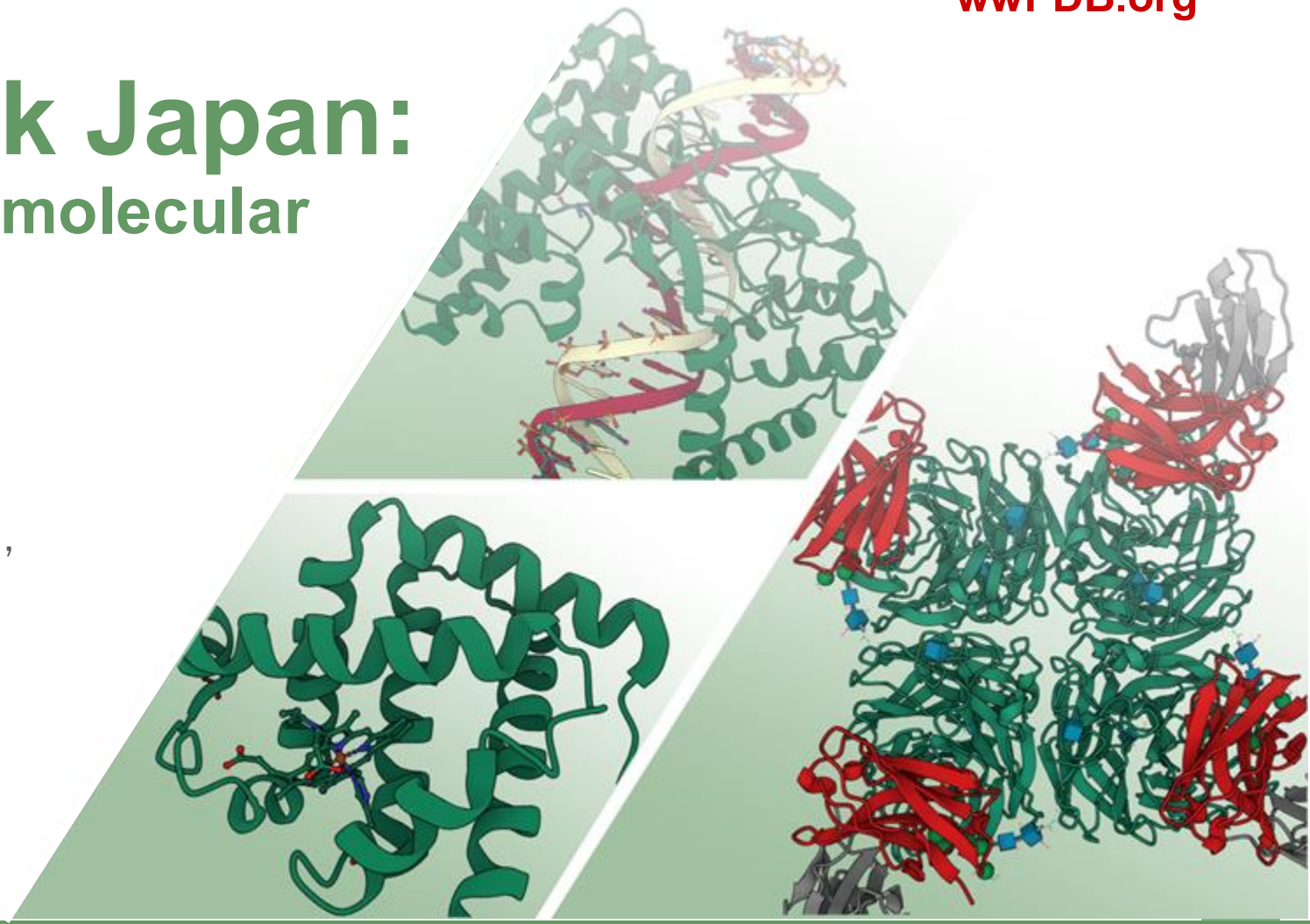
PDBj
Protein Data Bank Japan

WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB.org

Protein Data Bank Japan:
the Asian hub of 3D macromolecular structural data

Genji Kurisu, Ph.D.
Institute for Protein Research,
Osaka University



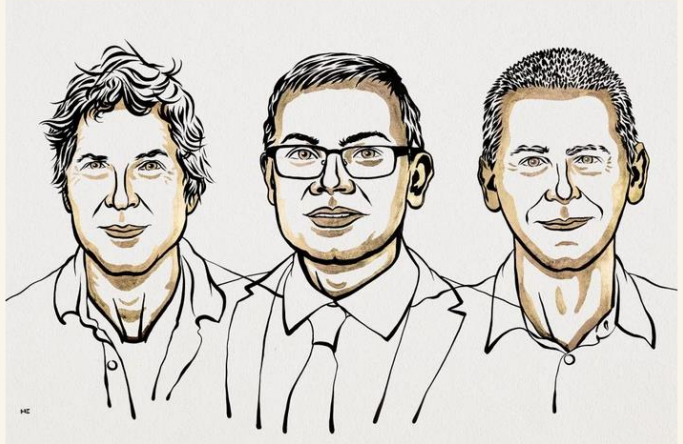
Congratulations!!

John Jumper said "I also want to really thank the giants on whose shoulders we stand. I thank the entire experimental community, the people that developed the ability to measure protein structures, **especially to Helen Berman and other pioneers of the Protein Data Bank, the PDB, who had the foresight to put these data together to make it available so that they would ultimately enable not just the insights of experimentalists, but the training on which we're able to--** our ability to train these models on the incredible work of the scientific community. It's humbling every time we train on years of effort. Each data point is years of effort from someone training to be a PhD student or for someone who has already gotten their PhD."

The 2024 chemistry laureates

The Nobel Prize in Chemistry 2024 was awarded with one half to David Baker "for computational protein design" and the other half jointly to Demis Hassabis and John M. Jumper "for protein structure prediction".

Demis Hassabis and John Jumper have successfully utilised artificial intelligence to predict the structure of almost all known proteins. David Baker has learned how to master life's building blocks and create entirely new proteins.



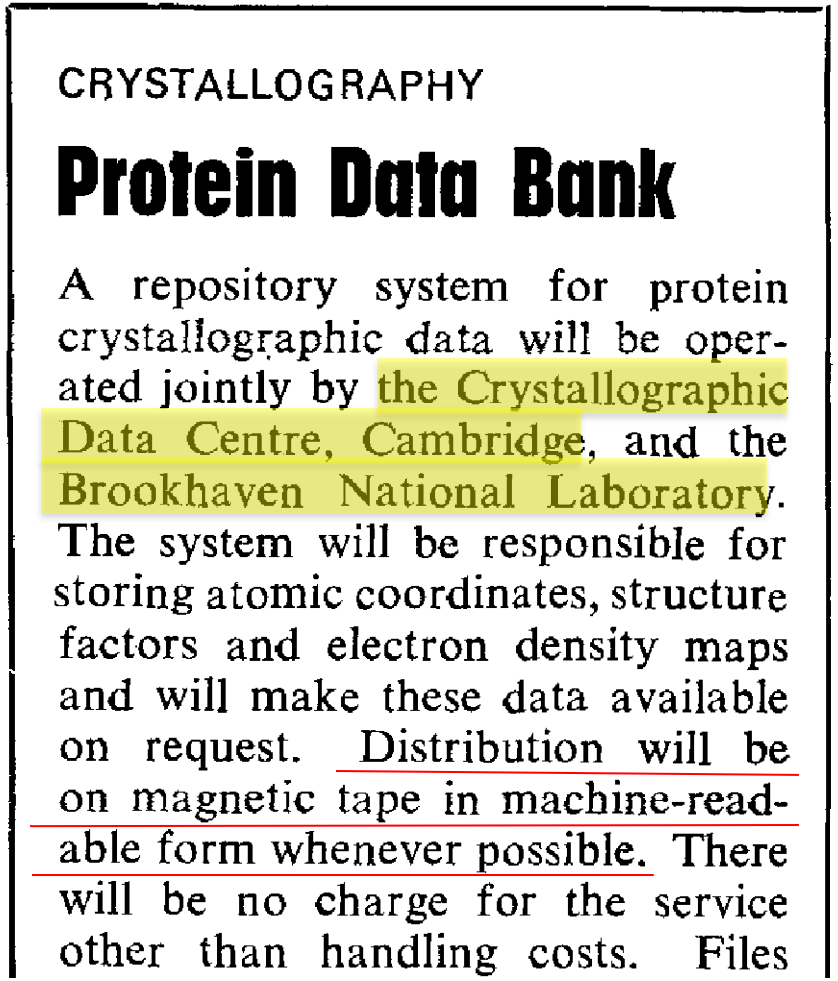
David Baker, Demis Hassabis and John Jumper. Ill. Niklas Elmehed © Nobel Prize Outreach

https://www.nobelprize.org/

Protein Data Bank was born in 1971

PDBj Protein Data Bank Japan
as a member of wwPDB PROTEIN DATA BANK

- PDB is the single global macromolecular structure archive.(est. in 1971 with 7 entries)
- From 1979, IPR Osaka University received the MT from BNL and distributed the PDB data to Japanese users.
- Since 2000, PDBj Protein Data Bank Japan has been managed at Institute for Protein Research, Osaka University as a member of the wwPDB, to curate and process the deposited data for an open and single archive.



