J. Mol. Biol. (1977) **112**, 535–542

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. α-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 10^7 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

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

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

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

TABLE 1

Protein data bank holdings

IDENT CODE	MOLECULE	DEPOSITOR	STATUS CODE
1ADK	ADENYLATE KINASE	G. SCHULZ	A
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I. BRANDEN	
2ADH	ALCOHOL DEHYDROGENASE (ORTHOPHEN)	C.-I. BRANDEN	
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	R
3CHA	ALPHA-CHYMOTRYPSIN	A. TULINSKY	
1FAB	ANTIGEN BINDING FRAGMENT (NEW)	R. POLJAK	
1REI	BENCE-JONES IMMUNOGLOBULIN REI	O. EPP, R. HUBER	
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	
1CAB	CARBONIC ANHYDRASE B	K. KANNAN	
1CAC	CARBONIC ANHYDRASE C	K. KANNAN	
1CPA	CARBOXYPEPTIDASE A	W. LIPSCOMB	
1CHG	CHYMOTRYPSINOGEN	J. KRAUT	
2CNA	CONCANAVALIN A	G. REEKE, G. EDELMAN	N
3CNA	CONCANAVALIN A	K. HARDMAN	R
1B5C	CYTOCHROME B5	F. S. MATHEWS	
1CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	R. DICKERSON	
2CYT	CYTOCHROME C (ALBACORE, REDUCED)	R. DICKERSON	
1CYC	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	
1C2C	CYTOCHROME C2	J. KRAUT	
155C	CYTOCHROME C550	R. TIMKOVICH	
1EST	ELASTASE	H. WATSON	
1FDX	FERREDOXIN	L. JENSEN	
1FXN	FLAVODOXIN (CLOSTRIDIUM MP)	M. LUDWIG	
1GCH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	P
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M. ROSSMANN	N
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	LADNER, HEIDNER, PERUTZ	RP
1DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	
1HHB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	
1LHB	HEMOGLOBIN (LAMPREY)	W. HENDRICKSON	
1YHX	HEXOKINASE (YEAST) BIII	T. STEITZ	B
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	
2LDH	LACTATE DEHYDROGENASE	M. ROSSMANN	PD
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	PD
1LYZ	LYSOZYME (HEN EGG-WHITE, SET W2)	R. DIAMOND	P
2LYZ	LYSOZYME (HEN EGG-WHITE, SET RS5D)	R. DIAMOND	P
3LYZ	LYSOZYME (HEN EGG-WHITE, SET RS6A)	R. DIAMOND	P
4LYZ	LYSOZYME (HEN EGG-WHITE, SET RS9A)	R. DIAMOND	P
5LYZ	LYSOZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND	P
6LYZ	LYSOZYME (HEN EGG-WHITE, SET RS16)	R. DIAMOND	P
1MDH	MALATE DEHYDROGENASE	L. BANASZAK	A
1MBN	MYOGLOBIN (SPERM WHALE)	H. WATSON	
2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	
3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	
3PTI	PANCREATIC TRYPSIN INHIBITOR	R. HUBER	R
8PAP	PAPAIN, NATIVE	J. DRENTH	R
2PAP	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)	J. DRENTH	
3PAP	PAPAIN (CYS DERIV OF CYS-25)	J. DRENTH	
4PAP	PAPAIN (OXIDIZED CYS-25)	J. DRENTH	
5PAP	PAPAIN (TOS-LYS, CYS-25)	J. DRENTH	
6PAP	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH	
7PAP	PAPAIN (BZOXY-PHE-ALA,CYS-25)	J. DRENTH	
1PGK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON	A
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, D. PHILLIPS	B
1PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, D. PHILLIPS	
1RNS	RIBONUCLEASE S	H. WYCKOFF	
2RXN	RUBREDOXIN	L. JENSEN	ND
1SNS	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	
1SGB	STREPTOMYCES GRISEUS PROTEINASE B	M. JAMES	A
1SBT	SUBTILISIN BPN'	J. KRAUT	
2SBT	SUBTILISIN NOVO	J. DRENTH	
1SOD	SUPEROXIDE DISMUTASE	J. AND D. RICHARDSON	A
1TLN	THERMOLYSIN (UNREFINED)	B. MATTHEWS	
2TLN	THERMOLYSIN (REFINED)	B. MATTHEWS	
1SRX	THIOREDOXIN	B.-O. SODERBERG	A
1TNA	TRANSFER RNA (YEAST, PHE)	J. SUSSMAN, S.-H. KIM	N
2TNA	TRANSFER RNA (YEAST, PHE)	M. SUNDARALINGAM	P
3TNA	TRANSFER RNA (YEAST, PHE)	JACK, LADNER, KLUG	P
1TIM	TRIOSE PHOSPHATE ISOMERASE	I. WILSON, D. PHILLIPS	
1PTN	TRYPSIN (NATIVE, PH8)	FEHLHAMMER, BODE, SCHWAGER	N
2PTB	TRYPSIN(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHWAGER	RN
1PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	BODE ET AL.	N

