## The Protein Data Bank: A Computer-based Archival File for Macromolecular Structures

The Protein Data Bank is a computer-based archival file for macromolecular 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. a-helix, RNA double-stranded helix) and representative computer programs of utility in the study and interpretation of macromolecular structures.

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, standardize, and distribute atomic co-ordinates and other data from crystallographic studies. As the number of solved protein and nucleic acid structures has grown to the point where some 10<sup>7</sup> characters are necessary to represent the co-ordinate information currently held, the need for such a computer-readable file has become very clear, and demands for the Bank's services have increased accordingly. The Protein Data Bank is one of several data base activities in the field of crystallography, e.g. the Bibliographic (Kennard et al., 1972) and Structural (Allen et al., 1973) Data Files for organic and organometallic compounds, the Atlas of Macromolecular Structure on Microfiche (AMSOM) (Feldmann, 1977), the Bond Index to the Determination of Inorganic Crystal Structures (BIDICS)‡ and the Powder Diffraction File.§

#### (a) Scope

The Protein Data Bank covers atomic co-ordinates, structure factors and phases from diffraction studies of macromolecules. Since most of this information is not generally published in the primary literature, the Bank depends for comprehensiveness on data supplied directly by the investigators. It is essentially a depository of data, held in computer-readable form, in contrast to other data banks that are based

<sup>§</sup> American Society for Testing Materials, 1916 Race St., Philadelphia, PA. 19103, U.S A.



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<sup>†</sup> Protein Data Bank is a misnomer of historical origin, since the file now contains entries for a nucleic acid.

<sup>‡</sup> I. D. Brown, Bond Index to the Determination of Inorganic Crystal Structures, McMaster University, Hamilton, Ontario, Canada, L8S 4M1.

