

Data Collection at SSRL: practical aspects



How Do I Become an SSRL User?

<http://smb.slac.stanford.edu/public/forms/becominguser/>

1. Submit a Proposal:

Standard General Use Proposals

- Single experiment or Program proposal
- Proposal deadlines are set for April 1, July 1 and December 1 of each year.
- Applications are reviewed for scientific merit and rated on a scale of 1 – 5.
- Proposals are eligible for beam time for a two-year period.
- http://www-ssrl.slac.stanford.edu/users/user_admin/px_proposal_guide.html

Rapid Access Proposals

- Normally ~5-8 shifts are reserved each scheduling period for Rapid Access time.
- Applications are reviewed for scientific merit and feasibility within 1 month
- The highest ranked proposal will be granted some or all of the shifts held in reserve.
- Other high ranking proposals are given consideration when cancellations occur.
- http://smb.slac.stanford.edu/forms/beamtime/rapid_access.html

How Do I Become an SSRL User?

2. Become a Participating Research Team

Though many of SSRL's beam lines are primarily devoted to general use access, several institutions have set up Participating Research Team agreements. For more information regarding macromolecular crystallography PRTs, contact Mike Soltis (soltis@slac.stanford.edu).

3. Collaborate with the SSRL Scientific Staff

If you are interested in establishing a collaboration with a member of the SSRL staff, have an unusual experimental set-up, or have inexperienced group members who need training, contact Mike Soltis (soltis@slac.stanford.edu).

A successful proposal

- A successful proposal has three components:
 1. **Important structural target/s, and/or a novel and useful experiment**
 2. **Sound justification of the need for synchrotron time**
 3. **Experience and previous results (can you carry out the experiment)**
- Make your proposal strong by balancing all three components
- Contact support staff beforehand for advice if you have any questions
- Make a reasonable estimate of time and determine the appropriate beamlines that could be used.

<http://smb.slac.stanford.edu/>

How much time does it take to screen, how much time does it take to collect data, how many samples do you have then ask for one shift extra?

- Look at other successful proposals if you can.

Justifications for synchrotron time

Some examples include:

- An energy (wavelength) not available in the home lab. Required for MAD/SAD experiments.
- Increased intensity to push the resolution limit. What resolution do you have, why do you need to extend it further? What question cannot be answered at the current resolution?
- The ability to resolve longer unit cells. What can the system at home resolve, what can you expect to resolve at the synchrotron? Look into the beamline instrumentation, do a quick calculation.
- In the robotic case, study many samples much faster than at home. What percentage of crystals provide good diffraction, how many do you need to screen efficiently? What time would that take at home.
- Does the experiment requires many measurements in a rapid as possible time?

Beam Time Requests

- Spokespersons with active proposals are notified via email to submit a request
- New beam time requests are required three times a year
- Beam time requests are due two months in advance each scheduling period
- Beam time request form:
http://smb.slac.stanford.edu/public/forms/beamtime/biobtrf_12-05.html
- For remote access: check that you “**want to collect data remotely**”

Other Paperwork:

A Use Agreement must be completed and turned in before your beamtime

http://www-ssrl.slac.stanford.edu/users/user_admin/useagreementmenu.html

New users are required to sign and submit the SSRL Computer Agreement Form:

<http://smb.slac.stanford.edu/public/facilities/computing/#Accounts>

Once you get beamtime



- Preparation



- Mounting



- Filling the cassette or puck



- Shipping
- Screening
- Planning
- Data collection
- Data backup

Beam Time Preparation

1. Read Online Documentation

User Guide: http://smb.slac.stanford.edu/public/users_guide/index.shtml

Blu-ice Manual: <http://smb.slac.stanford.edu/facilities/software/blu-ice/>

2. Acquire a Cassette Loading Kit or some Uni-pucks

available from: <http://www.crystalpositioningsystems.com/>

3. Acquire a Dry Shipping Dewar

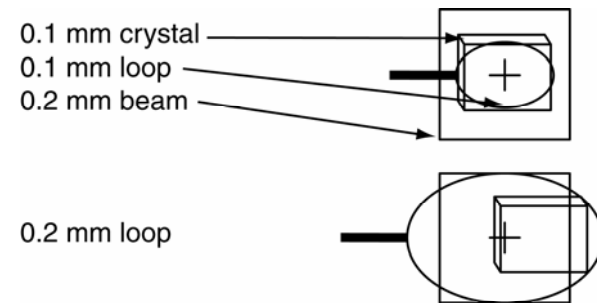
Dewars that fit cassettes: MVE model SC 4/2V (recommended), Taylor Wharton CP100 or CX100, or International Cryogenics IC-7VS

