
2.sfrm	59	0.02	-0.00	0.05	0.10	0.10	0.10
3.sfrm	118	0.01	-0.00	0.02	0.16	0.11	0.13
4.sfrm	110	0.01	-0.00	-0.01	0.11	0.11	0.11
5.sfrm	125	-0.01	-0.01	-0.01	0.12	0.11	0.13

#Ref

Number of reflections harvested

ErrX, ErrY, ErrZ

Average signed observed minus predicted position in pixels for the harvested reflections. ErrX and ErrY are average errors in plane of the frame, ErrZ is the average difference between observed and predicted frame number.

RmsX, RmsY, RmsZ

RMS difference in observed vs predicted positions for harvested reflections.

RmsX or RmsY values consistently above about 0.3 pixels indicate that there could be a problem with the orientation matrix.



SAINT – Listing (Log) File (for each run)

Background pixels updated = 90.83%

Port, connections: 51408, 1

# File	Inorm	#Sig	%>2s	<Cor>	%Ful	XSiz	YSiz	ZSiz	Beam
0.sfrm	0	0	0	0.00	0	0.58	0.52	0.31	1.006
1.sfrm	0	0	0	0.00	0	0.58	0.52	0.31	1.005
2.sfrm	1618	16	12	0.91	14	0.58	0.52	0.31	1.005
3.sfrm	1441.8	15	16	0.90	14	0.59	0.54	0.28	1.005
4.sfrm	1971.1	15	17	0.91	16	0.59	0.54	0.27	1.005
5.sfrm	1474.4	15	19	0.88	16	0.61	0.55	0.27	1.005

Inorm

Average intensity (normalised to 1 min / deg)

#Sig

Average I/sigma signed observed minus predicted position in pixels

%>2s

Percentage of harvested reflections having intensities less than twice its standard deviations.

<Cor>

Average coefficient (range -1 to 1) representing the degree of correlation between the 3D reflection profiles for the harvested reflections and the model 3D reflection profiles computed from strong spots.

Values consistently less than about 0.25 indicates a serious problem.

SAINT – Listing (Log) File (for each run)

Background pixels updated = 90.83%

Port, connections: 51408, 1

# File	Inorm	#Sig	%<2s	<Cor>	%Ful	XSiz	YSiz	ZSiz
0.sfrm	0	0	0	0.00	0	0.58	0.52	0.31
1.sfrm	0	0	0	0.00	0	0.58	0.52	0.31
2.sfrm	1618	16	12	0.91	14	0.58	0.52	0.31
3.sfrm	1441.8	15	16	0.90	14	0.59	0.54	0.28
4.sfrm	1971.1	15	17	0.91	16	0.59	0.54	0.27
5.sfrm	1474.4	15	19	0.88	16	0.61	0.55	0.27

%Ful

Average spot span in Z relative to the span of the frame queue. Spots which are wider than the frame queue are "rejected and not written to the output raw.

- 20 – 30 % ⇒ 😊 for "normal" crystals
- 50 – 60 % ⇒ 😐 still acceptable
- > 80 % ⇒ 😞 stop integration, change parameter

XSiz, YSiz, ZSiz

Real size of the reflections



SAINT – Listing (Log) File (for all - *_0m._ls)

Coverage Statistics for ins_0m.raw

.....Shell.....

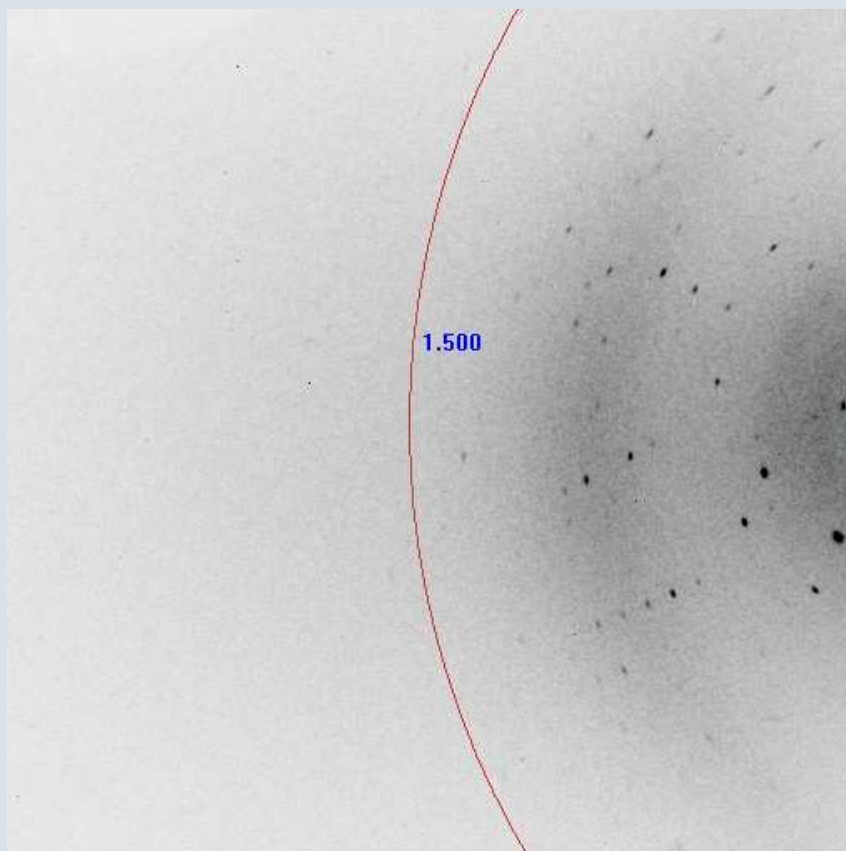
Angstrms	#Obs	Theory	%Compl	Redund	Rsym	Pairs	%Pairs	Rshell	#Sigma	%<2s
to 4.306	577	589	97.96	95.19	0.075	577	97.96	0.075	46.04	2.1
to 3.419	1133	1134	99.91	98.38	0.074	1133	99.91	0.073	36.55	2.5
to 2.987	1675	1676	99.94	99.50	0.074	1675	99.94	0.075	21.96	3.4
to 2.714	2224	2225	99.96	100.20	0.075	2224	99.96	0.082	12.83	9.7
to 2.519	2760	2763	99.89	100.77	0.076	2760	99.89	0.085	10.94	11.4
to 2.371	3300	3301	99.97	100.94	0.077	3300	99.97	0.094	8.35	17.5
to 2.252	3836	3837	99.97	101.04	0.078	3836	99.97	0.102	6.99	21.0
to 2.154	4362	4370	99.82	101.07	0.079	4362	99.82	0.114	5.73	26.8
to 2.071	4898	4899	99.98	101.09	0.081	4898	99.98	0.122	5.07	31.3
to 2.000	5438	5430	100.00	99.67	0.082	5437	100.00	0.148	3.78	40.5

Rsym Cumulative R(sym) on I for all reflections to the specified resolution

$$\langle |I - \langle I \rangle| / |\langle I \rangle| \rangle$$

Rshell R(sym) computed for the thin shell ending at this resolution.

Practical Example – Weak Diffraction Power



Goniometer				
Model				
Scan Axis	Omega			
Exposures / Correlation	2			
	Last Requested	Last Actual	Total (correlated)	
Exposure (sec.)	13.3333	13.36	120.403	
	2 Theta	Omega	Phi	Chi
Starting Angles	60	60	0	54.74
Ending Angles	60	59.5	0	54.74
Zero offsets	0.000	0.000	0.000	0.000

Practical Example – Integration with wrong ini-File



	Collect	Run #	First Image #	2-Theta	Omega	Phi	Chi / Kappa	Rotation Axis	# of Images	Expose Time (sec)
1	Yes	1	1	60	60	0	54.736	Omega	360	120
2	Yes	2	1	43	43	90	54.736	Omega	360	60
3	Yes	3	1	43	43	120	54.736	Omega	360	60
4	Yes	4	1	60	60	150	54.736	Omega	360	120
5	Yes	5	1	60	60	210	54.736	Omega	360	120
6	Yes	6	1	60	60	270	54.736	Omega	360	120
7	No	7	1	60	43	0	54.736	Phi	720	120
8										

SAINT settings

- Model Profile default
- Image Queue default
- Active Mask set

mb_0m_ls - Editor

Datei Bearbeiten Format ?

Coverage statistics for mb_0m.raw

Angstrms	#Obs	Theory	%Comp1	Redund	Rsym	Pairs	%Pairs	Rshell	#sigma	%<2s
to 2.222	8309	7846	100.00	3.76	0.873	4575	58.31	0.873	17.08	24.6
to 1.765	16541	15511	100.00	3.74	0.944	9911	63.90	1.008	14.68	30.0
to 1.542	24657	23089	100.00	3.67	0.946	15478	67.04	0.952	9.29	41.4
to 1.401	32803	30716	100.00	3.59	0.974	21220	69.08	1.064	11.71	47.9
to 1.301	40764	38328	100.00	3.50	0.995	26594	69.39	1.071	13.53	50.2
to 1.224	48796	45805	100.00	3.38	0.998	31677	69.16	1.013	14.49	50.9
to 1.163	56089	53445	100.00	3.22	0.992	35231	65.92	0.934	14.19	50.3
to 1.112	63203	60989	100.00	3.06	0.987	37707	61.83	0.860	13.77	48.3
to 1.069	70230	68493	100.00	2.92	0.982	39816	58.13	0.759	13.08	42.8
to 1.033	74942	76130	98.44	2.82	0.979	40973	53.82	0.695	14.62	39.8

Practical Example – Integration with wrong ini-File



SAINT log-file output

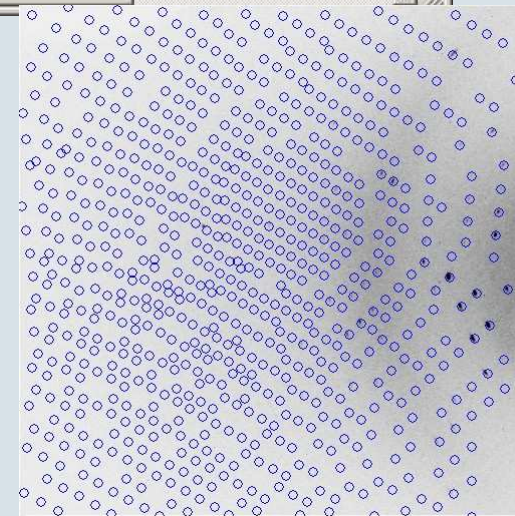
mb_01_ls - Editor

Datei Bearbeiten Format ?