### TABLE 1

## Protein data bank holdings

IDENT	ADENYLATE KINASE ALCOHOL DEHYDROGENASE (ADP-RIB) ALCOHOL DEHYDROGENASE (ORTHOPHEN) ALPHA-CHYMOTRYPSIN (TOSYL) ALPHA-CHYMOTRYPSIN (TOSYL) ALPHA-CHYMOTRYPSIN (NEW) BENCE-JONES IMMUNOGLOBUL IN REI CALCIUM-BINDING PARMALBUMIN SET 6A CALCIUM-BINDING PARWALBUMIN SET 6A CALCIUM-BINDING PARWALBUMIN SET 6A CALCIUM-BINDING PARWALBUMIN SET 6A CALCIUM-BINDING PARWALBUMIN SET 6A CARBONIC ANHYDRASE B CARBONIC ANHYDRASE C CARBONYEPTIDASE A CHYMOTRYPSINGEN CONCANAVALIN A CONCANAVALIN A CONCANAVALIN A CONCANAVALIN A CYTOCHROME C (ALBACORE, OXIDIZED) CYTOCHROME C (GENITO, HEART) CYTOCHROME C (GENITO, HEART) CYTOCHROME C (GENITO, HEART) CYTOCHROME CSS0 ELASTASE FERREDOXIN FLAVODOXIN (CLOSTRIDIUM MP) GAMMA-CHYMOTRYPSIN GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR HEMOGLOBIN (HORSE, AQUO MET) HEMOGLOBIN (HORSE, AQUO MET) HEMOGLOBIN (HUMAN, PETAL, DEOXY) HEMOGLOBIN (HUMAN, PETAL, DEOXY) HEMOGLOBIN (HUMAN, PETAL, DEOXY) HEMOGLOBIN (HUMAN, PETAL, DEOXY) HEMOGLOBIN (HUMAN, FETAL, DEOXY) HEMOGLOBIN (SUPERGENASE NAD/PYRUVATE LYSOZYME (HEN EGG-UHITE, SET RS5D) HYSOZYME (HEN EGG-UHITE, SET RS5D) PAPAIN (SYSOZYME, HEN EGG-UHITE, SET RS5D) PAPAIN (MORDENASE MYOGLOBIN (SPERM WHALE, MET) MYOGLOBIN (SPERM WHALE) MYOGLOBIN (SPERM WHALE) MYOGLOBIN (SPERM W	DEPOS I TOR	STATUS CODE
IADK IADH	ADENYLATE KINASE ALCOHOL DEHYDROGENASE (ADP-RIB)	G. SCHULZ C1. BRANDEN	A
2ADH 2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	R
3CHA 1EOR	ALPHA-CHYMDIRYPSIN	R. POLINSKY	
IREI	BENCE-JONES IMMUNOGLOBULIN REI	O. EPP, R. HUBER	
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	
3CPV	CALCIUM-BINDING PARVALBUMIN SET 61	R. KRETSINGER	
1CAB	CARBONIC ANHYDRASE B	K. KANNAN	
1CPA	CARBOXYPEPTIDASE A	W. LIPSCOMB	
1CHG	CHYMOTRYPS INOGEN	J. KRAUT	N
3CNA	CONCANAVAL IN A	K. HARDMAN	Ŕ
185C	CYTOCHROME B5	F. S. MATHEWS	
2CYT	CYTOCHROME C (ALBACORE, REDUCED)	R. DICKERSON	
ICYC	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	
155C	CYTOCHROME C250	R. TIMKOVICH	
IEST	ELASTASE	H. WATSON	
1FXN	FLAVODOXIN (CLOSTRIDIUM MP)	M. LUDWIG	
1GCH	GAMMA-CHYMOTRYPS IN	COHEN. DAVIES, SILVERTON	P
