

20年を迎えたPDBj - 50年を迎えようとするPDBでの位置づけ -

栗栖源嗣 大阪大学蛋白質研究所







2021年でProtein Data Bankは50年

PROTEIN DATA BANK



Structure **Meeting Review**

The Protein Data Bank at 40: Reflecting on the Past to Prepare for the Future

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A symposium celebrating the 40th anniversary of the Protein Data Bank archive (PDB), organized by the Worldwide Protein Data Bank, was held at Cold Spring Harbor Laboratory (CSHL) October 28-30, 2011. PDB40's distinguished speakers highlighted four decades of innovation in structural biology, from the early era of structural determination to future directions for the field.

when the race to the DNA double helix reached the finish line et al., 1953) and the first three-dimensional (3D) crystal structures of hemoglobin and myoglobin (Kendrew et al., 1958; Perutz et al., 1960) were determined. In the years that followed, a slow

Structural biology was born in Cambridge, England in the 1950s, of rain, snow (ves, snow in New York in October), and wind pelting on the tent in which they were displayed, they engen-(Franklin and Gosling, 1953; Watson and Crick, 1953; Wilkins dered lively discussions until the very last minute of the meeting. The program boasted 19 distinguished speakers. Several speakers who had been a part of that early era of structural biology described their experiences determining structures

Cel



Berman et al., Structure 20, 391-396 (2012)



最初期のアジアからの寄与

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1998

1997

1991 .

• 1989 •

1988 .

1982

• 1973 •----

1979 First DNA (Z-DNA) determined (Wang et al., 1979)

(Kim et al., 1973; Robertus et al., 1974)

First tRNA structures determined

. 2006 .

2009



Berman et al., Structure **20**, 391-396 (2012)

(Columbia Univ. Press, New York, 1966); C. L. Li, C. Cullen, H. Jasper, J. Neuro-physiol. 19, 111, 131 (1956). R. Lende, Sciencer 141, 730 (1963). 1938). L. Benevento and F. Ebner, J. Comp. Neurol. 143, 242 (1971); W. Hall, Anat. Rev. 166, 313 (1970); H. Kiluckey, ibid. 172, 345 (1972); and F. Ebner, Barin Behre, Evol., in press; R. Ravizza and I. T. Diamond, Anat. 55; R. Ravizza and I. T. Diamond, Anar. r. 172, 390 (1972). Walsh and R. Ebner, J. Anat. 107, 1 301 Morrison, Exp. Neurol. 26, (1970). 10. Supported by NINDS grant NS-06551 and fellowship NS-30714 (to H.P.K.). We thank E. W. Swick and E. DiPalma for antistance. (1970); E. Jones and T. Powell, Brain 13, 258 (1969); P. Strick, *ibid.* 20, 130 15 June 1972

Three-Dimensional Structure of Yeast Phenylalanine Transfer RNA: Folding of the Polynucleotide Chain

Abstract. At 4 Å resolution the polynucleotides in yeast phenylalanine transfer RNA are seen in a series of electron dense masses about 5.8 Å apart. These peaks are probably associated with the phosphate groups, while lower levels of electron density between segments of adjacent polynucleotide chains are interpreted as arising from hydrogen-bonded purine-pyrimidine base pairs. It is possible to trace the entire polynucleotide chain with only two minor regions of ambiguity The polynucleotide chain has a secondary structure consistent with the cloverleaf conformation; however, its folding is different from that proposed in any model. The molecule is made of two double-stranded helical regions oriented at right angles to each other in the shape of an L. One end of the L has the CCA acceptor; the anticodon loop is at the other end, and the dihydrowridine and TYC loops form the corner.

Transfer RNA (tRNA) has a key tide chain has been traced and its threedimensional folding is presented Yeast phenylalanine tRNA crystallizes in an orthorhombic unit cell, space group $P_{2_122_1}$, a = 33 Å, b = 56 Å, and c = 161 Å, with four molecules in the unit cell (2). The methods used in preparing crystals of yeast phenylalanine tRNA, and the chemistry of the isomorphous heavy atom replacements have been described (4). Three types of heavy atom derivatives containing plat.

at 4 Å Resolution



Nature Vol. 282 13 December 1976

future plankton production and fisheries harvests is not clear This study was supported by the US Department of Energy and the NSF. We thank C. J. Lorenzen and G. Rowe for unpublished data and S. Horrigan and B. Bowden for reviewing

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Molecular structure of a left-handed double helical DNA fragment at atomic resolution

Andrew H.-J. Wang*, Gary J. Quigley*, Francis J. Kolpak*, James L. Crawford*, Jacques H. van Boom[†], Gijs van der Marel[†] & Alexander Rich^{*}

Department of Biology, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139 Department of Organic Chemistry, Gorlaeus Laboratories, University of Leiden, The Netherland

The DNA fragment d(CpGpCpGpCpG) crystallises as a left-handed double helical molecule with Watson-Crick base pairs and an antiparallel organisation of the sugar phosphate chains. The helix has two nucleotides in the asymmetric unit and contains twelve base pairs per turn. It differs significantly from right-handed B-DNA.

Williams, P. J. LeB. in Chemical Oceanography Vol. 2 (eds Riley,) (Academic New York, 1975).
 Tappan, H. Pulkergeray: Palaeteclimatel, Palaetecic, 4, 187 (2048).