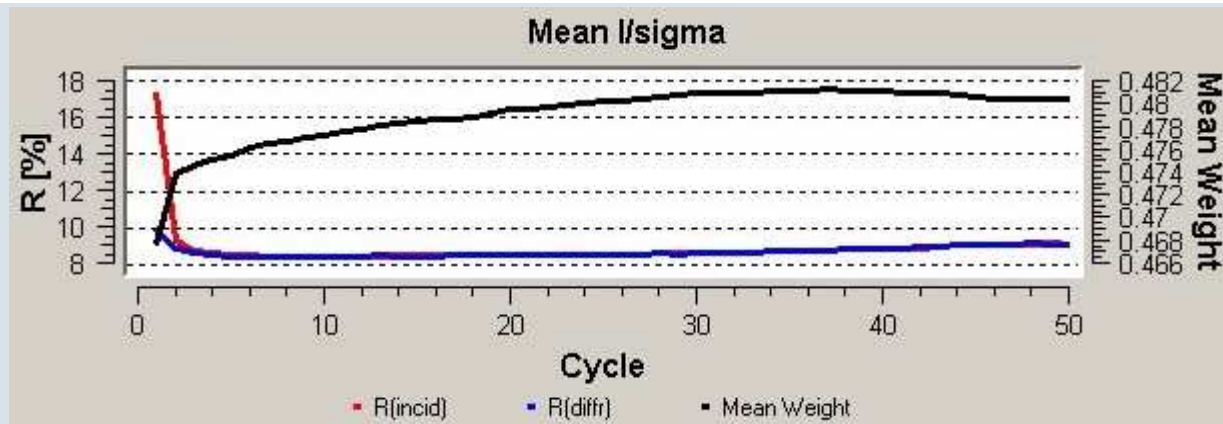
Background pixels updated = 84.10%

#	File	#Ref	ErrX	ErrY	ErrZ	RmsX	RmsY	RmsZ	Inorm	#Sig	%<2s	<Cor>	%Fu1	XSiz	YSiz	ZSiz	Beam
0.sfrm	0	0	0.00	0.00	0.00	0.00	0.00	0.00	0	0	0	0.00	0	1.01	1.03	0.73	1.003
1.sfrm	0	0	0.00	0.00	0.00	0.00	0.00	0.00	0	0	0	0.00	0	1.01	1.03	0.73	1.003
2.sfrm	73	0.17	-0.05	0.04	0.70	0.49	0.22	575.25	3	59	0.14	8	1.01	1.03	0.73	1.003	
3.sfrm	95	0.20	-0.11	0.00	0.70	0.70	0.26	437.6	3	71	0.21	10	1.05	1.04	0.74	1.003	
4.sfrm	97	0.04	0.04	-0.01	0.54	0.40	0.22	337.5	2	59	0.18	9	1.31	1.14	0.74	1.003	
5.sfrm	98	0.19	-0.01	0.02	0.66	0.43	0.23	376.02	2	68	0.20	9	1.31	1.14	0.74	1.003	
6.sfrm	108	-0.01	-0.01	-0.07	0.54	0.37	0.23	580.16	2	64	0.18	10	1.31	1.13	0.74	1.003	
7.sfrm	103	0.02	0.00	0.03	0.66	0.73	0.26	1201.5	5	64	0.17	9	1.30	1.13	0.74	1.003	
8.sfrm	97	-0.03	-0.01	-0.02	0.65	0.49	0.22	420.66	2	62	0.17	10	1.31	1.24	0.74	1.003	
9.sfrm	92	0.04	-0.04	0.00	0.68	0.40	0.21	1273.7	3	63	0.22	9	1.30	1.25	0.74	1.003	
10.sfrm	113	0.08	0.08	0.00	0.60	0.45	0.22	427.27	2	65	0.19	9	1.29	1.27	0.74	1.003	
11.sfrm	88	0.09	0.04	-0.04	0.73	0.49	0.23	654	3	67	0.21	9	1.29	1.27	0.75	1.003	
12.sfrm	112	0.00	-0.08	-0.01	0.61	0.58	0.24	1162.7	3	70	0.20	10	1.27	1.30	0.75	1.003	
13.sfrm	107	0.12	-0.17	0.02	0.68	0.75	0.25	851.88	4	59	0.18	10	1.26	1.32	0.75	1.003	
14.sfrm	85	-0.06	-0.08	-0.03	0.54	0.43	0.21	363.12	2	65	0.18	9	1.26	1.34	0.75	1.003	
15.sfrm	97	0.12	-0.01	-0.00	0.63	0.38	0.25	571.54	2	64	0.19	9	1.25	1.34	0.75	1.003	

Check orientation matrix
(Overlay in APEX2)



Practical Example – SADABS wrong ini-File



Initial Reflections

Total

Unique

Reflections after Outlier Rejection

Total

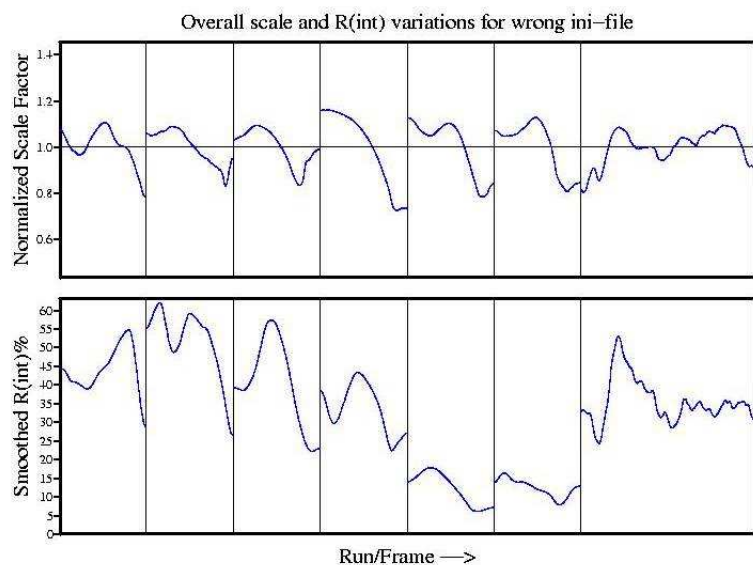
% Rejected

Unique

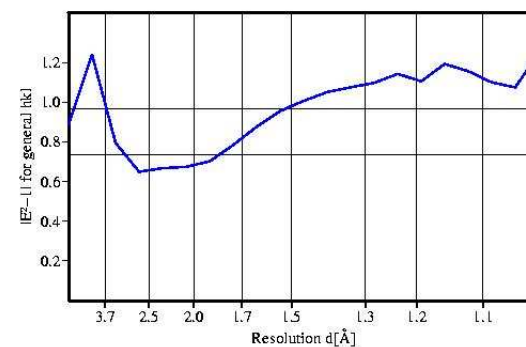
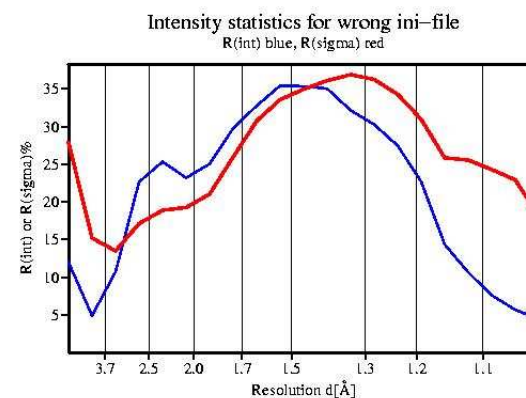
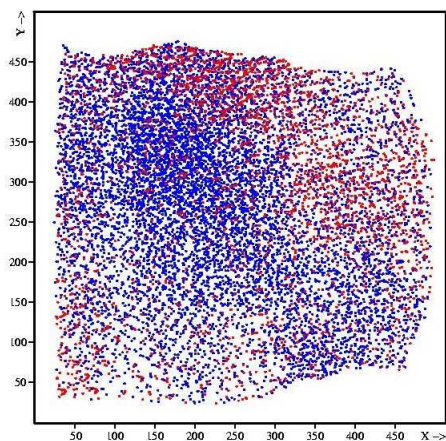
% Rejected

Batches	2-Theta	R(int)	Incid. factors	Diffr. factors	K	Total	I>2sig(I)
<input checked="" type="checkbox"/> 1	60.0	0.4330	0.845 - 1.192	0.645 - 2.531	2.010	16643	4956
<input checked="" type="checkbox"/> 2	43.0	0.5086	2.204 - 2.894	0.599 - 2.640	2.229	19789	4737
<input checked="" type="checkbox"/> 3	43.0	0.3991	1.210 - 1.589	0.605 - 2.567	2.116	15970	6984
<input checked="" type="checkbox"/> 4	60.0	0.3344	0.459 - 0.734	0.751 - 2.796	1.825	16669	6235
<input checked="" type="checkbox"/> 5	60.0	0.1163	0.351 - 0.503	0.757 - 2.788	1.671	14068	9378
<input checked="" type="checkbox"/> 6	60.0	0.1225	0.298 - 0.417	0.461 - 2.129	1.306	12932	6843
<input checked="" type="checkbox"/> 7	60.0	0.3529	1.608 - 2.194	0.578 - 2.468	2.015	22438	9693

Practical Example – SADABS Diagnostic Plots



Scan 1, detector 2-theta: 60.00°, $l-l > 3.00$ su (red+, blue-), errors (black)



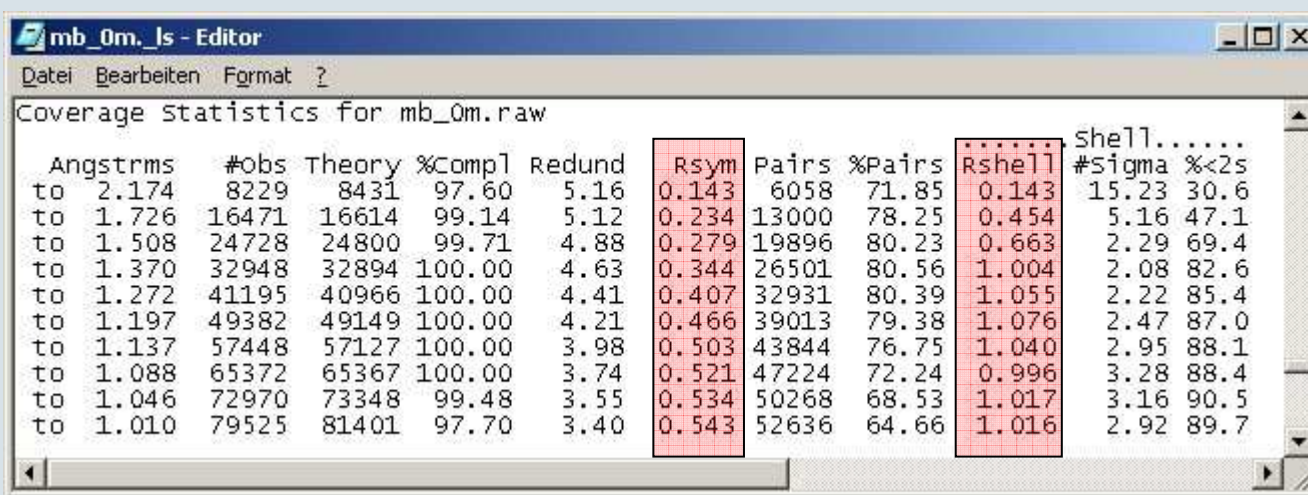
Practical Example – Integration of all Runs

Runs integrated

Run 1	1-360	360
run 2	1-360	360
run 3	1-360	360
run 4	1-360	360
run 5	1-360	360
run 6	1-360	360
run 7	1-720	720

