

SUPPORTING THE MX COMMUNITY  
DURING THE DARK PERIOD



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and GM/CA@APS Group Leader**

**Advanced Photon Source**

**APS UO PUC Meeting  
January 25, 2023**

# Outline

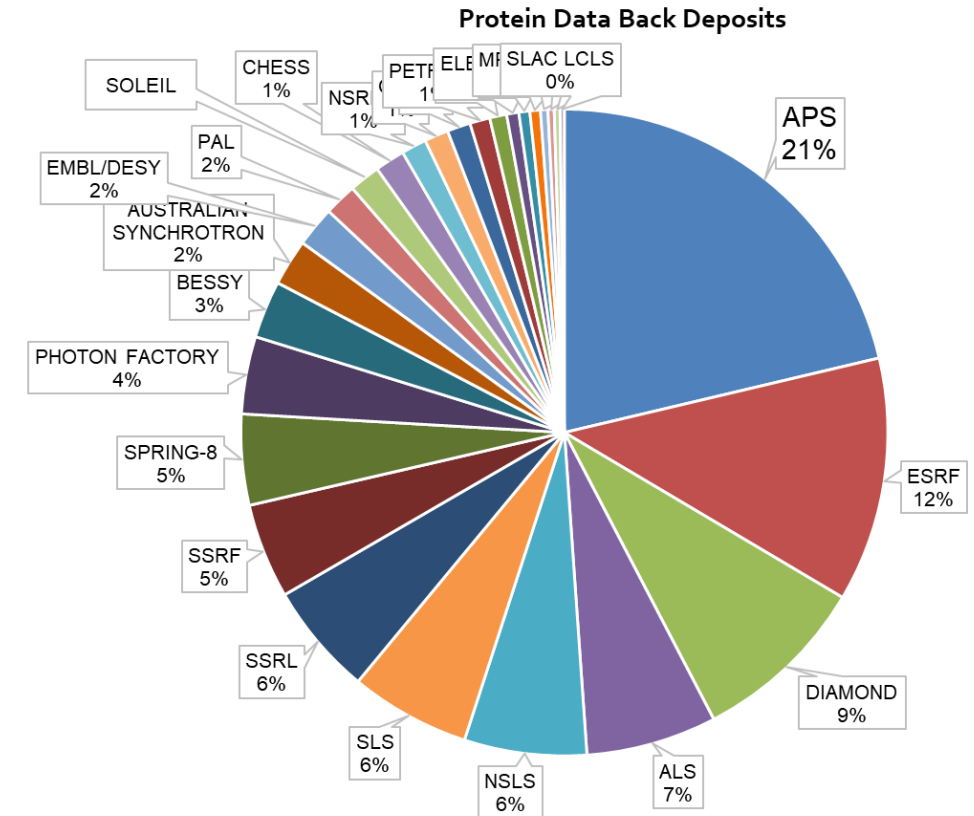
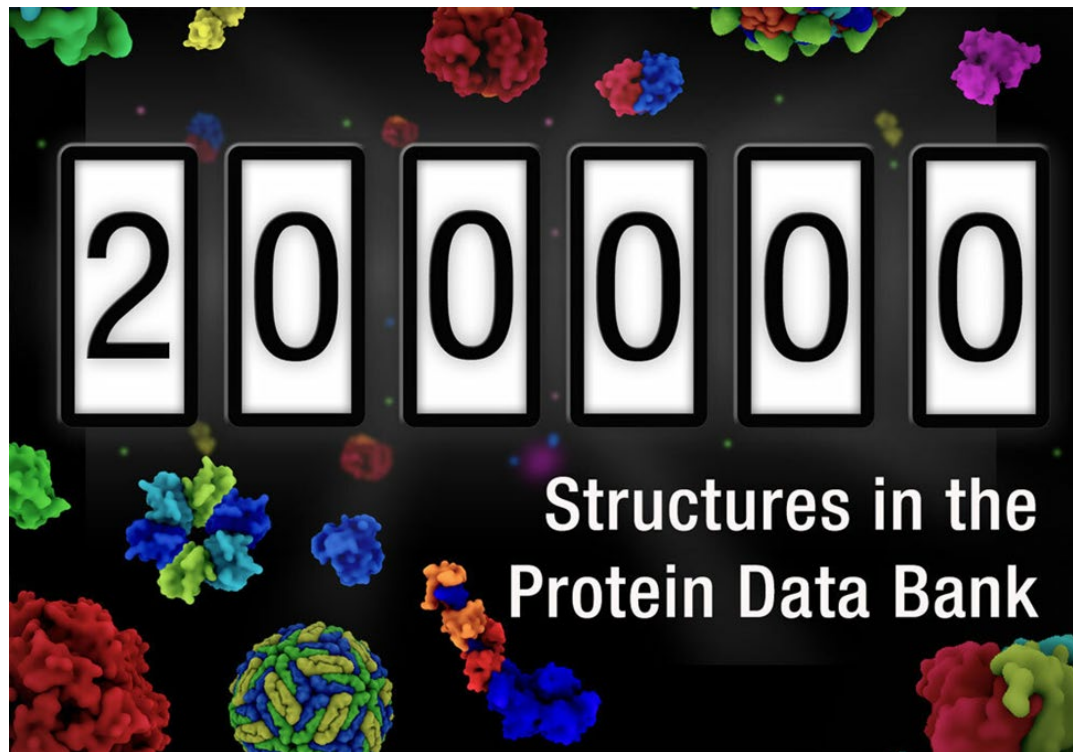
- Protein Data Bank Milestone
- Structural Biology at the Advanced Photon Source
- Planning for the dark period
- Beamtime at other facilities