4. Make sure you have plenty of loops and pins

available from: <http://www.hamptonresearch.com/>

Preparing pins

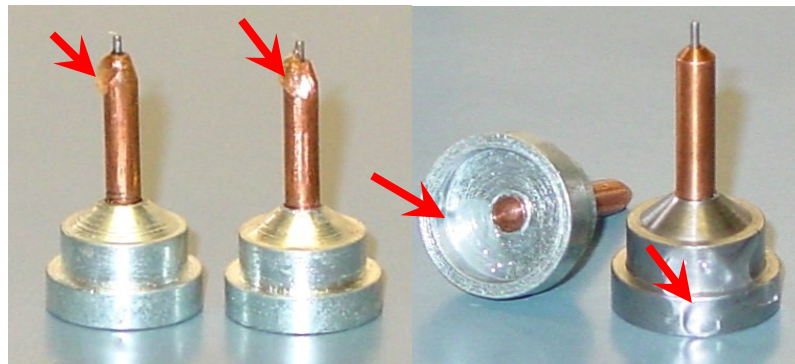
- Prepare a selection of pins and loops to suit crystal sizes – use loops roughly the same size as the crystal
 - Critical if using the robot for automated screening
 - At SSRL, automatic loop centering just does that, centers on the loop
 - If your crystal fills the loop, you will always hit it
 - BUT if it is much smaller than the loop, you could easily miss it



Preparing pins

- Prepare a selection of pins and loops to suit crystal sizes – use loops roughly the same size as the crystal
 - Glue the loop in the pin, 5 minute epoxy on the bottom of the loop holder to be inserted into the pin works well. Avoid getting epoxy on the outside of the copper mount.
 - Check the loop under a calibrated microscope, make sure it is intact then write the size on the magnetic base.