SAINT settings

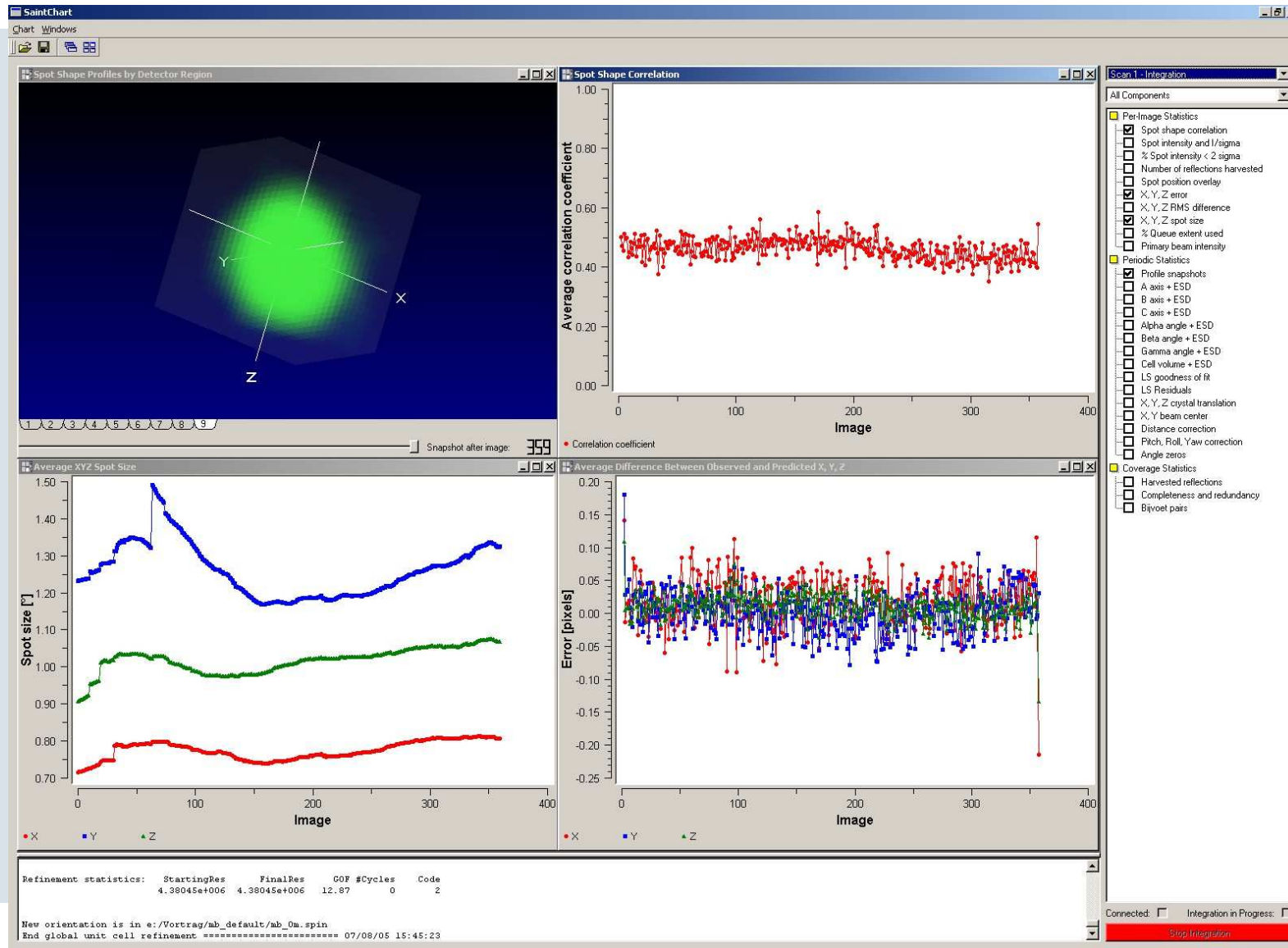
- **Model Profile** decreased
- **Image Queue** increased
- **Active Mask** set



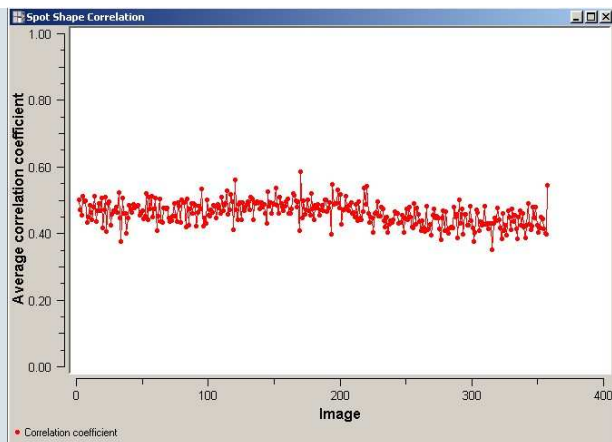
Coverage statistics for mb_0m.raw

Angstrms	#Obs	Theory	%Comp1	Redund	Rsym	Pairs	%Pairs	Rshell	#Sigma	%<2s
to 2.174	8229	8431	97.60	5.16	0.143	6058	71.85	0.143	15.23	30.6
to 1.726	16471	16614	99.14	5.12	0.234	13000	78.25	0.454	5.16	47.1
to 1.508	24728	24800	99.71	4.88	0.279	19896	80.23	0.663	2.29	69.4
to 1.370	32948	32894	100.00	4.63	0.344	26501	80.56	1.004	2.08	82.6
to 1.272	41195	40966	100.00	4.41	0.407	32931	80.39	1.055	2.22	85.4
to 1.197	49382	49149	100.00	4.21	0.466	39013	79.38	1.076	2.47	87.0
to 1.137	57448	57127	100.00	3.98	0.503	43844	76.75	1.040	2.95	88.1
to 1.088	65372	65367	100.00	3.74	0.521	47224	72.24	0.996	3.28	88.4
to 1.046	72970	73348	99.48	3.55	0.534	50268	68.53	1.017	3.16	90.5
to 1.010	79525	81401	97.70	3.40	0.543	52636	64.66	1.016	2.92	89.7

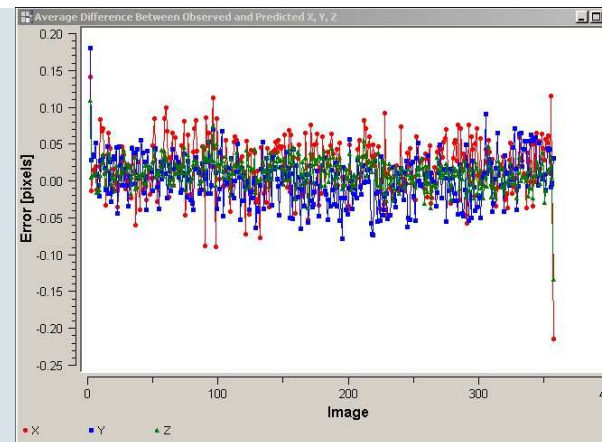
Practical Example – Graphics of SAINT Statistic



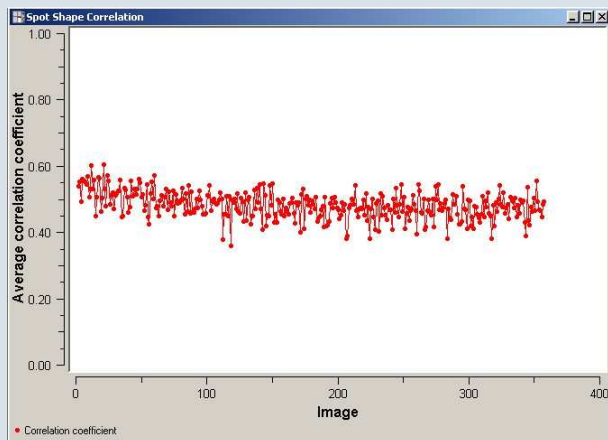
Practical Example – Graphics of SAINT Statistic



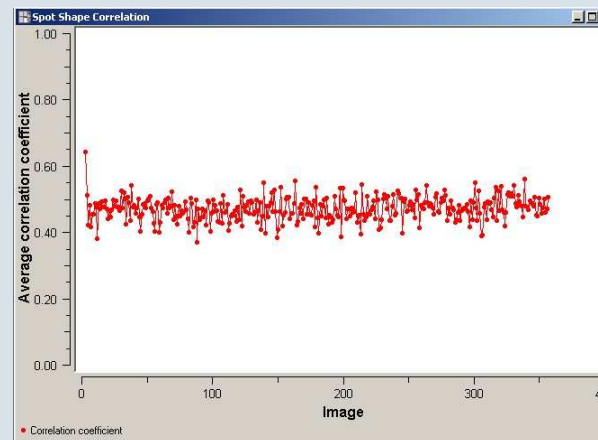
run 1 (correlation coefficient)



run 1 (position error)

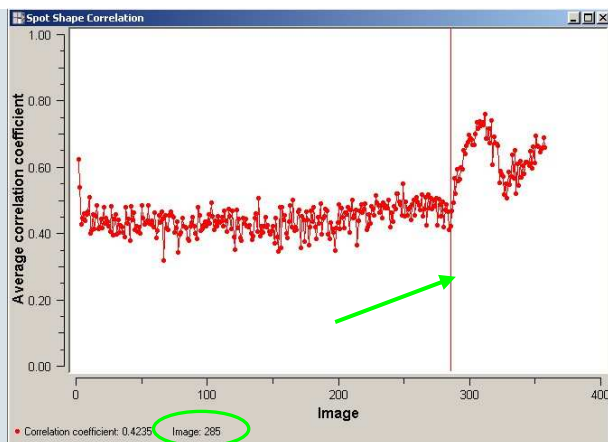


run 2 (correlation coefficient)

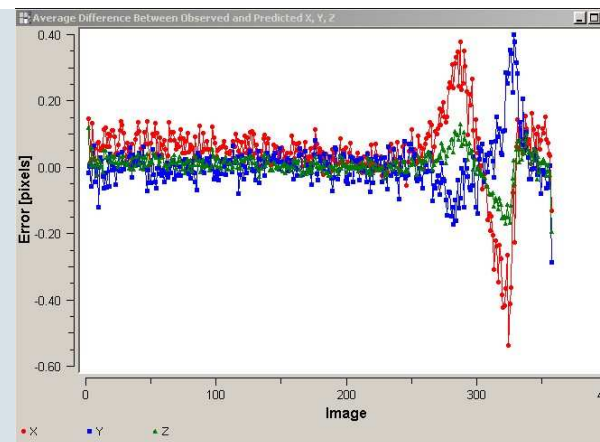


run 3 (correlation coefficient)

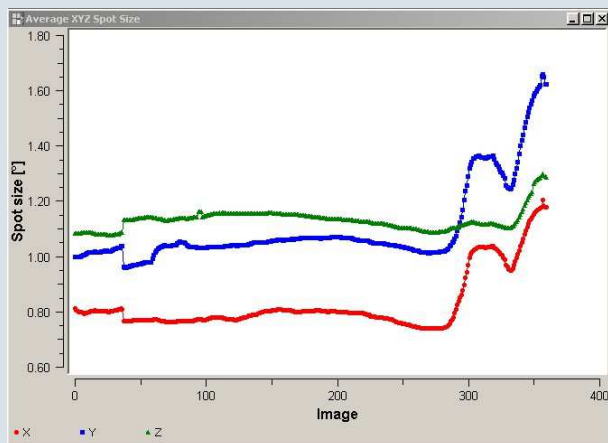
Practical Example – Graphics of SAINT Statistic



