ABBIX Closeout: A Retrospective

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LSBR Advisory Committee Meeting

March 29, 2017

With Gratitude to Our Colleagues and Sponsors

- ABBIX Project was funded by NIH (incl ARRA funding)
- Support was also provided by DOE BER and BES
- Critical support as well as operation and program management of the beamlines is provided by LSBR, co-sponsored by NIH and DOE BER

- John Lara
- Jean Jakoncic
- Dieter Schneider
- Stu Myers
- Tom Langdon
- Shirish Chodankar
- Bruno Seiva Martins
- Vivian Stojanoff
- John Skinner
- Hugo Slepicka
- Kun Qian
- Sean McSweeney
- Babak Andi
- Martin Fuchs
- Lin Yang
- Neil Whalen
- Dileep Bhogadi
- Rick Jackimowicz
- Edwin Lazo
- Bob Sweet
- Alexei Soares
- Grace Shea-McCarthy
- Wuxian Shi
- Yuan Gao
- Jim Magill
- Vito Graziano
- Jon DiFabio
- Sal Pjerov
- Oksana Ivashkeyvich
- Diego Omitto

Exact Promises We Made at the Start of LSBR Grant:

- We will deliver three state-of-the-art structural biology beamlines and experimental stations at NSLS-II to meet the LSBR P41 Center objectives
- ABBIX Project is well into construction and well-staffed, with organized management team
- Experienced Beamline Advisory Teams have met for AMX/FMX and LIX and will continue to meet periodically
- External teams have reviewed the project several times and will continue to do so periodically
- We will realize the desired capabilities of the beamlines and experimental stations
- **We have kept these promises, but …**
- **Keeping them didn't follow a straight line**

ABBIX Beamlines at NSLS-II
(Advanced Beamlines for Biological Investigations w/ X-rays)

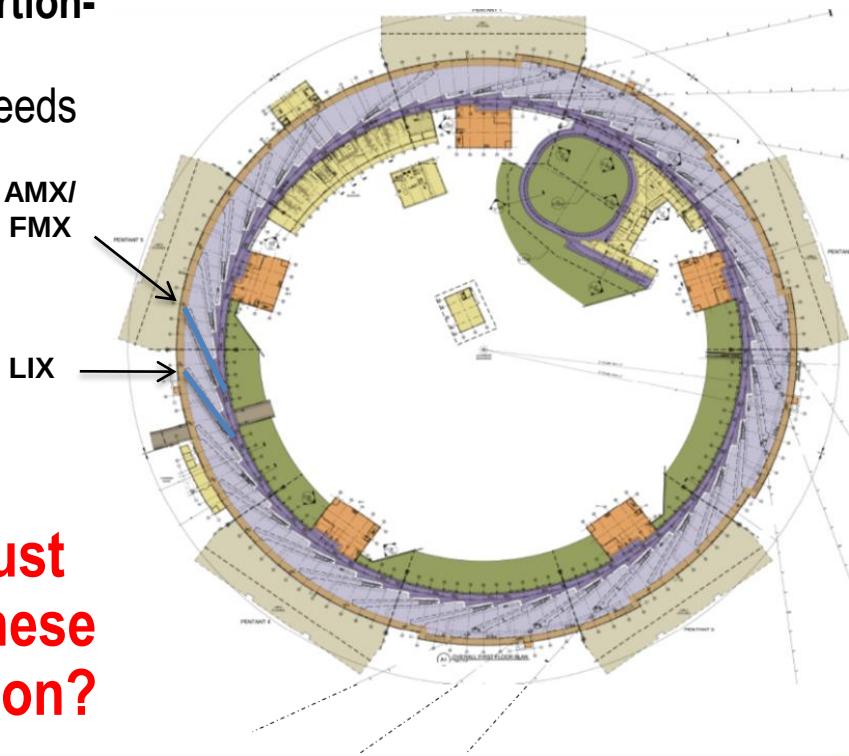
LIX -- High Brightness X-ray Scattering for Life Sciences
AMX -- Flexible Access and Highly Automated Macromolecular Crystallography Beamline
FMX -- Frontier Macromolecular Crystallography Beamline

