Screening Tab

The Screening tab in JBluIce-EPICS application is designed to accommodate automated screening of selected samples with limited or no human intervention. The Screening tab consists of various options to choose from and these are explained in detail.

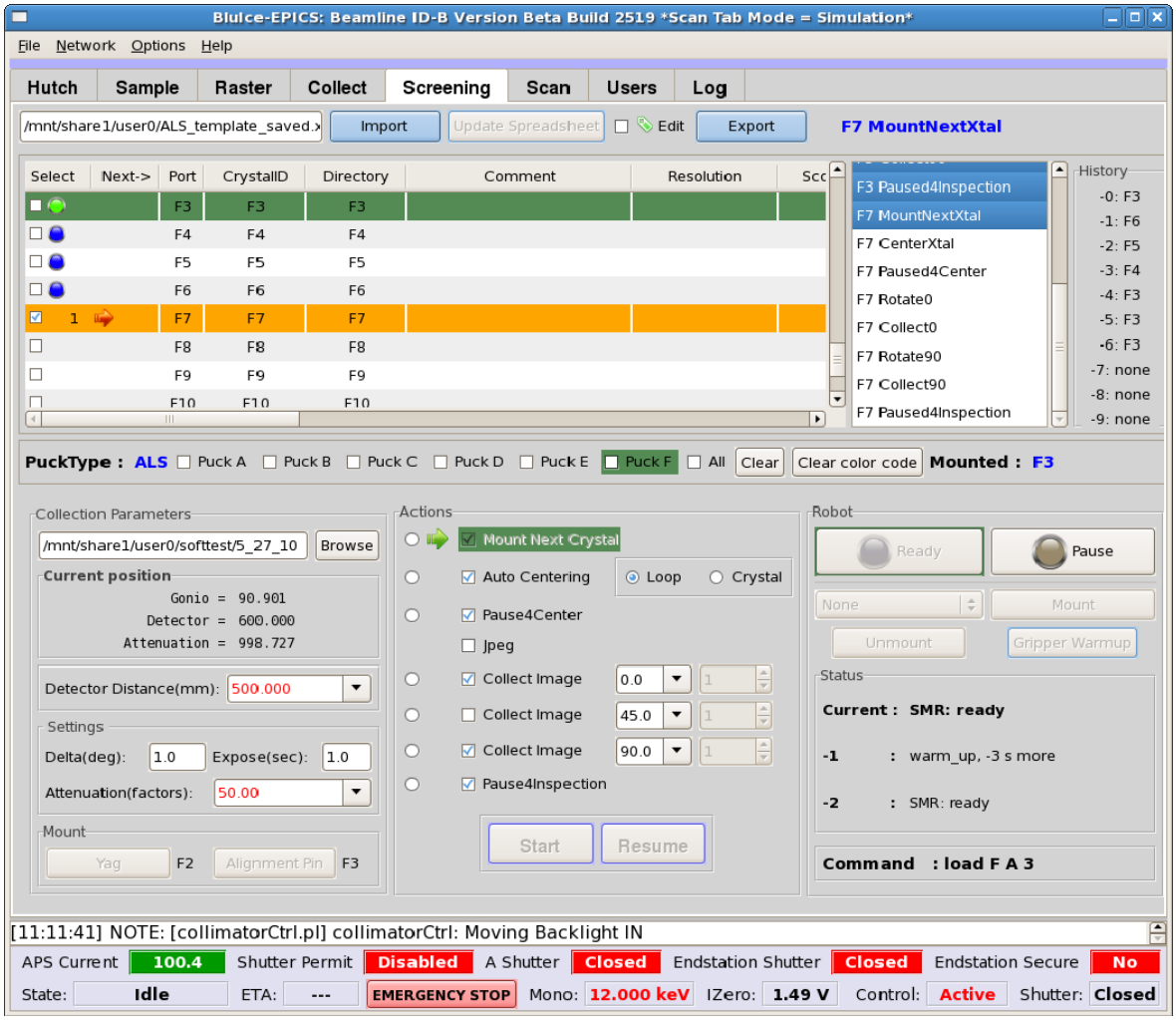


Fig 1: Screening tab in JBluIce-EPICS

Spreadsheet Instructions

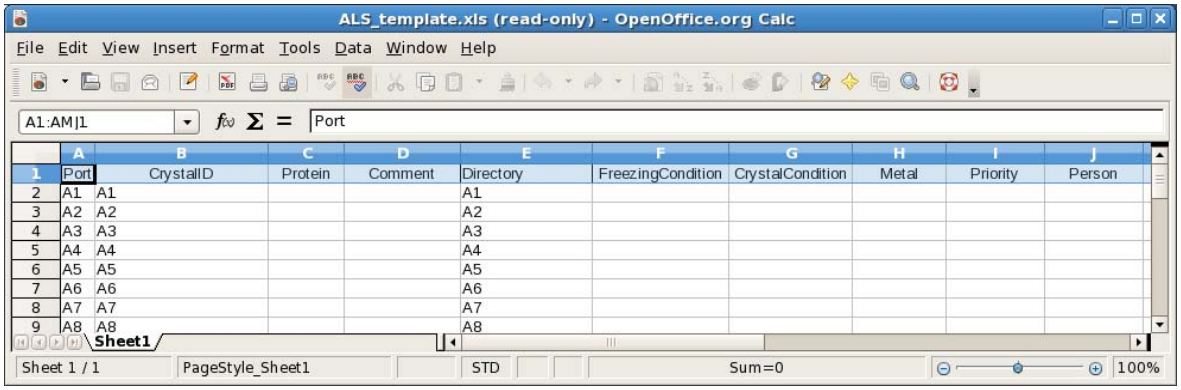
Screening in JBluIce-EPICS requires a Microsoft Excel Spreadsheet file to be loaded prior to using the automounter. Templates are available at the GM/CA CAT's website through the above link or in the user's home directory. The files are Rigaku_template.xls for Rigaku pucks and ALS_template.xls for ALS pucks or SSRL UniPucks respectively.

A typical spreadsheet is as shown in Fig 2. The ALS template consists of 96 rows while the Rigaku template consists of 72 rows. **Do not alter the number of rows in the spreadsheet** as this is used to determine the puck style that is loaded. Only three columns in the spreadsheet are essentially used by the screening system, namely, the Port, Crystal ID and the Directory (an explanation is given in the table). Other columns in the spreadsheet may either be populated with user information or left blank.

Port refers to a position in the puck. The robot will use this port to retrieve the sample. **Don't change this column**

