

RCSB PDB Advisory Committee

Virtual Meeting

April 21, 2020 2pm EDT, 11am PDT



Background Information Slides

Slides with a blue title are provided as background information and can be presented and discussed at the meeting by request.

Main Slides Appear with Red Titles

Agenda

2:00 pm ET	Welcome and Introductions	Stephen K. Burley
2:10	Response to COVID-19	Stephen K. Burley
2:15	2019 Overview	Stephen K. Burley
2:20	Deposition/Biocuration	Jasmine Young
2:35	New and Improved RCSB.org	John Westbrook
2:55	Outreach/Education	Christine Zardecki
3:05	Operations and Funding	Stephen K. Burley
3:15	PDB50 and AC Meetings	Stephen K. Burley
3:20	Discussion: PDB Format	John Westbrook
3:30	Executive Session	
3:55	Messages from AC	Stephen K. Burley, Andrej Sali, Christine Zardecki

Introductions to Meeting Participants

Advisory Committee

- Participating: Paul Adams (Chair), Peter Andolfatto, Judy Blake, Andy Byrd, Bridget Carragher, Wah Chiu, Kirk Clark, Paul Craig, Roland Dunbrack, Paul Falkowski, Thomas Ferrin, Mandë Holford, Cathy Peishoff, Sue Rhee, Torsten Schwede
- Not attending: Robert B. Darnell, Jill Trewhella,

RCSB PDB

- Stephen K. Burley, Helen M. Berman
- Rutgers: Robert Lowe, John Westbrook, Jasmine Young, Christine Zardecki
- UCSD: Jose Duarte
- UCSF: Andrej Sali

Summary of Questions for Consideration Today

- Any questions about our responses to the 2019 AC report?
- COVID-19: *Are there other projects in this area we could develop to support research and education?*
- Deposition/Biocuration: *Any concerns about the Deposition/Biocuration work underway with our wwPDB partners?*
- New and Improved RCSB.org: *Additional Site and Search Functionality requests?*
- Outreach/Education: *Suggestions for new materials and virtual venues for celebrating PDB50 throughout 2021?*
- Next Advisory Committee Meeting location?
- Discussion: *What advice do you have regarding PDB Legacy Format sunseting?*



Coronavirus, 2020
>25K views since Feb 6

Response to COVID-19

Stephen K. Burley

Question: Are there other projects in this area should we develop to support research and education?

Impact of COVID 19 on Operations

- Full team working remotely since mid-March
- Rutgers Undergraduate Honors Course taught *via* WebEx
 - Summer undergraduate research moved to remote experience; will focus on coronaviruses
- Biocuration of SARS-CoV-2 structures prioritized
 - Majority of authors have agreed to *Release Immediately*
 - Anticipating structures from worldwide efforts underway
- Monitoring is ongoing
- No service disruptions
- COVID-19 resources updated weekly at RCSB.org



Weekly Biocuration Meeting



Biocurating SARS-CoV-19

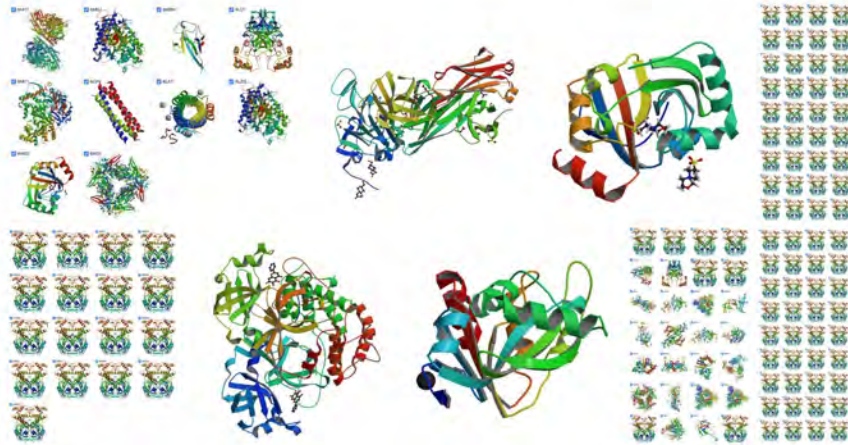
- Biocuration prioritized over other structures
 - Standard deadlines made more flexible for these structures
- Authors encouraged to *Release Immediately*
- Consistent Taxonomy name and ID (Severe acute respiratory syndrome coronavirus 2; 2697049)
- UniProt ID: Not yet assigned
- Related publications added ASAP

Our job as biocurators at the PDB is to receive these structures, examine them, validate them, then disseminate them to the world so that the data are freely available to and usable by all people everywhere in perpetuity.

It is a weighty responsibility made heavier in the case of COVID-19 by the knowledge that delays in advancing scientific understanding of the virus can be measured not just in days, but in lives lost.



Structural Coverage of SARS-CoV-2



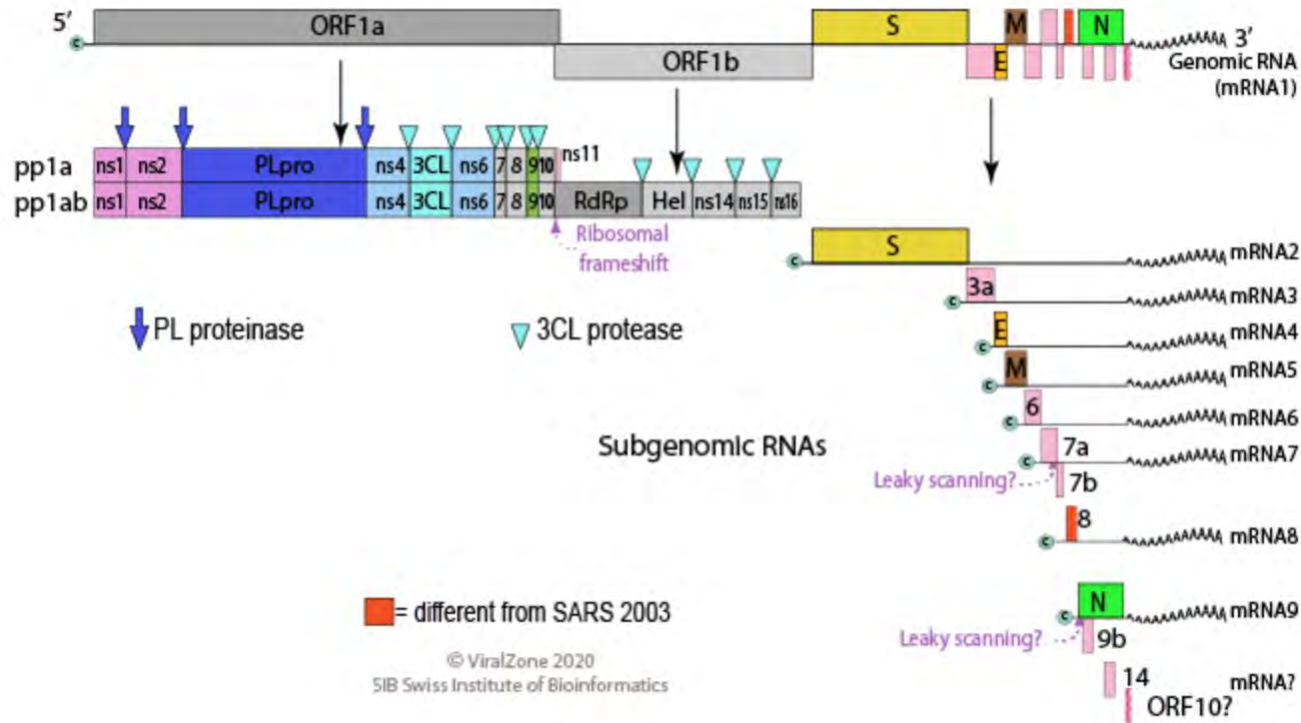
131 structures as of April 15, 2020

- 102 main protease
 - 93 PanDDA analysis-related
- 4 spike protein (some with ACE2)
- 1 papain-like protease
- 2 RNA-dependent RNA polymerase

Protein	PDB ID
Nsp1*	2gdt
Nsp2	-
PLpro	6w9c
Nsp4	-
3CL	6lu7
Nsp6	-
Nsp7*	2ahm
Nsp8*	2ahm
Nsp9	6w4b
Nsp10	6w61
Nsp11	-
RdRp	6m71
Helicase*	6jyt
Nsp14*	5nfy
Nsp15	6vww
Nsp16	6w61