1GPD 2MHB	GLYCERALDEHYDE-3-P-DEHYDRUGENASE(LUBS)	LADNER, HEIDNER, PERUTZ	, N RP
1 DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	
1HHB	HEMOGLOBIN (HUMAN, DEDXY)	M. PERUTZ, G. FERMI	
ILHB	HEMOGLOBIN (LAMPREY)	W. HENDRICKSON	420
IYHX	HEXOKINASE (YEAST) BIII	T. STEITZ	В
2LDH	LACTATE DEHYDROGENASE	M. ROSSMANN	PD
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	PD
2LYZ	LYSOZYME (HEN EGG-WHITE, SET RSSD)	R. DIAMOND	P
3LYZ	LYSOZYME (HEN EGG-WHITE, SET RS6A)	R. DIAMOND	P
5LYZ	LYSOZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND	P
6LYZ	LYSOZYME (HEN EGG-WHITE, SET RS16)	R. DIAMOND	P
1MBN	MYOGLOBIN (SPERM WHALE)	H. WATSON	н
2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	
3PTI	PANCREATIC TRYPSIN INHIBITOR	R. HUBER	R
8PAP	PAPAIN, NATIVE	J. DRENTH	R
3PAP	PAPAIN (CYS DERIV OF CYS-25)	J. DRENTH	
4PAP	PAPAIN (OXIDIZED CYS-25)	J. DRENTH	
6PAP	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH	
7PAP	PAPAIN (BZOXY-PHE-ALA, CYS-25)	J. DRENTH	^
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS. D. PHILLIPS	B
1PAB	PREALBUMIN (HUMAN, PLASMA)	S. DATLEY, D. PHILLIPS	
IRNS 2RXN	RIBONUCLEASE S	H. WYCKOFF	ND
ISHS	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	110
1SGB 1SBT	STREPTOMYCES GRISEUS PROTEINASE B	M. JAMES	A
2SBT	SUBTILISIN NOVO	J. DRENTH	
150D	SUPEROXIDE DISMUTASE THERMOLYSIN (UNREFINEN)	J. AND D. RICHARDSON	A
2TLH	THERMOLYSIN (REFINED)	B. MATTHEWS	
ISRX ITNA	THIOREDOXIN TRANSFER RNA (YEAST, PHE)	BO. SODERBERG J. SUSSMAN, SH. KIM	Ą
2TNA	TRANSFER RNA (YEAST, PHE)	M. SUNDARALINGAM	N P
3TNA 1TIM	TRANSFER RNA (YEAST, PHE) TRIOSE PHOSPHATE ISOMERASE	JACK, LADNER, KLUG	P
IPTN	TRYPSIN (NATIVE, PHB)	I. WILSON, D. PHILLIPS FEHLHAMMER, BODE, SCHWAG	ER N
2PTB 1PTC	TRYPSIN(BENZAMIDINE INHIBITED, PH?) TRYPSIN/TRYPSIN INHIBITOR COMPLEX	FEHLHAMMER. BODE, SCHWAG BODE ET AL.	ER RN
	TUS CODES	BODE ET HL.	н
BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUT	TON	
A	ALPHA CARBON ATOMS ONLY	1011	
B D	BACKBONE ONLY NEW DATA HAS BEEN PROMISED		
H	NEW ENTRY WITH DEPOSITOR FOR APPROVAL		
P R	IN PREPARATION REPLACES AN OUT OF DATE PARAMETER SET		
	THE PROPERTY OF		