CrystalID this label is used by the screening system to generate filenames. **A unique ID must be used for each sample.**

Directory If provided, this field will be used to generate subdirectories for each sample under the root screening directory. The default template Excel spreadsheet uses the **Port** as the subdirectory name.



	A	B	C	D	E	F	G	H	I	J
1	Port	CrystalID	Protein	Comment	Directory	FreezingCondition	CrystalCondition	Metal	Priority	Person
2	A1	A1			A1					
3	A2	A2			A2					
4	A3	A3			A3					
5	A4	A4			A4					
6	A5	A5			A5					
7	A6	A6			A6					
8	A7	A7			A7					
9	A8	A8			A8					

Fig. 2: A Typical spread sheet

Importing Spread Sheet

Fig. 3

A spreadsheet is loaded by clicking the “Import” button; it pops up a Webice login form (Fig. 4). Entering a password and hitting submit initiates the Webice software that can provide crystal scoring and data collection strategy. Detailed information on Webice is available at:

http://smb.slac.stanford.edu/facilities/remote_access/webice/

Users can proceed without initiating Webice by clicking on the Cancel button.

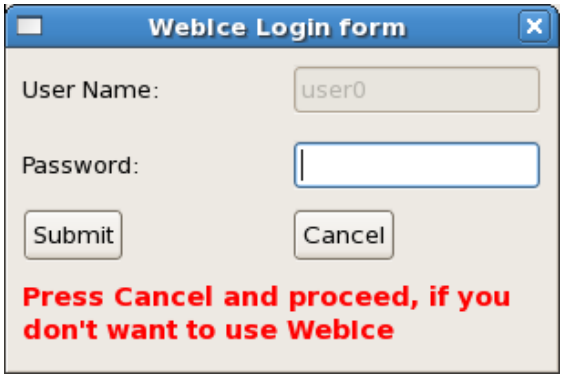


Fig. 4

In either case, you will be prompted to a window as shown in Fig. 5, for selecting the spreadsheet. Make sure that you are opening from your home directory and have the read/write permissions.