EXCESS GLUE OR GREASE



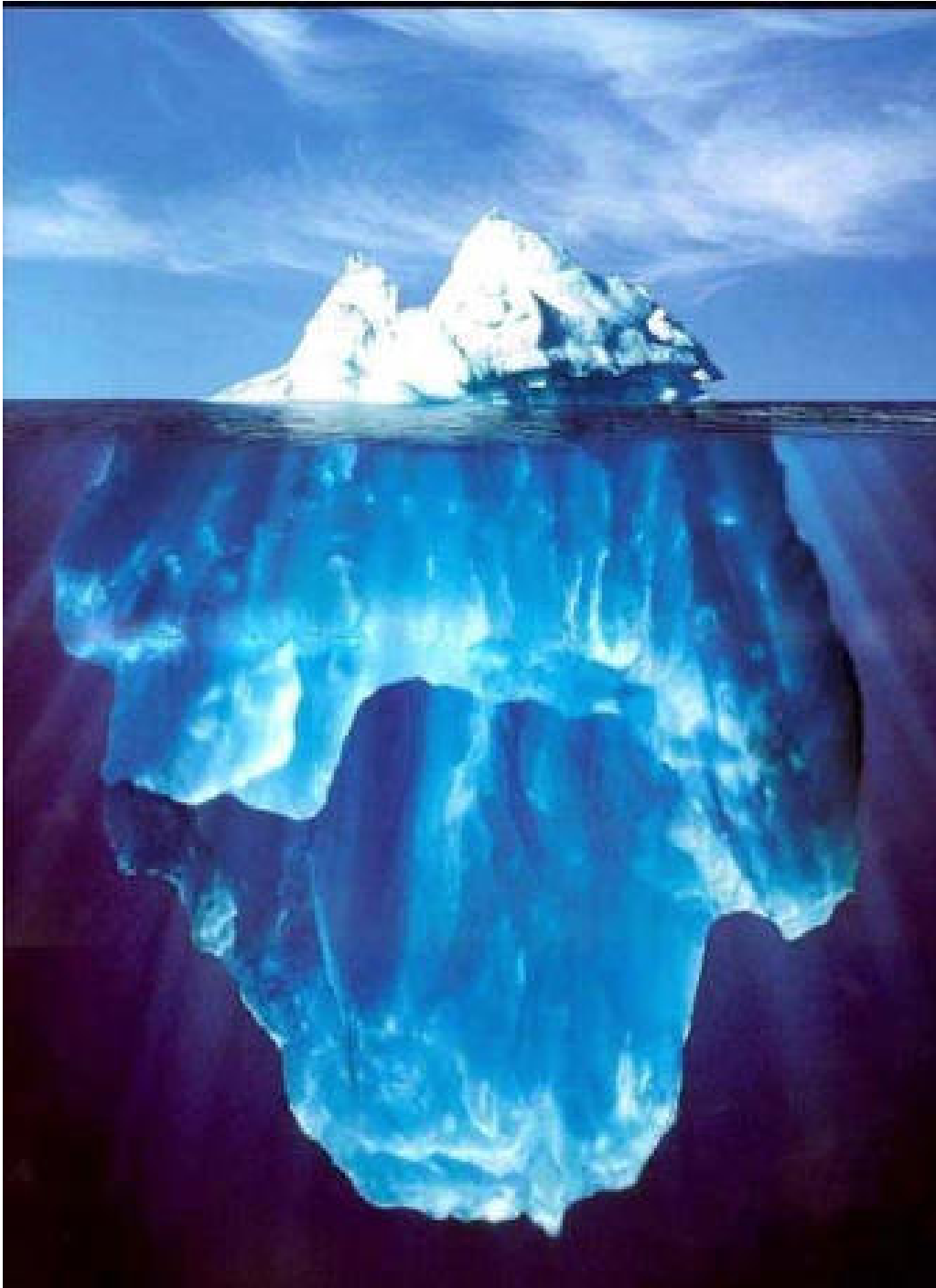
Cassette/puck filling

Don't procrastinate – Do not wait until the night before your shipping deadline to load all your samples! Crystals are perfectly happy to sit in the cassettes or pucks for several days to weeks.

- Note the cassette or puck number and the order to be used.
- Check the ports in the cassette or puck. Loops can break off and remain inside the port – this will cause problems with the robot.



- Each cassette contains 96 crystals and each puck holds 16. If several people are filling, the result could only be as good as the worst skilled. Training of inexperienced people with the cassettes, pucks, transfer tools and loading tools is probably a good thing!



The number
one practical
filling tip:

Ice is the Enemy!

**Filling should be done
as rapidly as possible.**

Ice is the Enemy!

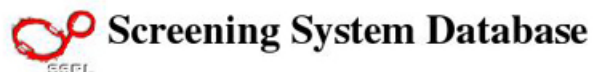
- **Make sure the nitrogen level is maintained.**
- The blue lid covers the filling reservoir, it does not prevent boil off of the liquid nitrogen.
- Try to load in a fume hood – this helps prevent ice buildup.
- If floating ice appears, put the cassette/puck in the full shipping Dewar, empty and dry the reservoir and then replace the nitrogen.
- If in doubt, use fresh nitrogen.
- If frost appears on the cassette/puck wash it by pouring liquid nitrogen over it.

- **Do not leave for a prolonged period, nitrogen boils off fast.**
- Use two tool sets if you have them. Dry one set as you use the other set. Swap over every 4 crystals or sooner if needed.
 - Ice on the end of the tool can cause the pin to stick to the tool.
 - Ice in the guide tool can cause the crystal to hit the cassette edge.
- Wash the cassettes/pucks in liquid nitrogen if necessary to remove ice prior to putting them in the shipping Dewar.

Keep track of your crystals as you load your cassette or puck.

Use the SSRL template excel files.