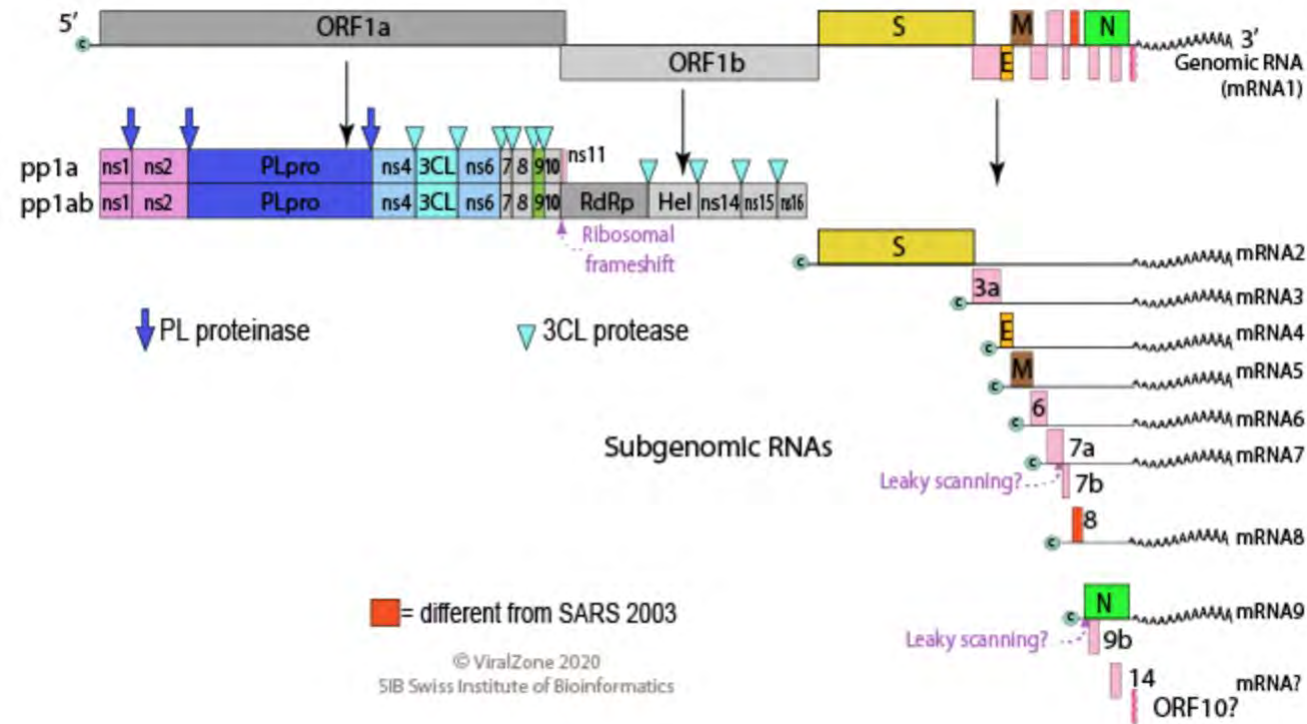
*SARS or MERS homolog

SAR-CoV-2 Genome Organization, 1



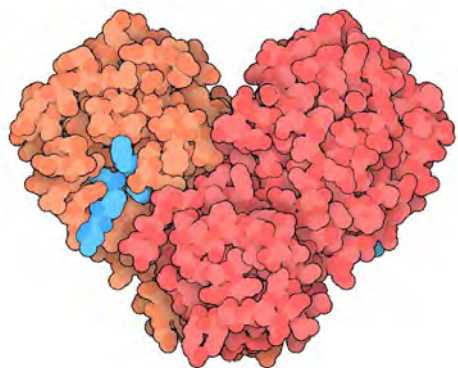
Protein	PDB ID
Nsp1*	2gdt
Nsp2	-
PLpro	6w9c
Nsp4*	3gzf
3CLpro	6lu7
Nsp6	-
Nsp7	6m71
Nsp8	6m71
Nsp9	6w4b
Nsp10	6w61
Nsp11	-
RdRp	6m71
Helicase*	6jyt
Nsp14*	5nfy
Nsp15	6vww
Nsp16	6w61

SAR-CoV-2 Genome Organization, 2



Protein	PDB ID
Spike pro	6vsb
Nsp3a*	2acf
Nsp3b*	2fav
Nsp3c	2w2g, 2kqv
Nsp3e	2k87
E pro*	5x29
M pro	-
Orf 6	-
Orf 7a	1yo4
Orf 7b	-
Orf 8	-
N pro*	1ssk, 2cjr
Orf 9b	-
Orf 14	-
Orf 10	-

Rapid COVID-19 Outreach Well-received

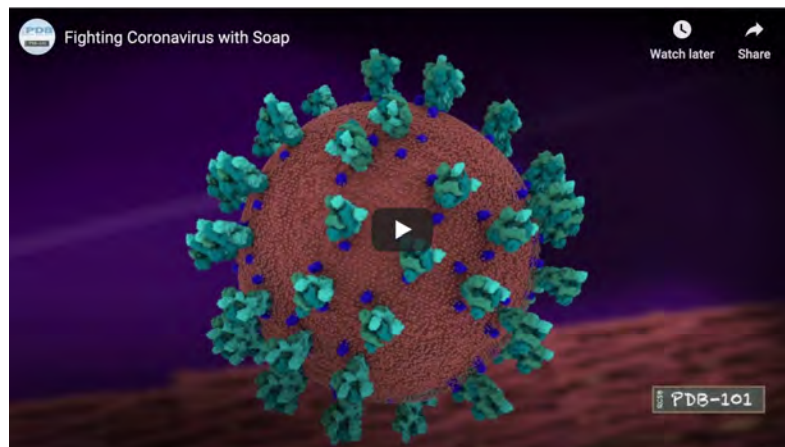


February Molecule of the Month:

[Coronavirus Proteases](#)

>54K views

Planned for June:
Coronavirus Spike Proteins



[Video](#)

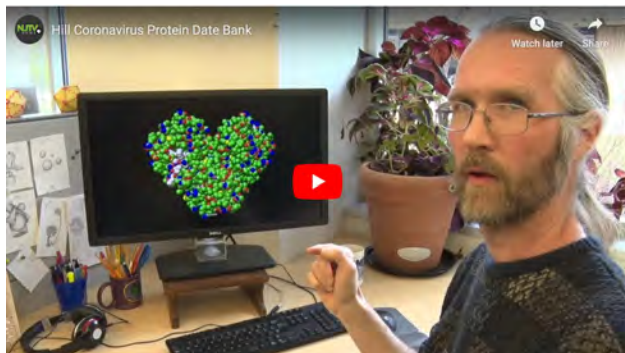
~165K views since March 18



[Coronavirus Coloring](#)

~11,800 views since March 17

PDB (and coronavirus) in the News



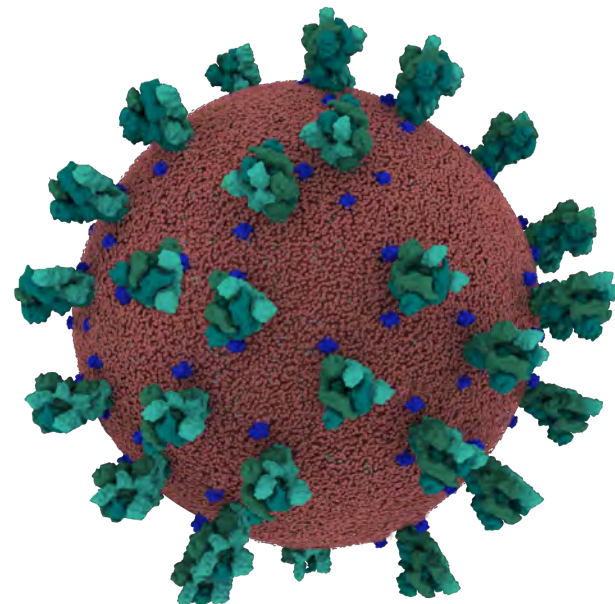
[NJTV News](#) talks with Rutgers University researchers Stephen Burley and Brian Hudson at the Protein Data Bank about finding the key to fighting COVID-19.

CALIFORNIA TODAY
The New York Times
Why Are California and New York Different in the Virus Crisis?
Monday: It's too early to say for sure, but some experts say early action by California leaders has helped. Also: Art during the pandemic.



WORLD VIEW · 24 MARCH 2020
nature
How to help the free market fight coronavirus
Share data, boost incentives and reduce red tape to identify drugs for use in emerging coronavirus epidemics.
[Stephen R. Burley](#)

About five weeks after cases of COVID-19 began to appear, scientists based in Shanghai, China, deposited the first 3D structure of a crucial protein from the virus causing the disease into the Protein Data Bank (PDB), an open-access repository for data on biological structures. As happened with severe acute respiratory syndrome (SARS) and Middle East respiratory syndrome (MERS) – both also caused by coronaviruses – scientists are sharing information in ways not typical for a competitive, commercial field. Knowing the shapes of proteins from the virus that causes COVID-19 could accelerate the discovery of drugs and vaccines. But that will not happen if other barriers – financial, regulatory or legal – get in the way. Lowering them is essential to defending against COVID-19 and preparing for the inevitable future outbreaks.



Questions and Comments?

Question: Are there other projects in this area should we develop to support research and education?

2019 Overview



March 19, 2019: PDB archive reaches 150,000 entries!

Impact of Publicly Available PDB Data

PDB Archive contains >1 TB of Structure Data for Proteins, DNA, and RNA

The cost to replicate the contents of the PDB archive is estimated at

\$16 billion (USD) ([Analysis](#))

The PDB Archive

- Grows at the rate of nearly 10% per year
- Used to download >2 million structure data files per day
- Managed by International collaboration US-Asia-Europe
- Manages “Big Data” as global Public Good

PDB Data

- Enable research in subject areas from [Agriculture to Zoology \(Analysis\)](#)
- Contributed data to nearly >1 million [published research papers](#)
- Used by >400 biological data resources

PDB Data Impact

- Basic and applied research
- Patent applications
- Discovery of lifesaving drugs
- Innovations that can lead to new product development and company formation
- STEAM education: [PDB-101](#) provides curricula and online tools for teachers and students

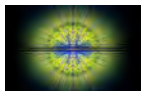
Millions of Data Consumers worldwide served every year

Researchers, scientists, educators, students, curious public, medical professionals, patients, and patient advocates

Public and Private sectors, including pharmaceutical and biotechnology companies

Generates return on investment of
~1,500 times federal funding
([Analysis](#))