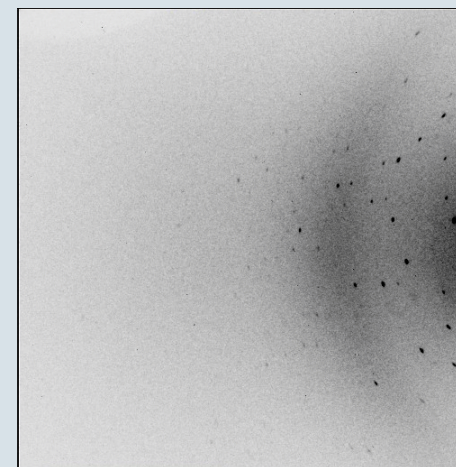
run 4 (correlation coefficient)



run 4 (position error)

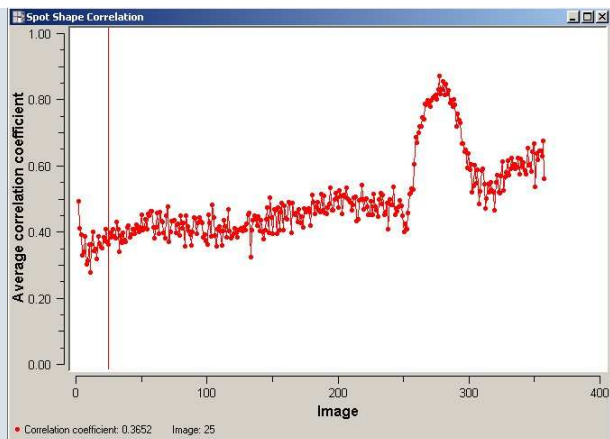


run 4 (spot size)

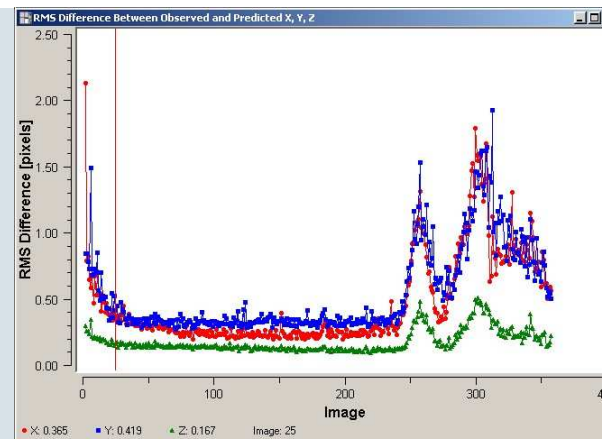


run 4 bad frames

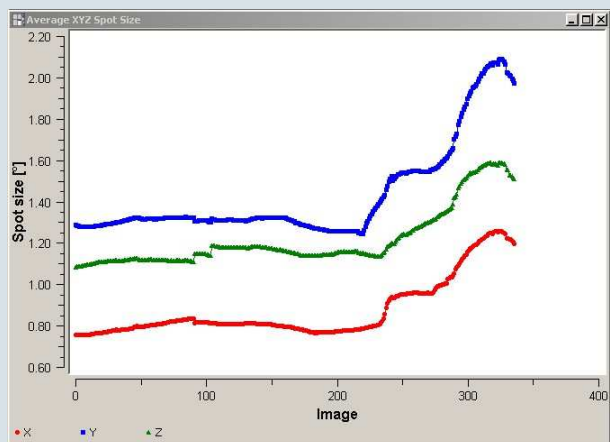
Practical Example – Graphics of SAINT Statistic



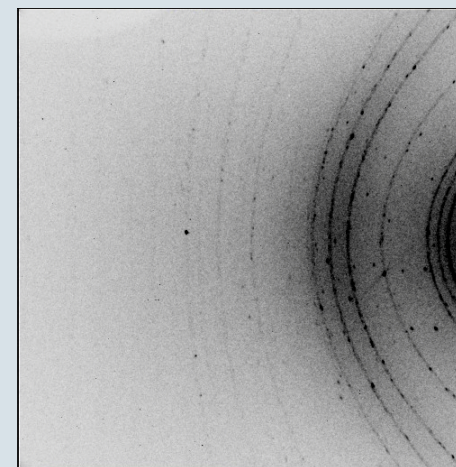
run 5 (correlation coefficient)



run 5 (position error)

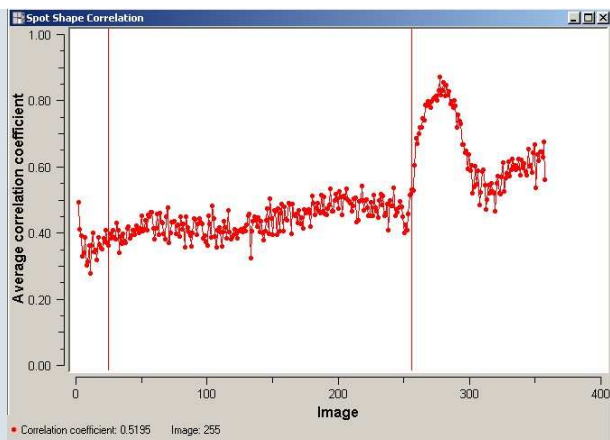


run 5 (spot size)

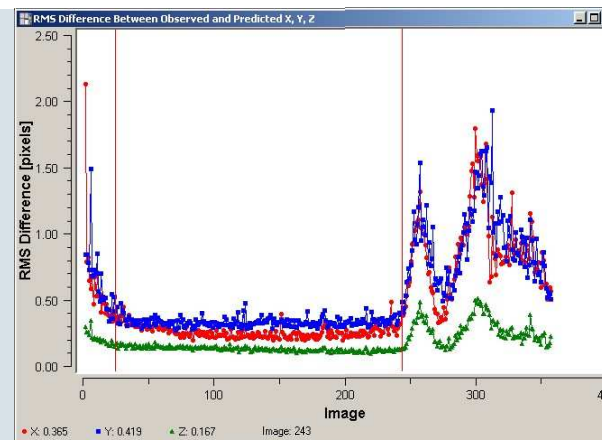


run 5 bad frames 1

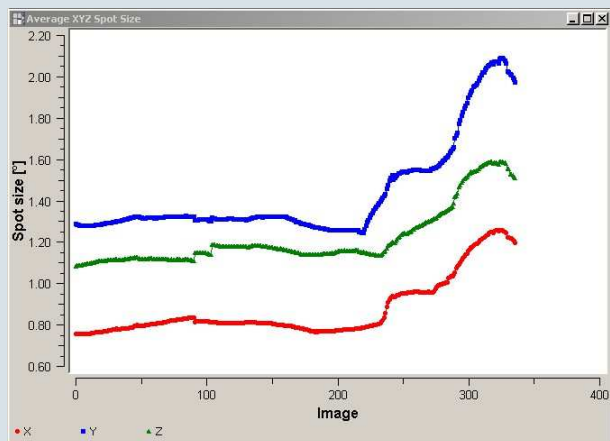
Practical Example – Graphics of SAINT Statistic



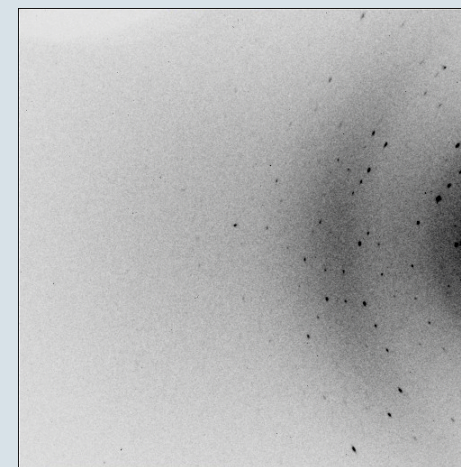
run 5 (correlation coefficient)



run 5 (position error)

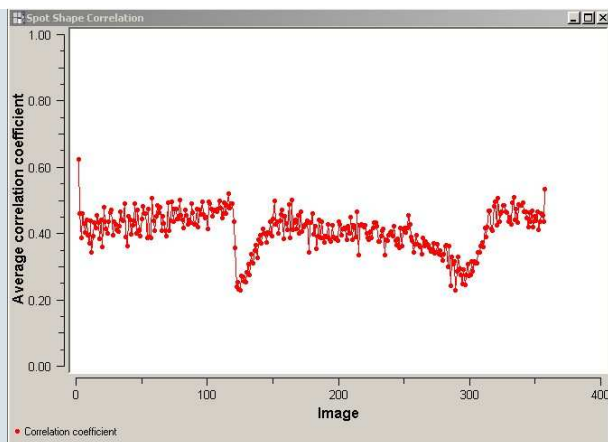


run 5 (spot size)

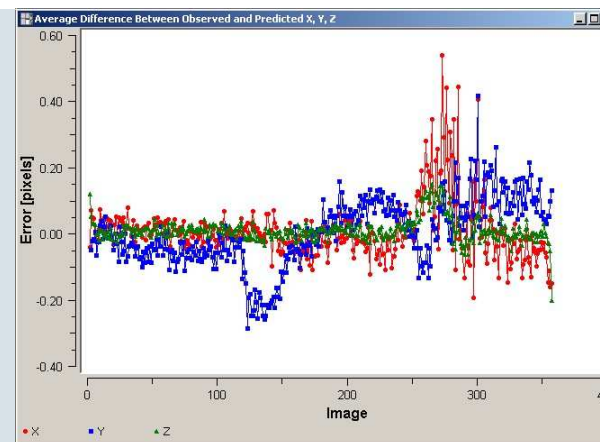


run 5 bad frames 2

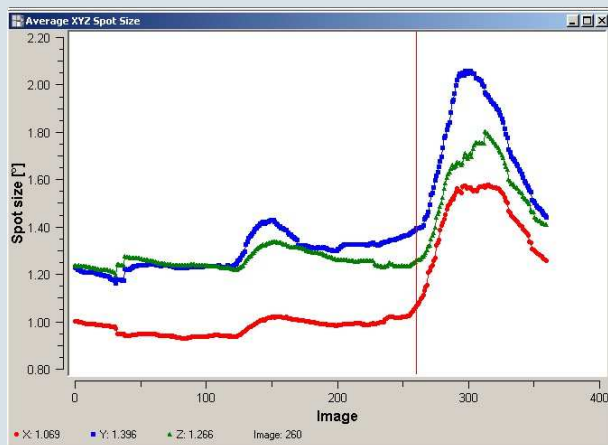
Practical Example – Graphics of SAINT Statistic



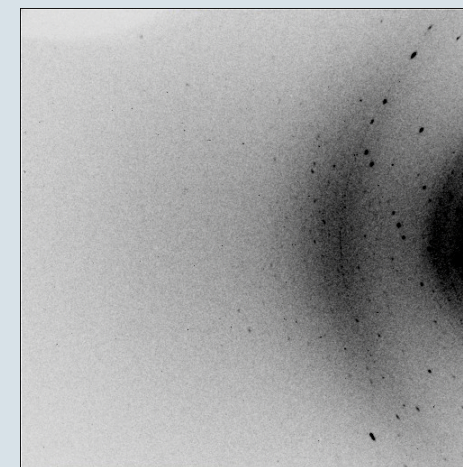
run 6 (correlation coefficient)



run 6 (position error)