<https://smb.slac.stanford.edu/crystals/>



User name:

Change the [Login](#) if your user name does not appear above.

Create New Entry:

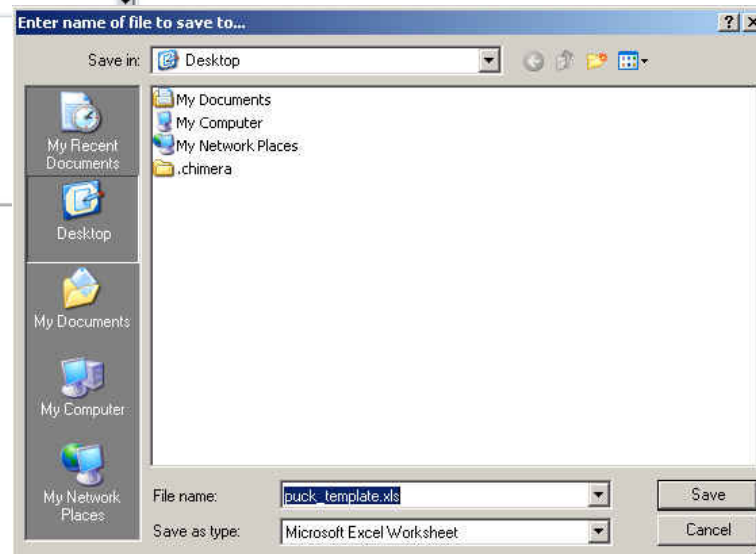
Cassettes 1 - 1 of 1 [start | prev | next | last]

Excel Spreadsheet	Cassette Pin	Possible Actions	Beamline
199 default.xls 2004-04-29 15:19:56 null		View/Edit Download Results Download Excel Delete	None

Download [SSRL cassette template](#) or [Puck adapter template](#)

For more information see the [Online Help](#).

Here is a page with all SMB [Beamlines](#).



Dewar shipping

Carefully Read and Follow the dewar shipping directions.

Remote Users are required to fill-out and follow the procedures described on our online dewar shipping form:

<http://smb.slac.stanford.edu/public/forms/shipping/DewarToSSRL.html>

After filling out the online form you should save the .pdf file that is created. This file contains shipping labels and a return shipping form.

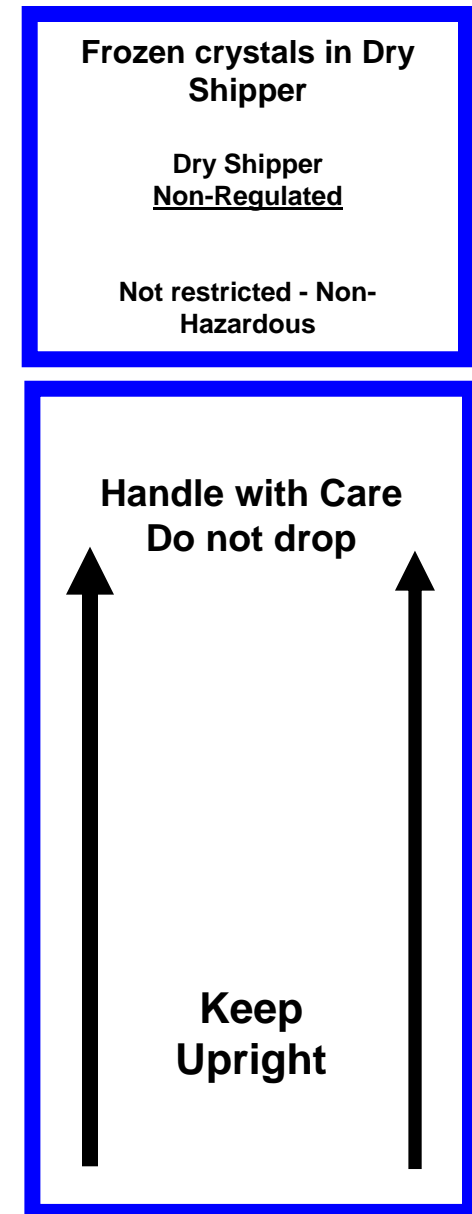
1. Attach a shipping label to each dewar.
2. Include a return shipping form inside the dewar.