on data abstracted from scientific publications. The Bank contains 77 atomic coordinate entries for 47 macromolecules (Table 1),† and 13 sets of structure factors and phases. The atomic co-ordinate entries, which include descriptive text and partial bond connectivities, conform to a uniform format (see below), but the structure factors and phases are stored in the format received from depositors. All co-ordinate entries are referred to depositors for verification, before being made available publicly through the Bank.

### (b) Record structure of atomic co-ordinate entries

Atomic co-ordinate entries consist of records each of 80 characters.‡ Using the punched card analogy, columns 1 to 6 contain a record type identifier, and columns 7 to 70 contain data.§ Columns 71 to 80 are normally blank, but may contain sequence information which is added by the library-file management program UPDATE¶ used to maintain the file on the Brookhaven CDC CYBER 70/76 computing system. In order to facilitate retrieval of data from the file, the first four characters of each record define the unique record type, and the syntax of each record is independent of the order of records within any entry for a particular macromolecule. (In the master file, this order is always fixed.) Atomic co-ordinate data contributed by depositors are processed into the standard format with program MACMOL, || which also subjects the data to certain nomenclature and connectivity checking procedures.

A sample partial entry for the protein ribonuclease S is shown in Table 2.<sup>††</sup> The unique code 1RNS identifying this entry is given in the HEADER record, along with the date these data were entered into the Bank, and a provisional classification based on function, intended for future use in indexing and subdividing the file. Text giving the name of molecule, species from which it has been obtained, authors, literature citations, and other general description are presented in records COMPND through REMARK. SEQRES gives the amino acid sequence, and FTNOTE records are footnotes keyed to particular residues or atoms. Records HELIX through TURN describe the secondary structure as stated or approved by the depositor. Record CRYST1 defines the unit cell, while ORIGX and SCALE respectively give transformations relating the orthogonal Angström co-ordinates stored in the file to those originally supplied by the depositor (these frequently are referred to an oblique or non-isometric system) and to standard crystallographic fractional co-ordinates. ATOM records give the IUPAC-IUB (1969) standard atom names (IUPAC-IUB, 1970), and residue abbreviations (IUPAC-IUB, 1971), along with sequence identifiers (cf. SEQRES, above), co-ordinates in Angström units, and occupancies and thermal

