

SER-CAT User Data Collection FAQ

1. “I started a data collection and I see blank images with no diffraction”.

If you started a data collection and see some images with no diffraction, you may go back and make sure that the crystal is properly aligned to the cross-hair. In some cases the pin may have slipped a bit after you had first aligned the sample. This can happen if there is some ice at the bottom of the pin base which sits on the goniometer. The ice may melt after some time and cause slippage of the pin. It is a good idea to make sure that the pin is completely stable before starting a data collection. In some rare cases, crystal loop may be loosely attached to the pin and may be unstable in the cryostream. In those cases, you may have to figure out the orientations in which the loop is most stable and try to collect a complete data set in the range of orientations in which the loop appears to be stable.

If you see blank images with no beam stop shadow, it is a good idea to first check whether the stored APS beam is lost. The information regarding the beam current and beam status is listed in the horizontal information bar at the bottom of Sergui page. If the beam current shows a value of zero and the beam status says “off”, it indicates that the APS beam is down. You would need to wait until the beam comes back (the beam current will go up to ~100 mA once the beam comes back). The beam status can be checked by accessing the following web page:

<https://www.aps.anl.gov/Machine-Status>

This web page may have information regarding the reason for loss of beam and the estimated time of beam return.

2. “APS stored beam was lost and it just came back. What should I do?”

Once the beam comes back (the beam current goes up to ~100 mA) and the shutter permit is enabled, you may open the A shutter by accessing ‘Setup→Shutter’ on Sergui.

It is a good idea to recheck the beam alignment once the beam comes back. When checking the beam alignment, no sample should be mounted on the goniometer. You may look at the beam by clicking the “Beam view→Out” option in the ‘Sample’ page on Sergui and then opening the beam shutter. If the beam looks misaligned with respect to the cross-hair, you may optimize the beam by running the optimization scans in ‘Hutch’ page one by one (Tune, Table, Pinhole Horizontal and Pinhole Vertical).

3. “I can not see my sample.”

If you mount a sample and can not see it on the Sample page camera on Sergui, the first step is to check whether the sample is actually mounted correctly on the goniometer. This can be done by accessing the following live camera feeds:

22ID: www.ser.aps.anl.gov/camera_idsq.html

22BM: www.ser.aps.anl.gov/camera_bmsq.html

If the sample has been mounted correctly on the goniometer, but you can not see the pin/loop on Sergui sample camera, it is possible that the sample may be out of the viewing range of the camera. If the camera zoom is not already at zoom level 1, change it to zoom level 1 to have a larger view to find your pin. You may then rotate your sample (omega) by 90 or 180 degree to see if you can locate the pin in any of the orientations. If you still do not see your sample loop, this may mean that you have a shorter pin than usual. To bring a short pin in the camera viewing range, you may click on the “small green pin” icon (located on the left-middle side on the sample view page for ID and right-middle side for BM). This should bring the pin/loop in the sample viewing area. You may then proceed to align the sample for your data collection.

While looking at the live camera feeds, if you see that the sample base is not sitting properly on the goniometer, DO NOT try to mount another sample (This can cause collision of one pin onto another when the gripper mounts a new sample). Please contact your user support immediately.

4. “I am not able to open Sergui.”

If you try to launch Sergui from a terminal window but Sergui fails to open, pay attention to the error message in the terminal window. If the message says:

The user “your_institution_name” is not scheduled for data collection OR The user “your_institution_name” is scheduled to use sergui nomar only.

You may first check whether you are logged in to the correct machine. Open a terminal window to see which machine you are logged into. If you are logged in for ID data collection, the terminal window should say “your_user_name@idc24”. If you are logged in for BM data collection, the terminal window should say “your_user_name@bmc83”. If you are logged into the correct machine and you believe you are scheduled for data collection on that day, contact your user support. The user support will enable your access once the beamline is ready for your use.

If Sergui fails to open due to a problem other than listed above, contact your user support.

5. “I collected some data sets and I would like to quickly look at auto-processing results”.

If you collected a data set and would like to quickly look at the results from SER-CAT auto-processing programs, you may go to the directory under which that particular data set was collected and type the following command in the terminal window:

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> zsum -b
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This will list a short summary of processing results from all the SER-CAT autoprocessing programs (cmdxds, Kylin and cmdDials). Please note that it may take a few minutes for the autoprocessing results to appear after you are done with collecting a dataset.

A summary of autoprocessing results for all the data sets collected can be found on Sergui page by accessing Processing→Auto Process Log. This summary is also available in a log file (“mysql_data_set_log_date”) under your data collection directory (/data/ID_user.raw).

6. “Where can I find the beam center values?”

The beam center values needed for different programs can be found in a file named ‘beamcenter_22ID.dat’ under your data collection directory (/data/ID_user.raw).

7. “I sent too many samples and I lost track of which crystals I have already mounted. Do you have that information somewhere?”

The information regarding the samples mounted using the robot can be found under your data directory (/data/ID_user.raw) in a file named ‘mysql_robot_usage_log_date’.

8. “My NX-client fails to connect to the SER-CAT computers”.

Make sure that you have the latest version of NX-client installed on your computer. If you are unable to connect to the data collection computer, check your NX-client settings. The IP address for ID computer is: 164.54.208.24, and for the BM computer is: 164.54.208.83. For data processing, you may connect to idc23 computer (164.54.208.23) or bmc93 computer (164.54.208.93). If your NX settings are correct, make sure that your internet connection is working. If you are still unable to connect, contact your user support.