If the online shipping form is used:

- You will be notified via email when your dewar arrives to SSRL
- Your dewar will be delivered to the beam line.
- If requested, your dewar will be filled with liquid nitrogen

Shipping Dry (magic words)

- To avoid delays in shipping your Dewar (shipping dry) should have a label with the magic words “**Non-regulated**”, “**Not-restricted**” and “**Non-Hazardous**”.
- Any label signifying liquid nitrogen should be **removed** if shipping dry.
- Ship to arrive at least a day in advance of the beamtime and arrange to have the Dewar filled on arrival.
- Shipments at SSRL are **not** accepted over the weekend so if your beamtime starts Monday aim to have the Dewar arrive on the Friday.



Final things before you arrive

Support Staff. Lookup the schedule for your support staff scientist.

This is your contact person.

http://smb.slac.stanford.edu/schedule/sch_staff.cgi

Email your friendly user-support staff person. Ensure they have your phone number and email address.

Jul 2006	1_5	11_1	11_3	7_1	9_1	9_2	Support Staff	
Sat 1	9b01-a.deacon	TD 7a78-s.tsai	TD 8851-m.toney	faci		1b52-e.snell	TD 1b57-n.horton	AC Aina Cohen
Sun 2		TD 9b01-a.deacon	TD 8851-m.toney	faci		1b52-e.snell	TD 1b57-n.horton	AD Ashley Deacon
Mon 3		AG 9a07-c.stout	GC 8851-m.toney	faci		1b29-p.pathuri	TD 9a65-k.zhang	AG Ana Gonzalez
Tue 4		AG 9a07-c.stout	GC 8851-m.toney	faci		1b29-p.pathuri	TD 9a40-a.villasenor	CS Clyde Smith
Wed 5	8837-a.cohen	AG 9a10-e.saphire	IM 8851-m.toney	faci		9a75-t.stout	TD 9a85-d.bussiere	CS Graeme Card
Thr 6	8054-m.soltis	AG 9a53-r.kornberg	GC 8851-m.toney	faci		1b16-h.noller	TD 1b16-h.noller	CS Irimpan Mathews (Mathews)
Fri 7	9b01-a.deacon	AG 9a53-k.garcia	GC	faci		1b28-j.vey	TD 1b28-j.vey	CS Mitch Miller
Sat 8	9b01-a.deacon	CS 9a52-a.brunger	CS	faci		1b28-j.vey	CS 1b28-j.vey	CS Mike Soltis
Sun 9		CS supr	CS	faci		1b28-j.vey	CS 1b28-j.vey	CS Pete Dunten
Mon 10	ma	AC ma	IM ma	faci		ma	PD ma	PD Tzanko Doukov
Tue 11	ap	AC ap	IM ap	faci		ap	PD ap	PD No Support
Wed 12	9b01-a.deacon	AC 9a01-i.wilson	GC	faci		1b50-e.bergmann	PD 8045-a.gonzalez	PD No Operation
Thr 13	9b01-a.deacon	AC 9a06-p.schummel	IM	faci		1b50-e.bergmann	PD 1b30-r.liddington	PD
Fri 14	9b01-a.deacon	AC 1b02-d.barondeau	IM	faci		1b25-e.pozharskiy	PD 1b23-s.turley	PD
Sat 15		GC 1b02-d.barondeau	GC	faci		1b25-e.pozharskiy	GC 1b23-s.turley	GC
Sun 16		GC 9b01-a.deacon	GC	faci		1b25-e.pozharskiy	GC 7a30-d.mckay	GC
Mon 17	1b00-w.scott	PD 9b01-a.deacon	IM	faci		9a85-d.bussiere	TD 9a65-k.zhang	GC
Tue 18	1b39-a.rosengarth	PD 9a53-k.garcia	IM 2899	faci		9a40-a.villasenor	TD 9a75-t.stout	GC
Wed 19	1b39-a.rosengarth	PD 9a02-g.chang	IM 2899	faci		9a97-m.malkowski	TD 7a27-d.rees	GC
Thr 20	1b39-a.rosengarth	PD 9a53-r.kornberg	IM 2899	faci		9a97-m.malkowski	TD 9a11-k.nettles	GC
Fri 21	1b63-c.raman	PD 1b63-c.raman	IM 2899	faci		7a90-e.baldwin	TD 7a59-e.baker	GC
Sat 22	1b63-c.raman	GC 1b63-c.raman	GC 2899	faci		7a90-e.baldwin	GC 7a59-e.baker	GC
Sun 23	1b63-c.raman	GC 1b63-c.raman	GC 2899	faci		7a90-e.baldwin	GC 7a59-e.baker	GC
Mon 24	ap	TD ap	CS ap	faci		ap	TD ap	GC
Tue 25	ap	TD ap	CS ap	faci		ap	TD ap	GC
Wed 26	7a70-m.hanson	TD 7a50-c.eigenbrot	CS 8051-m.toney	faci		1b43-c.stout	TD 7a83-s.choe	GC
Thr 27	9b01-a.deacon	TD 9a57-m.maduke	CS 8051-m.toney	faci		1b62-d.wilson	TD 1b61-m.murphy	GC
Fri 28	9b01-a.deacon	TD 9a05-e.getzoff	CS 8051-m.toney	faci		1b46	TD 1b59-s.roberts	GC
Sat 29	1b43-c.stout	CS 9a05-e.getzoff	CS 8051-m.toney	faci		1b46	CS 1b59-s.roberts	GC
Sun 30	1b43-c.stout	CS 9b01-a.deacon	CS 8051-m.toney	faci		1b46	CS 7a54-d.bushnell	GC
Mon 31	8054-m.soltis	GC 9a03-r.stevens	PD 2899	faci		7a73-l.brmen	TD 9a75-t.stout	GC