2019 in the Life of the RCSB PDB Community



Meeting: Visualizing molecules in action

New Jersey Science (Teacher) Convention



The New York Structural Biology Discussion Group Summer Meeting

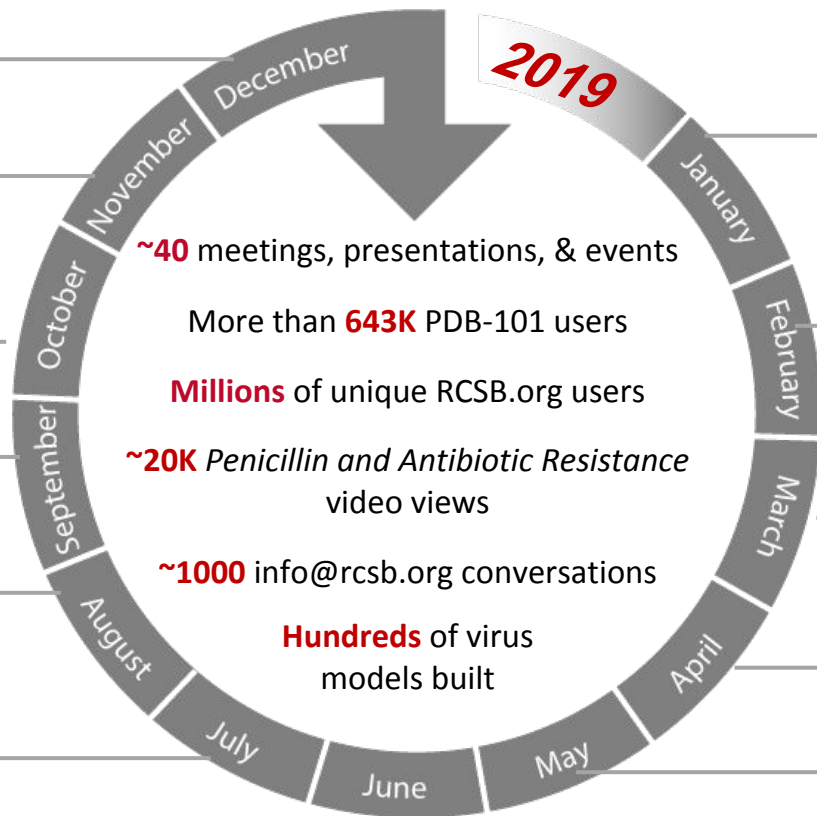


AMR Video Challenge



Carbohydrates Gordon Research Conference

RCSB PDB Advisory Committee



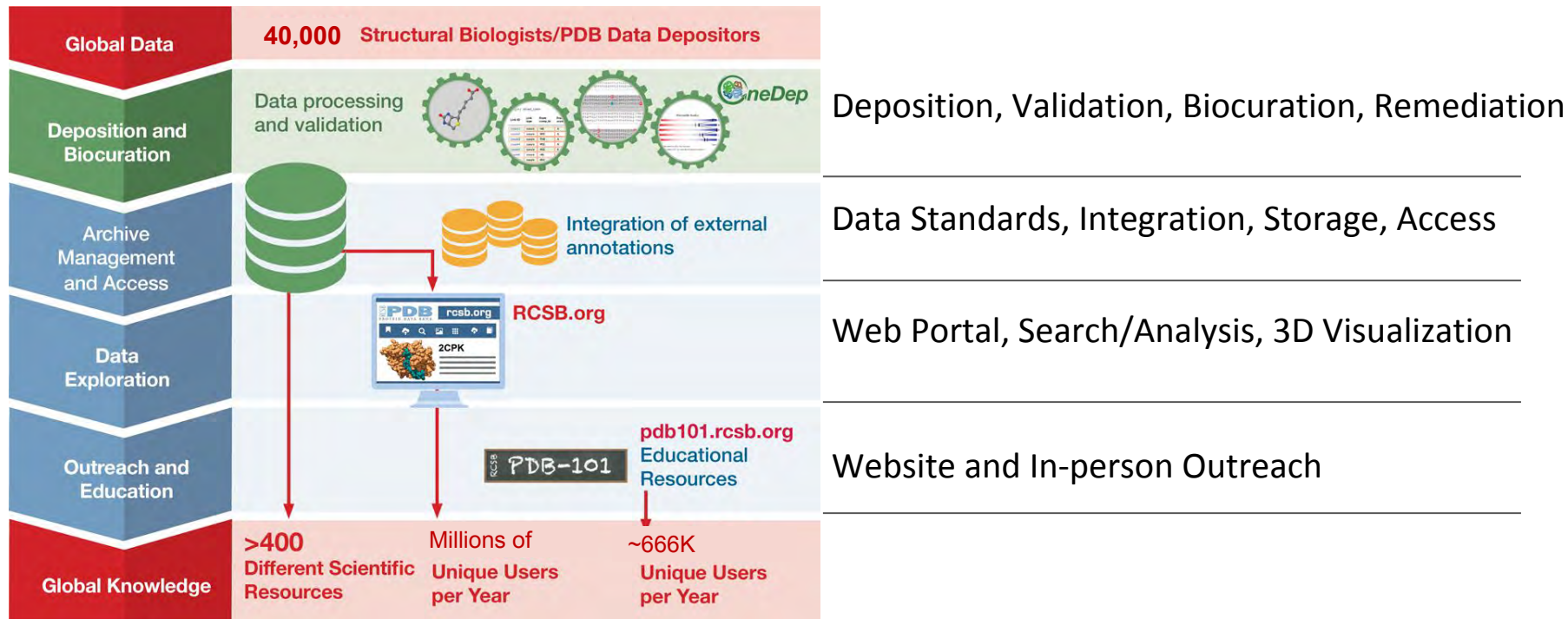
IQB Boot Camp
Single-Particle
Cryo-Electron Microscopy

The New York Structural Biology Discussion Group Winter Meeting

Undergraduate Course on Antimicrobial Resistance



RCSB PDB: Four Interoperating Services





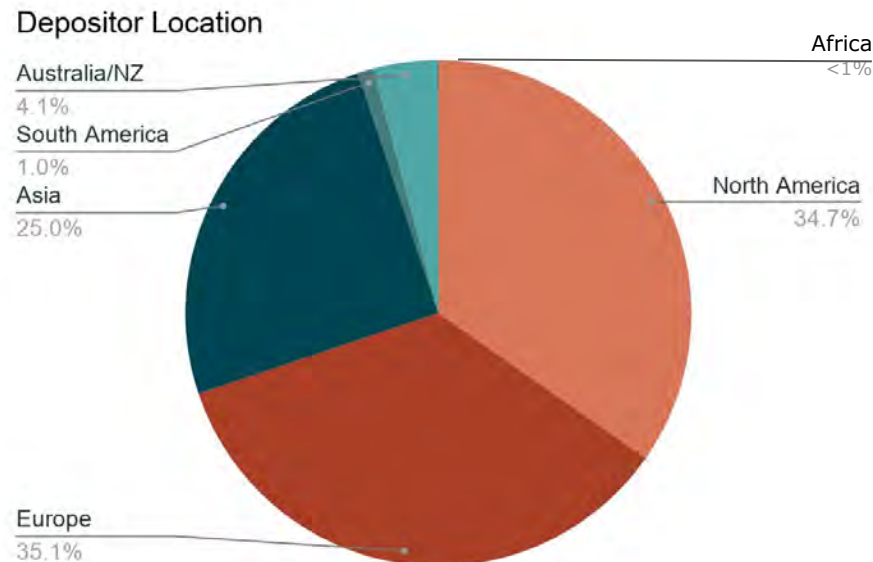
Deposition/Biocuration

Jasmine Young

Question: Any concerns about the Deposition/Biocuration work underway with our wwPDB partners?

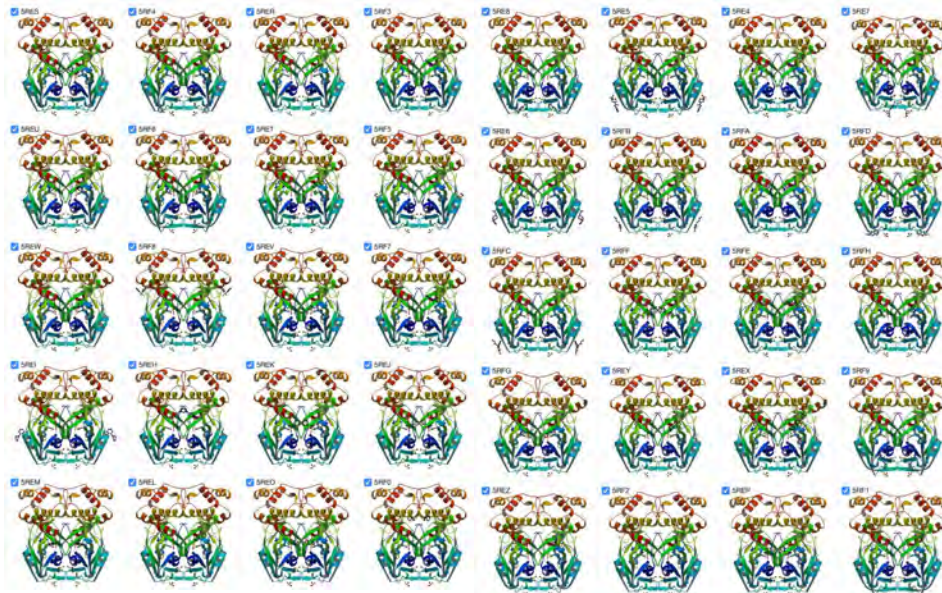
2019 wwPDB Deposition/Biocuration Statistics

- 13,377 new depositions
 - 5,531 RCSB PDB-biocured
 - 12,179 deposited in 2018
 - On track for >13K depositions in 2020
- Biocuration workload balanced geographically
 - 41% Americas, Oceania
 - 34% Europe, Africa
 - 25% Asia



GroupDep Enables Effective Deposition/Biocuration

- Depositors can submit multiple, similar structures *via* GroupDep
- Total of 92 SARS-CoV-2 structures with 91 novel ligands from PanDDA fragment screening
- All processed and released within one week from date of deposition