CRYSTALLOGRAPHY

Protein Data Bank

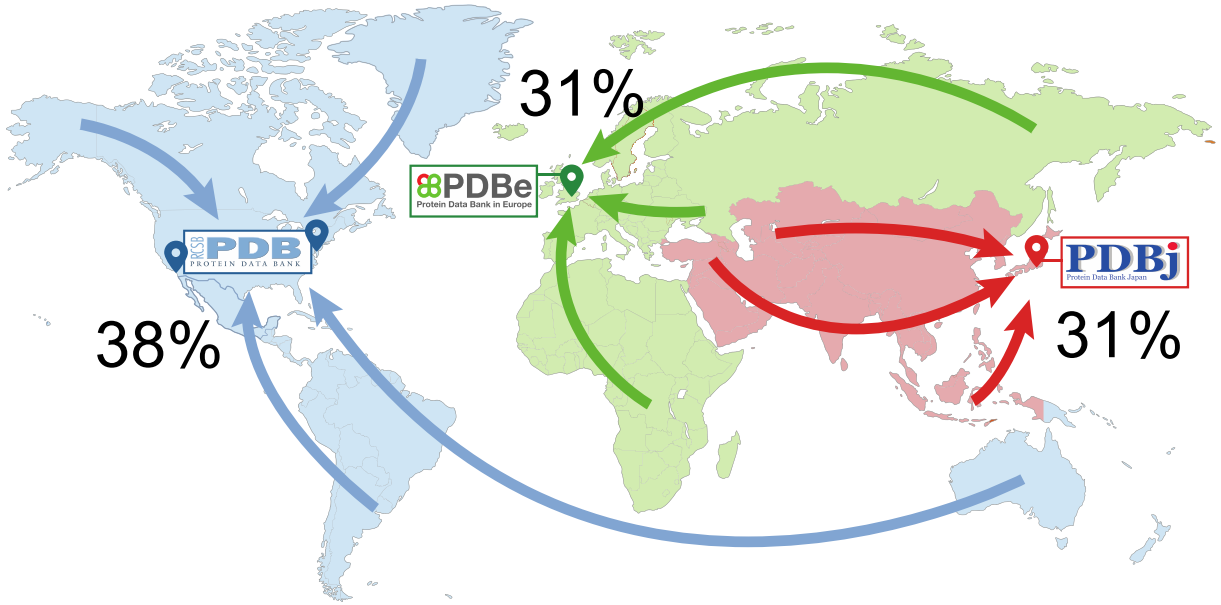
A repository system for protein crystallographic data will be operated jointly by the Crystallographic Data Centre, Cambridge, and the Brookhaven National Laboratory. The system will be responsible for storing atomic coordinates, structure factors and electron density maps and will make these data available on request. Distribution will be on magnetic tape in machine-readable form whenever possible. There will be no charge for the service other than handling costs. Files

Nature New Biology **233**, page 223 (1971)

PDB is jointly managed by wwPDB

PDBj Protein Data Bank Japan
as a member of wwPDB PROTEIN DATA BANK

Geographical deposition in 2023



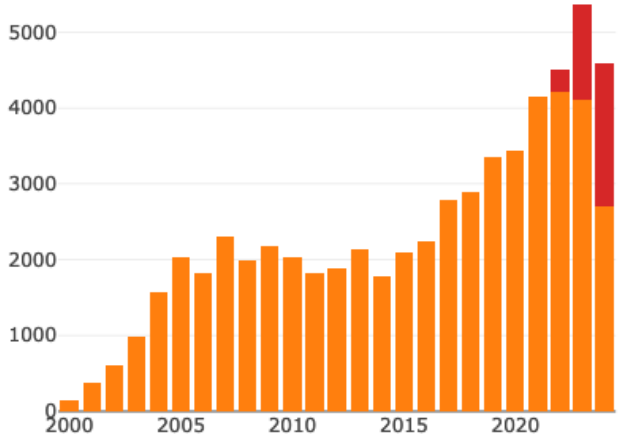
wwPDB PROTEIN DATA BANK

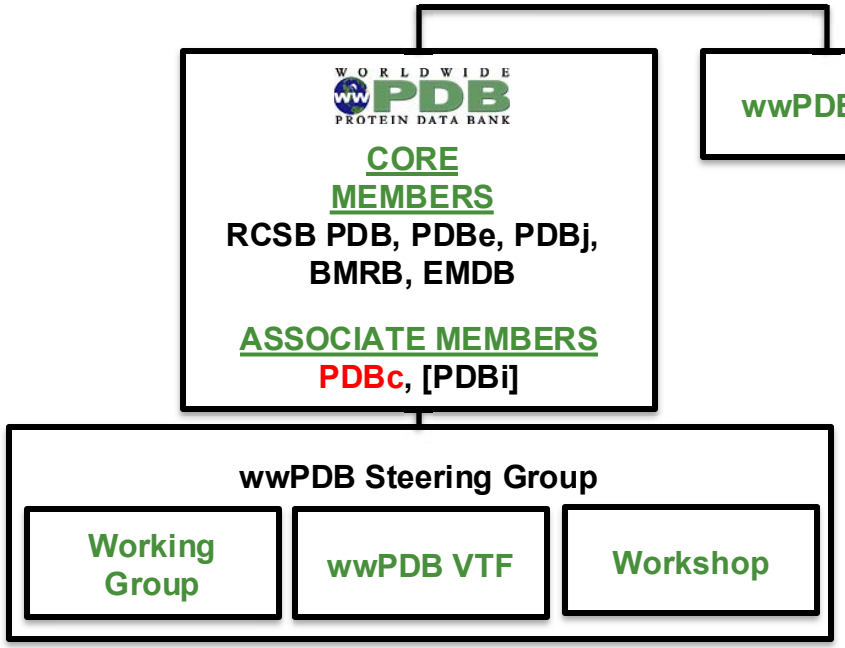
RCSB PDB PROTEIN DATA BANK | PDBe Protein Data Bank in Europe | PDBj Protein Data Bank Japan | BMRB Biological Magnetic Resonance Data Bank | EMDB Electron Microscopy Data Bank

Launch of Protein Data Bank China

PDBj Protein Data Bank Japan
as a member of wwPDB PROTEIN DATA BANK

Deposited to PDBj
Processed by PDBj and PDBc





letters to the editor

Acta Cryst D STRUCTURAL BIOLOGY
ISSN 2059-7983

Announcing the launch of Protein Data Bank China as an Associate Member of the Worldwide Protein Data Bank Partnership

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Accepted 21 July 2023

Edited by R. J. Read, University of Cambridge, United Kingdom

This paper is dedicated to the International Union of Crystallography on the occasion of its 75th anniversary.

Keywords: macromolecular crystallography; nuclear magnetic resonance; three-dimensional cryo-electron microscopy; Protein Data Bank; Biological Magnetic Resonance Bank; Electron Microscopy Data Bank; Worldwide Protein Data Bank.

The Protein Data Bank (PDB) is the single global archive of atomic-level, three-dimensional structures of biological macromolecules experimentally determined by macromolecular crystallography, nuclear magnetic resonance spectroscopy or three-dimensional cryo-electron microscopy. The PDB is growing continuously, with a recent rapid increase in new structure depositions from Asia. In 2022, the Worldwide Protein Data Bank (wwPDB; https://www.wwpdb.org/) partners welcomed Protein Data Bank China (PDBc; https://www.pdbc.org.cn) to the organization as an Associate Member. PDBc is based in the National Facility for Protein Science in Shanghai which is associated with the Shanghai Advanced Research Institute of Chinese Academy of Sciences, the

Current PDB Archive Status

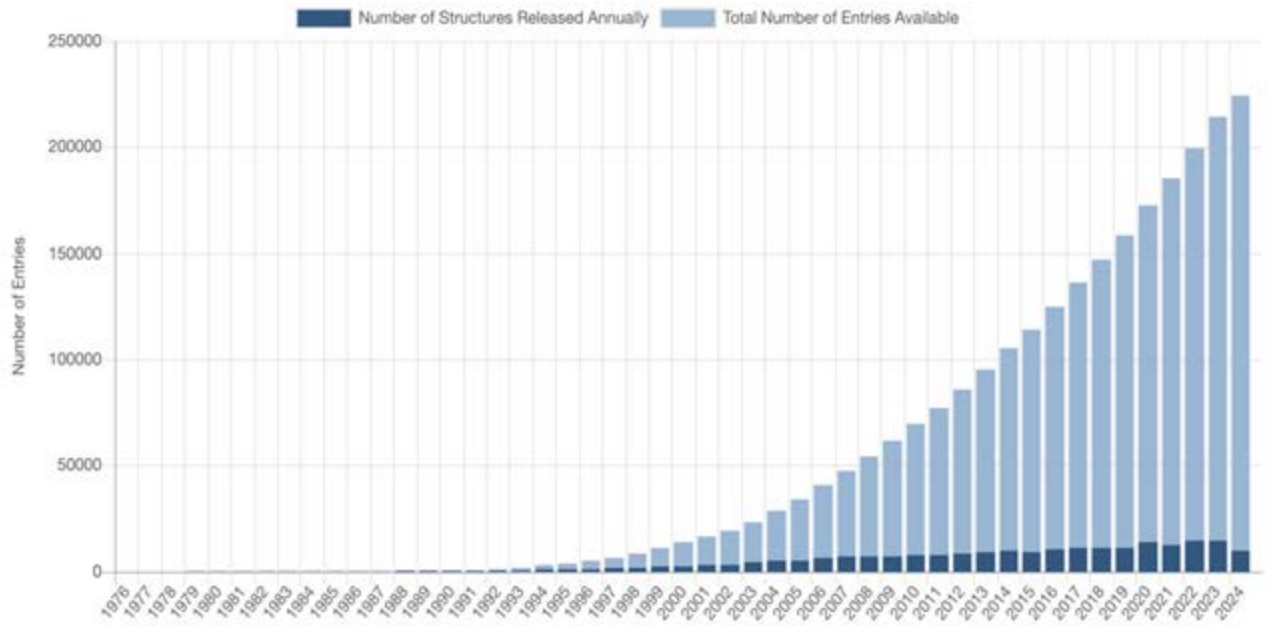
- Total Entries=224,201
  (as of 8/29/2024)

- Core Archive Storage
  - OneDep Sessions: ~96 TB
  - ftp(legacy + versioned): ~1.7 TB
  - ftp snapshots: ~13.6TB
  - EMDB ftp: ~18.5 TB

- **PDB-IHM data now being served alongside PDB structures**

- Both PDB and PDB-IHM data also being housed and delivered by Amazon Web Services (AWS) with no storage or egress fees

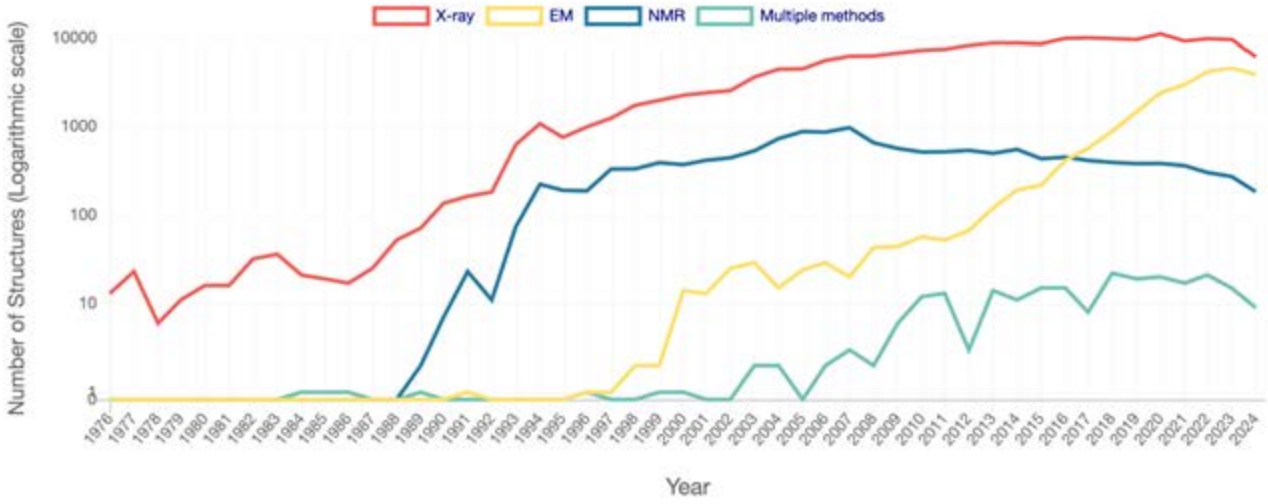
- NextGen archive now serving enriched annotation in the atomic coordinate files (https://files-nextgen.wwpdb.org)