# Protein Data Bank Milestone

On January 10, 2023, the number of structures deposited in the PDB crossed 200,000

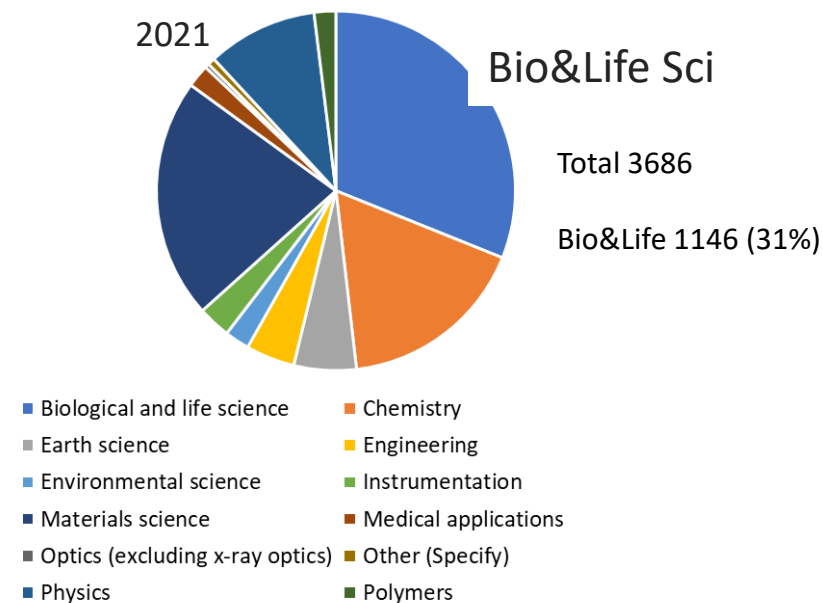
PDB deposits based on data collected at APS beamlines

- 21% of all structures from synchrotron sources
- 60% of all structures from US synchrotron sources



# Argonne's Advanced Photon Source (APS) a DOE Office of Science User Facility

- The APS provides high-energy, high-brightness X-ray beams that are ideal for studying the arrangements of molecules and atoms
- Use of the APS (and other Office of Science user facilities) is free for open research intended for publication
- There are **68** beamlines at the APS where over **5300** researchers do their work every year
- Scientists use **16** of these specialized beamlines for macromolecular crystallography (MX), to examine molecular structures and interactions that could yield lifesaving medicines for various diseases
- Biological & Life Sciences accounts for  $\sim 1/3$  of APS users. Most are MX users.
- Users have studied many diseases and drugs – cancer, influenza, Type 2 diabetes, HIV/AIDS, Ebola, Zika, COVID-19



# Preparing for the dark period

In 2017, we formed a working group of life sciences representatives for U.S. light sources

ALS	Paul Adams and Corie Ralston
APS	Bob Fischetti
NSLS-II	Sean McSweeney
SSRL	Britt Hedman and Keith Hodgson
LCLS	Soichi Wakatsuki
CHESS	Rick Cerione, Marian Szebenyi and Richard Gillian

## Outcome

- Initial white paper describing the problem – shared with DOE light source Directors
- Update white paper included some steps to reduce the impact – shared with NIH and DOE program managers
- NIH and DOE provided supplemental funds to facilities for equipment in 2022
- NIH and DOE may provide supplemental funds to facilities for additional staffing at other facilities

## Outreach

- Workshop on biological science opportunities provided by the APS Upgrade, Argonne, August 20-11, 2018
- APS Structural Biology Town Hall meeting, Argonne, June 21, 2022
- ACA 2022 meeting, Traversing the APS Dark Period, July 31, 2022
- Pittsburg Diffraction Conference, Argonne, October 2, 2022
- Email to over 2200 APS MX users about accessing beamtime at NSLS-II





# Beamtime arrangements at other facilities

Most CATs have formed partnerships or submitted a **Block Allocation Group (BAG)** proposal to domestic and international light sources

## NSLS-II

- Has seen a large influx of single PI and BAG proposals

## SSRL

- Recently introduced BAGs to their proposal system - APS CATs can apply for time
- We are working with SSRL to establish a set aside of 50% of the time on BL14-1 (a bending magnet beamline) for APS General Users.

Diamond Light Source (DLS) - APS and DLS have established a reciprocal agreement.