Evolving Experimental Methods: Growth in EM

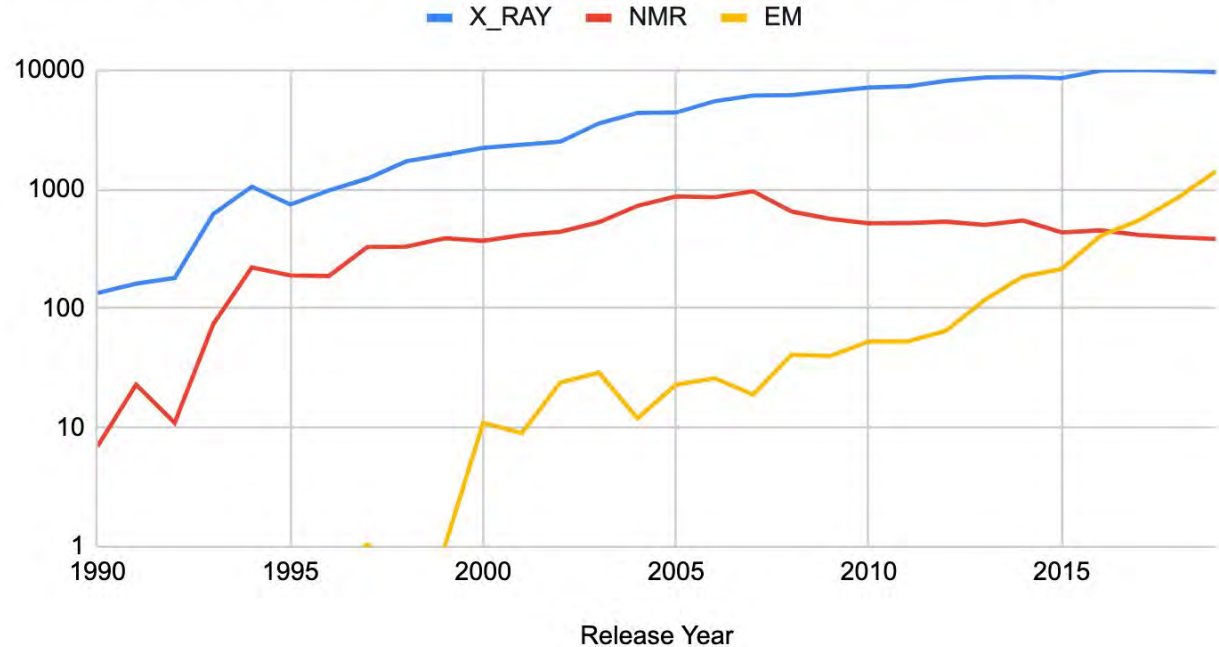
nature

NEWS • 10 FEBRUARY 2020

Revolutionary cryo-EM is taking over structural biology

The number of protein structures being determined by cryo-electron microscopy is growing at an explosive rate.

New Structures Annually by Method (logarithmic scale)



Evolving Experimental Methods: Growth in XFEL

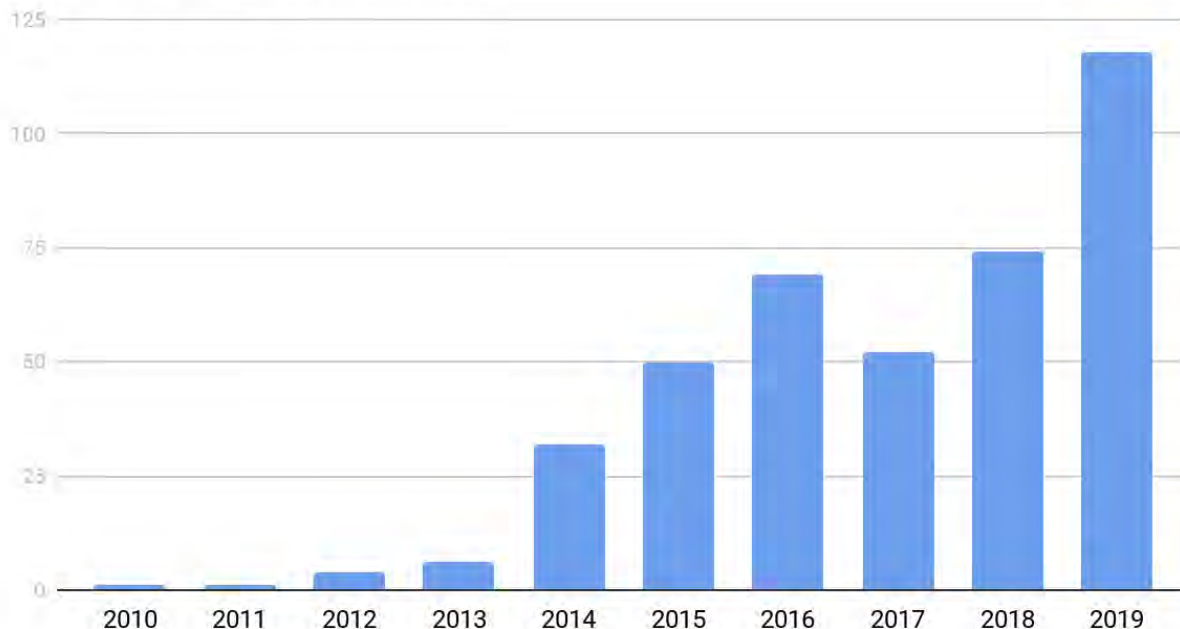
PHYSICS TODAY

24 Jul 2018 in Research & Technology

Smaller, faster, harder: Crystallography with XFELs

The latest generation of free-electron laser x-ray sources can produce molecular movies with even higher time resolution than before.

Growth in XFEL Depositions



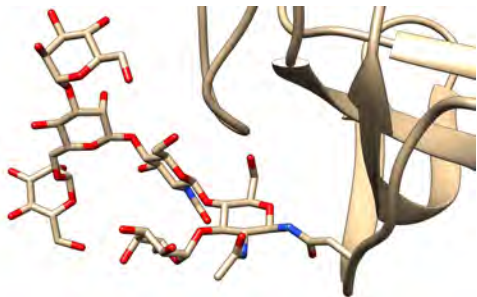
Deposition/Biocuration in 2019

- Better software management *via* GitHub
- Molecular views of ligand validation in validation reports
- Mandatory submission of PDBx/mmCIF Coordinates for MX
- wwPDB DOI landing page
- Author-initiated coordinate replacement enabled
- Ongoing biocuration efficiency improvements
- Carbohydrate remediation
- 3DEM map validation for depositors

July 2020: Release of Updated Carbohydrates

Scope

- 970 monosaccharides in the Chemical Component Dictionary
- ~9% of PDB structures that contain carbohydrates remediated
 - ~14,000 PDB structures
 - ~15,000 oligosaccharides



Status

Communicated with glycoscience, PDB, and software developer communities *via* conferences/virtual meetings

Standardized nomenclature following IUPAC/IUBMB

Adopted glycoscience community software

Provided uniform representation for oligosaccharides with community linear descriptor(s)

wwPDB Highlights

Improved DOI Landing Page



The screenshot shows the wwPDB landing page for entry 6QW9. At the top, the 'WORLDWIDE PDB PROTEIN DATA BANK' logo is visible. Below it, the entry is identified as 'PDB Entry - 6QW9' with a status of '(Status - Released)'. A 'Summary information' section follows, containing the title 'Crystal structure of KPC-2 complexed with relebactam (16 hour soak)', the DOI '10.2210/pdb6qw9/pdb', the primary publication DOI '10.1128/AAC.00564-19', and the entry authors 'Tooke, C.L., Hinchliffe, P., Spencer, J.'. It also lists the initial deposition on '5 March 2019', initial release on '21 August 2019', and latest revision on '2 October 2019'. A 'Downloads' section provides links for 'Structure coordinates (PDBx/mmCIF)', 'Structure coordinates (PDBML)', 'Structure coordinates (PDB)', 'X-ray diffraction data (PDBx/mmCIF)', and 'Validation report (PDF)'. At the bottom, it says 'Links to more resources for 6QW9 at:' and features logos for 'PDB', 'PDBj', and 'PDBe'.

DOI: [10.2210/pdb6Q9W/pdb](https://doi.org/10.2210/pdb6Q9W/pdb)

Author-initiated Coordinate Replacement

- OneDep entries enabled in August 2019
- Legacy entries enabled in February 2020
- 43 replacements so far
 - 38 X-ray
 - 3 3DEM
 - 2 NMR
- Back-end legacy code improved as a side outcome

wwPDB Highlights

Mandatory Submission of PDBx/mmCIF Coordinates

- Successfully implemented for MX structures July 2019
- Transition to PDBx/mmCIF
 - Publicly announced
 - Improved PDBx/mmCIF conversion tools
 - Collaborated with community software developers to help improve their software packages
- Will follow this successful path for 3DEM and NMR structures



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England

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data dictionary; data archiving; biocuration;
validation; macromolecular crystallography;
data standards; PDBx/mmCIF format; Protein
Data Bank; Worldwide Protein Data Bank.

letters to the editor

Announcing mandatory submission of PDBx/mmCIF format files for crystallographic depositions to the Protein Data Bank (PDB)