- † In addition to current co-ordinate entries shown in Table 1, the Bank contains obsolete entries (for adenylate kinase tosyl,  $\alpha$ -chymotrypsin, concanavalin A, lactate dehydrogenase, horse methemoglobin, papain, rubredoxin, benzamidine-inhibited trypsin and pancreatic trypsin inhibitor), which have been superseded by later, more accurate data. These obsolete data are available on special request.
- † Originally, the Bank used a 140-character format, similar to that employed in the protein refinement programs of Diamond (1966,1971). The 140-character format has been superseded by the 80-character format.
  - § A detailed description of the file formats is available from Brookhaven on request.
- ¶ Control Data Corporation, UPDATE Reference Manual, Publication No. 60342500, Control Data Corporation, Arden Hills, Minnesota, 1974.
- $\parallel$  G. J. B. Williams, unpublished. For the 140-character data, program PROIN by E. F. Meyer was utilized.
- †† The file is organized in a similar way for proteins and nucleic acids, although certain differences exist, e.g. with regard to details of atom and residue names.



Table 2
Abbreviated sample atomic co-ordinate entry (ribonuclease S)

```
HEADER
           HYDROLASE (PHOSPHORIC DIESTER, RNA)
                                                         01-APR-73
                                                                      IRNS
           RIBONUCLFASE-S (E.C. 3.1.4.22)
BOVINE (BOS TAURUS) PANCREAS
COMPND
SOURCE
AUTHOR
           F. M. RICHARDS AND H. W. WYCKOFF
           R.J. FLETTERICK AND H. W. WYCKOFF, PRELIMINARY REFINEMENT
JRNL
JRNL
           OF PROTEIN COORDINATES IN REAL SPACE, ACTA CRYST. . VOL. A31,
JRNL
           P698 (1975) .
REMARK
          I REFERENCE 1. F. M. RICHARDS AND H. W. WYCKOFF, ATLAS OF
REMARK
             STRUCTURES FOR MOLECULAR BIOLOGY, VOL. 1. RIBONUCLEASE-S, CLARENDON PRESS (1973).
REMARK
REMARK
          1 REFERENCE 2. F. M. RICHARDS AND H. W. WYCKOFF, BOVINE
REMARK
             PANCREATIC RIBONUCLEASE. THE ENZYMES, EDITED BY P. D.
REMARK
          1 BOYER, VOL. IV. THIRD EDITION, P647, ACADEMIC PRESS (1971)
1 REFERENCE 3. F. M. RICHARDS, H. W. WYCKOFF, W. D. CARLSON,
REMARK
REMARK
             N. M. ALLEWELL, B. LEE AND Y. MITSUI, PROTEIN STRUCTURE, RIBONUCLEASE-S AND NUCLEOTIDE INTERACTIONS, COLD SPRING
REMARK
REMARK
REMARK
             HARBOR SYMPOSIA ON QUANTITATIVE BIOLOGY. VOL. XXXVI. P35
REMARK
REMARK
          1 REFERENCE 4. N. M. ALLEWELL AND H. W. WYCKOFF.
             CRYSTALI OGRAPHIC ANALYSIS OF THE INTERACTION OF CUPRIC
REMARK
REMARK
             ION WITH RIBONUCLEASE S. J. BIOL. CHEM. . VOL. 246, P4657
REMARK
              (1971)
REMARK
          1 REFERENCE 5. H. W. WYCKOFF, D. TSEKNOGLOU, A. W. HANSON,
             J. R. KNOX. B. LEE AND F. M. RICHARDS. THE THREE-
REMARK
REMARK
             DIMENSIONAL STRUCTURE OF RIBONUCLEASE-S. INTERPRETATION
             OF AN FLECTRON DENSITY MAP AT A NOMINAL RESOLUTION OF 2 ANGSTROMS. J. BIOL. CHEM., VOL. 245, P305 (1970).
REMARK
REMARK
REMARK
          1 REFERENCE 6. H. W. WYCKOFF, K. D. HARDMAN, N. M. ALLEWELL.
             T. INAGAMI, D. TSERNOGLOU, L. N. JOHNSON AND F. M. RICHARDS. THE STRUCTURE OF RIBONUCLEASE-S AT 6 ANGSTROM
REMARK
REMARK
REMARK
            RESOLUTION, J. BIOL. CHEM., VOL. 242, P3749 (1967).
REMARK
REMARK
          2 RESOLUTION. 2.0 ANGSTROMS.
REMARK
REMARK
          3 REFINEMENT. BY A STEEPEST-DESCENTS PROCEDURE. REFER TO THE
REMARK
          3
            JRNL CITATION ABOVE.
REMARK
REMARK
          4 THIS COORDINATE SET IS DESIGNATED OF BY THE DEPOSITOR.
REMARK
REMARK
          5 THE *S-PEPTIDE* (RESIDUES 1-20) WHICH FORMS A SEPARATE
REMARK
            CHAIN FROM THE REMAINDER OF THE MOLECULE IS GIVEN THE
REMARK
          5 CHAIN INFITTIFIER S.
SEGRES
          1 5
                20 LYS GLU THR ALA ALA ALA LYS PHE GLU ARG GLN HIS MET
SEGRES
                20
                     ASP SER SER THR SER ALA ALA
SEGRES
               104
                     SER SER ASN TYR CYS ASN GLN MET MET LYS SER ARG
SEGRES
               104
                     ASN LEU THR LYS ASP ARG CYS LYS PRO VAL ASN THR PHE
SEGRES
               104
                     VAL HIS GLU SER LEU ALA ASP VAL GLN ALA VAL CYS SER
SEGRES
               104
                     GLY LYS ASN VAL ALA CYS LYS ASN GLY GLN THR ASN CYS
SEGRES
          5
               104
                     TYR GLN SER TYR SER THR MET SER ILE THR ASP CYS ARG
SEGRES
               104
                     BLU THR GLY SER SER LYS TYR PRO ASN CYS ALA TYR LYS
SEORES
               104
                     THR THR GLN ALA ASN LYS HIS ILE ILE VAL ALA CYS GLU
SFORES
               104
                     GLY ASN PRO TYR VAL PRO VAL HIS PHE ASP ALA SER VAL
FINOTE
FINOTE
         1 THE MAIN CHAIN AND MOST OF THE ASSOCIATED SIDE CHAINS ARE
FINOTE
         1 NOT WELL-DEFINED IN THE REGIONS OF RESIDUES 2, 65-72 AND
FINOTE
          1 119-123
FINOTE
FTNOTE
          2 THE MAIN CHAIN IS VERY POORLY DEFINED OR NOT VISIBLE AT ALL
FTNOTE
            IN THE FLECTRON DENSITY MAP IN THE REGIONS OF RESIDUES 1.
         2 18-20,21-23 AND 124.
1 H1 THR & 3 MET S
FTNOTE
            H1 THR q
HELIX
                                       13
           HZ ASN
HELIX
                         24 ASN
                                       34 1
```