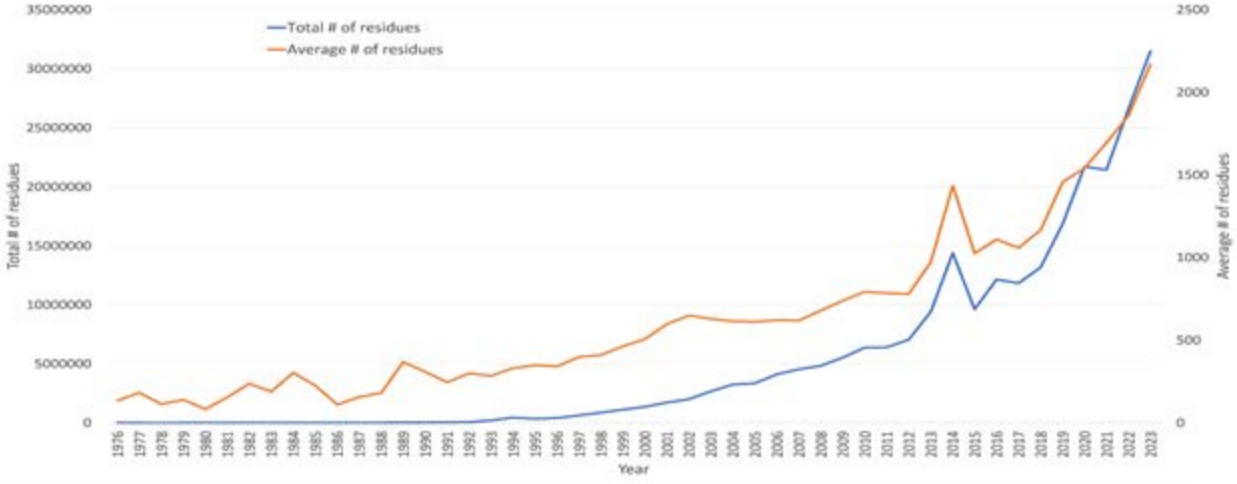
PDB Archive Growth

- Year-end holdings 224,201
- 14,468 new entries released
- Archival entries growing in both size and complexity
- Record 4,579 new 3DEM entries released
  - ~12% increase *versus* 2022

Growth of PDB Archive



Growth of Residues



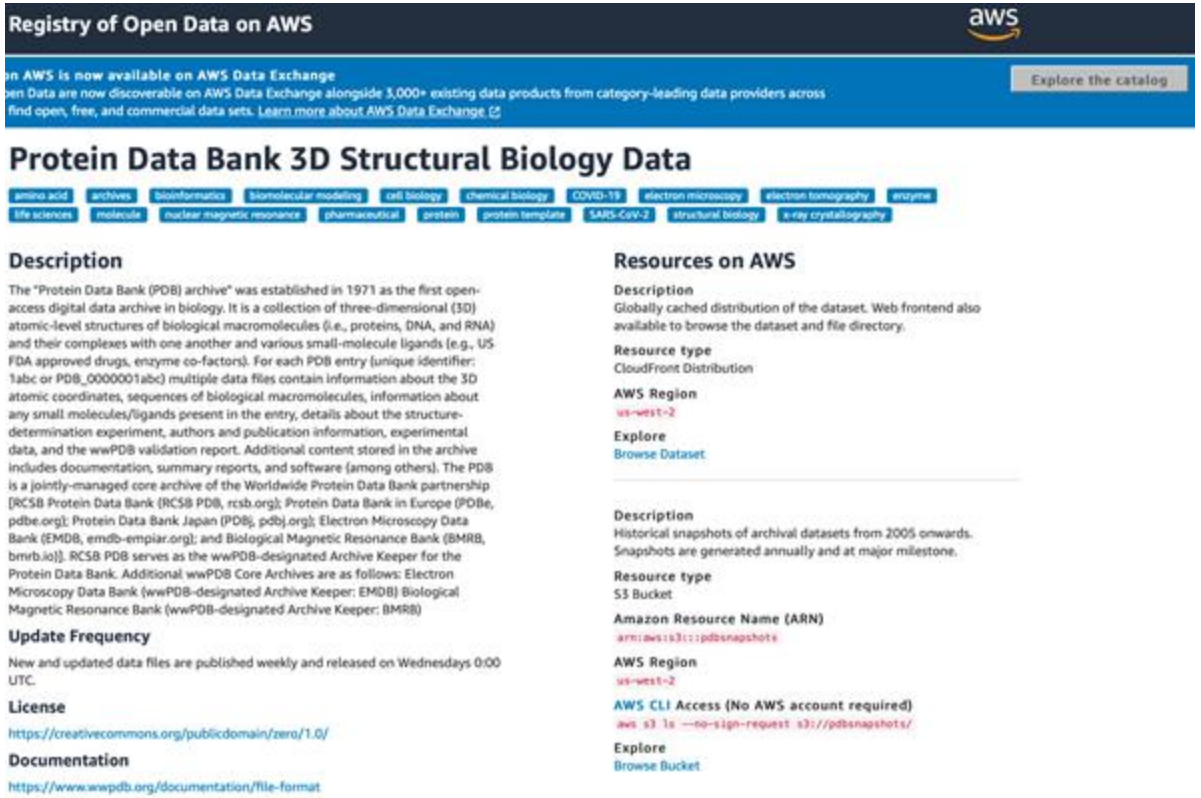
PDB Data Delivery by AWS

- **Exactly Same Data** are distributed from RCSB PDB, PDBe and PDBj

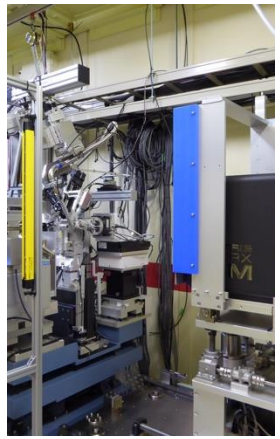
- Amazon Web Services (AWS) Open Data Sponsorship Program now housing and delivering PDB data
  - No storage fees charged to wwPDB
  - No egress fees charged to PDB users

- Current AWS holdings include:
  - Annual PDB Archive Snapshots
  - Current PDB FTP Archive (updated weekly)

- AWS can deliver PDB data faster than RCSB PDB, PDBe, or PDBj!



Data are Curated, Validated and Processed into PDB, BMRB or EMDB Archives

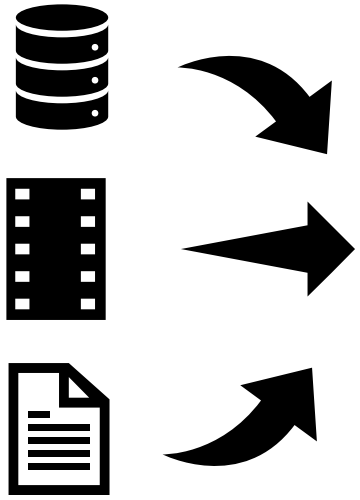


Crystallography

Cryo-Electron Microscopy

NMR Spectroscopy

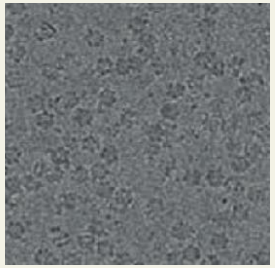
Experimental Data
Experimental Condition,
Sample information,
Related Information



PDB

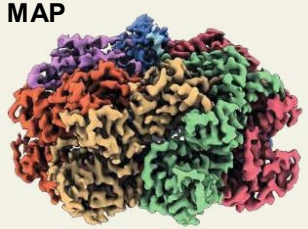
Biocuration
Link to External Data
Validation
Standardlization

RAW IMAGE



Where to share data
Electron Microscopy Public Image Archive (EMPIAR)

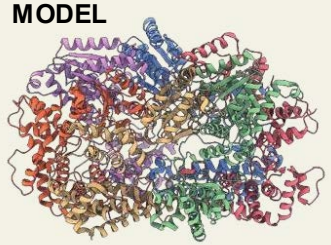
MAP



Electron Microscopy Data Bank (EMDB)

This is then combined with the known pr otein sequence to create a nal model showing the placement of atomic groups.