Goals

- **Design and build 3 NIH-funded state-of-the-art insertion-device-based beamlines for NSLS-II**
- Uphold scientific programs that address NIH mission needs
- Build first biological sciences beamlines at NSLS-II
- Increase usage of NSLS-II in early operations phase

Execution Benefits Derived

- Leveraged by extensive auxiliary supporting infrastructure developed by NSLS-II Project
- Timeline was similar to NEXT Project, with symbiotic benefits (e.g. some shared procurements)

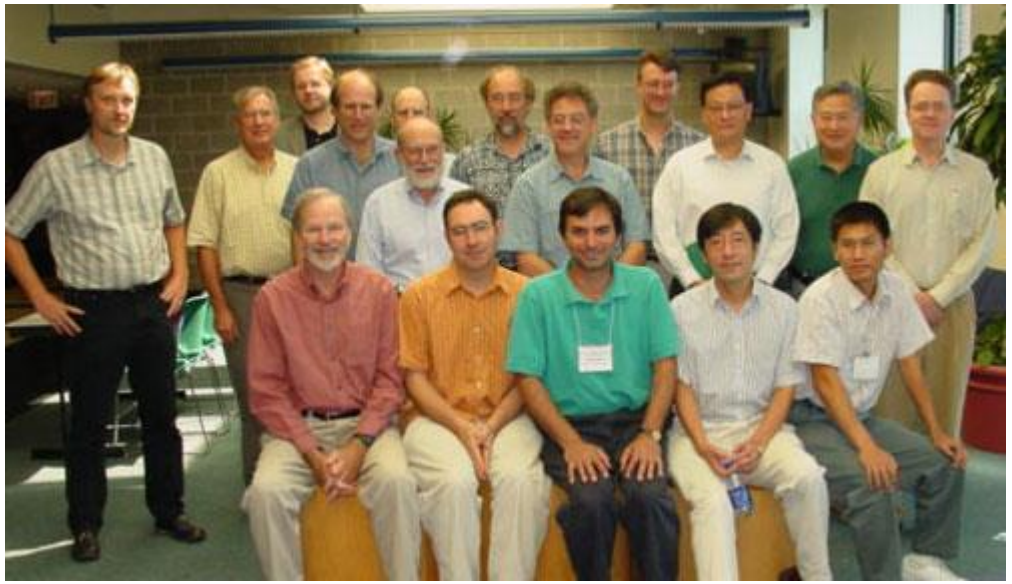


The above are general considerations; just what was it that was really special in these beamlines that merited their construction?

What was to become ABBIX began in 2003:

Scientific Opportunities in Macromolecular Crystallography at NSLS-II
Cold Spring Harbor, July 2003
(progenitor of what became AMX & FMX)

Scientific Opportunities in Soft Matter and Biophysics at NSLS-II
Stony Brook, September 2003
(progenitor of what became LIX)



More workshops of a general nature occurred in 2004-8:

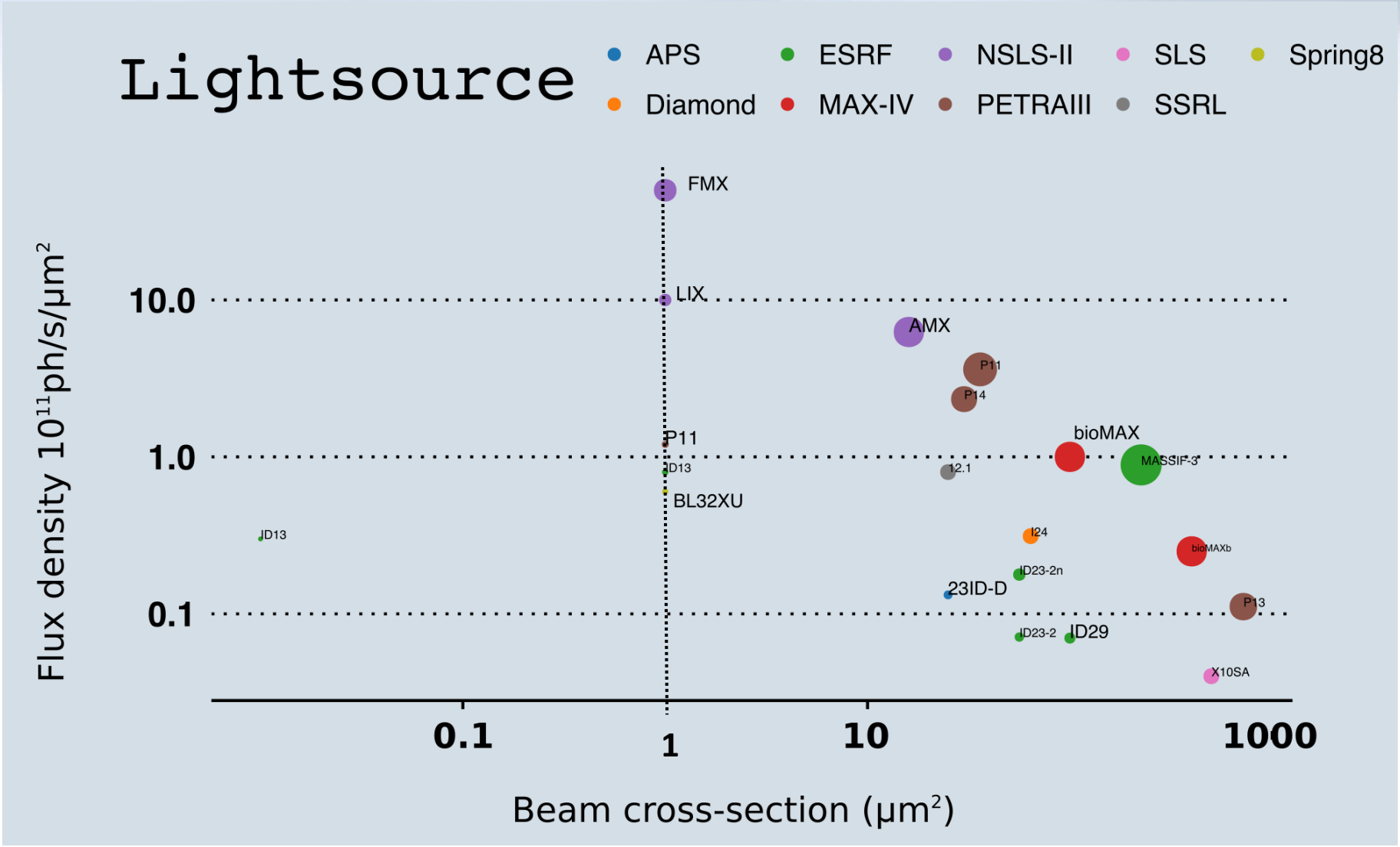
- March 15, 2004: Workshop for NSLS-II
- May 25, 2005: Applications of Small Angle X-Ray Scattering to Biological Structures
- July 17-18, 2007: NSLS-II User Workshop
- January 15-16, 2008: Scientific Strategic Planning Workshop for Life Sciences
- February 11-12, 2008: Scientific Strategic Planning Workshop for Soft and Biomolecular Materials

Starting in 2009, layers of opportunities were studied that pointed to potential unique virtues of NSLS-II for biology:

- July 23-24, 2009: MX Frontiers at the One Micron Scale

- Trends toward smaller crystals, and new approaches such as serial crystallography data collection, highlighted the importance of microbeams for MX, for which NSLS-II would be uniquely positioned

Beam size and flux density:



- Low synchrotron emittance translates into bright beamlines

And more specific opportunities which could capitalize on the unique virtues of NSLS-II for biology were identified via:

- Various thematic workshops occurring from 2009 onward:
  - Solution studies of macromolecules
  - Self-assembly of soft and biomolecular materials
  - Automated crystal handling and visualization
- **These led to April 21-22, 2015: First Science at the ABBIX Beamlines Meeting**
  - Scanning serial crystallography, LCP jet serial crystallography
  - RNA molecules and Ser/Thr phosphatases
  - Very small crystals, weak diffraction, large unit cells
  - SAD multi-crystal crystallography
  - Nuclear pore complexes and huge complexes
  - 10 μs resolution time-resolved solution scattering
  - Scattering-based scanning probe imaging