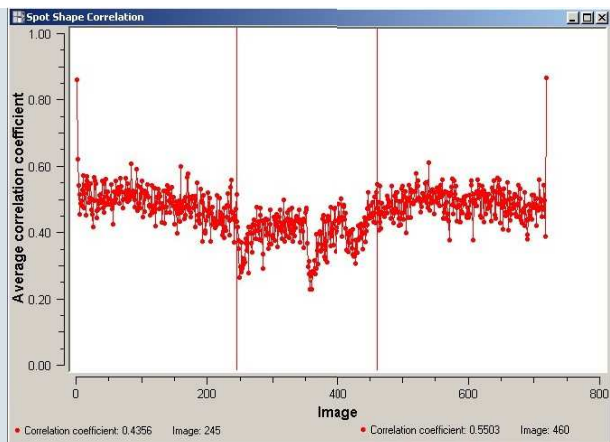


run 6 (spot size)

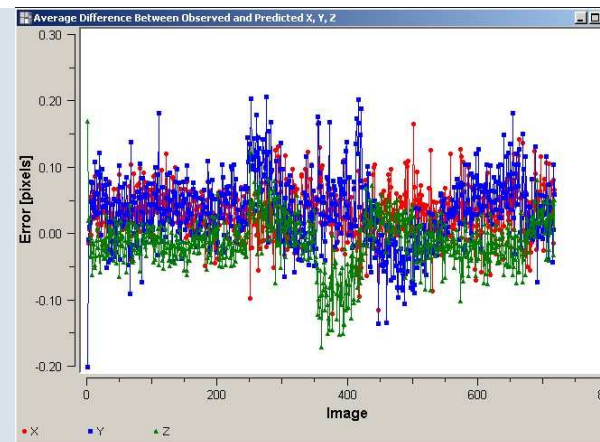


run 6 bad frames

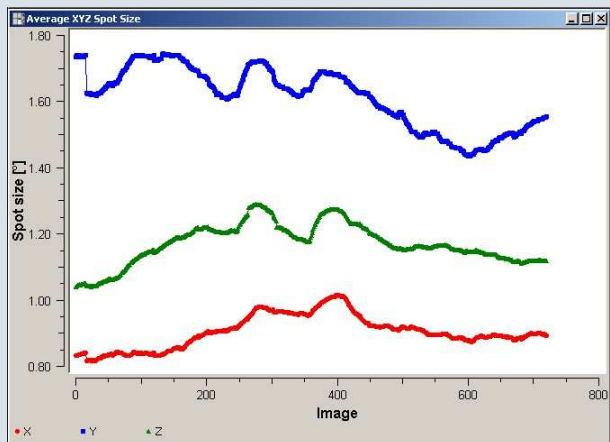
Practical Example – Graphics of SAINT Statistic



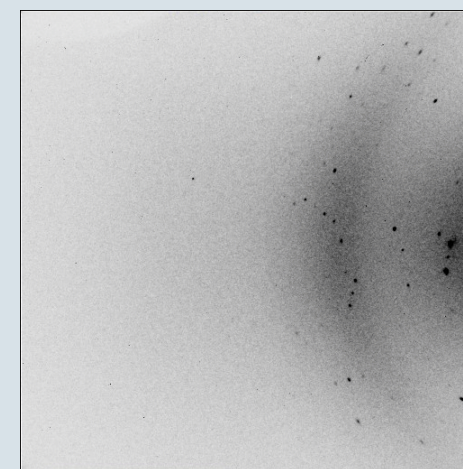
run 7 (correlation coefficient)



run 7 (position error)

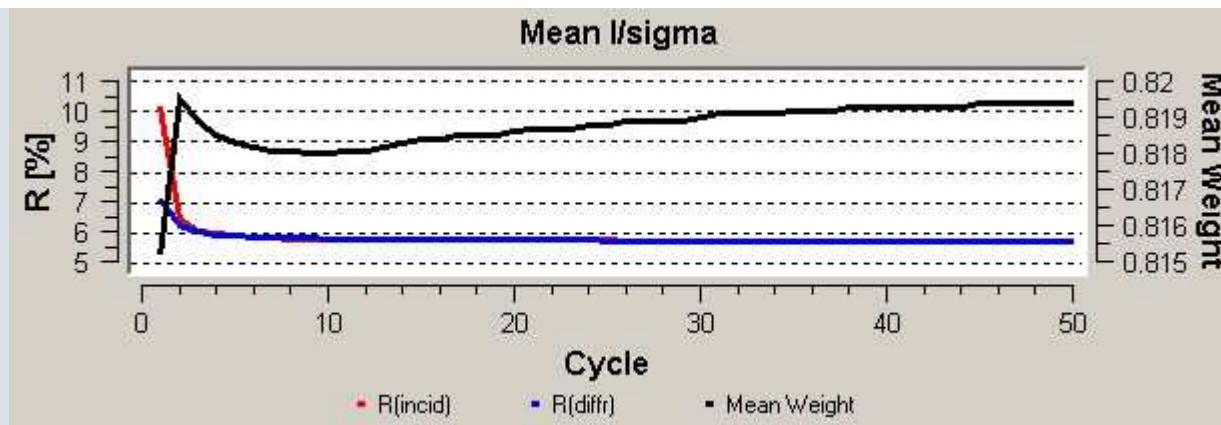


run 7 (spot size)



run 7 bad frames ?

Practical Example – SADABS all Runs



Initial Reflections

Total

Unique

Reflections after Outlier Rejection

Total

% Rejected

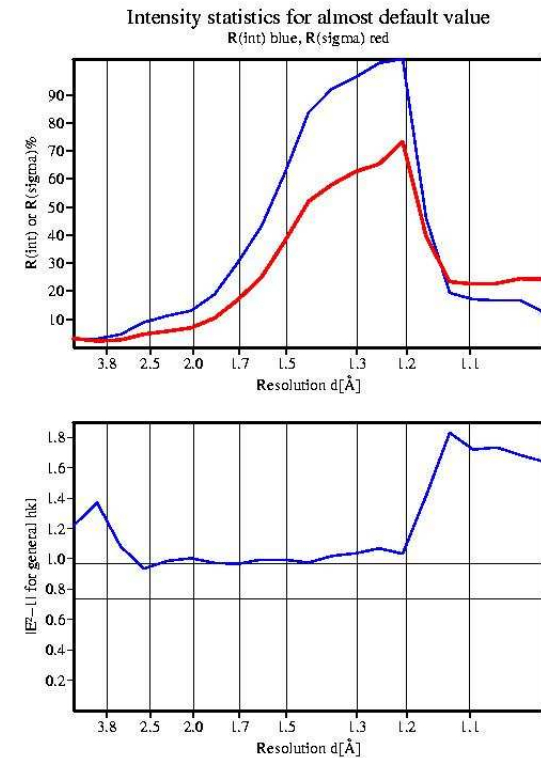
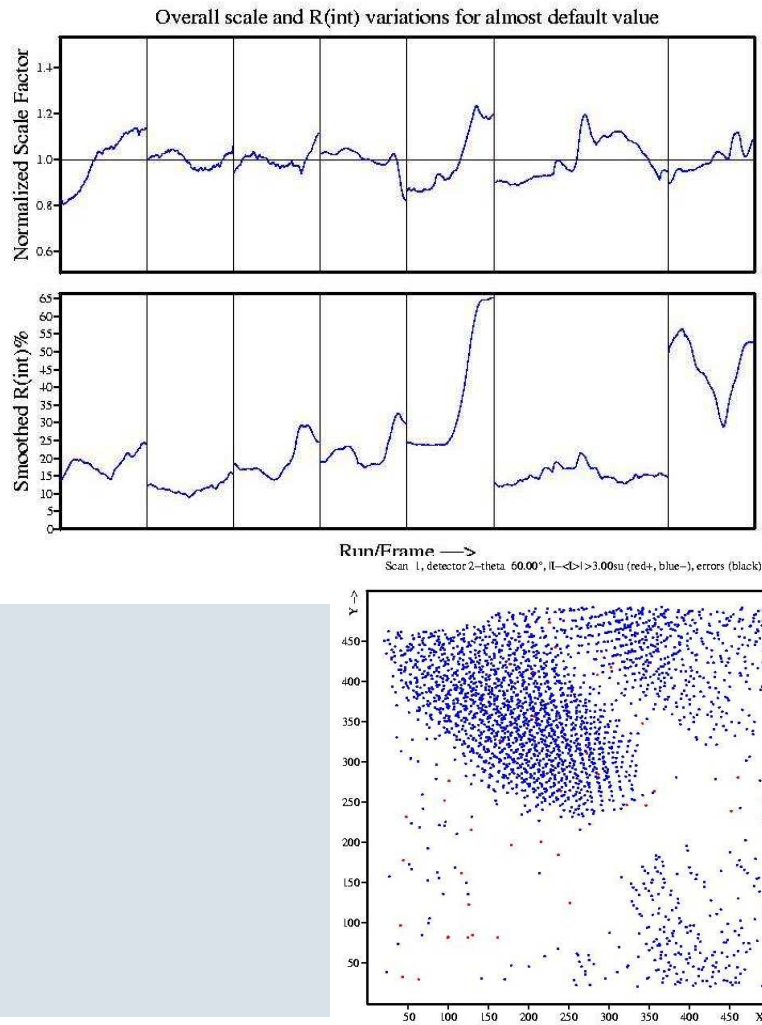
Unique

% Rejected

Batches	2-Theta	R(int)	Incid. factors	Diffr. factors	K	Total	I>2sig(I)
<input checked="" type="checkbox"/> 1	60.0	0.1842	0.713 - 1.007	0.907 - 1.330	0.785	39561	13066
<input checked="" type="checkbox"/> 2	43.0	0.1152	0.977 - 1.090	0.925 - 1.311	0.730	29712	10756
<input checked="" type="checkbox"/> 3	43.0	0.1965	0.811 - 0.964	0.925 - 1.205	0.929	29971	10116
<input checked="" type="checkbox"/> 4	60.0	0.2207	0.707 - 0.903	0.931 - 1.329	0.940	32447	9160
<input checked="" type="checkbox"/> 5	60.0	0.3583	0.526 - 0.754	0.907 - 1.237	1.214	35682	8306
<input checked="" type="checkbox"/> 6	60.0	0.1525	0.660 - 0.887	0.907 - 1.269	0.729	44481	15781
<input checked="" type="checkbox"/> 7	60.0	0.4504	0.705 - 0.879	0.906 - 1.265	1.384	29519	7624