Crystallisation and structure solution The ammonium salt of the deoxy hexamer d(CG)1 was prepared In a mimonium stario the decxy nexamer (a)(Cs), was prepared by a slight modification of the recently developed" phospho-triester approach. The crystals were grown from a solution containing 30 mM sodium cacodylate buffer (pH 7.0), 10 mM spermine tetrachloride, 15 mM MgCJ, and 2 mM d (CG), samp the vapour diffusion method as developed for tRNA crystalon*. The precipitating agent was 5% ison anol. Crystal s over a period of .7 × 0.5 mm were

J. Biochem., 70, 913-924 (1971)

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Tamaichi ASHIDA, Tatzuo UEKI,* Tomitake TSUKIHARA,** Akio SUGIHARA,*** Tsunehiro TAKANO and Masao KAKUDO

Institute for Protein Research, Osaka University, Osaka

The Crystal Structure of Bonito (Katsuo) Ferrocytochrome c

Received for publication, March 10, 1971

The crystal structure of bonito ferrocytochrome c has been studied at 4Å resolution on the basis of two isomorphous heavy atom derivatives (K₃UO₂F₅ and K₂PtCl₄). The crystal of bonito ferrocytochrome c belongs to an orthorhombic system with a space group of $P2_12_12_1$. The unit cell dimensions are: a=57.54, b=84.71 and c=37.74 Å. The crystal contains two kinds of molecules which are nearly equivalent to each other via the pseudo-twofold axis along the a axis.

The main structural features of bonito ferrocytochrome c molecule, such as the size and shape, the pathway of the polypeptide chain, and the orientation and the environment of the heme group, appear to be similar to those of horse ferricytochrome c, although it is suggested that the side-chain conformation at the surface



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Nature New Biology 233, page 223 (1971)

CRYSTALLOGRAPHY

Protein Data Bank

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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 will be updated as new material is received. The total holding will be announced annually in the organic



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structures. The Bank stores in a uniform format atomic co-ordinates and partial bond connectivities, as derived from crystallographic studies. Text included in each data entry gives pertinent information for the structure at hand (e.g. species from which the molecule has been obtained, resolution of diffraction data, literature citations and specifications of secondary structure). In addition to atomic co-ordinates and connectivities, the Protein Data Bank stores structure factors and phases, although these latter data are not placed in any uniform format. Input of data to the Bank and general maintenance functions are carried out at Brookhaven National Laboratory. All data stored in the Bank are available on magnetic tape for public distribution, from Brookhaven (to laboratories in the Americas), Tokyo (Japan), and Cambridge (Europe and worldwide). A master file is maintained at Brookhaven and duplicate copies are stored in Cambridge and Tokyo. In the future, it is hoped to expand the scope of the Protein Data Bank to make available co-ordinates for standard structural types (e.g. α -helix, RNA double-stranded helix) and representative computer programs of utility in the study and interpretation of macromolecular structures.

BNL

The Protein Data Bank[†] (1971,1973) was established in 1971 as a computer-based archival file for macromolecular structures. The purpose of the Bank is to collect,

Bernstein et al., J. Mol. Biol., 112, 535-342, 1979



TABLE	1	

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5311, Yamada-Kami, Suita

Osaka, Japan

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Brookhaven National Laboratory









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PDBjのあゆみ





PDBjが積み上げた20年の実績





PDBjは3つのwwPDBデータを管理





wwPDBにおけるRDF化の現状

wwPDB/RDF http://rdf.wwpdb.org/

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



<rdf:Description rdf:about="http://rdf.wwpdb.org/pdb/1BY4"> <rdf:type rdf:resource="http://purl.uniprot.org/core/Structure_Resource"/> <database rdf:resource="http://purl.uniprot.org/database/PDB"/> <method rdf:resource="http://purl.uniprot.org/core/X-Ray_Crystallography"/> <resolution rdf:datatype="http://www.w3.org/2001/XMLSchema#float">2.10</resolution> </rdf:Description>



wwPDBでPDBjがRDFファイルを公開



<http://www.w3.org/2004/02/skos/core#>

Subject: https://rdf.wwpdb.org/pdb/1E6E

Predicate	Object				
dcterms:identifier	1E6E				
skos:altLabel	1e6e				
dc:title	ADRENODOXIN REDUCTASE/ADRENODOXIN COMPLEX OF MITOCHONDR IAL P450 SYSTEMS				



wwPDB DOI landing page

Data-In



WORLDWIDE

PDB entry - 5AT1

(Status - Released)

Summary information

Title:

STRUCTURAL CONSEQUENCES OF EFFECTOR BINDING TO THE T STATE OF ASPARTATE CARBAMOYLTRANSFERASE CRYSTAL STRUCTURES OF THE UNLIGATED AND ATP-, AND CTP-COMPLEXED ENZYMES AT 2.6-ANGSTROMS RESOLUTION

DOI: 10.2210/pdb5at1/pdb

Primary publication DOI: 10.1021/bi00485a019

Entry authors: R.C. Stevens, J.E. Gouaux, W.N. Lipscomb

Initial deposition on: 1 January 1990

Initial release on: 15 October 1990

Latest revision on: 13 July 2011

Latest revision number: 1.3

Downloads:

Structure coordinates (PDBx/mmCIF) Structure coordinates (PDBML) Structure coordinates (PDB) Structure coordinates (RDF) X-ray diffraction data (PDBx/mmCIF) Validation report (PDF)

Links to more resources for 5AT1 at :



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Nature Structural Biology 10, 980 (2003) doi: 10.1038/nsb1203-980 More publications

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- wwPDB landing pageを 作成し直接redirectする よう変更
- 各Journalに新しいリンク の更新を依頼

PDBj構成員と協力者



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https://www.miraikikin.osaka-u.ac.jp/916/

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