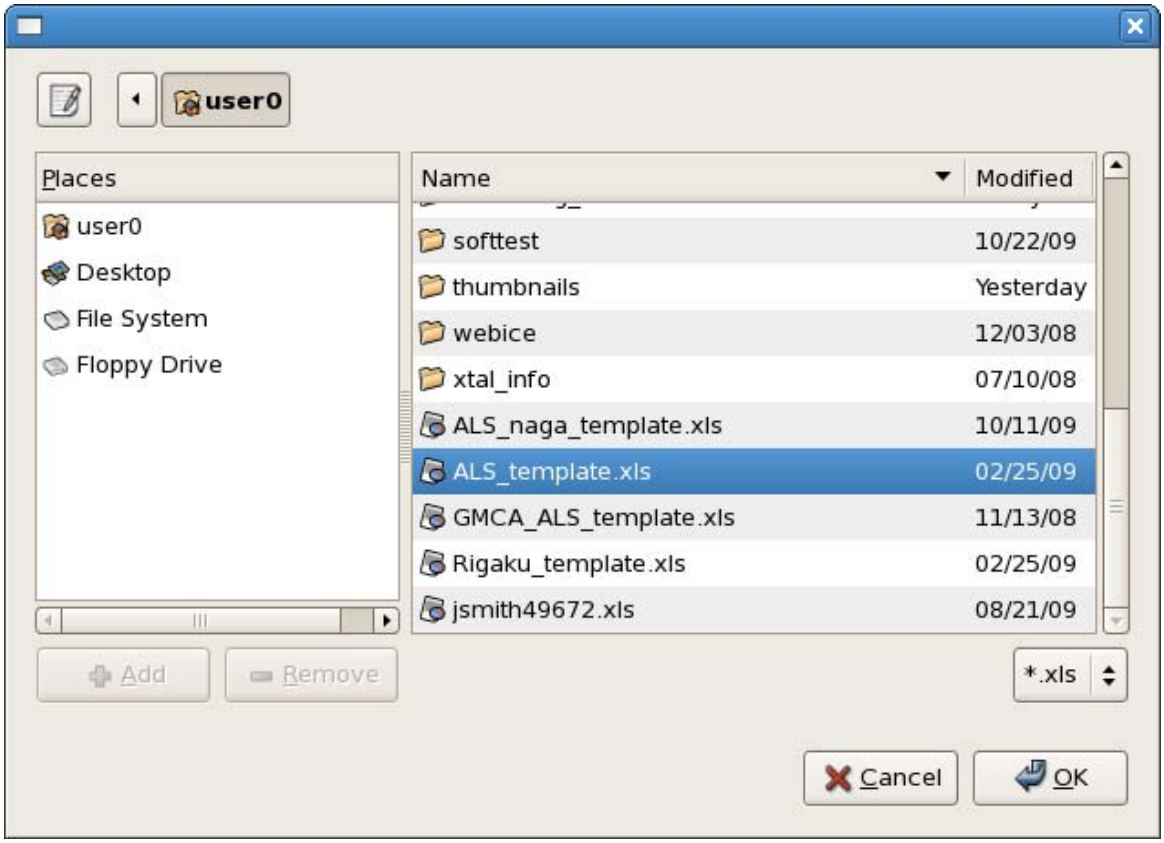
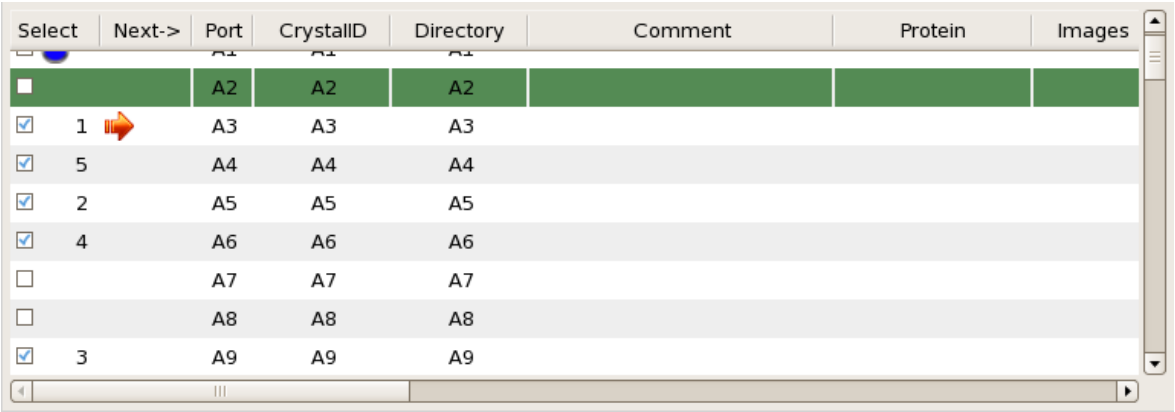


Fig. 5

Choosing samples for screening

Once the spreadsheet is loaded users can choose to mount the samples in any order. The order of clicking the check box determines the order of sample selection. A number appears next to the check box indicating the order in which the samples will be screened. For example, according to sample selection on Fig. 6, samples will be screened in the order A3, A5, A9, A6, and A4.