Practical Example – SADABS Diagnostic Plots

all Runs

Practical Example – Integration without bad Frames / nine Profiles



Runs integrated

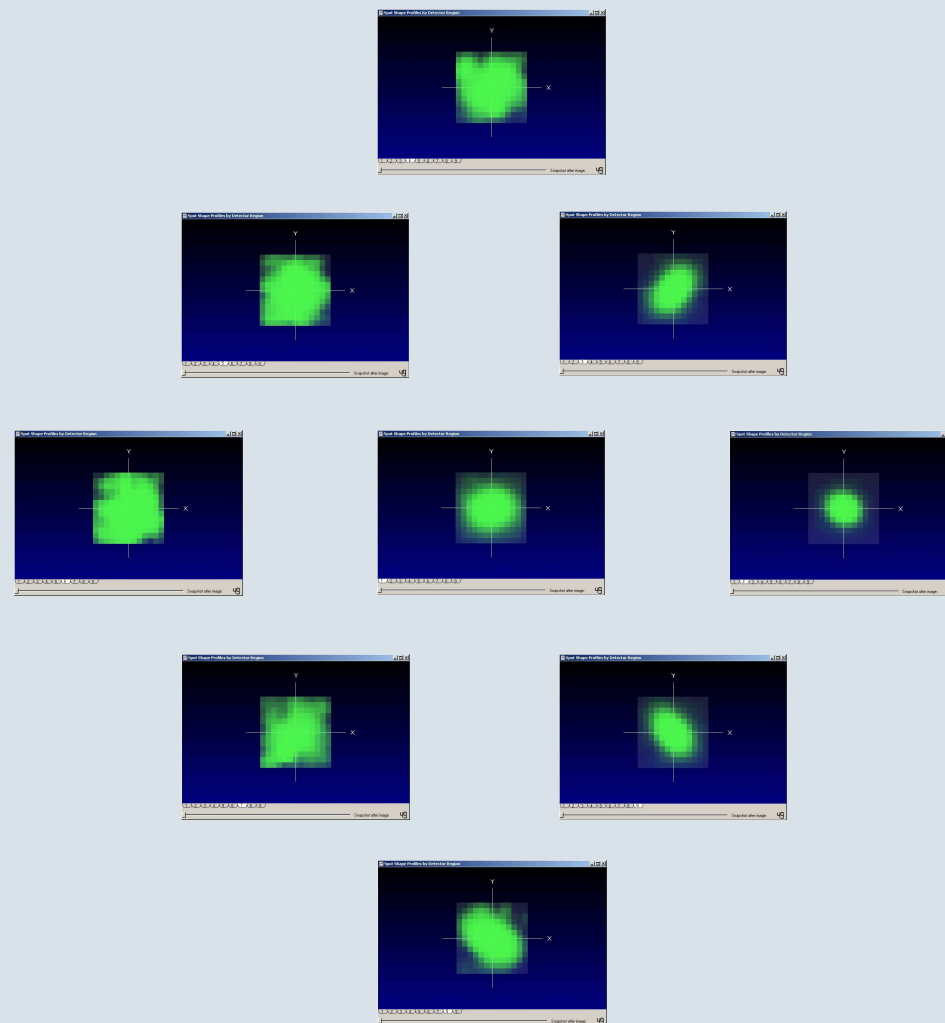
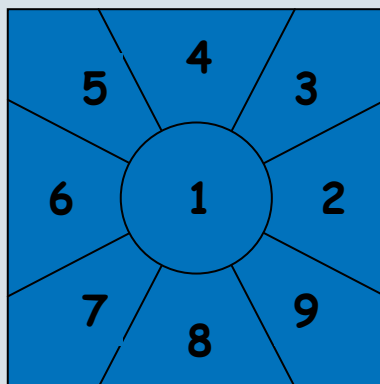
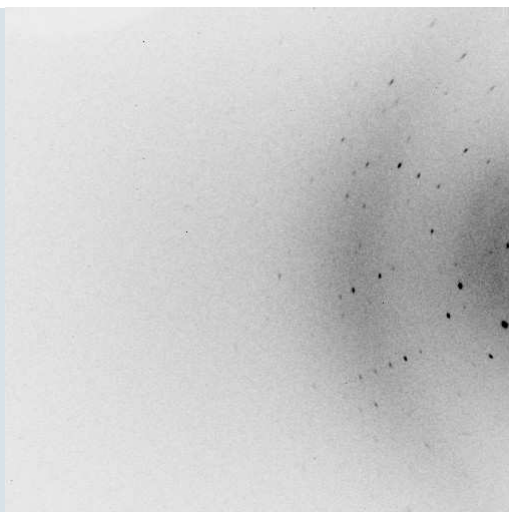
Run 1	1-360	360
run 2	1-360	360
run 3	1-360	360
run 4	1-270	270
run 5	25-255	230
run 6	1-250	250
run 7	1-720	720

SAINT settings

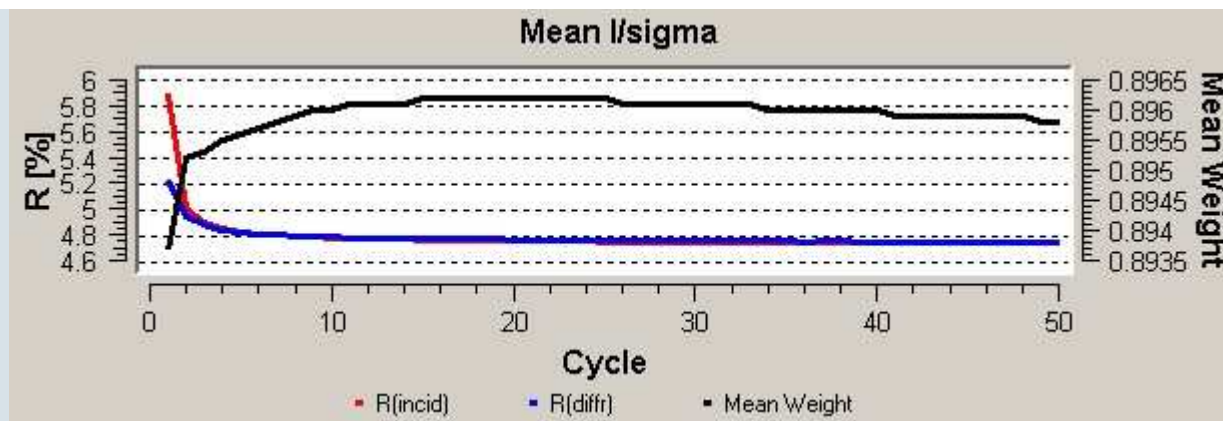
- **Model Profile** decreased
- **Image Queue** increased
- **Active Mask** set

Angstrms	#Obs	Theory	%Comp1	Redund	Rsym	Pairs	%Pairs	Rshell	#sigma	%<2s
to 2.175	8233	8427	97.70	4.62	0.079	4399	52.20	0.079	15.06	31.4
to 1.726	16463	16609	99.12	4.59	0.098	9502	57.21	0.153	4.23	48.9
to 1.508	24727	24783	99.77	4.38	0.116	14509	58.54	0.312	1.59	72.2
to 1.370	32974	32879	100.00	4.18	0.134	19461	59.19	0.516	0.78	86.5
to 1.272	41151	40945	100.00	3.99	0.152	24250	59.23	0.585	0.63	89.8
to 1.197	49326	49128	100.00	3.82	0.168	28888	58.80	0.646	0.52	91.9
to 1.137	57234	57096	100.00	3.62	0.178	32275	56.53	0.641	0.42	94.0
to 1.088	64786	65295	99.22	3.41	0.183	34214	52.40	0.571	0.30	95.5
to 1.046	72019	73310	98.24	3.25	0.187	36003	49.11	0.648	0.17	98.0
to 1.010	78081	81347	95.99	3.12	0.190	37393	45.97	0.669	0.14	98.5

Practical Example – Profiles 1 – 9 in SAINT



Practical Example – SADABS nine Profiles



Initial Reflections

Total

Unique

Reflections after Outlier Rejection

Total

% Rejected

Unique

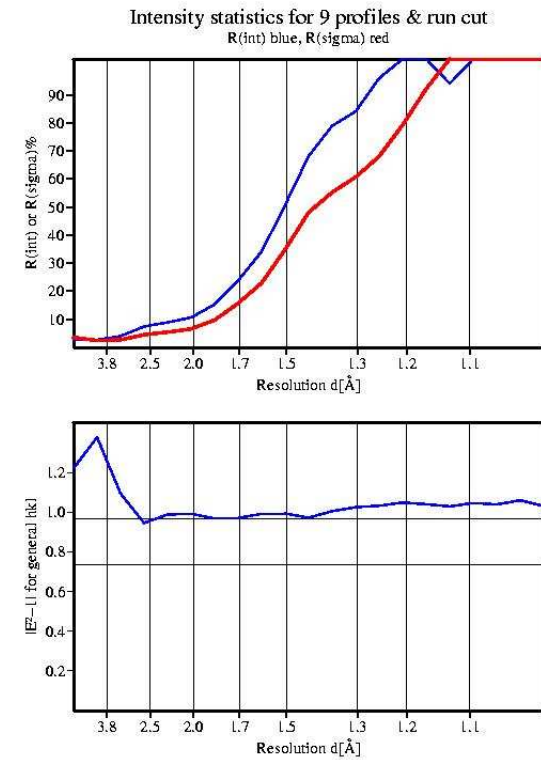
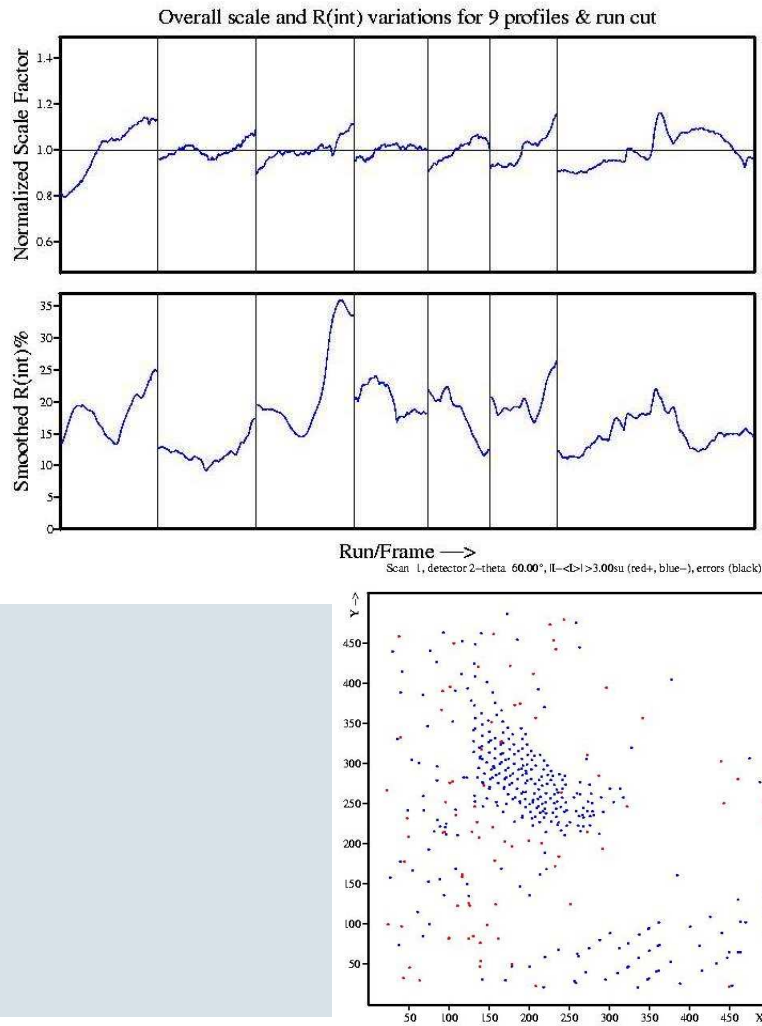
% Rejected