MODEL

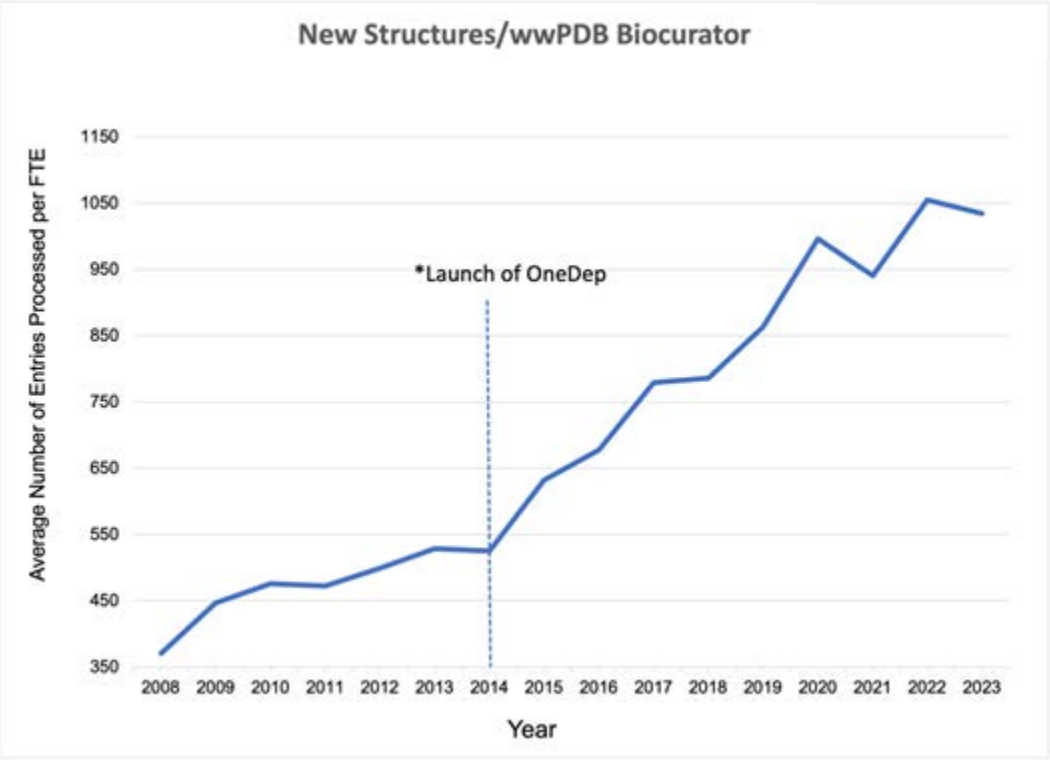


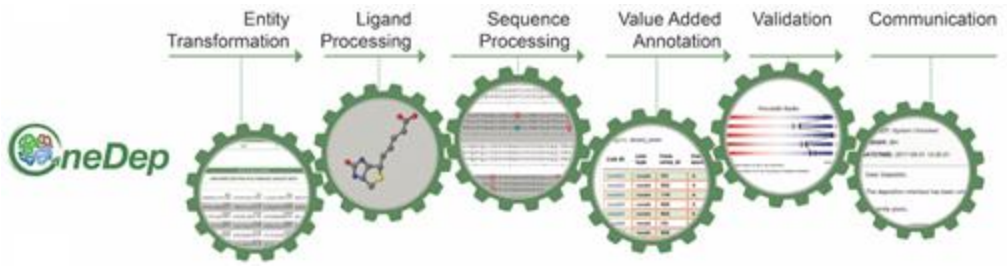
Protein Data Bank (PDB)

Chemical Compounds

wwPDB Biocurator Productivity

- 17,064 depositions in 2023
- Improved efficiency for biocurating incoming depositions
  - Auto-approve entries w/o corrections
  - Automated validation runs without UI access
  - Provide site specific setting on automated assembly annotation without UI access
  - Improved automation of ligand processing for unambiguous ligand cases
  - Improve efficiency by skipping PISA calculations for NMR, EM and large X-ray entries
- New sequence builder tool supports chimeric proteins
- Improved use of author-provided ligand restraints for graph search





wwPDB Validation

http://www.wwpdb.org/task/validation-task-forces

- Adopted recommendations from VTFs and workshops (e.g., LVW, EM)
- Validation report offered at four different stages
- Provided anonymous standalone validation server and API
  - Server: validate.wwpdb.org
  - API: wwpdb.org/validation/onedep-validation-web-service-interface
- Submission of **wwPDB-official Validation Report** during manuscript review process is mandatory (Nature, Cell, Science, Structure, Acta D & F, NAR, FEBS, J Biol Chem, J Immunology, eLIFE, PLoS One, Protein Sci, Angew Chem Int Ed Engl, SCI Rep)

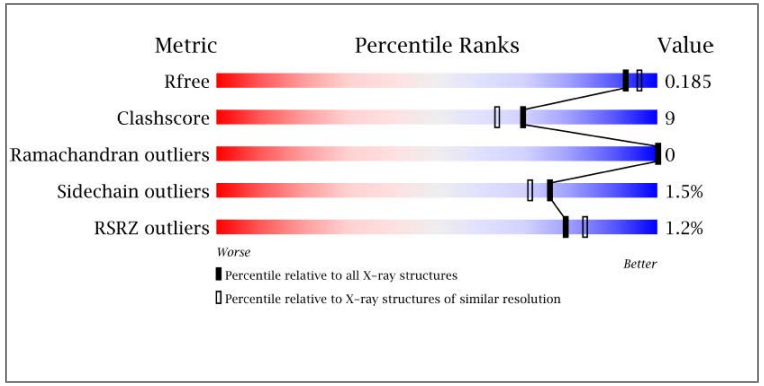
1. **Structure Determination**
   Pre-validate data independently before deposition
2. **Deposition**
   Mandatory acknowledgement of report produced during deposition
3. **Biocuration**
   wwPDB-official report for journal submission
4. **Public Release**
   Report available for all released PDB entries

Quality Control by Validation Report

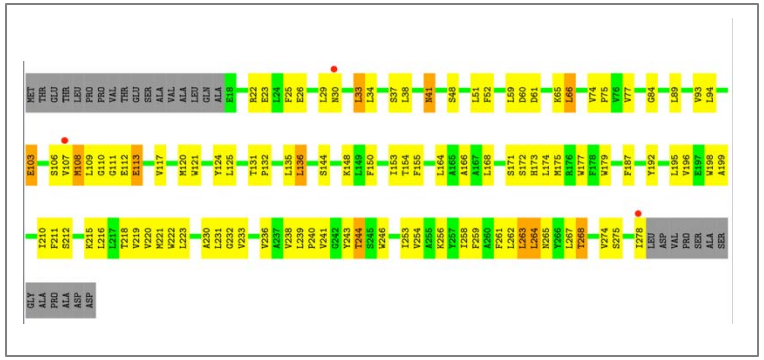
- Model Quality
  - Bond lengths and angles (outlier info, RMS-Z)
  - Chirality, planarity
  - Close contacts (including worst clashes, MolProbity clash score)
  - Torsion angles (Ramachandran statistics, protein rotamers)
  - Ligand geometry (Mogul analysis)

- Residue Plots
  - Residues with model-quality outliers (0, 1, 2, >2)
  - Residues with RSR-Z > 5 are highlighted
  - Residues not observed

Overall Quality Summary

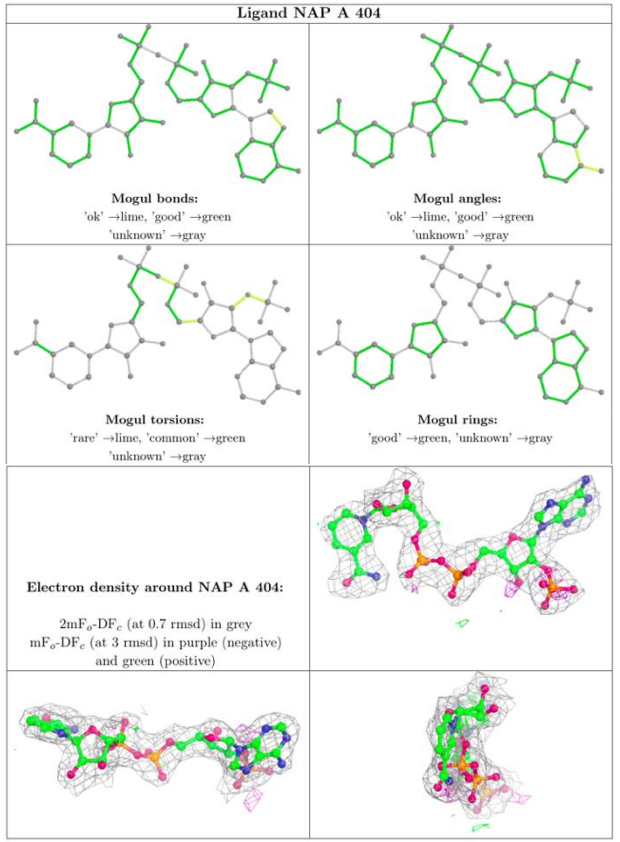


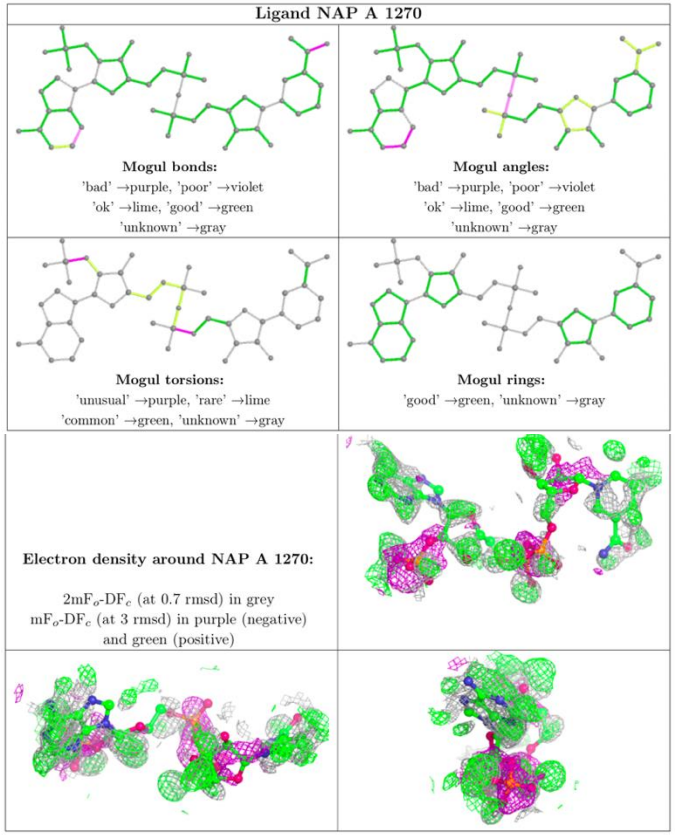
Residue Plots



wwPDB Validation Improvements: Ligands

- Partnership with Global Phasing Ltd. and CCDC
- Ligand of Interest (LOI) highlighted
- 2D views of geometrical quality
- 3D views of electron density fits for X-ray