Meantime, interest in developing these beamlines was expressed by NIH in several meetings:

- April 28, 2008: with NSLS-II management and an ad hoc panel
  - Discussion of life sciences opportunities and needs at NSLS-II
- June 4-5, 2009: with NSLS-II management and a different ad hoc panel
  - Further discussion of life sciences opportunities at NSLS-II and associated costs
- May 24, 2010: with a new external advisory committee
  - Discussion of desired characteristics of life sciences beamlines
- February 24, 2011: with same external advisory committee
  - Recommendation that NIH proceed with the planning and construction of two MX beamlines and one x-ray scattering beamline
- In addition, substantial efforts were pursued within NIH and DOE in regard to identifying and committing the funding as well as in preparing NIH-DOE interagency agreements and MOUs

And proposals to develop these beamlines were submitted, reviewed, and approved by NSLS-II:

- June 2010: preparation workshops and proposals submission
- October 2010: approval of proposals for AMX, FMX, and LIX
- May 2011: following the recommendation that NIH proceed with these beamlines, and with DOE-NIH interagency agreements and MOUs enacted, ABBIX formally began with this funding profile:

($M)	FY10	FY11	FY12	FY13	FY14	Total
IDs/FEs (NIH ARRA)	12.0	0.0	0.0	0.0	0.0	12.0
Beamlines (NIH)	0.0	23.4	5.5	4.1	0.0	33.0
Total ABBIX Project Funds	12.0	23.4	5.5	4.1	0.0	45.0
Common Beamline Systems (Funded by NSLS-II Project)	0.0	0.0	0.0	1.0	2.0	3.0
Total ABBIX + NSLS-II Funds	12.0	23.4	5.5	5.1	2.0	48.0

- Significant front-loading of funds, removed any cash-flow concern

$48M was what these beamlines were projected to cost, but $48M could not be authorized; funds had to be held for:

- **Risks!** Contingency funds needed to be set aside to address.

Risk ID	Risk Name	Date started	Date to Complete	$ Value ($M)	Likelihood (V = very likely, L = likely, U = unlikely)	$ Value Weighted by Likelihood (V = 0.9, L = 0.7, U = 0.5) ($M)
1	Underestimated effort	Jan-12	Jan-15	1.8	L	1.26
2	Higher-than-expected worldwide demand for beamline components	Jan-12	Jan-14	0.75	V	0.675
3	Higher-than-expected optic quality required	Jan-12	May-13	1.35	L	0.945
4	Required optic quality is closer to state-of-the-art than expected	Jan-12	Jan-14	1.1	L	0.77
5	Higher-than-expected inflation rate	Jan-12	Jan-15	0.4	L	0.28
6	Design Changes	Jan-12	May-13	0.8	L	0.56
7	Market-driven price fluctuations	Jan-12	Jan-14	0.4	L	0.28
8	Changes to EESE requirements/designs	Jan-12	Jan-14	0.11	U	0.055
9	Insufficient mechanical stability of optical components	Jan-12	Aug-13	0.72	L	0.504
10	Higher-than-expected thermal deformation of optics	Jan-12	May-13	0.36	L	0.252
11	Underperforming equipment brought from NSLS	Jan-12	Jan-14	0	U	0
12	Underestimated component costs	Jan-12	Jan-14	0.8	L	0.56
13	Personnel recruitment delays	Jan-12	Dec-14	0.25	U	0.125
14	Accidents and injuries	Jan-12	Sep-15	0.5	U	0.25
15	Limited availability of specialized effort	Jan-12	Jan-14	0.5	L	0.35
16	Late installation of EESEs	Jan-12	Jan-14	1	L	0.7
17	Installation of beamlines during facility operations	Jan-12	Sep-15	0.5	U	0.25
18	Insertion Device Field Quality does not meet NSLS-II requirements	Jan-12	Jan-15	0.54	U	0.27
				Total 11.88		**8.086**

ABBIX RISK REGISTRY

So it was necessary to create a base scope:

- Insertion devices and front ends (including commissioning)
- Design and engineering of all beamlines (optics, vacuum system, diagnostics, controls)
- **Acquisition of FMX and LIX (and a portion of AMX) photon delivery systems** (optics, vacuum system, diagnostics, controls)
- Design, engineering, and acquisition of all radiation enclosures
- Design and engineering of all endstation components, and **acquisition of FMX endstation components only**
- **This seemed to indicate the possibility that just one complete beamline and endstation, plus portions of the others, might be built**

ABBIX Base Scope Cost Estimates

WBS #	WBS Name	Base Scope ($M)		
		Labor	M&S	Total
5.01	Project Management	3.1	1.0	**4.1**
5.02	Conceptual Design	0.1	0.0	**0.1**
5.04	AMX Beamline	0.5	1.6	**2.1**
5.05	FMX Beamline	1.7	9.6	**11.3**
5.06	LIX Beamline	1.8	3.8	**5.6**
5.07	Insertion Devices	2.0	5.4	**7.4**
5.08	Front Ends	0.7	1.6	**2.3**
5.09	Beamline Control Systems	1.6	0.7	**2.3**
	Total Project Cost ($M)	11.4	23.7	**35.1**

Note: amount of funds that were available for contingency were **$9.9M** when the project was baselined in 2013 (about 30% of the ABBIX baseline costs remaining).

And we devised a prioritized spending plan for the items still needed to complete three whole beamlines:

Scope Contingency Item	Decision Date	Labor Cost Estimate (K$)	M&S Cost Estimate (K$)	Grand Total (K$)
(1) LIX Flight Path and Vacuum Chamber	Nov. 2013	204	451	655
(2) LIX Experimental Apparatus	Jan. 2014	353	699	1,053
(3) LIX Computation and Storage HW Phase 1	Sep. 2014	127	114	240
(4) LIX Sample Prep Space	Sep. 2014	79	190	270
(5) LIX Detector System	Feb. 2014	94	889	983
(6) LIX Computation and Storage HW Phase 2	Dec. 2014		199	199
(7) AMX Deflecting Mirrors	Apr. 2014	33	598	631
(8) AMX KB Mirrors	Apr. 2014	171	1,166	1,337
(9) AMX Controls Infrastructure	Apr. 2014	210	120	330
(10) AMX Detector	Jan. 2015	150	2,451	2,601
(11) AMX Diffractometer	Sep. 2015	456	1,149	1,605
Scope Contingency - ABBIX Total		1,877	8,026	**9,903**

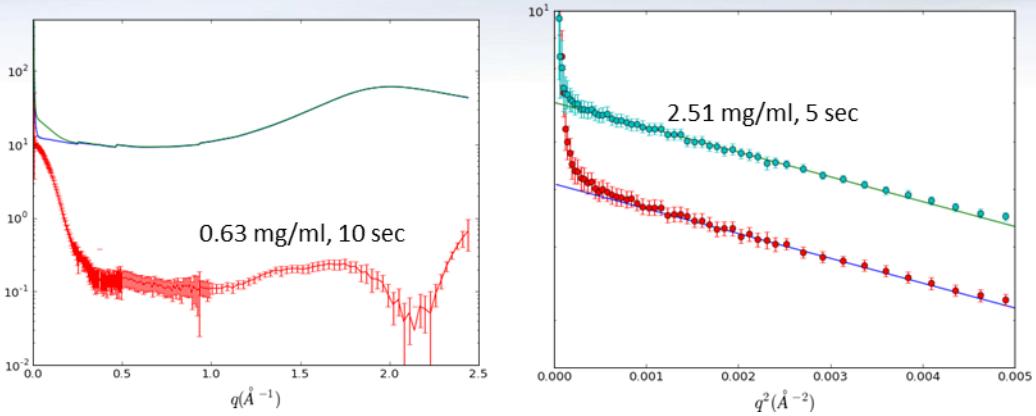
- Most of the above were achieved using ABBIX Project contingency funds
- The detectors for LIX and AMX were exceptions
- For LIX, the detectors (three PILATUS3 PADs) were obtained through a separate NIH SIG grant via Stony Brook
- For AMX, a substitute from NSLS acquired in 2011 (PILATUS 6M) was offered, and was upgraded using ABBIX funds
- An Eiger 9M detector for AMX was eventually obtained, sponsored through LSBR

How did ABBIX add millions of dollars of scope while retiring risks at relatively modest cost?