If you plan to use the remote access facilities:

Install the NX client software on your data collection computer

www.nomachine.com/download.php

Contact your support scientist to arrange to test your NX connection and the **Blu-Ice** software before you beamtime.

The screenshot shows the NoMachine website's download page. At the top, there is a navigation menu with links for Products, Download, Support, Customers, Developers, Partners, Store, and Home. The main content area features a large 'Download' section with the text 'Get NX software from NoMachine' and a sub-section for 'Screenshots'. Below this, there is a 'TestDrive' section with a 'Test Drive' button. On the left side, there are three product categories: 'NX Free Edition' (with links for Linux and Solaris), 'NX Server' (with links for Linux and Solaris), and 'NX Node'. On the right side, there is a 'Technology Brief' section with links for 'Windows file sharing support' and 'Data encryption and security'.

The screenshot shows the Blu-Ice software interface for BLI-5. The window title is 'NX - imathew@smblx2.slac.stanford.edu:1097 - web'. The interface is divided into several sections. At the top, there is a menu bar with options: Hutch, Collect, Screening, Scan, Users, and Setup. Below the menu bar, there is a 'Cassette' dropdown menu set to 'left: cassette_0215_10_20_2004'. To the right of the cassette menu are buttons for 'Update', 'Load File', and 'Web'. The main area contains a table with columns for 'Port', 'ID', 'Protein', and 'Comment'. The table lists 13 rows of data, with the first row being 'Mount Next' and the second row being 'A1 test'. Below the table, there is a 'Screening Status' section with a 'Begin' button and a 'Screening done' indicator. To the right of the 'Begin' button is a 'Rotate by' dialog box with fields for 'Delta: 1.000' and 'Time: 30.000'. Below the 'Begin' button are buttons for 'Start', 'Stop', 'Disrupt', 'Reset', and 'Abort'. At the bottom of the interface, there is a 'Crystal selection OK' section with a 'Sample' dropdown menu and a 'Hutch' dropdown menu. Below these are buttons for 'Select Zoom Level' (Low, Med, High), 'Move Sample', and 'Rotate Phi' (-50, +50, +180). At the very bottom, there is a status bar with 'Idle', 'Hutch: open', 'Abort', 'Energy: 12657.695 eV', 'Network: Active', 'Shutter: closed', and '04:24:37 PM'.