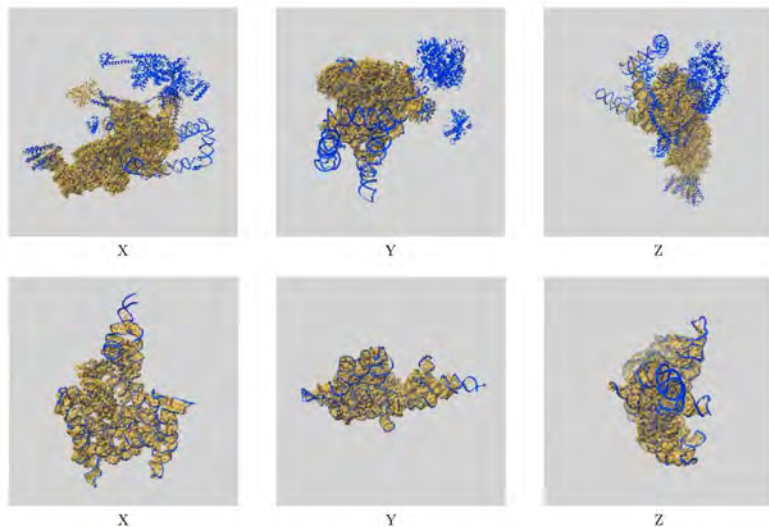
Paul D. Adams,^{a,b} Pavel V. Afonine,^a Kumaran Baskaran,^c Helen M. Berman,^d John Berrisford,^e Gerard Bricogne,^f David G. Brown,^g Stephen K. Burley,^{h,i,j,k} Minyu Chen,^j Zukang Feng,^g Claus Flensburg,^l Aleksandras Gutmanas,^e Jeffrey C. Hoch,^{h,k} Yasuyo Ikegawa,^j Yumiko Kengaku,^j Eugene Krissinel,^l Genji Kurisu,^l Yuhe Liang,^d Dorothee Liebschner,^a Lora Mak,^e John L. Markley,^{h,k} Nigel W. Moriarty,^a Garib N. Murshudov,^m Martin Noble,ⁿ Ezra Peisach,^d Irina Persikova,^d Billy K. Poon,^a Oleg V. Sobolev,^a Eldon L. Ulrich,^c Sameer Velankar,^{h,k} Clemens Vornrhein,^j John Westbrook,^d Marcin Wojdyr,^{l,j} Masashi Yokochi^o and Jasmine Y. Young^d

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wwPDB Validation Highlights

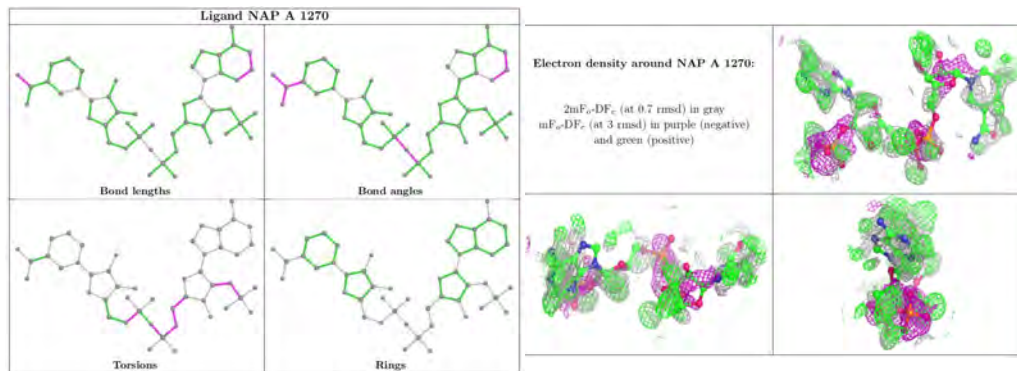
Improved EM Map Validation

Fit of model to the map volume



2D Ligand Visualization

Geometry and density fit for X-ray

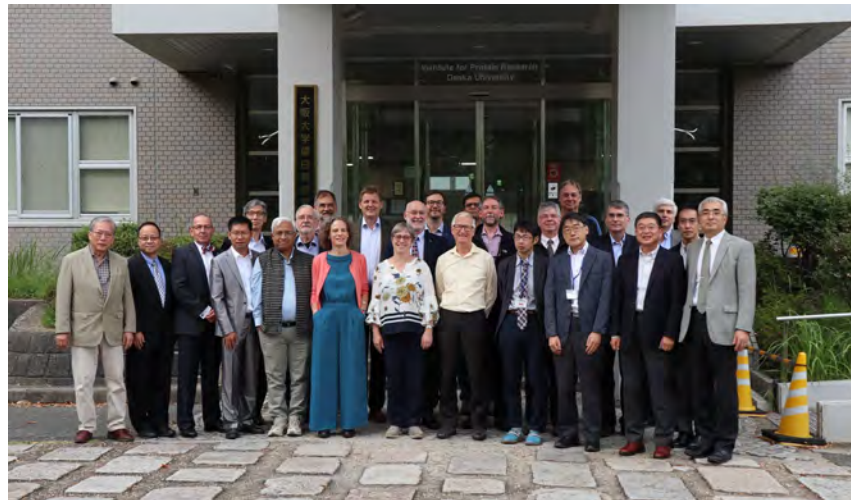


Deposition/Biocuration Goals for 2020

Goal	Impact/Gain
Validation enhancements: NMR restraints, EM Maps	Improve data quality Increase Biocuration efficiency
Supporting NEF format from NMR technique	Enable restraint validation Improve data quality
Carbohydrate remediation	Enable FAIR Better data validation
Provide ED map coefficients at FTP	Enable data reproducibility
Assembly Annotation by Depositor and Biocuration Automation	Increase Biocuration efficiency
Chemical Component Versioning	Better data management Automated tracking on changes
Streamlining EMDB release process with PDB	Enhance wwPDB collaboration Simplify weekly releases
Infrastructure Upgrade	Improve system maintenance
Improve Workflow for Ligand Validation	Improve data quality Increase Biocuration efficiency
Recalculation of wwPDB validation reports	Better data validation

Meeting Highlights wwPDB AC

- Plans endorsed for
 - Next Generation FTP Archive
 - PDBx/mmCIF for 3DEM
 - PDBx/mmCIF for Micro ED
 - PDBx/mmCIF for NMR
 - PDB China roadmap
 - PDB India roadmap
- Future role of BMRB in evolution



October 18, 2019 PDBj, Osaka University

Integrative Methods

PDB-Dev

- New website launched March 3rd at pdb-dev.wwpdb.org
 - ABI Development Building a Pipeline for Integrative/Hybrid Models (NSF DBI 1756248 to Brinda Vallat; funding ends August 2021)
 - Federating Structural Models and Data: Outcomes from A Workshop on Archiving Integrative Structures (2019) Structure 27: 1745-1759 doi: 10.1016/j.str.2019.11.002
- Integrated new validation developed by RCSB PDB at UCSF

PDB-Dev
Prototype Archiving System for Integrative Structures

Released Entries: 37

Home About Deposit Contact FAQ Browse Structures Keyword Search (e.g., NPC AND 306M) Search Tips

Welcome to PDB-Dev

PDB-Dev is a prototype archiving system for structural models obtained using integrative or hybrid modeling and is funded by the NSF ABI Development Program. Structural characterization of many complex macromolecular assemblies is increasingly carried out using integrative modeling, where a combination of complementary experimental and computational techniques is used to determine the structure. The structural models obtained through integrative modeling are collected, archived and disseminated to the public through PDB-Dev. Once the mechanisms for processing integrative models are fully established through PDB-Dev, key components will be integrated with the existing PDB and the PDB-Dev holdings will be moved into the PDB.

Released PDB-Dev Structures



News

Welcome to the new PDB-Dev website

The PDB-Dev web interface has been revamped to provide dynamic, responsive and mobile-friendly web pages. The newly designed website has been made possible due to an overhaul of our backend infrastructure. PDB-Dev website now includes a new service that facilitates search and retrieval of integrative structures archived in PDB-Dev. Simple search using macromolecular names, entry identifiers, experimental methods used, author names, software used and several other keywords are now supported. [Read more...](#)

Whitepaper from the integrative modeling community

In March 2019, a satellite workshop titled "Working towards federating structural models and data" was held at the Biophysical Society Annual meeting in Baltimore, Maryland to assess current progress and discuss further requirements for archiving integrative structures. The primary goal of the workshop was to bring together experts from different scientific communities contributing to integrative structural biology and build consensus for addressing the challenges involved in archiving integrative structures. A whitepaper summarizing the outcomes of the workshop was recently published in the journal *Structure*. [Read more...](#)

PDB-Dev
Prototype Archiving System for Integrative Structures

Released Entries: 36

Validation Report for PDBDEV_00000001

Overview Model details Data quality Model quality Fit to data used for modeling Fit to data not used for modeling Uncertainty

PDBDEV_00000001

This entry has 0 distinct model fits.

Fit of model to data used for modeling: SAS data
Fit of model to SAS data

Radius of gyration (R_g) estimates

R_g estimates were obtained from SASBOB.

R _g from Guinier analysis	R _g from P(r) plot
2.0	2.1

Questions and Comments?

Question: Any concerns about the Deposition/Biocuration work underway with our wwPDB partners?