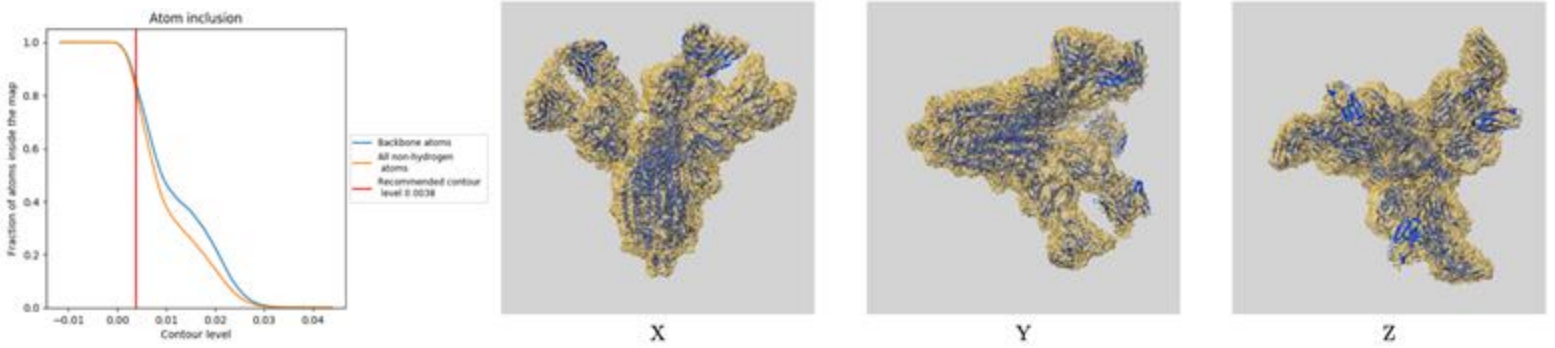




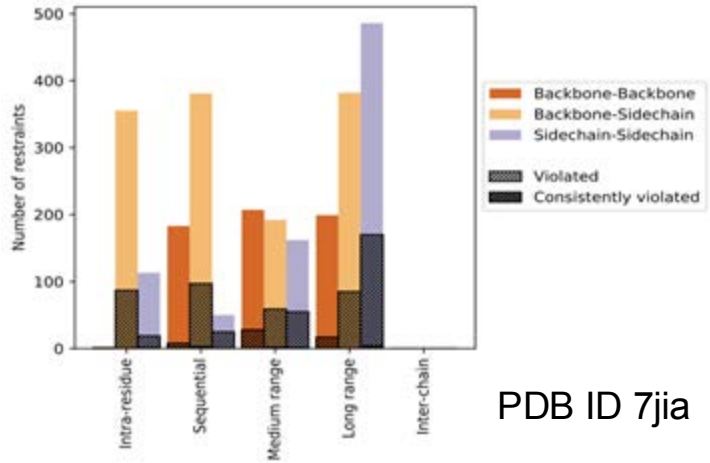
Feng, Z. *et al.*, Structure, 2021 doi: 10.1016/j.str.2021.02.004

wwPDB Validation Improvements: 3DEM and NMR Structures

- EM map volume analysis
  - The fit of model to the map at residue level and global visual overlay
  - Map analysis and visualization
- NMR restraints assessments
  - Distance and dihedral angle restraints with graphical and tabular statistics
  - Available for restraints deposited in single NEF/NMR-STAR formats



PDB ID 7cwu



PDB ID 7jia

Linked Data by Knowledge Graph (RDF)

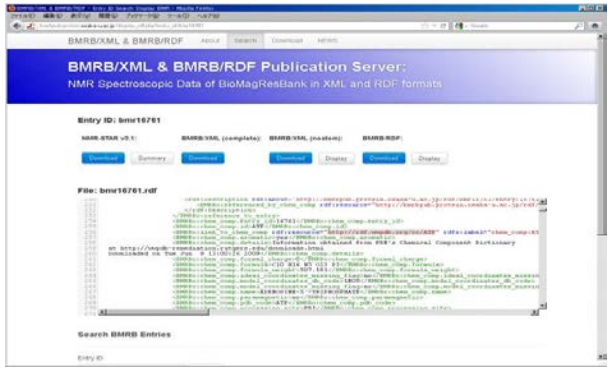
PDBj Protein Data Bank Japan
as a member of wwPDB PROTEIN DATA BANK

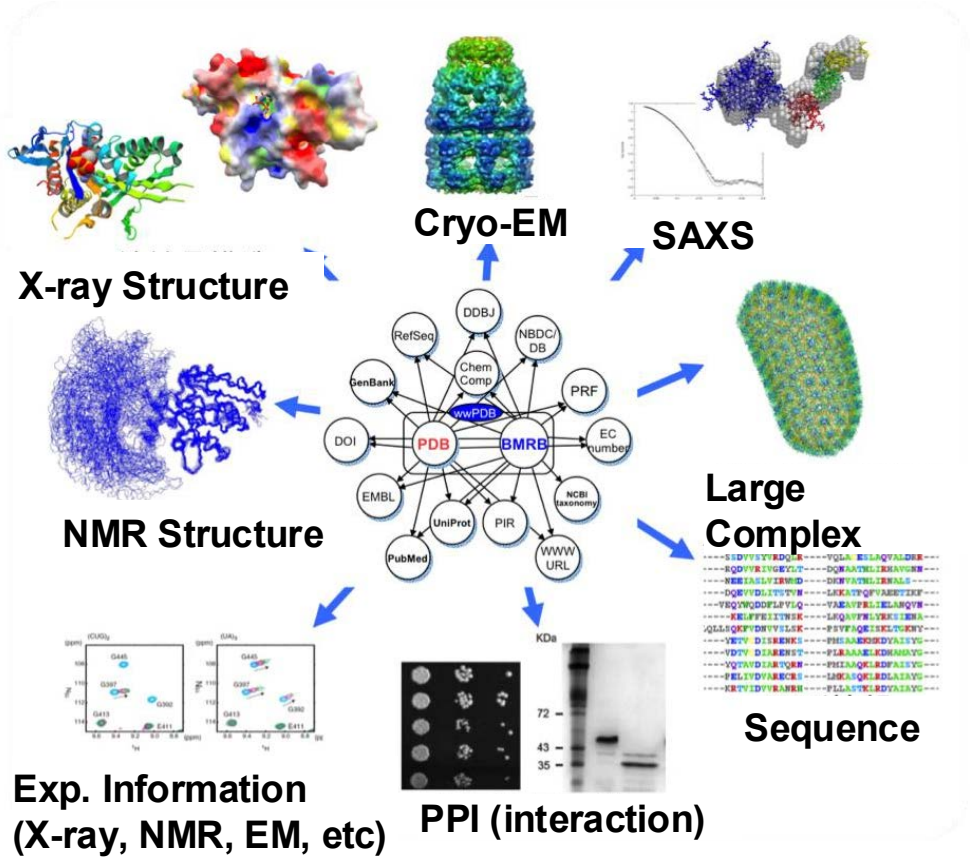
wwPDB/RDF

http://rdf.wwpdb.org/

BMRB/RDF

http://bmrbpub.protein.osaka-u.ac.jp



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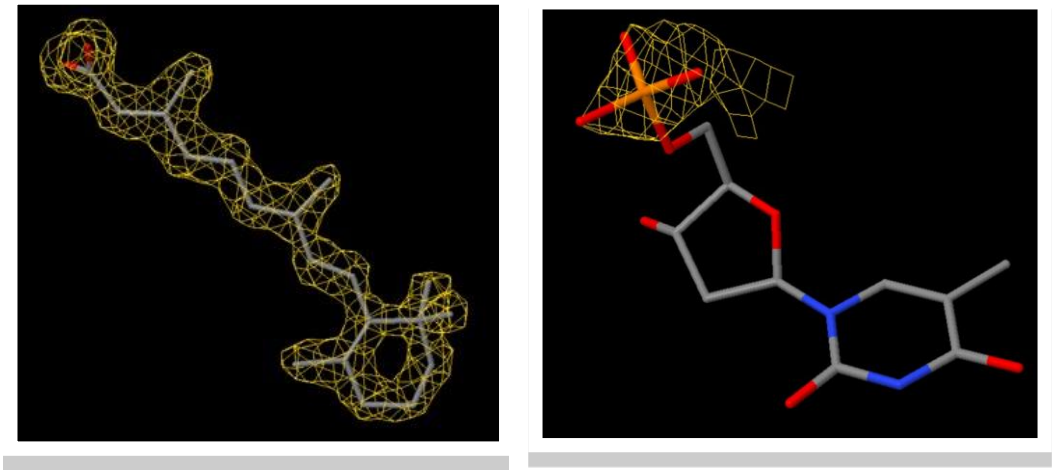
Kinjo et al. (2012) Nucl. Acids Res. 40, D453-D460.
Yokochi et al. (2016) J. Biomed. Semantics, 7:16.

Validation Report and Linked Data enable Machine-based entry selection

- Users can filter the entries with the bound chemical compounds by biological function
- Users can select the best/better entries with the validation parameters calculated by the corresponding experimental data stored in PDB, BMRB or EMDB.



Both entries are at 2.0 Å resolution
Left : RSR=0.10, CC=0.95
Right : RSR=0.41, CC=0.70

Muti-language service in PDBj.org

208844
数据于2023-08-23公开中

PDBj
Protein Data Bank Japan

English 日本語 简体中文 繁體中文 한국어

Search pdbj.org

RCSB PDB PDBe BMRB Adv. Search Search help

8I5E
Latest new entries

CHINESE

- Home
- 数据登记 (OneDep)
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- 标准格式
- Quick links
- 搜索
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- 衍生数据库

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- Previous workshop
- Games
- Papermodels

关于PDBj
- 帮助

关于PDBj

日本蛋白质结构数据库（PDBj: Protein Data Bank Japan), 是一个依托大阪大学蛋白质研究所，与其联合开发及共同研究的重点项目。在运营维护全球统一的生物大分子立体结构数据库的同时，还提供各种与结构解析相关的应用工具及数据库。 PDBj由JST-NBDC (JPMJND2205) 和AMED-BINDS联合提供支持，其徽标的设计灵感来自于细胞色素c（PDBID：1cyc）的立体结构，它也是第一个在日本成功解析的蛋白质分子结构。

Find the service you need

Choose a keyword listed below or input keywords into the textbox at the right of the keyword list. The brief explanation of the matched services will be displayed.

- Click the 'Show all services' button to display the explanation for all services.
- Input some keywords into the 'Word Search Box' to narrow down the search results.