- DLS will construct and operate a beamline at the APS which DLS users could access during the DLS down time. During this period, the beamline will be exclusively used by Diamond users (academia and industry), applying through the Diamond user office.
- APS General Users and CATs would have access to 12.5% of each of four high-throughput MX beamlines (I03, I04, I04-1, and I24) at DLS during the APS-U downtime, and for the 6 months after startup. Access is for Unattended Data Collection (remote access is possible) for nonproprietary research on BLS-1 samples.





# How to get beamtime at Diamond - General Users

## Key points

- Only nonproprietary research
- Only samples that fall within BioSafety Level One (BSL-1) category are accepted (dry shippers)
- Only **Unipucks** and **spine pins** are accepted for the Diamond high-throughput beamlines

## Process for General Users (GUs)

- APS issues a call for beamtime at Diamond for a specific period - **1st call tentatively February 1, 2023, open for one week**
- General Users submit a Rapid Access Proposal to APS for beamtime on “Diamond Beamlines (I03, I04, I04-1, and I24)”
- The proposal is active for only one period at Diamond
- APS proposal system programming changes are complete and ready to be activated for a call
- APS sends the proposals out for peer review
- Diamond notifies APS how much beamtime is available for a given period
- APS Beamtime Oversight Committee allocates beamtime based on the priority score and distribution between GUs and CATs
- APS (Fischetti) submits a BAG proposal to Diamond for APS GUs. (Need to know the list of users.)
- APS notifies users of their allocation
- Each PI within the APS GU BAG or a designee must register with DLS, complete safety training, and fill out the Experimental Risk Assessment (ERA) form (equivalent to ESAF) 2 weeks in advance
- APS or DLS notifies users when and where to ship their samples
- Initially data will be queued for unattended Data Collection (equivalent to APS mail-in)
- In subsequent calls, Diamond will schedule Remote-access data collection

# How to get beamtime at Diamond - CATs

## Key points

- Only nonproprietary research
- Only samples that fall within BioSafety Level One (BSL-1) category are accepted (dry shippers)
- Only **Unipucks** and **spine pins** are accepted for the Diamond high-throughput beamlines

## Process for APS MX CATs (non-proprietary)

- APS issues a call for beamtime at Diamond for a specific period - **1st call tentatively February 1, 2023, open for one week**
- Each CAT forms one (or more if necessary) BAGs from their CAT members
- The CAT submits a BAG proposal to Diamond (How is the proposal identified as part of the APS allocation?)
- The duration of the BAG proposal needs to be determined
- CAT proposals do not need to be reviewed for access to the APS allocation of time
- Diamond notifies APS how much beamtime is available for a given period
- APS Beamtime Oversight Committee allocates beamtime based on the priority score and distribution between GUs and CATs
- CATs notify members of their allocation
- CATs allocate beamtime to their members within the CAT allotment
- CAT PI or designee can assign roles to members to see data based on experiment ID
- Each PI within the CAT BAG(s) or a designee must register with DLS, complete safety training, and fill out the Experimental Risk Assessment (ERA) form (equivalent to ESAF) 2 weeks in advance
- CATs coordinate members shipping within their BAG(s)
- Initially data will be queued for unattended Data Collection (equivalent to APS mail-in)
- In subsequent calls, Diamond will schedule Remote-access data collection

## *MX Allocation and Oversight Committee (MX-AOC) Charter (Draft name)*

User operations of the APS will terminate on April 17, 2023, for a year-long storage ring replacement. The new and upgraded ring (APS-U) will prove at least two orders of magnitude increase in brightness. After startup, the APS-U and beamlines will need to be commissioned. The APS macromolecular crystallography (MX) community is almost one-third of the entire APS community, and APS MX beamlines account for nearly 60% of the U.S. Protein Data Bank Deposits. APS management has established agreements with other U.S. and international light sources to provide beamtime during the transition period.

The *MX Allocation and Oversight Committee (MX-AOC)* committee will be responsible for advising the APS Associate Laboratory Director in the following areas:

- To ensure equitable and transparent management of beam time resources for the MX community during the dark time in collaboration with partner facilities
- To provide a framework for APS MX general users and CAT members to access beamtime at partner facilities
- To distribute beamtime amongst GUs and CATs based on the APS GU access model and agreements with partner facilities
- To allocate beamtime for APS MX GU proposals based on peer review scores and agreements with participating facilities
- CAT members will be responsible to allocated time to their members based on agreements with participating facilities
- The committee may assist in resolving disputes amongst CAT members that can not be resolved within the CAT
- CAT members are not permitted to submit GU proposals
- Committee composition includes each MX CAT Director or designee
- A quorum shall be defined as a simple majority at any virtual, in-person meeting, or electronic voting if necessary
- Life Sciences Advisory to the APS Director shall be chair

# Acknowledgements

## APS

- Laurent Chapon
- Denny Mills
- Mark Langguth
- Susan White de Pace
- Connie Vanni
- Arvin Ramanathan

## Diamond

- Dave Stuart
- Dave Hall
- Linda Gregory
- Paul Barret
- Laura Williams
- Elizabeth Shotton

## SSRL

- Aina Cohen
- Lisa Dunn