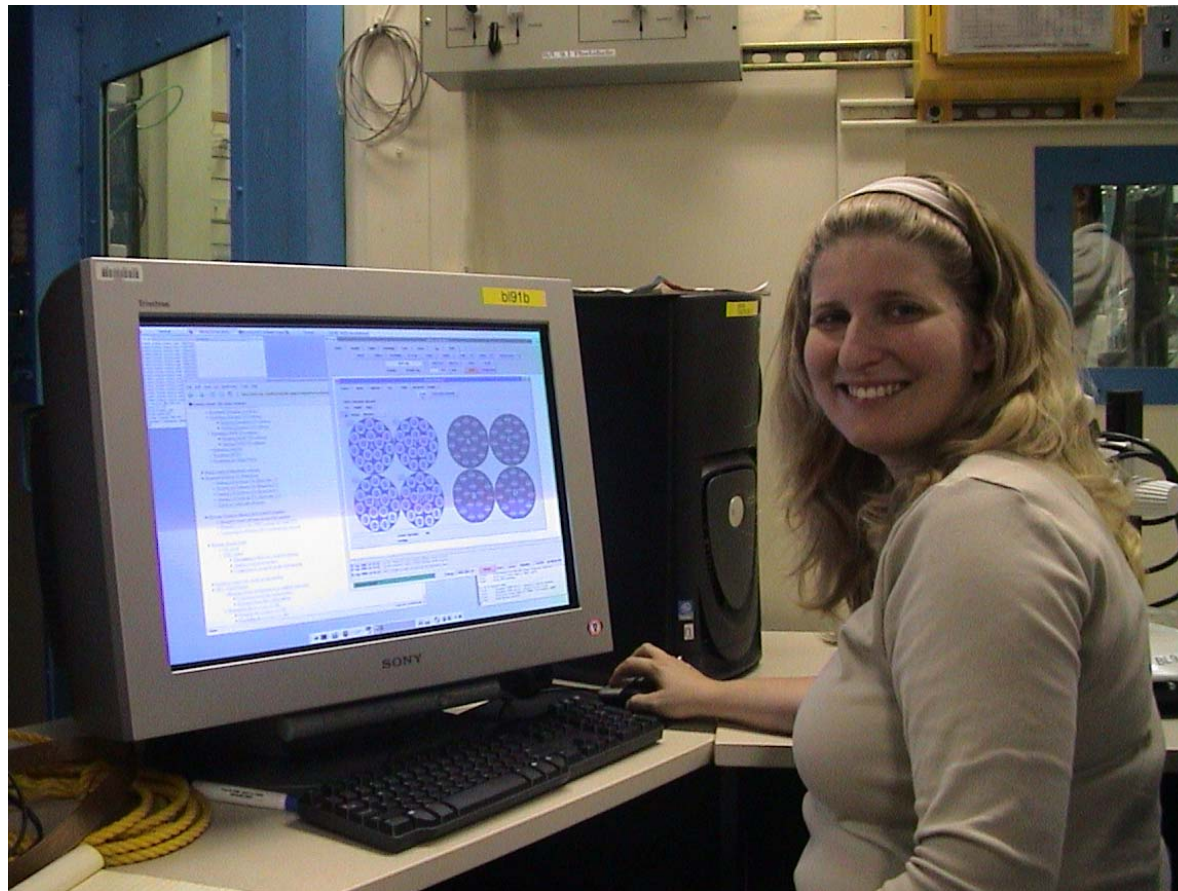
During your beam time

Support Staff will load your cassettes or pucks into the robot dewar. If you are present onsite, you can be shown how to do this for yourself.



Probing your pucks

Support Staff will then probe your cassette or puck with the robot to check for port jams.