☐ PDB	☐ BMRB	☐ EMDB	
☐ search	☐ deposition	☐ viewer	☐ education/dictionary
☐ NMR	☐ electron microscopy	☐ secondary structure	☐ sequence
☐ similarity	☐ function prediction	☐ chemical component	☐ structure prediction
☐ binding site	☐ surface structure	☐ 3D structure	☐ genome
☐ RDF	☐ SPARQL	☐ gene	☐ disease
☐ drug			

Show all services

e.g. motif, mole

Reset

最新消息

2023-08-23	142 new PDB entries have been released on 2023-08-23.
2023-08-17	[wwPDB] wwPDB Events at IUCr
2023-07-27	[wwPDB] Updated Annotation and Standardization of Peptide Residues
2023-07-11	Some hostnames have been deprecated
2023-07-10	[wwPDB] Celebrating 20 Years of the wwPDB
2023-07-05	[wwPDB] PDB NextGen Archive Now Provides Intra-molecular Connectivity

当月的分子

284: ATM和ATR激酶

文章列表

最新冠状病毒结构

EM Navigator

BMRBj Biological Magnetic Resonance Data Bank Japan

EMPIAR PDBj

BSM-Arc BINDS Biological Structure Model Archive

XRDa Xtal Raw Data Archive

208844
數據於2023-08-23公開中

PDBj
Protein Data Bank Japan
Worldwide Protein Data Bank Foundation
WORLDWIDE PDB PROTEIN DATA BANK

English 日本語 简体中文 繁體中文 한국어

Search pdbj.org

RCSB PDB PDBe BMRB Adv. Search Search help

8PU9
Latest new entries

CHINESE

- Home
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- 查詢
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- 服務&軟體
- 衍生資料庫

教材
- 幫助
- eProtS
- 本月的分子
- Previous workshop
- Games
- Papermodels

關於PDBj
- 幫助

關於PDBj

日本蛋白質結構數據庫（PDBj: Protein Data Bank Japan), 是一個依託大阪大學蛋白質研究所，與其聯合開發及共同研究的重點項目。在運營維護全球統一的生物大分子立體結構數據庫的同時，還提供各種與結構解析相關的應用工具及數據庫。 PDBj由JST-NBDC (JPMJND2205) 和AMED-BINDS聯合提供支持，其徽標的設計靈感來自於細胞色素c（PDBID: 1cyc）的立體結構，它也是第一個在日本成功解析的蛋白質分子結構。

Find the service you need

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- Click the 'Show all services' button to display the explanation for all services.
- Input some keywords into the 'Word Search Box' to narrow down the search results.

☐ PDB	☐ BMRB	☐ EMDB	
☐ search	☐ deposition	☐ viewer	☐ education/dictionary
☐ NMR	☐ electron microscopy	☐ secondary structure	☐ sequence
☐ similarity	☐ function prediction	☐ chemical component	☐ structure prediction
☐ binding site	☐ surface structure	☐ 3D structure	☐ genome
☐ RDF	☐ SPARQL	☐ gene	☐ disease
☐ drug			

Show all services

e.g. motif, mole

Reset

最新消息

2023-08-23	142 new PDB entries have been released on 2023-08-23.
2023-08-17	[wwPDB] wwPDB Events at IUCr
2023-07-27	[wwPDB] Updated Annotation and Standardization of Peptide Residues
2023-07-11	Some hostnames have been deprecated
2023-07-10	[wwPDB] Celebrating 20 Years of the wwPDB
2023-07-05	[wwPDB] PDB NextGen Archive Now Provides Intra-molecular Connectivity

當月的分子

284: ATR和ATR激酶

文章列表

最新冠狀病毒結構

EM Navigator

BMRBj
Biological Magnetic Resonance Data Bank Japan

EMPIAR PDBj

BSM-Arc
BINDS Biological Structure Model Archive

XRDa
Xtal Raw Data Archive

208844
건을2023-08-23부터공개중

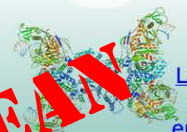
English 日本語 简体中文 繁體中文 한국어

PDBj Protein Data Bank Japan

Search pdbj.org

RCSB PDB PDBe BMRB Adv. Search Search help

8FFI



Latest new entries

KOREAN

- 홈
- 데이터 등록 (OneDep)
- 다운로드
- 표준 포맷
- Quick links
- 검색
- Molecular Viewers
- 서비스와 소프트웨어
- 다른 데이터베이스
- 교재
  - 도움말
  - eProtS
  - 이달의 분자
  - Previous workshop
  - Games
  - Papermodels
- PDBj 정보
  - 도움말
  - 출판물

PDBj 정보

일본 단백질구조 데이터 뱅크(PDBj : Protein Data Bank Japan)는 오사카 대학 단백질 연구소의 공동 이용·공동 연구 거점 활동으로써 운영되고 있으며, 국제적으로 통일화 된 생체 고분자의 입체 구조 데이터베이스를 운영함과 동시에, 분석 툴 및 관련 데이터베이스를 제공하고 있습니다. PDBj는 JST-NBDC (JPMJND2205) 와AMED-BINDS의 지원으로 개발되고 있습니다. PDBj의 로고는 일본에서 최초로 결정된 구조인 시토크롬C (PDBID: 1cyc) 로 부터 디자인 되었습니다.

Find the service you need

Choose a keyword listed below or input keywords into the textbox at the right of the keyword list. The brief explanation of the matched services will be displayed.

- Click the 'Show all services' button to display the explanation for all services.
- Input some keywords into the 'Word Search Box' to narrow down the search results.

☐ PDB	☐ BMRB	☐ EMDB	
☐ search	☐ deposition	☐ viewer	☐ education/dictionary
☐ NMR	☐ electron microscopy	☐ secondary structure	☐ sequence
☐ similarity	☐ function prediction	☐ chemical component	☐ structure prediction
☐ binding site	☐ surface structure	☐ 3D structure	☐ genome
☐ RDF	☐ SPARQL	☐ gene	☐ disease
☐ drug			

Show all services

e.g. motif, mole

Reset

새로운 뉴스

2023-08-23	142 new PDB entries have been released on 2023-08-23.
2023-08-17	[wwPDB] wwPDB Events at IUCr
2023-07-27	[wwPDB] Updated Annotation and Standardization of Peptide Residues
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2023-07-05	[wwPDB] PDB NextGen Archive Now Provides Intra-molecular Connectivity

이달의 분자

284: ATM 및 ATR 키 나제

기사 목록

신종 코로나바이러스 최신구조정보

EM Navigator

BMRBj Biological Magnetic Resonance Data Bank Japan

EMPIAR PDBj

BSM-Arc BINDS Biological Structure Model Archive

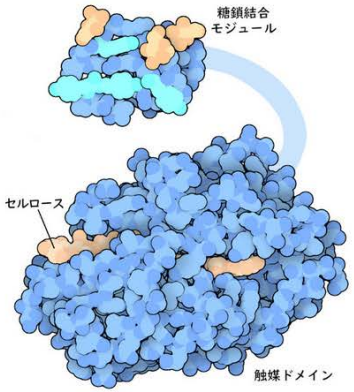
XRDa Xtal Raw Data Archive

281 セルラーゼとバイオエネルギー

Cellulases and Bioenergy

著者: David S. Goodsell　翻訳: 工藤 高裕（PDBj）

石油に由来する燃料は減ってきていて、気候変動の主な原因ともなっている。そこでバイオエネルギーの研究者たちは自然界に目を向け、人類に提供するよりクリーンで再生可能な燃料を探している。ている。**エタノール**（ethanol）は、燃料として、あるいは持続可能な航空燃料を製造するための中間体として魅力的な解決策の一つになるのではないかと考えられている。アルコール飲料は有史以前から糖を発酵して製造されていたが、現在これと同じ技術を使って燃料となるエタノールがつくられている。現在、糖のほとんどはトウモロコシとサトウキビでまかなわれているが、このやり方は食糧生産に適した土地をエネルギー用に転用してしまうことになり、また作物を生産するときに多くエネルギーを消費するので理想的とは言えない。そこで、スイッチグラス、ポプラ、トウモロコシの茎など、より丈夫で食用にならない作物の**セルロース**（cellulose）をエタノールに変換する方法を探す努力が続けられている。



真菌類の一種トリコデルマ・リーゼイ（*Trichoderma reesei*）のCel7Aは、糖鎖結合モジュール（上）と触媒ドメイン（下、セルロースは茶色で表示）が柔軟なリンカーでつながっている。糖鎖結合モジュールは、いくつかのチロシン（水色）とグリコシル化部分（薄茶色）を含み、セルロース繊維の表面をつかむことができる。高解像度TIFF画像は こちら。

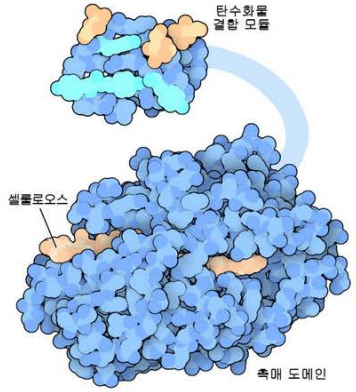
セルロースの分解

セルロースは**ブドウ糖**（glucose）からできているが、ブドウ糖同士が強固に結合し安定したポリマーとなっている。**セルロース合成酵素**（cellulose synthase）がセルロースの鎖を何本も積み重ね、さらに丈夫な繊維にすることで、セルロースは作られている。そのため、セルロースを発酵しエタノールを工業的に製造する場合、あらかじめセルロースの鎖を分離し、小さな糖へと切断しておく必要がある。通常、植物原料は、化学薬品や「水蒸気爆発」などの強力な過程を使って前処理しておき、植物の細胞壁を破壊することで酵素がセルロース繊維に作用できるようにする。次に、セルラーゼ酵素群を組み合わせて作用させることにより、セルロース繊維を個々の糖へと分解していく。このセルラーゼ酵素の原料となるのが、**トリコデルマ・リーゼイ**（*Trichoderma reesei*、別名ハイポクリア・ジェコリナ *Hypocrea jecorina*）という真菌である。これは第二次世界大戦中にソロモン諸島で発見された種で、綿生地に生えていたものである。現在では、バイオエタノール製造のほか、ストーンウォッシュジーンズのデニムを柔らかく

281 셀룰라아제와 바이오에너지 (Cellulases and Bioenergy)

Author: David S. Goodsell　Translator: PDBj

석유에서 유래한 연료는 줄어들고 있고 기후변화의 주요 원인이 되기도 한다. 그래서 바이오에너지 연구자들은 자연계로 눈을 돌려 인류에게 제공할 보다 깨끗하고 재생 가능한 연료를 찾고 있다. 에탄올(ethanol)은 연료로서 혹은 지속가능한 항공연료를 제조하기 위한 중간체로서 매력적인 해결책의 하나가 되지 않을까 생각되고 있다. 알코올 음료는 유사 이전부터 당을 발효해 제조됐으나 현재 이와 같은 기술을 사용해 연료가 되는 에탄올이 만들어지고 있다. 현재 당의 대부분은 옥수수와 사탕수수로 조달되고 있는데, 이 방식은 식량 생산에 적합한 토지를 에너지용으로 전용하게 되어버리고, 또한 작물을 생산할 때 많은 에너지를 소비하므로 이상적이라고 할 수 없다. 이에 스위치글라스, 포플러, 옥수수 줄기 등 보다 튼튼하고 식용이 되지 않는 작물인 셀룰로오스(cellulose)를 에탄올로 변환하는 방법을 찾는 노력이 계속되고 있다.