Batches	2-Theta	R(int)	Incid. factors	Diffr. factors	K	Total	I>2sig(I)
<input checked="" type="checkbox"/> 1	60.0	0.1812	0.710 - 1.023	0.888 - 1.417	0.737	41774	14270
<input checked="" type="checkbox"/> 2	43.0	0.1191	0.999 - 1.134	0.928 - 1.341	0.705	33789	11666
<input checked="" type="checkbox"/> 3	43.0	0.2195	0.791 - 0.981	0.928 - 1.269	0.955	32575	10506
<input checked="" type="checkbox"/> 4	60.0	0.2028	0.737 - 0.801	0.910 - 1.430	0.700	30960	9076
<input checked="" type="checkbox"/> 5	60.0	0.1747	0.695 - 0.821	0.889 - 1.252	0.712	26658	7866
<input checked="" type="checkbox"/> 6	60.0	0.1999	0.581 - 0.732	0.889 - 1.244	0.835	28628	7559
<input checked="" type="checkbox"/> 7	60.0	0.1501	0.659 - 0.854	0.888 - 1.331	0.697	48817	17231

Practical Example – SADABS Diagnostic Plots

BRUKER

nine Profiles



Practical Example – Integration without bad Frames One Profile (Blend Profiles)



Runs integrated

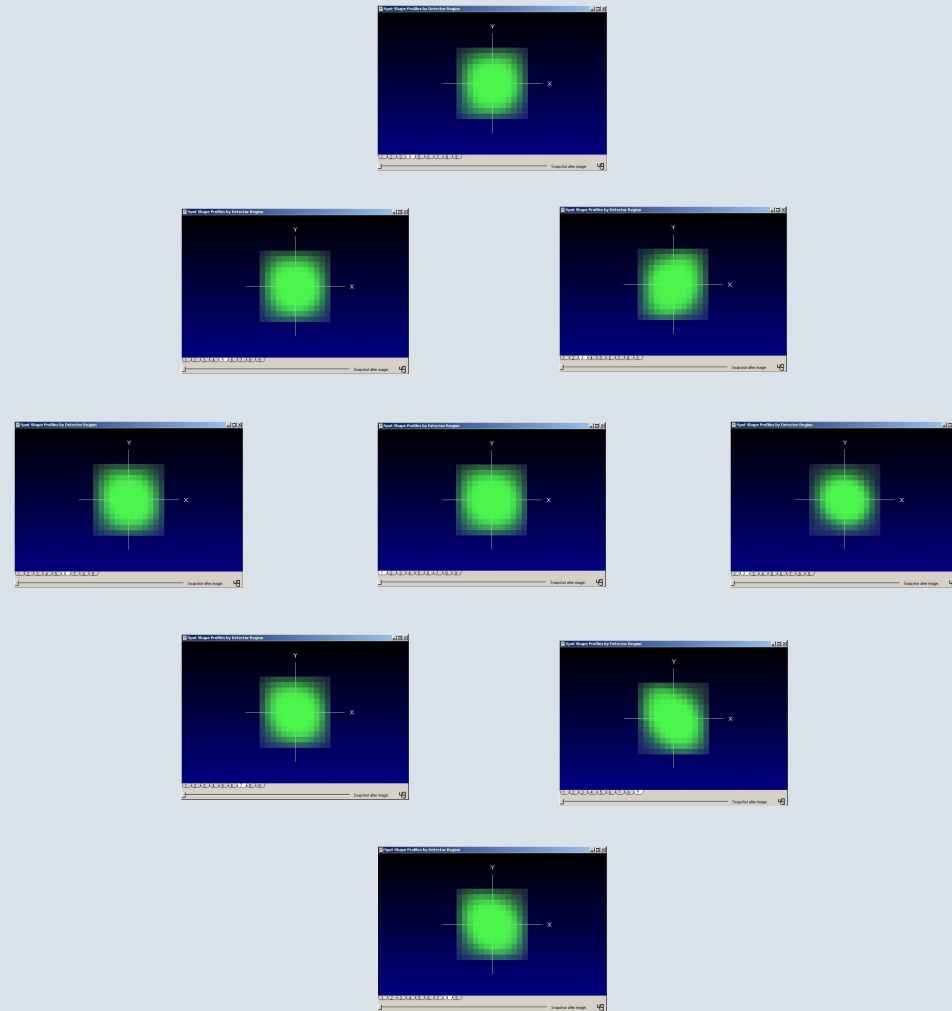
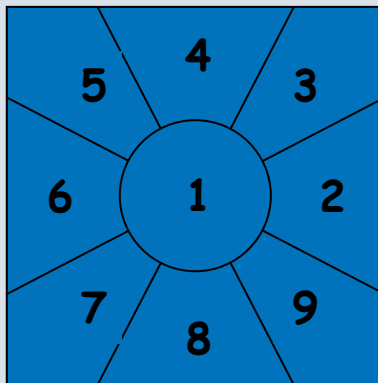
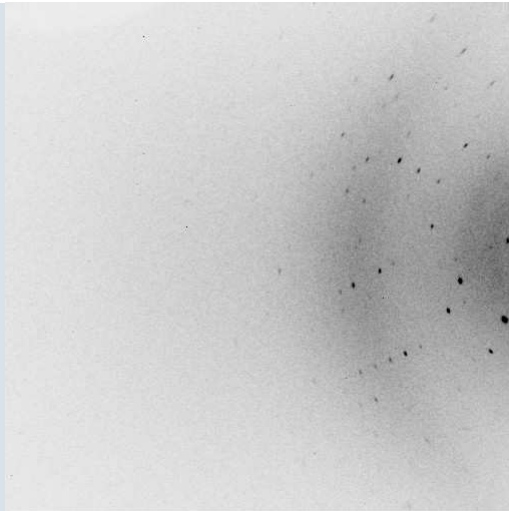
Run 1	1-360	360
run 2	1-360	360
run 3	1-360	360
run 4	1-270	270
run 5	25-255	230
run 6	1-250	250
run 7	1-720	720

SAINT settings

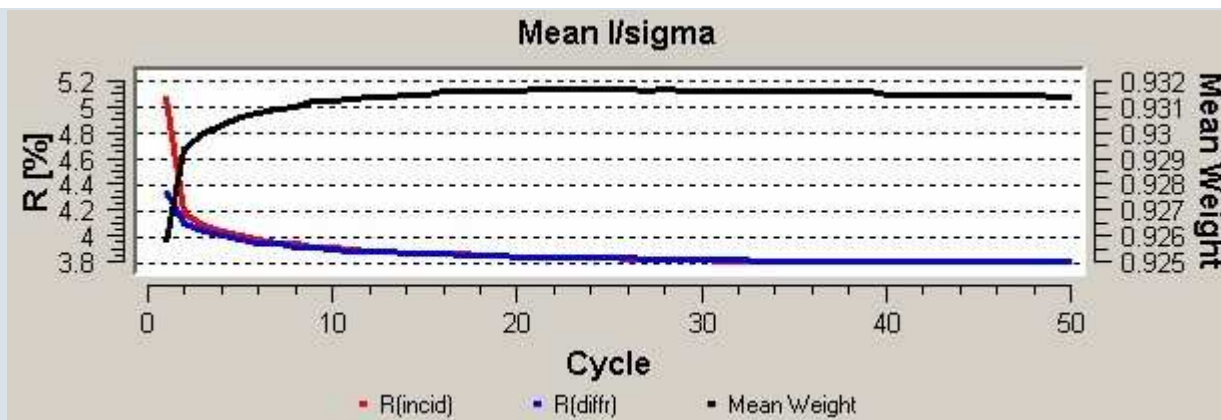
- **Model Profile** decreased
- **Image Queue** increased
- **Active Mask** set
- **Blend Profiles** enabled

Angstrms	#Obs	Theory	%Comp1	Redund	Rsym	Pairs	%Pairs	Rshell	#Sigma	%<2s
to 2.169	8299	8472	97.96	4.69	0.071	4516	53.31	0.071	18.71	30.0
to 1.722	16607	16714	99.36	4.64	0.087	9715	58.12	0.147	4.50	49.7
to 1.504	24890	25006	99.54	4.43	0.099	14768	59.06	0.290	1.43	75.4
to 1.367	33239	33162	100.00	4.22	0.111	19842	59.83	0.492	0.58	90.5
to 1.269	41466	41269	100.00	4.03	0.121	24713	59.88	0.566	0.40	93.8
to 1.194	49746	49504	100.00	3.86	0.130	29455	59.50	0.613	0.29	95.7
to 1.134	57738	57579	100.00	3.66	0.137	32877	57.10	0.636	0.21	97.2
to 1.085	65402	65797	99.40	3.45	0.140	34895	53.03	0.626	0.16	97.9
to 1.043	72772	73911	98.46	3.27	0.143	36724	49.69	0.690	0.06	99.4
to 1.007	78706	82029	95.95	3.15	0.145	38129	46.48	0.707	0.01	99.7

Practical Example – One Profile in SAINT (Blend Profiles)



Practical Example – SADABS one Profile (Blend Profiles)



Initial Reflections

Total: 247991

Unique: 78706

Reflections after Outlier Rejection

Total: 247892

% Rejected: 0.0

Unique: 78706

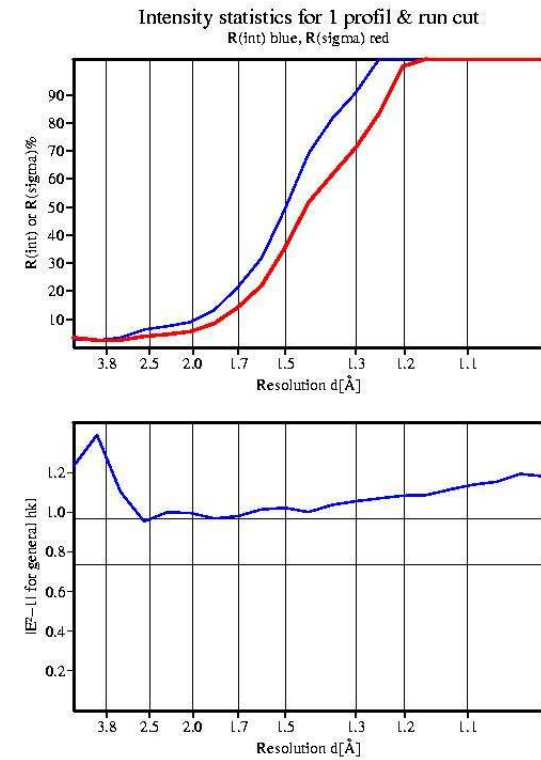
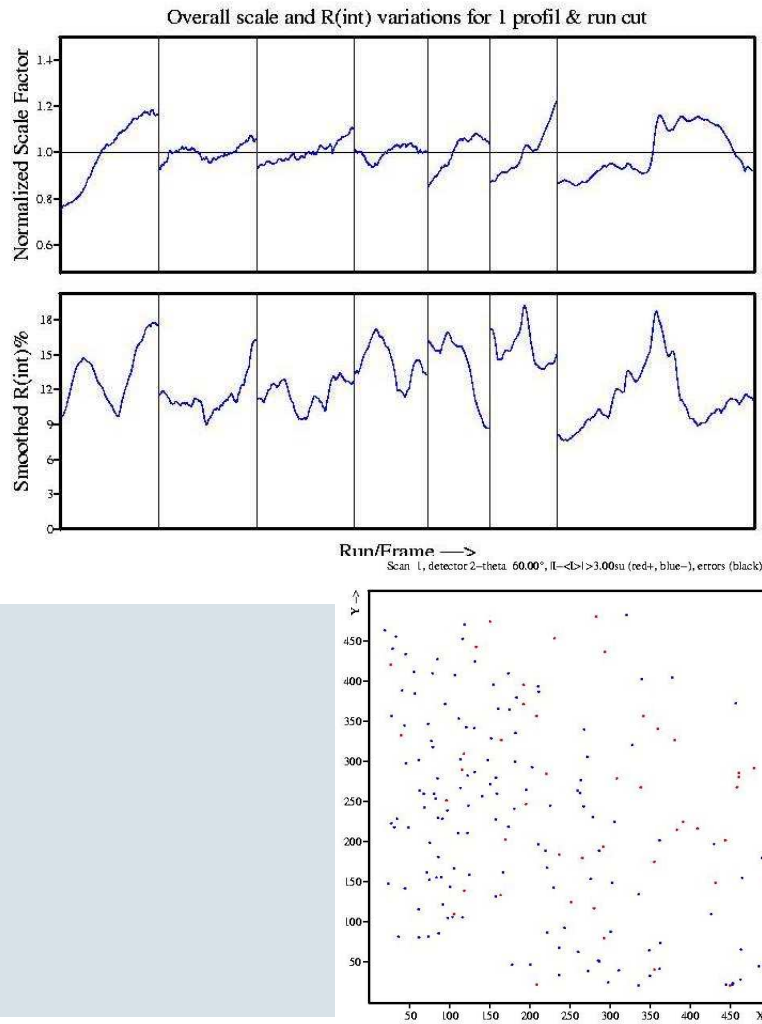
% Rejected: 0.0