Select	Next->	Port	CrystalID	Directory	Comment	Protein	Images
☐		A2	A2	A2			
☑	1	A3	A3	A3			
☑	5	A4	A4	A4			
☑	2	A5	A5	A5			
☑	4	A6	A6	A6			
☐		A7	A7	A7			
☐		A8	A8	A8			
☑	3	A9	A9	A9			

Fig. 6

Editable Spreadsheet

	This symbol appears on the table columns when 'Edit' option selected, Those columns are editable

Certain columns could be edited after the spreadsheet has been imported. Checking the edit box highlights the columns editable in the loaded spreadsheet shown with the green ‘tag’ symbol. Modified and updated spreadsheet could be saved in the xls format by clicking on the “export” button. Screening spreadsheet also saves the edited content automatically, it is achieved in two different ways depending on whether Webice is invoked or not.

If Webice is invoked - every time a cell/row is edited it will post the information to Webice. The user has to click on “Update Spreadsheet” to get back both edited information as well as Webice information.

If Webice not invoked – Upon editing, the information is automatically saved in the file with extension "_saved.xls“. The user will have to import this saved file to see all the edits.

Upon clicking the “export” button, it pops up a window (Fig 7), to rename the file and to choose the directory to save. Also when ever the spreadsheet is edited the spreadsheet is saved into the home directory with extension “_saved.xls”. In the above example the name of the saved file is ALS_template_saved.xls

