Proposal MX-2480 (98268 - (continuation of MX-2480))

Advanced Photon Source, Sector 21 - The Life Sciences Collaborative Access Team (LS-CAT) - CAT Member Macromolecular Crystallography

Introduction:

This BAG Proposal was intended to provide beamtime to laboratories of Member Institutions of the Life Sciences Collaborative Access Team (LS-CAT) at Sector 21 of the Advanced Photon Source during the APS Upgrade Dark Period. We have approximately 80 Principal Investigators whose laboratories use Macromolecular Crystallography in CAT Member Universities, though not were all included during the proposal process due to not having provided necessary information or registering with ESRF in time for the submission deadline. However, it was always the intention that the four LS-CAT Staff Crystallographers would be the operators of the beamlines during each Remote Experiment, in order to streamline the process for both our CAT Members, and for the Staff of Lightsources to which we applied for access to beam time.

***Shift usage*:** The following remarks were added (in part) in the comments box in the Experimental Summaries section of the Submit Experimental Report page, expanded here.

There are a few discrepancies compared to ISPyB summaries in which beamline was used for time allocated. For 17 June/ID30A-3 our results indicate it was ID30B, for 7 July/ID30A-3 our results indicate it was ID30B, for 16 July/ID30B, there was no summary in ISPyB. In addition, there are ISPyB results for 29 July and 31 July/ID30A-1 not represented in the shifts to check the boxes for. I think these mismatches might have been due to our Beamline Scientist Hosts rescheduling or finding extra beamtime for us when there may have been some sort of a problem on the assigned beamline, however I did not participate in every experiment, and did not keep track this as carefully as I should have.

***BAG PIs*:** All co-proposers given in the proposal form are already listed – but as mentioned above, only our four LS-CAT Staff Crystallographers have been collecting all of the data. We are Joseph Brunzelle, Zdzislaw Wawrzak, Spencer Anderson, Pamela Focia.

***PDBs and Publications*:**

It is too early for work using any data collected for members of this BAG to have been published or deposited in the PDB, however all of our CAT Members are aware that any data used that was measured at ESRF will give full acknowledgment to the synchrotron, beamlines and Staff that were involved. *(See last section below called Note:)*

Summary of results :

By my count using information provided by ISPyB, we have measured 3,452 datasets, and 1,380 tests from 1,190 samples. In general, the feedback from the laboratories for which we have collected diffraction data is very positive. The researchers are grateful to be able to further their research whether they learn that some crystal forms do not diffract at all, diffract to low or to high resolution, importantly, they are getting information that they need. Those who are getting high quality moderate to high resolution data, may have additional goals, such as locating ligands they have synthesized in the electron density. We are doing, and they have done, a lot of screening in their studies, both past and present.

***Beamtime request justification*:**
We made a guess at how many shifts to request during the proposal submission process. We are pleased that ESRF has generously given us the number of 2 shift visits they have, visits that work well for our time zone, and also want to thank the scheduler, Deborah Davison for her excellent help when we have needed to reschedule a visit when the schedule first comes out.

***Beamline Performance*:**

We have been very impressed with the beamline operations at ESRF, including the automated features in MXCube3, the automated data collection at times, and the autoprocessing routines and the summary of results in ISPyB. These all provide advanced features we would like to adopt and implement at our beamlines after the APS-U is complete and we have received and commissioned all of our new equipment (which unfortunately will not all be simultaneous due to backlogs of the delivery of some of the new equipment). ESRF does a wonderful job in all ways.

We had to cancel some beamtime we were awarded on BM07 after using it once. It performed very well, but due to the need for sending SC3-SPINE pucks, we could not justify sending a dewar that could only hold 60 samples due to the cost of shipping a dewar to Europe. Once BM07 begins to use Unipucks, we will be happy to collect data there again.

Note:

We have only had beamtime for 6 months of our 2-year proposal, so no new PDB depositions or publications have been related to data collected at ESRF. However, due to the need for a PDB entry and a publication in order to fully submit this Progress Report and BAG Proposal Continuation, I have been instructed by the User Office to note 1 PDB entry, and cite the following article associated with beamline ID30B:

McCarthy A.A., Barrett R., Beteva A., Caserotto H., Dobias F., Felisaz F., Giraud T., Guijarro M., Janocha R., Khadrouche A., Lentini M., Leonard G.A., Lopez Marrero M., Malbet-Monaco S., McSweeney S., Nurizzo D., Papp G., Rossi C., Sinoir J., Sorez C., Surr J., Svensson O., Zander U., Cipriani F., Theveneau P., Mueller-Dieckmann C. - ID30B – a versatile beamline for macromolecular crystallography experiments at the ESRF. J Synchrotron Radiat. 2018 Jul 1; 25(Pt 4): 1249–1260. Published online 2018 Jun 27. doi: 10.1107/S1600577518007166 PMCID: PMC6038607, PMID: 29979188

Which I could not find in your database, so will use this one:

J Synchrotron Radiat 2022 Mar 1;29(Pt 2):581-590.
doi: 10.1107/S1600577522000984.Epub 2022 Feb 22.
ID23-2: an automated and high-performance microfocus beamline for macromolecular crystallography at the ESRF
Max Nanao [1], Shibom Basu [2], Ulrich Zander [2], Thierry Giraud [1], John Surr [1], Matias Guijarro [1], Mario Lentini [1], Franck Felisaz [2], Jeremy Sinoir [2], Christian Morawe [1], Amparo Vivo [1], Antonia Beteva [1], Marcus Oscarsson [1], Hugo Caserotto [1], Fabien Dobias [1], David Flot [1], Didier Nurizzo [1], Jonathan Gigmes [1], Nicolas Foos [1], Ralf Siebrecht [3], Thomas Roth [1], Pascal Theveneau [1], Olof Svensson [1], Gergely Papp [1], Bernard Lavault [3], Florent Cipriani [2], Ray Barrett [1], Carole Clavel [1], Gordon Leonard [1] PMID: 35254323, PMCID: PMC8900849 DOI: 10.1107/S1600577522000984