Batches	2-Theta	R(int)	Incid. factors	Diff. factors	K	Total	I>2sig(I)
<input checked="" type="checkbox"/> 1	60.0	0.1325	0.678 - 1.062	0.872 - 1.367	0.640	42551	14207
<input checked="" type="checkbox"/> 2	43.0	0.1116	1.037 - 1.206	0.910 - 1.414	0.655	34009	11323
<input checked="" type="checkbox"/> 3	43.0	0.1142	0.919 - 1.092	0.916 - 1.284	0.661	33879	11329
<input checked="" type="checkbox"/> 4	60.0	0.1407	0.749 - 0.833	0.885 - 1.368	0.639	31742	9087
<input checked="" type="checkbox"/> 5	60.0	0.1359	0.655 - 0.829	0.873 - 1.358	0.640	26937	7664
<input checked="" type="checkbox"/> 6	60.0	0.1538	0.545 - 0.764	0.873 - 1.329	0.702	29106	7729
<input checked="" type="checkbox"/> 7	60.0	0.1099	0.612 - 0.830	0.873 - 1.363	0.615	49668	17446

Practical Example – SADABS Diagnostic Plots



One Profile



Practical Example – Integration best up to 1 Å One Profile



Runs integrated

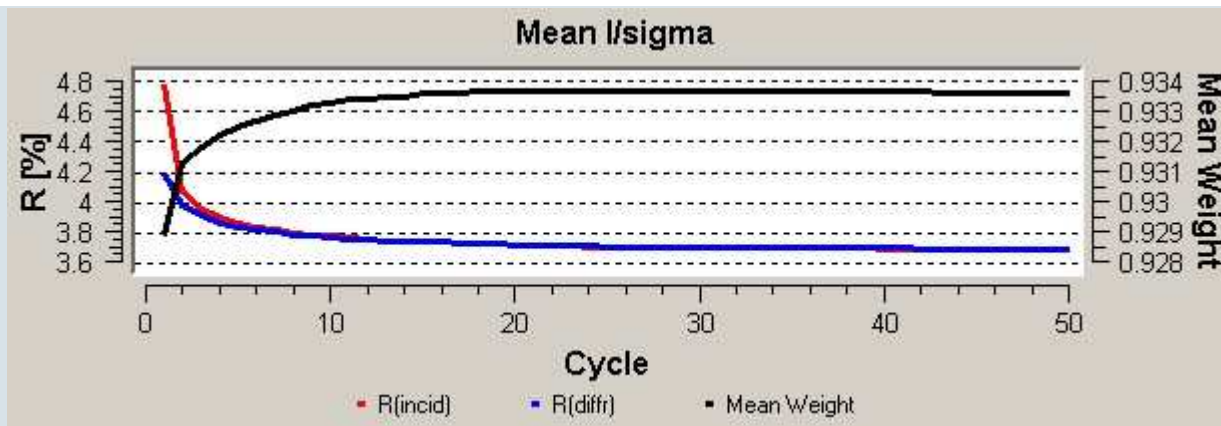
run 1	1-360	360
run 2	1-360	360
run 3	1-360	360
run 4	1-270	270
run 5	25-255	230
run 6	1-250	250
run 7a	1-244	244
run 7b	460-720	230

SAINT settings

- **Model Profile** decreased
- **Image Queue** increased
- **Active Mask** set
- **Blend Profiles** enabled

Angstrms	#Obs	Theory	%Comp1	Redund	Rsym	Pairs	%Pairs	Rshell	Shell..... #sigma	%<2s
to 2.169	8285	8472	97.79	4.45	0.066	4508	53.21	0.066	18.80	29.8
to 1.722	16580	16714	99.20	4.39	0.083	9707	58.08	0.145	4.53	49.6
to 1.504	24867	25006	99.44	4.19	0.095	14758	59.02	0.289	1.43	75.4
to 1.367	33212	33162	100.00	3.99	0.106	19832	59.80	0.484	0.58	90.3
to 1.269	41437	41269	100.00	3.80	0.116	24700	59.85	0.558	0.40	93.8
to 1.194	49695	49504	100.00	3.64	0.125	29432	59.45	0.602	0.29	95.6
to 1.134	57654	57579	100.00	3.45	0.131	32876	57.10	0.626	0.22	97.1
to 1.085	65310	65797	99.26	3.24	0.134	34894	53.03	0.619	0.16	97.7
to 1.043	72640	73911	98.28	3.08	0.137	36723	49.69	0.681	0.06	99.4
to 1.007	78595	82029	95.81	2.96	0.138	38128	46.48	0.711	0.02	99.7

Practical Example – SADABS best up to 1 Å One Profile



Initial Reflections

Total

Unique

Reflections after Outlier Rejection

Total

% Rejected

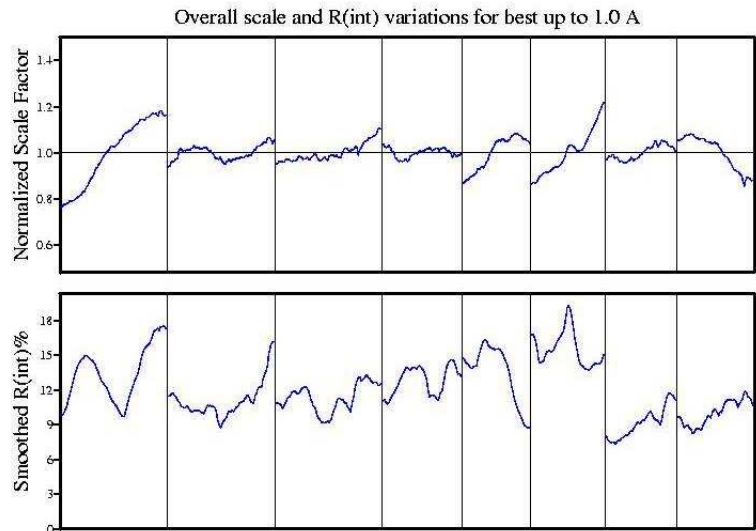
Unique

% Rejected

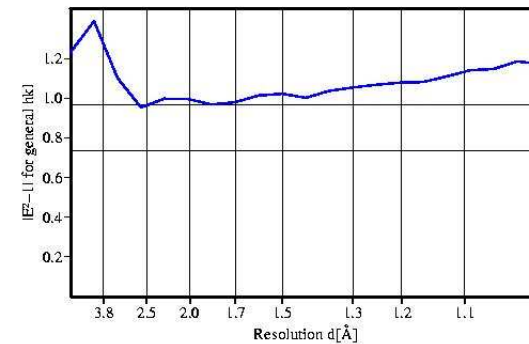
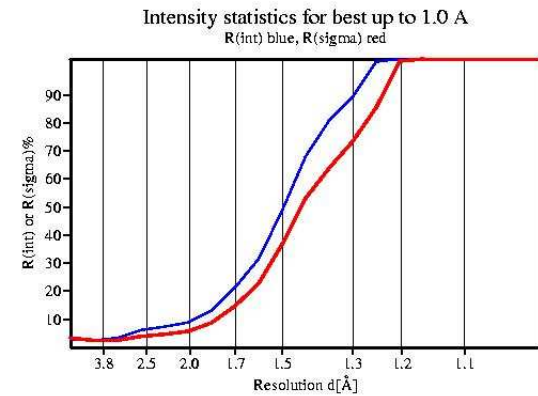
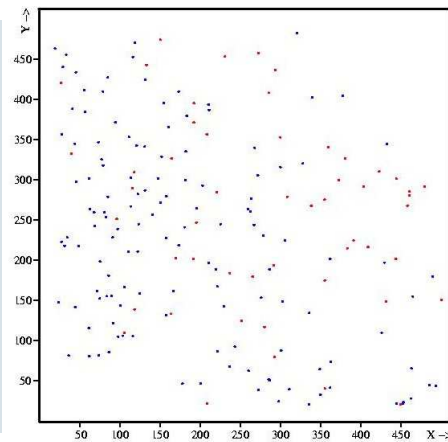
Batches	2-Theta	R(int)	Incid. factors	Diffr. factors	K	Total	I>2sig(I)
<input checked="" type="checkbox"/> 1	60.0	0.1328	0.706 - 1.096	0.887 - 1.316	0.644	42553	14153
<input checked="" type="checkbox"/> 2	43.0	0.1093	1.087 - 1.239	0.914 - 1.463	0.655	34010	11325
<input checked="" type="checkbox"/> 3	43.0	0.1118	0.970 - 1.130	0.921 - 1.310	0.663	33884	11307
<input checked="" type="checkbox"/> 4	60.0	0.1274	0.798 - 0.862	0.898 - 1.306	0.633	31742	9156
<input checked="" type="checkbox"/> 5	60.0	0.1320	0.683 - 0.852	0.887 - 1.393	0.641	26937	7663
<input checked="" type="checkbox"/> 6	60.0	0.1537	0.557 - 0.785	0.887 - 1.366	0.705	29107	7710
<input checked="" type="checkbox"/> 7	60.0	0.0903	0.530 - 0.586	0.887 - 1.335	0.590	16573	6477
<input checked="" type="checkbox"/> 8	60.0	0.0996	0.567 - 0.716	0.887 - 1.212	0.602	17599	6811

Practical Example – SADABS Diagnostic Plots

best up to 1 Å



Run/Frame →
Scan 1, detector 2—theta 60.00°, II—$\langle I \rangle > 3.00\text{su}$ (red+, blue—), errors (black)



Practical Example – Comparison of different Integrations



	wrong ini	all runs	blend N	blend Y	best up to 1 Å
total no. of refl.	211518	271117	243739	247991	232456
unique refl.	74942	79101	78080	78706	78595
R(int) input	58.69	21.68	7.42	6.58	6.10
R(int) output	9.14	5.73	4.76	3.82	3.69
after rejection					
total no. of refl.	118509	241373	243201	247892	232405
% rejected	44.0	11.0	0.2	0.0	0.0
unique refl.	64729	73570	78074	78706	78595
% rejected	13.6	7.0	0.0	0.0	0.0