Probing your pucks

The screenshot shows the Robot Control software interface. The main window displays a 4x2 grid of pucks labeled A, B, C, and D. Each puck is represented by a circular diagram with a grid of points. The status bar at the bottom indicates "Current Operation: robot_config probe" and "warning:". The log window at the bottom left shows the following text:

```
22 Sep 2006 14:40:23 server reports: port status change event called
22 Sep 2006 14:40:28 server reports: port status change event called
22 Sep 2006 14:40:32 server reports: port status change event called
```

The status bar also shows "Detector Ready", "Energy: 12647.850 eV", "Abort", "User: Active", "Shutter: closed", and "02:40:25 PM".

The screenshot shows the Robot Control software interface. The main window displays a 4x2 grid of pucks labeled A, B, C, and D. Each puck is represented by a circular diagram with a grid of points. The status bar at the bottom indicates "Current Operation: idle" and "warning:". The log window at the bottom left shows the following text:

```
22 Sep 2006 14:49:33 server reports: current event id 0
22 Sep 2006 14:49:33 Bluice reports: SII 4767 2
22 Sep 2006 14:49:33 server reports: SII 4767 2
```

The status bar also shows "Detector Ready", "Energy: 12647.850 eV", "Abort", "User: Active", "Shutter: closed", and "02:30:41 PM".

Beginning your screening

Your pucks can be viewed in the **Sample** Tab in **Blu-Ice**. You can also mount crystals from this tab.



If you want to use the robot to screen the crystals automatically, you need to assign a spreadsheet to the correct beamline

Screening System Database

User name:

Change the [Login](#) if your user name does not appear above.

Create New Entry:

Excel Spreadsheet	Cassette Pin	Possible Actions	Beamline
199 default.xls 2004-04-29 15:19:56	null	View/Edit Download Results Download Excel Delete	None
4767 puck_template.xls 2006-09-22 14:45:12	unknown_pin	View/Edit Download Results Download Excel Delete	BL9-1 right

Download [SSRL cassette template](#) or [Puck adapter template](#)

For more information see the [Online Help](#).

Here is a page with all SMB [Beamlines](#).

Beginning your screening

The screenshot displays the Blu-Ice 4.5 for BL9-1 software interface. The main window is titled "Blu-Ice 4.5 for BL9-1" and features a menu bar with options: Hutch, Sample, Collect, Screening, Scan, Users, Log, Staff. Below the menu bar, there are buttons for "Web", "Import", "Export", "Edit", and a dropdown for "Strategy(just_moun)".

The central part of the interface is a table listing samples. The columns are: View, Custor, Port, Containe, CrystallID, Protein, Comment, and SystemWarning. The table contains 17 rows of data, with row 41 highlighted in pink and row 42 in green. Row 41 is labeled "Mounted->" and row 42 is labeled "Mount Next->".

Below the table, there are control panels for "Sample", "Hutch", "Robot", and "Panel". The "Sample" panel includes "Select Zoom Level" (Low, Med, High), "Move Sample" (directional arrows), "Rotate Phi" (-90, +90, +180), and "Center Loop". The "Hutch" panel includes "Sample Lights Control" (Back Light, Turn Off) and "Side Light Intensity".

On the right side, there is a "Directory" field (set to /data/blct), a "Detector" dropdown (set to binned), and a list of tasks with checkboxes: Mount Next Crystal, Loop Alignment, Stop, Collect Image, Collect Image, Collect Image, Stop. Below this are buttons for "Start", "Stop", "Dismount", and "Reset Parameters".

The "Screening Tasks" panel shows a list of tasks for C10, C11, C12, C13, C14, and C15. The tasks are: Stop, JPEG Snapshot, Collect Image, Mount Next Crystal, Loop Alignment, Stop, JPEG Snapshot, Collect Image, Mount Next Crystal, Loop Alignment, Stop, JPEG Snapshot, Collect Image, Mount Next Crystal, Loop Alignment, Stop, JPEG Snapshot, Collect Image, Mount Next Crystal, Loop Alignment, Stop, JPEG Snapshot, Collect Image.

At the bottom, there is a status bar showing the date and time: "22 Sep 2006 15:09:47 robot reports: drvina tong". Below this, there are indicators for "Detector Ready" (green), "Energy: 12647.850 eV", "Abort" (red), "User: Active", "Shutter: closed", and "03:10:09 PM".