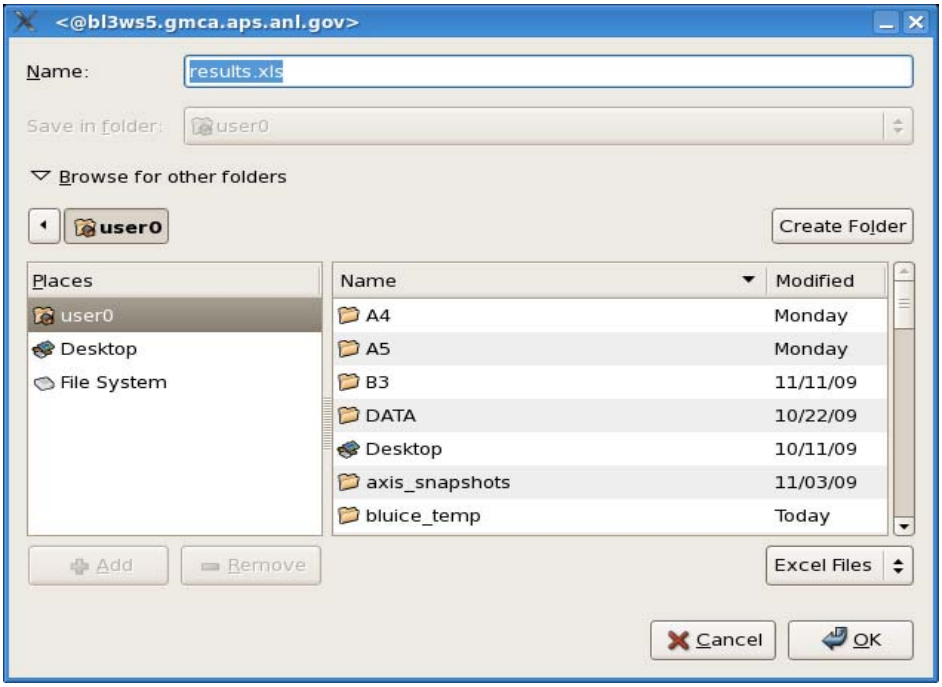


Fig. 7

Choosing a parent data directory and data collection parameters

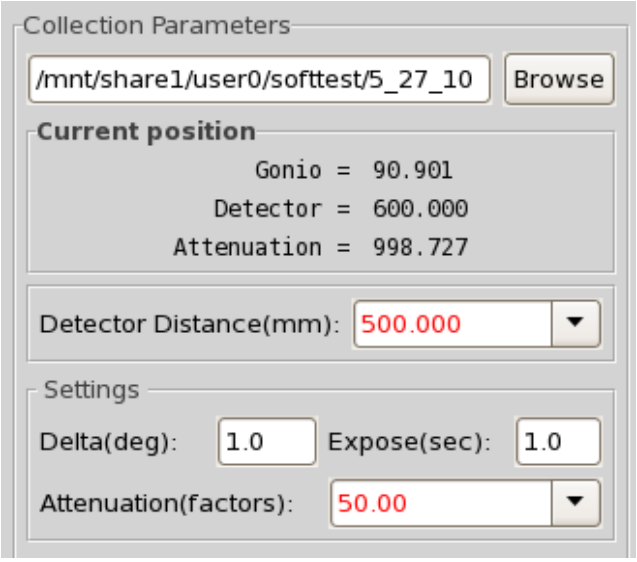


Fig. 8

Data collection directory could be chosen by having the appropriate path specified in directory field. By default the directory displayed will be the home directory for your username which in general is "/mnt/share#/user". The path chosen will be the parent data directory and the directory information specified in the spread sheet in the "Directory" column will become the subdirectory of this parent directory where the diffraction images will be saved. Data collection parameters such as Detector distance, Delta (oscillation angle), exposure time and Attenuation can be specified in the respective fields as shown in Fig 8.

Tasks to be performed on any given sample

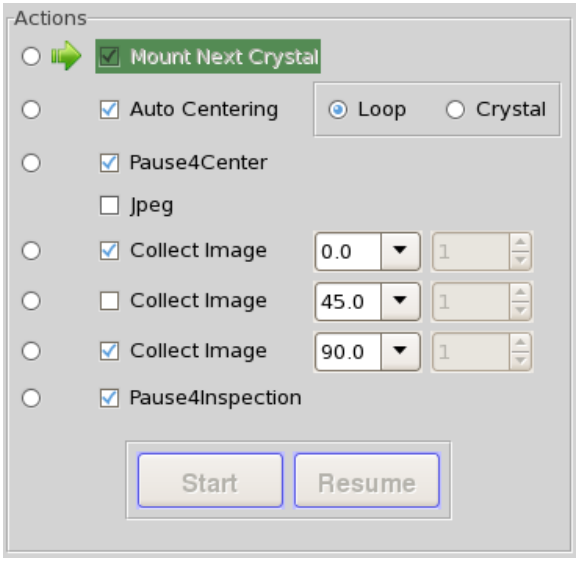


Fig. 9a

Fig 9b

As shown in Fig 9a, you could choose the tasks that you want the system to perform on any given sample. "Mount Next Crystal" is the default option. "Auto Center crystal" will use the software "XREC" to center the loop or the crystal (as chosen) in the beam. If you prefer to center the crystal yourself, you should de-select the "Auto Center" option and choose "Pause4center", this way the system will wait for the user to center the sample. Up to 3 diffraction images at desired angles could be collected. In addition to taking diffraction images, snapshots of the crystal (High-resolution camera only) at the desired angles are taken if 'Jpeg' option (Fig. 9a) is checked. A complete list of tasks that will be carried out for each sample can be seen as listed in Fig. 9b.

Fig. 10

The puck type indicator informs the user of the current Robot setup, if this is different from your puck type contact the support staff before you start anything. Warning: Puck type mismatch could cause severe damage to the automounter gripper. Puck type should show "ALS" for ALS/Unipuck style pucks and "Rigaku" for Rigaku (MSC) style pucks.

Choosing "pause4inspection" waits for the user to decide whether or not to move to the next crystal. Clicking "Resume" will mount the next crystal, if you want to continue on the mounted crystal then you have 2 options. a) If you want to collect data on the mounted crystal, go to the collect tab and set up for data collection. b) If you want to redo one or several tasks from the "Actions" task list just click on the left side of the task of interest (the green arrow will move to the task of interest) and hit "Resume", this will redo the selected task of interest and the subsequent checked tasks until it reaches "pause4inspection" again. This way you can recollect individual diffraction images with a new set of parameters than previously taken.

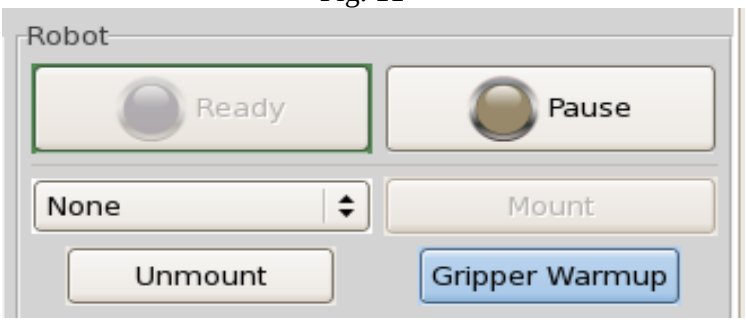
The users have the ability to modify the sequence of the tasks being done even while the system is in operation. So be careful in what you do.