New and Improved RCSB.org

Archive Management/Access
Data Exploration

John Westbrook

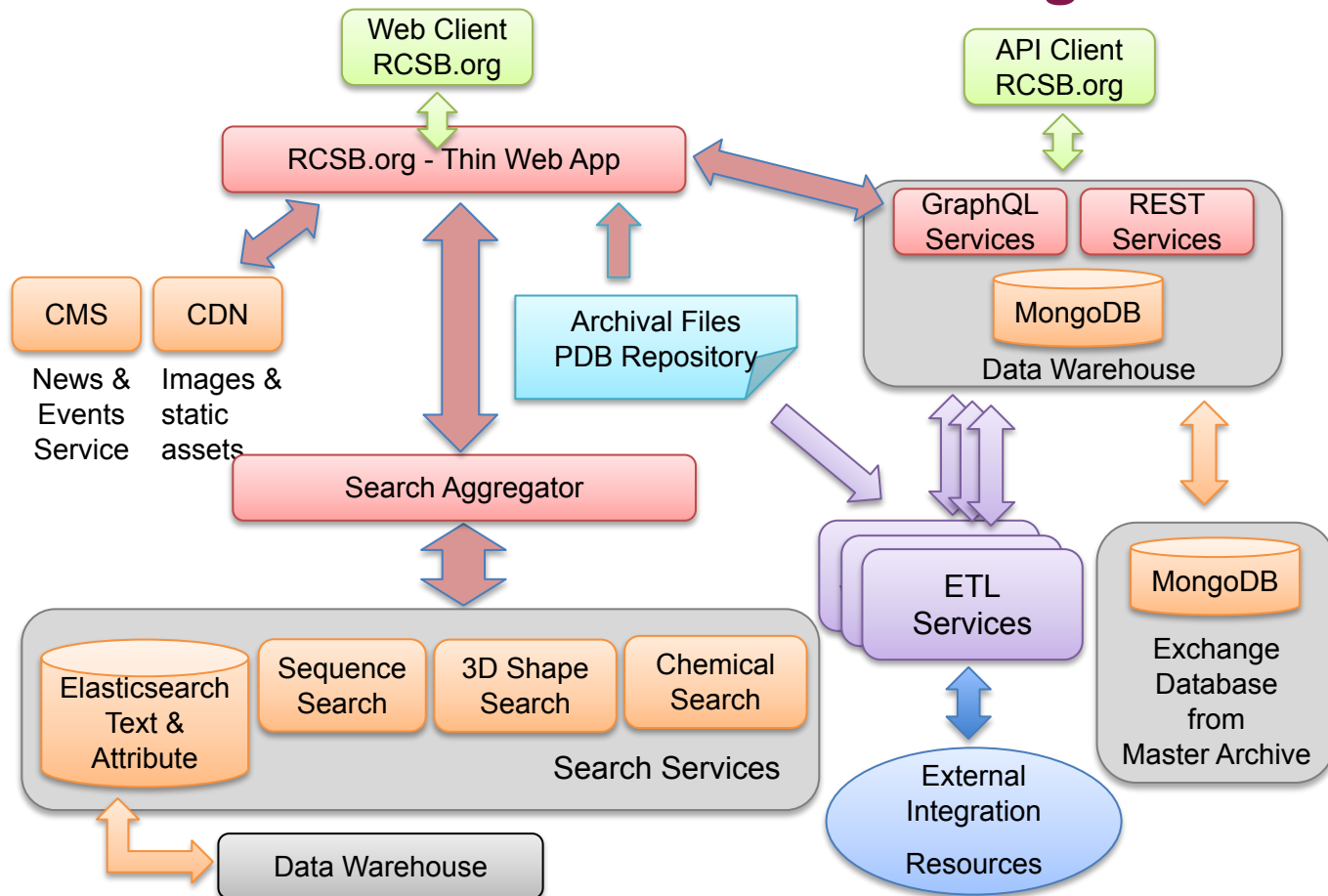
Questions: Additional Site and Search Functionality requests?



Archive Management/Access Highlights

- Upgraded Archive Management data storage system
- Continued productionization of new service architecture to support new RCSB.org and expanded programmatic data access
- Continued targeted remediation (carbohydrates) and extended data integration (NIH Common Fund Resources, PubChem)
- Continued OpenStack cloud migration of the weekly updates
- Migrating to more portable software packaging using Docker and Kubernetes

New Search Architecture Drives RCSB.org



Data Exploration in 2019: Improved RCSB.org

- Development of website design utilizing APIs for delivery of data to RCSB.org users
- New APIs supporting programmatic access to RCSB.org data for power users, external resources
- New website capabilities supporting
 - Enhanced Search and Delivery Backend Services (Elasticsearch/GraphQL)
 - Categorical Auto Suggest
 - Multi-Select Drill Down Refinement
 - New Advanced Search Query Builder UI
 - Integrated Full-Text, Attribute, Browsing, Sequence and Structure Search
 - Multiple types of results (*e.g.*, Assemblies, Entries, Polymer & Non-Polymer Entities)
 - Bookmarkable Search History integrated with MyPDB
 - Tabular Reporting
 - Batch Data Download

Timeline from Development to Deployment

- 2019
 - May: Demonstration at RCSB PDB AC meeting
 - Summer 2019: Coding
 - Fall 2019: Internal Alpha Testing
- 2020
 - January: Beta Testing begins
 - April 8, 2020: First Public Release
 - April: Bug fixes
 - May onwards: Feature Releases



Demonstrating the Power of Next Gen RCSB.org

Scenario: Find all PDB X-ray structures better than 2.5Å resolution (acceptable cutoff for structure guided drug discovery) of proteins that are >35% identical in amino acid sequence to SARS-CoV-2 Main Protease that have the same mechanism based inhibitor N3 bound to the target protein.

Outcome: Returned 6 Coronavirus Main Protease structures dating from 2005 (SARS: 2amq) to 2020 (SARS-CoV-2: 6lu7) all with N3 covalently attached to the active site Cys residue.

New Advanced Search Query Builder UI

[Search](#) [History](#) [Browse Annotations](#) [MyPDB](#) [Help](#)

Query: (Experimental Method equals "X-RAY DIFFRACTION" **AND** Data Collection Resolution (Å) < 2.5 **AND** Chemical ID(s) equals PRD_002214) **AND** Sequence = SLSGFRKMAFPSGKVEGCMVQVTCGTTTLNGLWLDDTVYCPRHVICTAEDMLNPNYEDLLIRKSNHSFLVQAGNVQLRVIGHSMQNCLLRKVDTSNPKTPKYKFVRIQPGQTFSVLACYNGSPSGVYQCAMRPNHTIKGSFLNGSCGSGVGFNIDYDCVSFCYMHMELPTGVHAGTDLEGKFYGPFDVDRQTAQAAGTDTTITLNVLAWLAAVINGDRWFLNRFITTLNDFNLVAMKYNYEPLTQDHVDILGPLSAQTGIAVLDMCAALKELLQNGMNGRTILGSTILEDEFTPFVDVWRQCQSGVTEG **AND** Target = Protein **AND** E-Value Cutoff = 1000000 **AND** Identity Cutoff = 0.35

Open In Query Builder  Save to MyPDB

Advanced Search Query Builder ?

Text ?

Experimental Method ▼ X-RAY DIFFRACTION ⬆ Add + NOT Count ×

AND Data Collection Resolution (Å) ▼ < ⬆ 2.5 + NOT Count ×

AND Chemical ID(s) ▼ PRD_002214 + NOT Count ×

AND / OR Add Field Add Subgroup Remove Group

Add Group

Sequence ?

SLSGFRKMAFPSGKVEGCMVQVTCGTTTLNGLWLDDTVYCPRHVICTAEDMLNPNYEDLLIRKSNHSFLVQAGNVQLRVIGHSMQNCLLRKVDTSNPKTPKYKFVRIQPGQTFSVLACYNGSPSGVYQCAMRPNHTIKGSFLNGSCGSGVGFNIDYDCVSFCYMHMELPTGVHAGTDLEGKFYGPFDVDRQTAQAAGTDTTITLNVLAWLAAVINGDRWFLNRFITTLNDFNLVAMKYNYEPLTQDHVDILGPLSAQTGIAVLDMCAALKELLQNGMNGRTILGSTILEDEF

Count Clear

PDB ID Target Protein ⬆ ? E-Value Cutoff ? Identity Cutoff % (Integer only) ?

Structure Similarity ?

Display Results as ? Structures ⬆

Count Clear 

39

Search Results Presented in Tabular Form

Displaying 1 to 6 of 6 **Structures**

Page 1 of 1

Display 25 per page

Structure Report

PDB ID	Structure Title	Experimental Method	Release Date	Structure Keywords	Structure Author	Resolution (Å)	Molecular Weight (Structure)	Number of Polymer Residues	Number of Atoms	
2AMQ	Crystal Structure Of SARS_CoV Mpro in Complex with an Inhibitor N3	X-RAY DIFFRACTION	2005-09-13	HYDROLASE	Yang, H., Xue, X., Yang, K., Zhao, Q., Bartlam, M., Rao, Z.	2.3	69.94	634	5111	☒
2HOB	Crystal structure of SARS-CoV main protease with authentic N and C-termini in complex with a Michael acceptor N3	X-RAY DIFFRACTION	2007-04-03	VIRAL PROTEIN	Xue, X., Yang, H., Shen, W., Zhao, Q., Li, J., Rao, Z.	1.95	34.56	312	2728	☒
2Q6F	Crystal structure of infectious bronchitis virus (IBV) main protease in complex with a Michael acceptor inhibitor N3	X-RAY DIFFRACTION	2008-02-12	HYDROLASE	Xue, X.Y., Yang, H.T., Xue, F., Bartlam, M., Rao, Z.H.	2	68.63	630	5039	☒
5EU8	Structure of FIPV main protease in complex with dual inhibitors	X-RAY DIFFRACTION	2015-12-30	HYDROLASE/HYDROLASE INHIBITOR	Wang, F., Chen, C., Liu, X., Yang, K., Xu, X., Yang, H.	2.447	34.31	313	2465	☒
5GWZ	The structure of Porcine epidemic diarrhea virus main protease in complex with an inhibitor	X-RAY DIFFRACTION	2017-03-29	HYDROLASE/HYDROLASE INHIBITOR	Wang, F., Chen, C., Yang, K., Liu, X., Liu, H., Xu, Y., Chen, X., Liu, X., Cai, Y., Yang, H.	2.444	67.69	626	4857	☒
6LU7	The crystal structure of COVID-19 main protease in complex with an inhibitor N3	X-RAY DIFFRACTION	2020-02-05	VIRAL PROTEIN	Liu, X., Zhang, B., Jin, Z., Yang, H., Rao, Z.	2.16	34.51	312	2500	☒

Displaying 1 to 6 of 6 **Structures**

Page 1 of 1

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Searches Saved and Shared in the Cloud *via* MyPDB

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[Search Queries](#) [Documentation](#) [Saved Queries](#) [Account Settings](#) [Sign out](#)