TABLE 2—continued

_								_									_
	HELIX	3	H3 5	FR	50	ALA	56	1									
	SHEET	ī		Lys	41	HIS	48	0									
	SHEET	ż	51 3		79	THR	87	-1	N	ASN		44	0	CYS		84	
	SHEET	3	S1 3		96	LYS	104	-1	N	ASP	•	83	0	THR	1	0 0	
	SHEET	1	52 4		61	ALA		0						- 1			
	SHEET	2	52 4	ASN	71	SER		-1		VAL	-	63	0	CYS		72	
	SHEET	3	52 4	HIS	105	GLIJ		-1	N	TYH		73	0	VAL		80	
	SHEET	4	52 4	VAL	116	VAL		-1	0	ALA	77	109	N.	VAL	1.	18	
	TURN	1	1200	AL	-	VAL	57		PSEU								
	TURN	2		LA		SER	59		PSEU					·ueer			
	TURN	3	T3 C		10 <del>7</del> 3753	GLY	68							SHEET			
	TURN	4	T4 T			SER	90						31	SHEET	31	6	
	CRYST1	44.	.650		650	97.1		.00			120.		- 31	2 1		0	
	ORIGXI		1.00		0.00		0.000				.000	SOLD WINDS					
	ORIGXZ		0.00		1.00		1.000				.000						
	ORIGX3		0.00		0.00	2021	0.000				.000						
	SCALEI			2396	.01	2931 5861	0.000				.000						
	SCALE2			0000	0.00	2001	.010				.000						
	SCALE3			0000		0000	-15.39		7.9		20.2		1.0	0 0.	00	2	
	ATOM	1	N CA	LYS	•		-15.14		7.6		18.		1.0		00	2	
	ATOM	3	C		5 1		-14.98		6.1		18.		1.0		.00	2	
	ATOM	4	ŏ	Lys			-15.14		5.3		19.		1.0		.00	2	
	ATOM	5	СВ	LYS			-13.87		8.2		18.		1.0		.00	2	
	ATOM	6	CG	Lys	350		-12.69		7.6	54	18.		1.0	0 0.	.00	2	
	へきれたいまれたかい!					n.An.An.	******		****	*****			*****	tututu	***	オルオル	
	ATOM	927	N	ASP	121		-6.79	5	-9.2	47	7.0	034	1.0	0 0.	00	1	
	ATOM	928	CA	ASP	121		-5.81	3	-9.4	25		935	1.0		.00	1	
	ATOM	929	C	ASP	121		-6.21					789	1.0		.00	1	
	ATO4	930	0	ASP	121		-5.82		-9.8			552	1.0		.00	1	
	ATO4	931	CB	ASP	121		-4.52					6,48	1.0		.00	1	
	ATOM	932	CG	ASP	121		-3.47		-9.5			587	1.0		.00	1	
	ATOM	933	001	2505 9175000	121		-3.32		-8.0			636	1.0		.00	1	
	ATOM	934	002	1000	121		-2.71					799	1.0		00	1	
	ATOM	935	N	AL.A	122		-7.04					013	1.0		00	1	
	ATOM	936	CA	AI A	122		-7.96					084	1.0		00	1	
	ATOM	937	С	ALA	122		-8.55					724	1.0		00	1	
	ATOM	938	0	AL.A	122		-8.49					925	1.0		.00	1	
	MOTA	939	CB	ALA	122		-6.99					881	1.0		.00	1	
	ATOM	940	N	SFR	123		-8.88					717	1.0		.00	1	
	ATOM	941	CA	SFP	123		-9.75 -8.91					627 880	1.0		.00	1	
	ATOM	942	c	SEP	123 123		-8.37					810	1.0		.00	i	
	ATOM	943	O CB	SFR	123		-10.87					597	1.0		.00	î	
	ATOM	944	OG	SFR	123		-10.15					530	1.0		.00	î	
	ATOM	946	N	VAL	124		-8.84					438	1.0		.00	Š	
	ATOM	947	CA	VAL	124		-8.59					596	1.0		00	S	
	ATOM	948	c	VAL	124		-9.23					209	1.0		00	S	
	ATOM	949	ŏ	VAL.	124		-8.58					377	1.0		.00	2	
	ATOM	950	СВ	VAL	124		-8.93					162	1.0		00	2	
	ATOM	951	CG1	VAL	124		-9.13					012	1.0		.00	2	
	ATOM	952	CG2	~ ~	124		-7.78					226	1.0		.00	2	
	ATOM	953	OXT		124		-10.41				1.	046	1.0	0 0	.00	2	
	TER	954		VAL.	124												
	CONECT	196	195														
	CONECT	312	311														
	CONECT	448	447														
	CONECT	498	497														
	CONECT	549	498	548													
	CONECT	644	196	1,1	3												
	CONECT	729	312		3												
	CONECT	844	448			1500	0.250			-	0,57			_	_	12020	
	MASTER		36	1 0	0	3	7	4		0	6	952	00	2	8	10	
	END																
_		_															_



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