Robot

Robot section indicates the current status of the Robot. The Robot will have to be in the "Ready" state to perform any action; the Ready button with green border indicates the robot is ready. The Robot switches to "Pause" state automatically if it encounters any Errors (ERR).

Manual options are available for users who do not wish to use the spreadsheet. The user can select the sample of interest from the drop down box shown in Fig 11 (showing "None" with up and down arrows) and click on mount button. Unmounting the sample is obviously done by clicking on the Unmount button. A manual gripper warm up can be performed by clicking on the Gripper warm-up button.

Fig. 11



Automounter Status

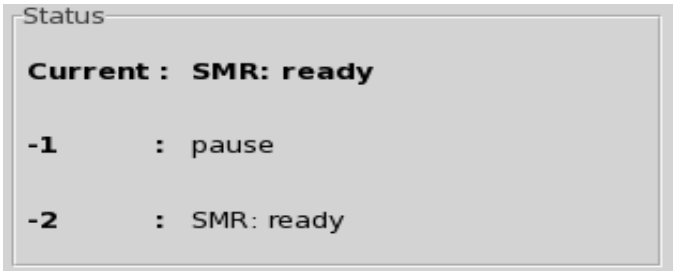


Fig. 12

Current automounter task and the previous two tasks of the Automounter are displayed in the Screening tab for the benefit of the users. Current status according to the example shown in Fig 12 is that the gripper is getting warmed up and the warm up cycle has 3 seconds more. The -1 and -2 are the two previous tasks. The following error status will be seen if the automounter encounters any problems, as mentioned earlier the Robot will in "Pause" state when this happens. Explanation on the automounter errors will be handled in the later part of the manual. .

Fig. 13

Mounted History

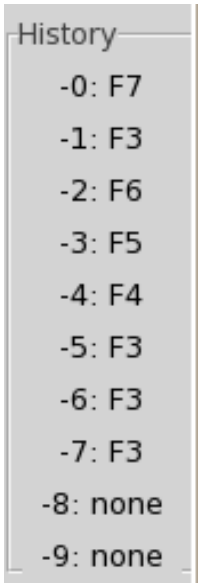


Fig. 14

Mount history of the past 10 mounts are shown for the benefit of the users. -0 represents the last mounted sample.

Mount YAG and Alignment pins

Separate buttons are available for easy mounting of YAG and alignment pin placed inside the Dewar. YAG crystal is used for the alignment of the beam and the alignment pin is used for correcting the center of rotation of the goniometer. The positions of these are predetermined by the Staff.