Signed in via Google as John Westbrook

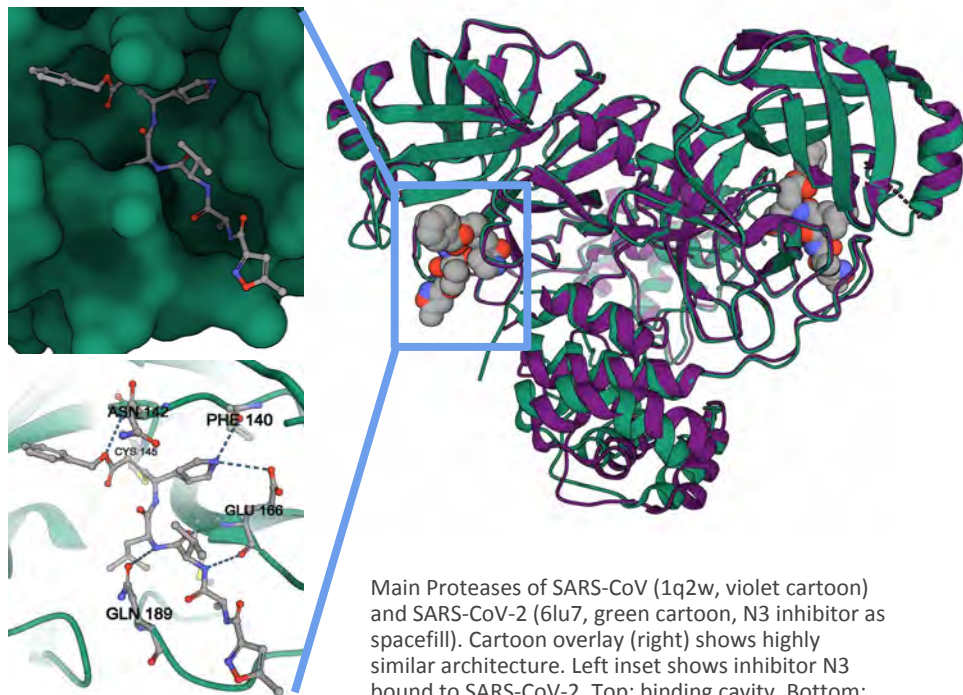
Query	Result Type	Count	Saved	Notify	Delete All
 (Experimental Method equals "X-RAY DIFFRACTION" AND Data Collection Resolution (Å) < 2.5 AND Chemical ID(s) equals PRD_002214) AND Sequence = SLSGFRKMAFPSGKVEGCMVQVTCGTTTLNGLW LDDTVYCPRHVICTAEDMLNPNYEDLLIRKSNHSLVQAGNVQLRVIGHSMQNCLLRKVDTSNPKTPKYKFV RIQPGQTFSVLACYNGSPSGVYQCAMRPNHTIKGSFLNGSCGSGVGFNIDYDCVSFCYMHMELPTGVHAGT DLEGKFYGPFDVRQTAQAAGTDTTITLNLVLAWLAAVINGDRWFLNRFTTTLNDFNLVAMKYNIEPLTQDHVDI LGPLSAQTGIAVLDMCAALKELLQNGMNGRTILGSTILEDEFTPFVVRQC SGVTEG AND Target = Protein AND E-Value Cutoff = 1000000 AND Identity Cutoff = 0.35	Structure	6	4/13/2020, 5:30:28 PM		

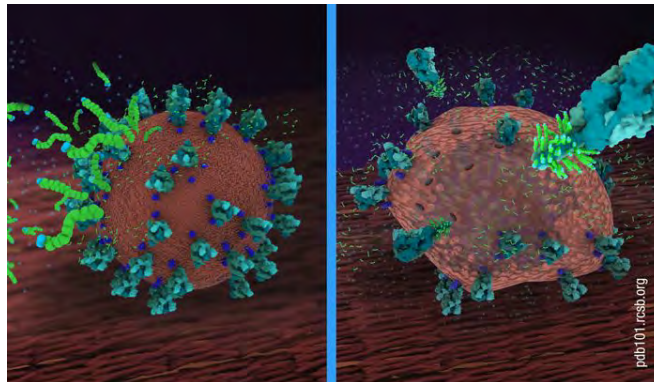
Contact Us

[Link to Search](#)

Mol* Released for Improved 3D Visualization

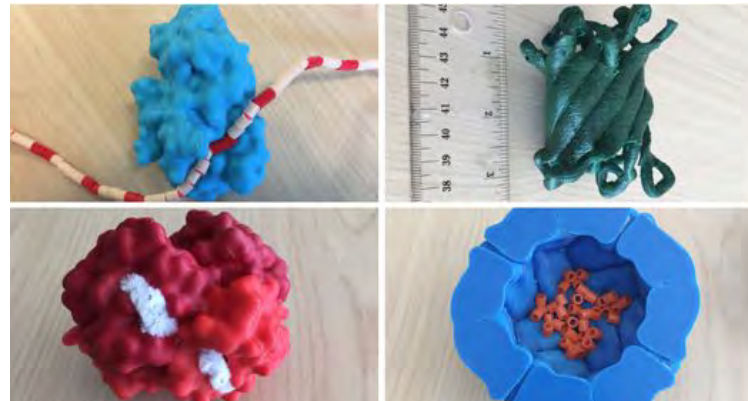
- Mol* (mol-star) community graphics library extends and supersedes NGL capabilities
 - Sequence Panel
 - Ligand Focus
 - 3D Validation Report
 - Assembly Symmetry
 - X-Ray and EM Density Maps
 - 3D Measurements
 - Custom Colors and Representations
- Available from RCSB.org and PDBe.org
- Collaborative wwPDB project





Questions and Comments?

Question: Additional Site and Search Functionality requests?



Outreach/Education

Question: Suggestions for new materials and virtual venues for celebrating PDB50 throughout 2021?

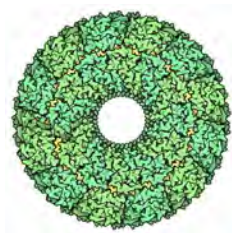
PDB-101 in 2019: ~666K users, ~2M page views

- 2019 calendar
- 12 Molecules of the Month
- Gallery of David Goodsell's Art
- Video Challenges
 - Antimicrobial Resistance completed
 - Content for Drugs & Brain
- Video: *Penicillin and Antibiotic Resistance*

[Measles Virus Proteins](#)

March 2019

14,721 views



- Flyer: *Antibiotics in Action*
- Poster/Animation: *Superbugs! How Bacteria Evolve Resistance to Antibiotics*
- Global Health pages
- GPCR Paper Model
- Guide: *PDBx for Beginners*
- PDB & Data Archiving Curriculum
- MotM User Survey



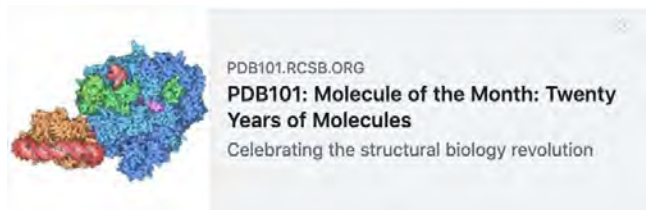
[Penicillin and Antibiotic Resistance](#)

21,306 views on YouTube

Celebrating 20 Years of *Molecule of the Month*

2019 [Survey](#): 339 responses

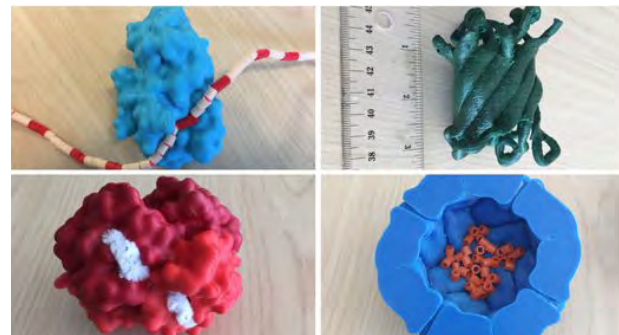
- ~50% use MOTM for teaching
- ~60% work at a college/university
- ~78% work in Biology & Biochemistry



[January 2020](#)



Image of Measles Virus Proteins
(on cover) selected as 2019
FASEB BioArt Winner



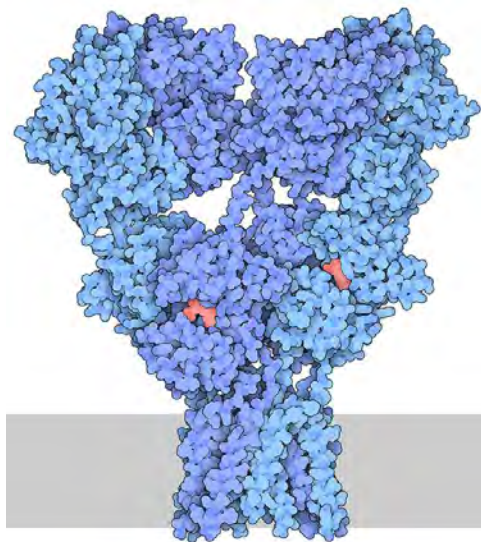
[3D print files for popular MOTMs released Q1 2020](#)

- alpha-amylase, ferritin, GFP, and hemoglobin.
- Highlights a special molecular feature
- Suggested modeling e.g., making heme molecules, to help tell a molecular story

Health Focus (2020-21): Drugs and the Brain



Molecular origami: [GPCR](#)



[AMPA Receptor](#), MOTM July 2019



[Video Challenge for High School Students: Molecular Mechanisms of Opioid Action \(Fall 2019 - Spring 2020\)](#)