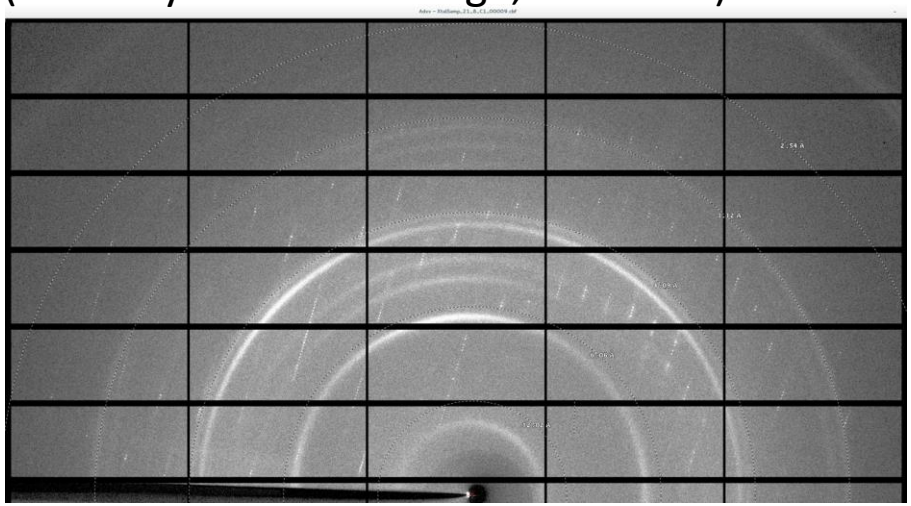
- A dedicated pool of talented staff, ranging from scientific to technical, even administrative
- Favorable contract terms, as well as lumped procurements with other (non-ABBIX) projects, e.g. for the hutches
- Expensive detectors provided or funded outside the project
- Resources planning to capture particular specialized labor pools at critical junctures when they became available (e.g. rolled off from the NSLS-II Project)
- Reliance on expert advice from the BATs and a sound review process, as well as a partnership with Case (for AMX/FMX)
- Excellent relationships with NSLS biology beamline groups and LSBR as well as with other portfolios such as the NSLS-II Project, all of which made investments in the ABBIX beamlines
- Engagement and transparency with our sponsors at NIH, BER, and BES

It culminated in these first data in summer 2016:

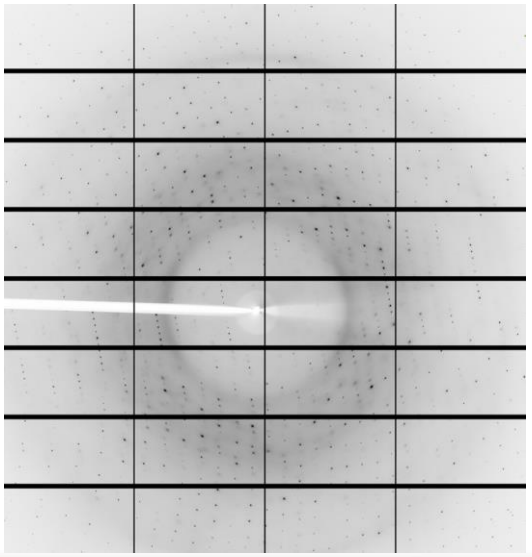
Test data from ribonuclease A (13.7 kDa) to explore the LIX beamline capability to measure low-concentration solutions of small molecules.



Room-temp diffraction from crystal having a unit cell of dimensions 480 Å × 60 Å × 60 Å at AMX (courtesy of Rebecca Page, Brown U.)



Diffraction from lysozyme single crystal recorded on Eiger 16M detector at FMX.



And so, with some help from our friends,
I'd like to say thank you on behalf of the group and ourselves, and I hope we passed the audition!