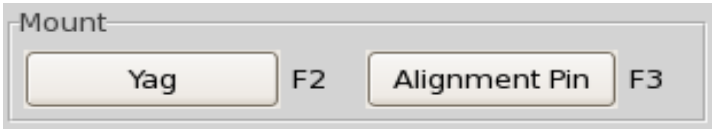


Fig. 15

Sample Screening

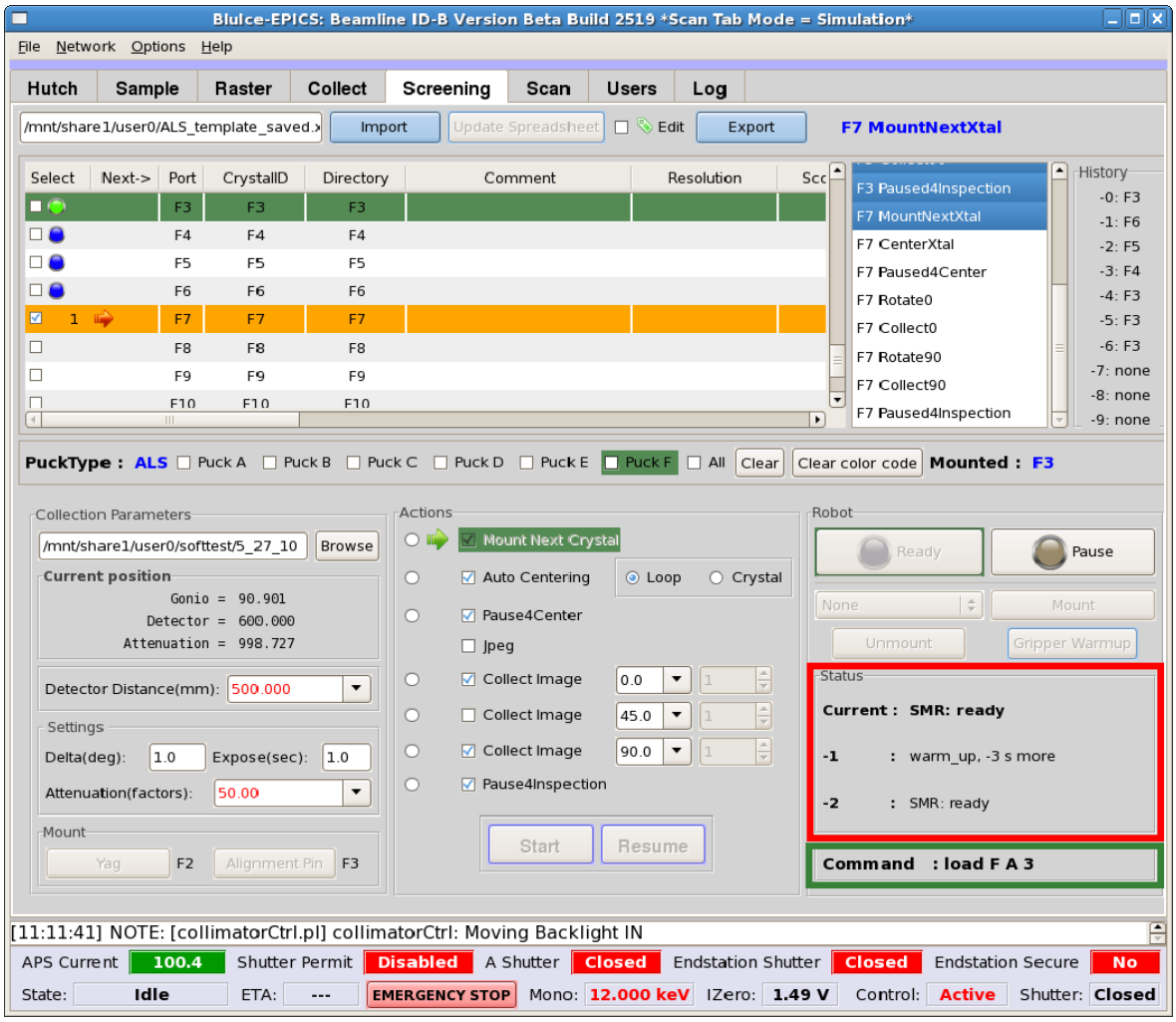


Fig. 17

Choose the samples to be screened, choose the tasks, screening is initiated by clicking on the "Start" button. Automounter status will give you information on the current task performed by the automounter (area within red border of Fig 17). The current sample mounted will be highlighted in green (Fig 17) on the spreadsheet. The current screening task being performed will be highlighted in green in the task list (Fig 17). If "pause4center" or "pause4inspection" have been chosen, the system will wait for user intervention with the "Resume" button. A yellow bar in the spread sheet means that sample has been chosen to be mounted next and the command line also has "load ##" (area within green border of Fig 17). As shown in the figure 17 the present sample mounted is A4 (green background on the spread sheet, sample status mounted: A4).

Color codes are assigned to screened samples and the following table explains the meaning of the color code associated with a sample.

	Red symbol indicates robot tries to mount the sample and failed
	Blue symbol indicates sample successfully mounted and proceeded to next sample with out collecting

	Green symbol indicates sample successfully mounted and collected two or more images

Several sets of images can be collected on a certain mounted sample. While the automounter is awaiting user input during “pause4center” or “pause4inspection”, it is possible to recollect diffraction images on this sample by moving the arrow mark to the task of interest and clicking on the 'Resume' button (in the action window). The sets are named according to the order of collection. Ex : First set of images will be named test_1_0.####, second set image named test_2_0.####.

Robot Errors

Any time a Robot error occurs, the automounter will switch to the PAUSE state with error message displayed in the Robot status area (marked with red border in fig. 18). Error messages appear in red, ex:. ERR:recover:pin@gonio. When communicating with your host, report the status or problems with the robot by reading these messages. You or your host will then be able to focus in and resolve the problem.

Common Problems and Solutions:

1) Problem: The robot stops working and goes to pause.
Solution: Try switching from Pause to Ready by pressing the Ready button. Often times this resolves simple problems.

2) Problem: Robot consistently has problems in mounting or dismounting the bases into the Dewar.
Solution: Inform your host of this problem. You could also check to see if the pucks were loaded correctly and that you are using the correct pin bases.

3) Problem: Gripper repeatedly fails to unmount the sample on the Goniostat.
Solution: Contact host and notify him of this problem. The host might be able to solve this problem by adjusting the gripper warm-up parameters.