Working with Teachers and Students



RCSB PDB at the New Jersey Science Convention for teachers



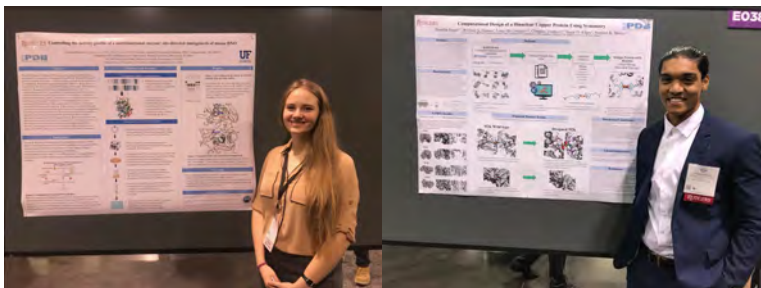
High School PDB Depositors:
PDB 6PEY: MTHFR with mutation



QUBES/BioQuest Meeting for
UG Educators



Systems/Network Medicine
Conference for Clinicians and
Medical Researchers

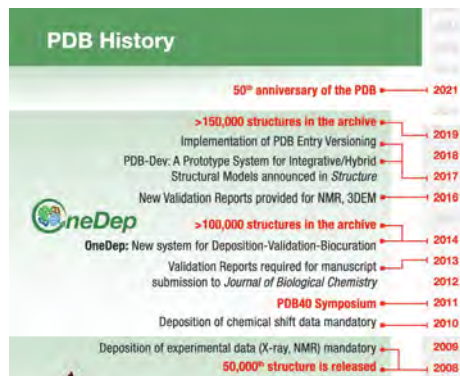


Galyna and Jitendra presented at
Annual Biomedical Research Conference for Minority Students (ABRCMS)



Buffalo Case Studies
Conference for
UG Educators & HS Teachers

PDB50: Celebrating a Golden Anniversary in 2021



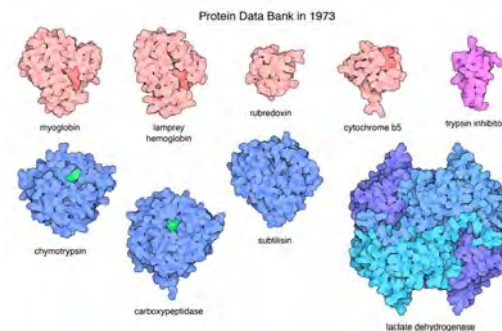
Historical Retrospectives



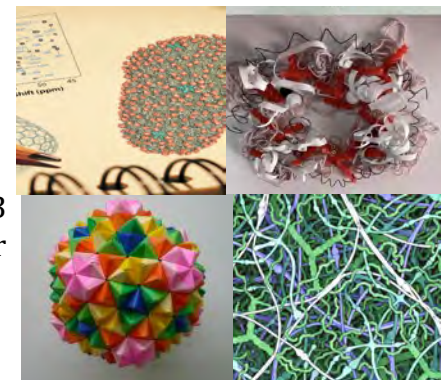
PDB-themed issue of *Journal of Biological Chemistry* in development

Shown: Coronavirus issue

Molecule of the Month article



Joint wwPDB 2021 calendar





Questions and Comments?

Question: Suggestions for new materials and virtual venues for celebrating PDB50 throughout 2021?



Operations and Funding

Questions:

- *Other federal funding sources we should target?*
- *Any philanthropic organization suggestions?*
- *Suggestions for financial support for wwPDB PDB50 Symposia?*

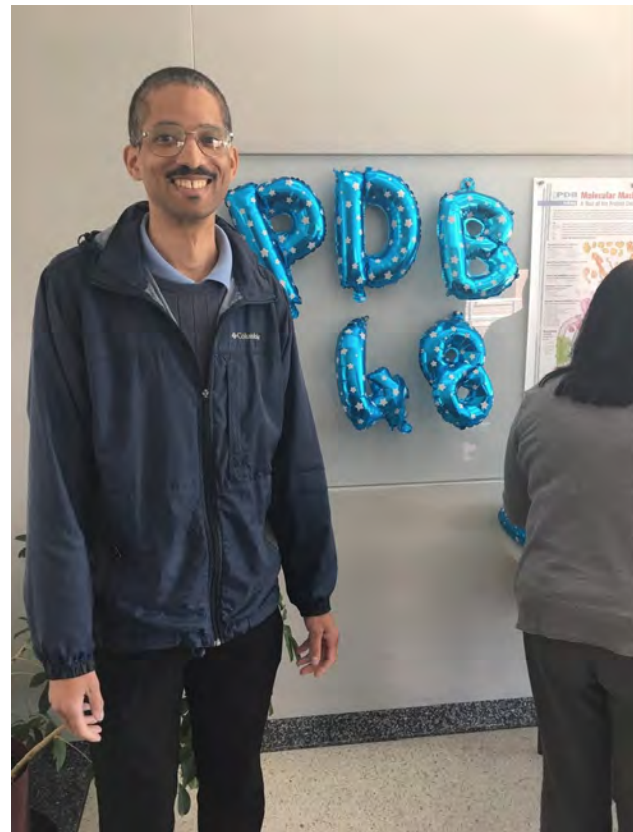
Operations: Team Advancements/Transitions

Rutgers

- New Biocurator: Gregg Crichlow
- New Hires Pending
- Departures: Wendy Tao (Developer),
Luigi Di Constanzo (Biocurator)

UCSD

- Promotion to Site Manager: Jose Duarte
- Departures: Chris Randle (DevOps),
Dmytro Guzenko (PostDoc)
- New Hires Pending



Questions and Comments?

- *Other federal funding sources we should target?*
- *Any philanthropic organization suggestions?*
- *Suggestions for financial support for wwPDB PDB50 Symposia?*

Celebrating PDB Golden Anniversary in 2021

- Wed May 5, 2021, following ASBMB Meeting in Indianapolis, IN

Confirmed Speakers: Eddy Arnold, Helen Berman, Wah Chiu, Johann Deisenhofer, Juli Feigon, Angela Gronenborn, Jenny Martin, Tom Blundell, Alexandre Bonvin, Zihe Rao, Stephen L. Mayo, Hao Wu

- Sat July 31, 2021, beginning of ACA Meeting in Baltimore, MD

Confirmed Speakers: Frances H. Arnold, Squire J. Booker, Rafael M. Couñago, Wayne A. Hendrickson, Eva Nogales, Erica Ollman Saphire, John Rubinstein, Andrej Sali, Chris Sander, Cynthia Wolberger

- October 20-21, 2021, EMBL Heidelberg

Invited Speakers: Bissan Al Lazikani, Cheryl Arrowsmith, Madan Babu, Drew Berry, Patrick Cramer, Don Hilvert, Martin Jinek, Alwyn Jones, Christine Orengo, Lori Passmore, Jane Richardson, Andrew Senior, Dave Stuart, Janet Thornton, Nicolas Tomae

- December 2021: AsCA, Malaysia (TBD)

- JBC Reviews Special Issue March 2021
(Co-Editors: Lila Gierasch and Helen M. Berman)

Funds being raised by

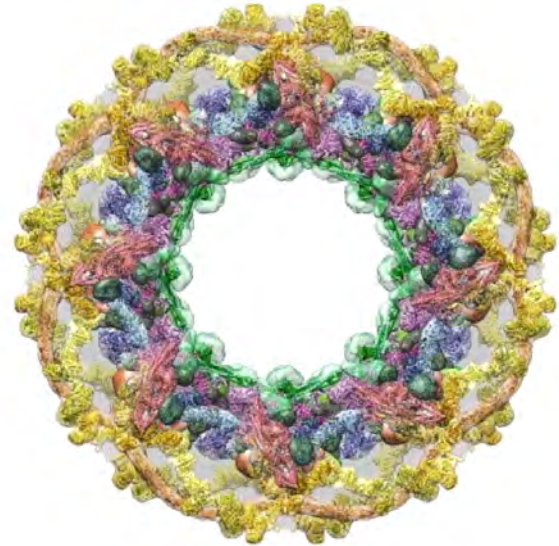


Worldwide
Protein Data Bank
Foundation

2019-2023: Meeting the Challenges Ahead

Structural biology is evolving

1. Growth/Complexity
2. Evolving Experimental Methods (SFX/XFEL, 3DEM)
3. Emerging Integrative/Hybrid Met



I/H Methods Structures

552-protein yeast Nuclear Pore Complex

Kim et al. (2018) *Nature* 555, 475-82

PDBDEV_00000010; PDBDEV_00000011; PDBDEV_00000012

Acknowledgements



RCSB.ORG

info@rcsb.org

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Disease, and National Cancer Institute,
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US Department of Energy (DE-SC0019749)

RCSB PDB is hosted by:

RUTGERS

UC San Diego

SDSC SAN DIEGO
SUPERCOMPUTER CENTER

UCSF
University of California
San Francisco



Member, Worldwide Protein Data Bank (wwpdb.org)



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Group Screenshot Photo



Additional Question: Sunsetting PDB Legacy Format

- Legacy PDB Format Files are increasingly un-FAIR vehicles for content delivery
- Worked with software developers to enable PDBx/mmCIF adoption
- PDB Legacy Format deprecated for X-ray structure deposition (July 2019)
- As a transitional measure, PDB converts PDBx/mmCIF entries that cannot be represented in PDB Format to one (or more) PDB Format Files with limited record types using an automated nomenclature re-mapping strategy
- Continued production and delivery of these 'tar' file bundles of PDB Format Files (w/ limited records) will NOT support adoption of coming extensions for:
 - Branched entities that improve carbohydrate remediation
 - Identifier code character expansion (PDB and Chemical Component IDs)
- Delivery of PDB Legacy Format files is slowing adoption of PDBx/mmCIF
- *What advice do you have regarding sunsetting of PDB Legacy Format?*

**Thank you for your
contributions**