진균류의 일종인 트리코더마 리세이(*Trichoderma reesei*)의 Cel7A는 당사슬 결합 모듈(위)과 촉매 도메인(아래, 셀룰로오스는 갈색으로 표시)이 유연한 링커로 연결되어 있다. 당사슬 결합 모듈은 여러 티로신(하늘색)과 글리코실화 부분(연갈색)을 포함하여 셀룰로오스 섬유의 표면을 잡을 수 있다. 고해상도 TIFF 이미지는이쪽。

셀룰로오스 분해

셀룰로오스는 포도당(glucose)으로 이루어져 있는데 포도당끼리 견고하게 결합하여 안정적인 폴리머로 되어 있다. 셀룰로오스 합성효소(cellulose synthase)가 셀룰로오스 사슬을 여러 개 중첩하여 더욱 튼튼한 섬유로 만들면서 셀룰로오스가 만들어진다. 따라서 셀룰로오스를 발효하여 에탄올을 공업적으로 제조할 경우 미리 셀룰로오스 사슬을 분리하여 작은 당으로 절단해 둘 필요가 있다. 일반적으로 식물 원료는 화학약품이나 '수증기 폭발' 등 강력한 과정을 통해 전처리를 해놓고 식물의 세포벽을 파괴함으로써 효소가 셀룰로오스 섬유에 작용할 수 있도록 한다. 다음으로 셀룰라아제 효소군을 조합하여 작용시킴으로써 셀룰로오스 섬유를 개개의 당으로 분해하여 나간다. 이 셀룰라제 효소의 원료가 되는 것이 트리코더마 리세이(*Trichoderma reesei* , 일명 히포크레아 제코리나 (*Hypocrea jecorina*))라는 진균이다. 이는 제2차세계대전 중 솔로몬제도에서 발견된 종으로 면 원단에 자라고 있던 것이다. 현재는 바이오에탄올 제조 외에도 스톤워시 청바지의 데님을 부드럽게 하는 등의 작업에도 널리 이용되고 있다.

셀룰라아제의 과학

E-mail or slack-friendly Mol Viewer in PDBj.org

PDBj Protein Data Bank Japan
as a member of WORLDWIDE PDB PROTEIN DATA BANK

208844
件を2023-08-23に公開中

PDBj Protein Data Bank Japan

English 日本語 简体中文 繁體中文 한국어

Search pdbj.org

RCSB PDB PDBe BMRB Adv. Search Search help

- ホーム
- データ登録（OneDep）
- ダウンロード
- 標準フォーマット
- クイックリンク
- 検索サービス
- 分子ビューア
- サービス&ソフトウェア
- 二次データベース
- 教材
  - ヘルプ
  - eProtS

概要 | 構造情報 | 実験情報 | 機能情報 | 相同蛋白質 | 履歴 | ダウンロード

8I3J

Crystal structure of human inner-arm dynein heavy chain d stalk and microtubule binding domain

8I3J の概要

エントリーDOI	10.2210/pdb8i3j/pdb
分子名称	Dynein axonemal heavy chain 1 (1 entity in total)
機能のキーワード	contractile protein, motor protein
由来する生物種	Homo sapiens (human)
タンパク質・核酸の鎖数	1
化学式量合計	31487.84

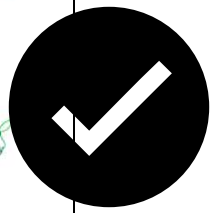
ダウンロード

- Sequence (fasta)
- PDBx/mmCIF
- PDBML (ヘッダのみ (no-atom))
- PDB形式 (全ての情報)
- 検証レポート (PDF)
- EDMap 2fo-fc (MTZ)

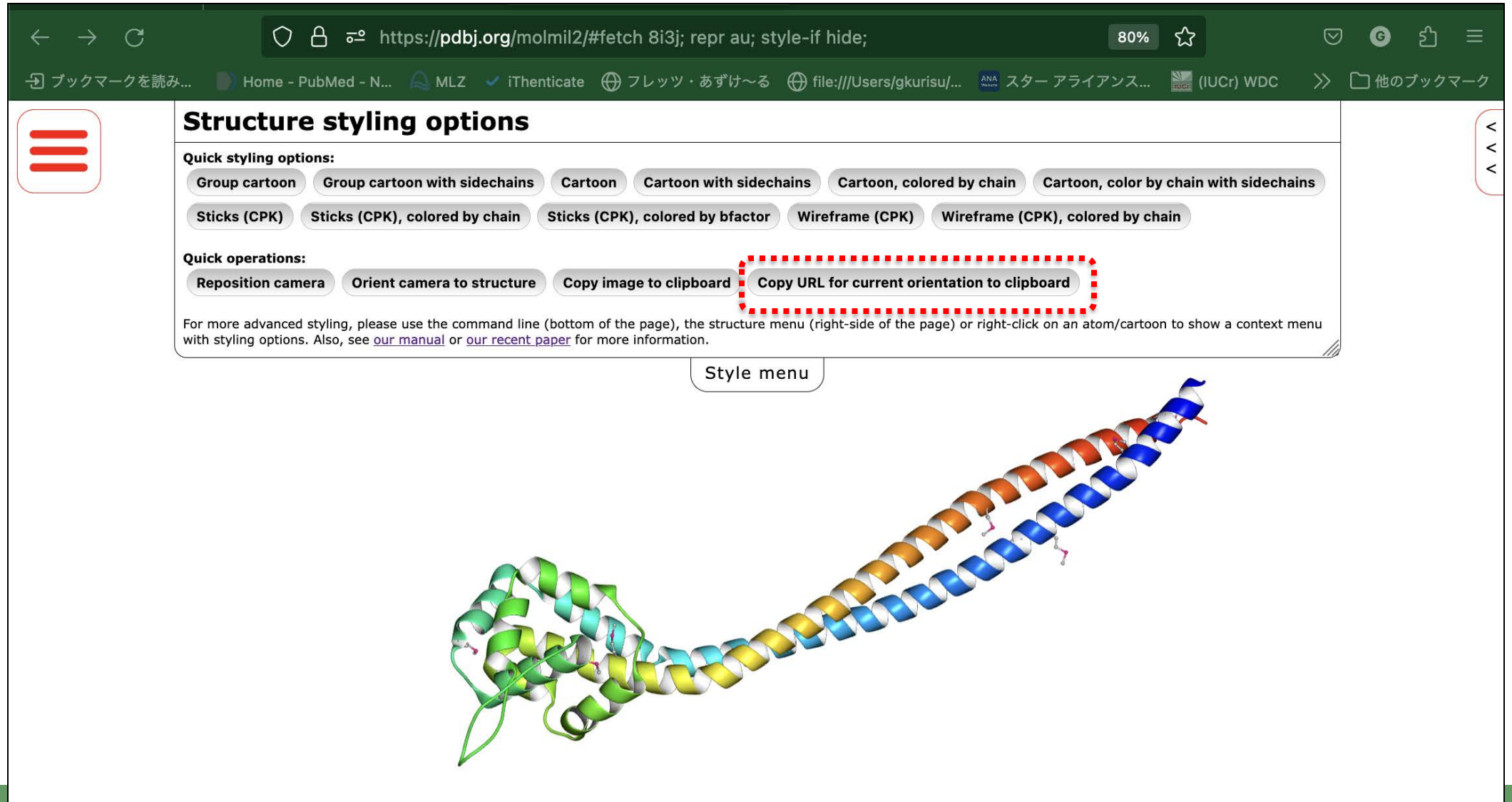
More...

構造

非対称単位を表示



“Copy URL for current orientation to clipboard”



PDBx/mmCIF format

- Format is based on the Self-defining Text Archive and Retrieval, developed by Hall et al. 1991 (DOI: 10.1021/ci00002a020)
- No more fixed-width columns
- Still uses a keyword-value based format, but one that is very extensible
- Comes with a dictionary

PDBx/mmCIF: 5zno

```
data_5ZNO
#
_entry.id   5ZNO
#
_audit_conform.dict_name       mmcif_pdbx.dic
_audit_conform.dict_version    5.296
_audit_conform.dict_location   http://mmcif.pdb.org/dictionaries/ascii/mmcif_pdbx.dic
#
loop_
_database_2.database_id
_database_2.database_code
PDB   5ZNO
WWPDB D_1300007412
#
_pdbx_database_status.status_code                     REL
_pdbx_database_status.status_code_sf                  REL
_pdbx_database_status.status_code_mr                  ?
_pdbx_database_status.entry_id                        5ZNO
_pdbx_database_status.recvd_initial_deposition_date   2018-04-10
_pdbx_database_status.SG_entry                        N
_pdbx_database_status.deposit_site                    PDBJ
_pdbx_database_status.process_site                    PDBJ
_pdbx_database_status.status_code_cs                  ?
_pdbx_database_status.methods_development_category    ?
_pdbx_database_status.pdb_format_compatible           Y
#
loop_
_audit_author.name
_audit_author.pdbx_ordinal
_audit_author.identifier_ORCID
'Numoto, N.'   1  ?
'Inaba, S.'    2  ?
'Yamagami, Y.' 3  ?
'Kamiya, N.'   4  ?
'Bekker, G.J.' 5  ?
'Ishii, K.'    6  ?
'Uchiyama, S.' 7  ?
'Kawai, F.'    8  ?
'Ito, N.'      9  ?
'Oda, M.'      10 ?
#
_citation.abstract                  ?
_citation.abstract_id_CAS           ?
_citation.book_id_ISBN              ?
_citation.book_publisher            ?
_citation.book_publisher_city       ?
_citation.book_title                ?
_citation.coordinate_linkage        ?
_citation.country                   US
_citation.database_id_Medline       ?
```

PDBx/mmCIF format

- All-in-all: a very structured format suitable for proper annotation of the meta-data and extensible to allow now only large structures, but also many different experimental sources

data item = name + value

```
data_5ZNO
#
_entry.id   5ZNO
#
_audit_conform.dict_name       mmcif_pdbx.dic
_audit_conform.dict_version    5.296
_audit_conform.dict_location
http://mmcif.pdb.org/dictionaries/ascii/mmcif_pdbx.dic
#
loop_
_database_2.database_id
_database_2.database_code
PDB    5ZNO
WWPDB D_1300007412
#
_pdbx_database_status.status_code                     REL
_pdbx_database_status.status_code_sf                  REL
_pdbx_database_status.entry_id                        5ZNO
_pdbx_database_status.recvd_initial_deposition_date   2018-04-10
_pdbx_database_status.SG_entry                        N
_pdbx_database_status.deposit_site                    PDBJ
_pdbx_database_status.process_site                    PDBJ
_pdbx_database_status.pdb_format_compatible           Y
#
loop_
_audit_author.name
_audit_author.pdbx_ordinal
_audit_author.identifier_ORCID
'Numoto, N.'    1  ?
'Inaba, S.'     2  ?
'Yamagami, Y.'  3  ?
'Kamiya, N.'    4  ?
'Bekker, G.J.'  5  ?
'Ishii, K.'     6  ?
'Uchiyama, S.'  7  ?
'Kawai, F.'     8  ?
'Ito, N.'       9  ?
'Oda, M.'       10 ?
#
_citation.country                   US
_citation.id                        primary
_citation.journal_abbrev            Biochemistry
_citation.journal_id_ASTM           BICHAW
_citation.journal_id_CSD            0033
_citation.journal_id_ISSN           1520-4995
_citation.journal_volume            57
```