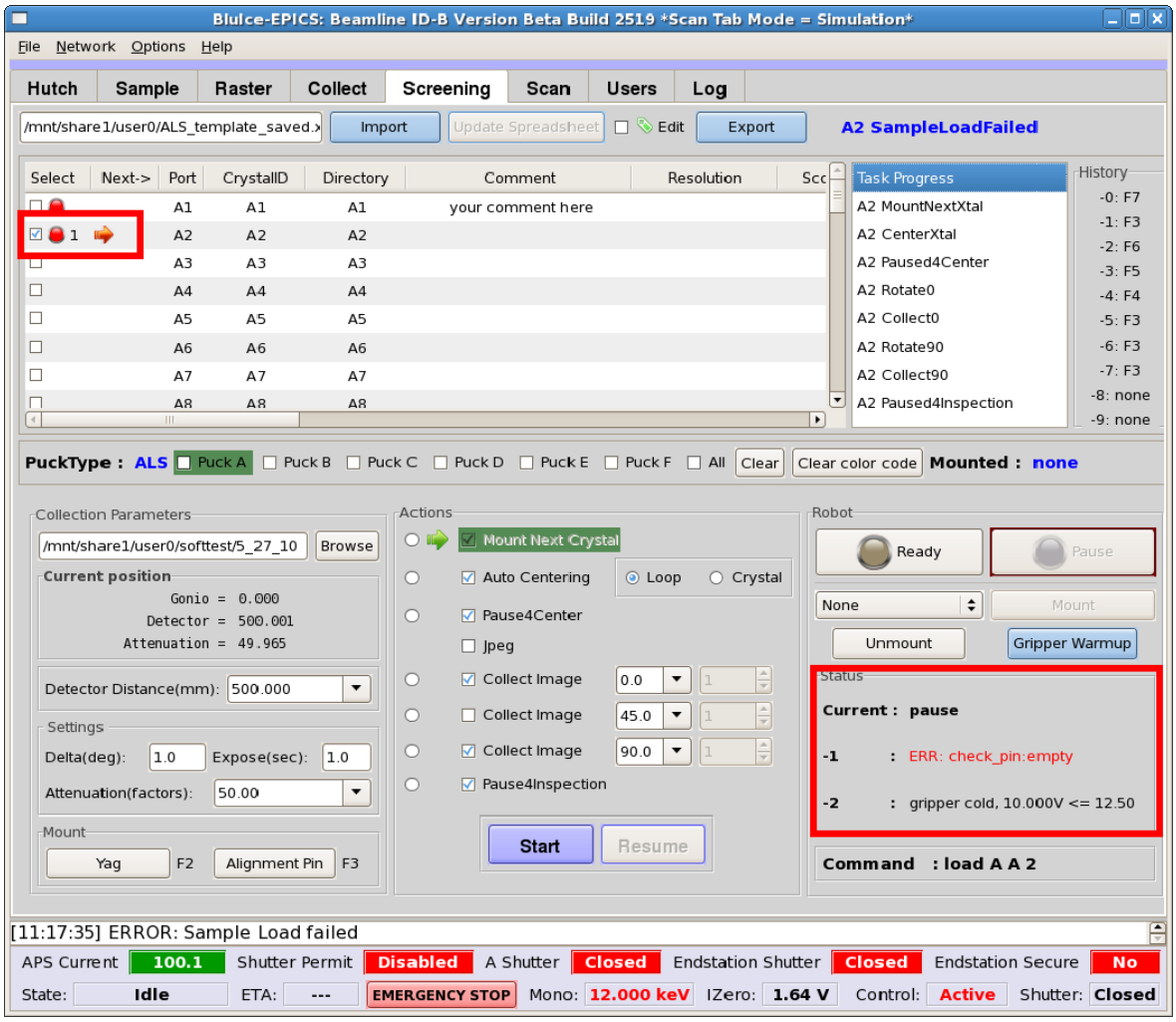


Fig 18

Webice

Screening Tab is integrated with Webice (Crystal scoring/Data collection strategy). The software queries for a password (same as user password) on hitting the 'Import' button, given the correct password Webice is authenticated. After the successful data collection of 2 diffraction images which are apart by at least 5 degrees, Webice autoindexes and calculates parameters like cell, mosaicity, predicted resolution, crystal score, etc. The Webice information is updated to the screening spreadsheet on clicking the "**update spreadsheet**" button. Detailed information on Webice is available at http://smb.slac.stanford.edu/facilities/remote_access/webice/

The edited information and Webice results can be exported to an Excel file by clicking on 'Export' Button