Web-based mmCIF editor

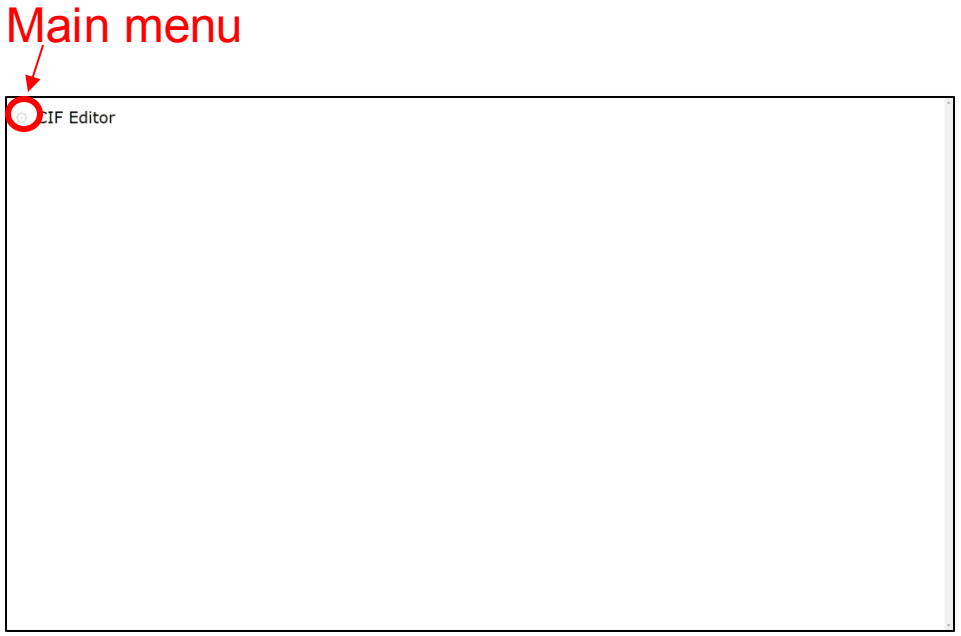
- It's not easy to edit mmCIF files, especially when used to PDB flat files
- PDBj has developed an mmCIF editor:
  - Available at: **https://pdbj.org/cif-editor/**
  - Help page: https://gitlab.com/pdbjapan/cif-editor/wikis/home
  - Bekker *et al.* 2019, DOI: 10.5940/jcrsj.61.159
- Multiple methods to edit are supported
- New features can be added

If you have any requests, please contact us at https://pdbj.org/contact

  - Or create an issue at https://gitlab.com/pdbjapan/cif-editor/issues

How-to: Load a file

- Looks very plain on first load (right)



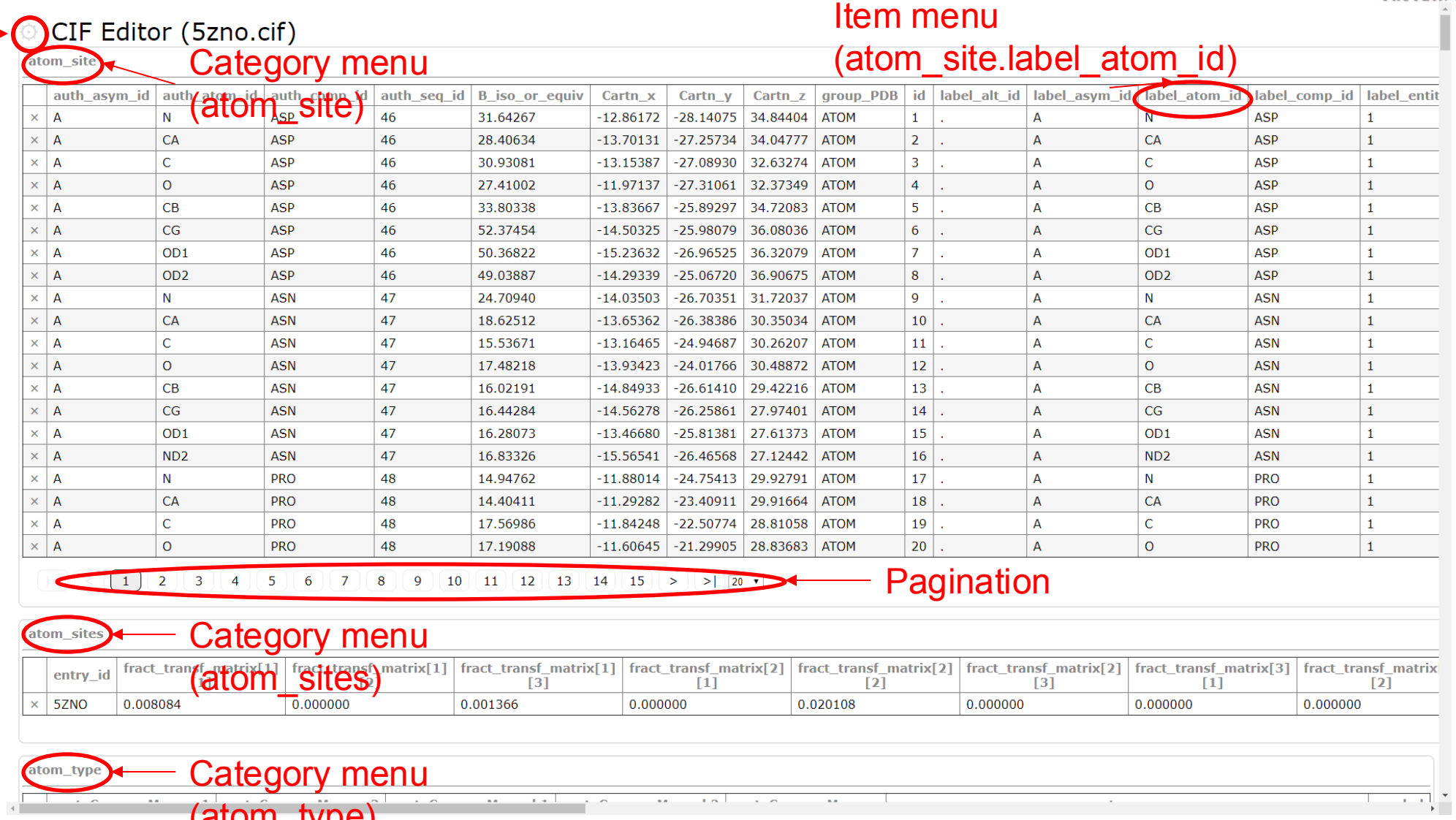
- Three options:
  - Main menu ( ) → Open mmCIF file → Select file in dialogue
  - Drag file from local file system into the CIF Editor and drop the file
  - Load a publicly available file via URL: https://pdbj.org/cif-editor/#https://pdbj.org/rest/displayPDBfile?format=mmcif&id=1crn

High-level overview

Main menu

Table for the atom_site category

Table for the atom_sites category



atom_site

	auth_asym_id	auth_atom_id	auth_comp_id	auth_seq_id	B_iso_or_equiv	Cartn_x	Cartn_y	Cartn_z	group_PDB	id	label_alt_id	label_asym_id	label_atom_id	label_comp_id	label_entit
×	A	N	ASP	46	31.64267	-12.86172	-28.14075	34.84404	ATOM	1	.	A	N	ASP	1
×	A	CA	ASP	46	28.40634	-13.70131	-27.25734	34.04777	ATOM	2	.	A	CA	ASP	1
×	A	C	ASP	46	30.93081	-13.15387	-27.08930	32.63274	ATOM	3	.	A	C	ASP	1
×	A	O	ASP	46	27.41002	-11.97137	-27.31061	32.37349	ATOM	4	.	A	O	ASP	1
×	A	CB	ASP	46	33.80338	-13.83667	-25.89297	34.72083	ATOM	5	.	A	CB	ASP	1
×	A	CG	ASP	46	52.37454	-14.50325	-25.98079	36.08036	ATOM	6	.	A	CG	ASP	1
×	A	OD1	ASP	46	50.36822	-15.23632	-26.96525	36.32079	ATOM	7	.	A	OD1	ASP	1
×	A	OD2	ASP	46	49.03887	-14.29339	-25.06720	36.90675	ATOM	8	.	A	OD2	ASP	1
×	A	N	ASN	47	24.70940	-14.03503	-26.70351	31.72037	ATOM	9	.	A	N	ASN	1
×	A	CA	ASN	47	18.62512	-13.65362	-26.38386	30.35034	ATOM	10	.	A	CA	ASN	1
×	A	C	ASN	47	15.53671	-13.16465	-24.94687	30.26207	ATOM	11	.	A	C	ASN	1
×	A	O	ASN	47	17.48218	-13.93423	-24.01766	30.48872	ATOM	12	.	A	O	ASN	1
×	A	CB	ASN	47	16.02191	-14.84933	-26.61410	29.42216	ATOM	13	.	A	CB	ASN	1
×	A	CG	ASN	47	16.44284	-14.56278	-26.25861	27.97401	ATOM	14	.	A	CG	ASN	1
×	A	OD1	ASN	47	16.28073	-13.46680	-25.81381	27.61373	ATOM	15	.	A	OD1	ASN	1
×	A	ND2	ASN	47	16.83326	-15.56541	-26.46568	27.12442	ATOM	16	.	A	ND2	ASN	1
×	A	N	PRO	48	14.94762	-11.88014	-24.75413	29.92791	ATOM	17	.	A	N	PRO	1
×	A	CA	PRO	48	14.40411	-11.29282	-23.40911	29.91664	ATOM	18	.	A	CA	PRO	1
×	A	C	PRO	48	17.56986	-11.84248	-22.50774	28.81058	ATOM	19	.	A	C	PRO	1
×	A	O	PRO	48	17.19088	-11.60645	-21.29905	28.83683	ATOM	20	.	A	O	PRO	1

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 > >| 20

atom_sites

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×	5ZNO	0.008084	0.000000	0.001366	0.000000	0.020108	0.000000	0.000000	0.000000

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