STATUS CODES

BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
D	NEW DATA HAS BEEN PROMISED
N	NEW ENTRY WITH DEPOSITOR FOR APPROVAL
P	IN PREPARATION

on data abstracted from scientific publications. The Bank contains 77 atomic co-ordinate 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.[††] 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 Ångström 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 Ångström 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, α-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.

[‖] 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   1RNS
COMPND    RIBONUCLEASE-S (E.C. 3.1.4.22)
SOURCE    BOVINE (BOS TAURUS) PANCREAS
AUTHOR    F. M. RICHARDS AND H. W. WYCKOFF
JRNL      R.J. FLETTERICK AND H. W. WYCKOFF, PRELIMINARY REFINEMENT
JRNL      OF PROTEIN COORDINATES IN REAL SPACE, ACTA CRYST., VOL. A31,
JRNL      P698 (1975).
REMARK   1
REMARK   1 REFERENCE 1. F. M. RICHARDS AND H. W. WYCKOFF, ATLAS OF
REMARK   1  STRUCTURES FOR MOLECULAR BIOLOGY, VOL. 1. RIBONUCLEASE-S,
REMARK   1  CLARENDON PRESS (1973).
REMARK   1 REFERENCE 2. F. M. RICHARDS AND H. W. WYCKOFF, BOVINE
REMARK   1  PANCREATIC RIBONUCLEASE, THE ENZYMES, EDITED BY P. D.
REMARK   1  BOYER, VOL. IV, THIRD EDITION, P647, ACADEMIC PRESS (1971)
REMARK   1 REFERENCE 3. F. M. RICHARDS, H. W. WYCKOFF, W. D. CARLSON,
REMARK   1  N. M. ALLEWELL, B. LEE AND Y. MITSUI, PROTEIN STRUCTURE,
REMARK   1  RIBONUCLEASE-S AND NUCLEOTIDE INTERACTIONS, COLD SPRING
REMARK   1  HARBOR SYMPOSIA ON QUANTITATIVE BIOLOGY, VOL. XXXVI, P35
REMARK   1  (1971).
REMARK   1 REFERENCE 4. N. M. ALLEWELL AND H. W. WYCKOFF,
REMARK   1  CRYSTALLOGRAPHIC ANALYSIS OF THE INTERACTION OF CUPRIC
REMARK   1  ION WITH RIBONUCLEASE S, J. BIOL. CHEM., VOL. 246, P4657
REMARK   1  (1971).
REMARK   1 REFERENCE 5. H. W. WYCKOFF, D. TSERNOGLOU, A. W. HANSON,
REMARK   1  J. R. KNOX, B. LEE AND F. M. RICHARDS, THE THREE-
REMARK   1  DIMENSIONAL STRUCTURE OF RIBONUCLEASE-S. INTERPRETATION
REMARK   1  OF AN ELECTRON DENSITY MAP AT A NOMINAL RESOLUTION OF 2
REMARK   1  ANGSTROMS. J. BIOL. CHEM., VOL. 245, P305 (1970).
REMARK   1 REFERENCE 6. H. W. WYCKOFF, K. D. HARDMAN, N. M. ALLEWELL,
REMARK   1  T. INAGAMI, D. TSERNOGLOU, L. N. JOHNSON AND F. M.
REMARK   1  RICHARDS, THE STRUCTURE OF RIBONUCLEASE-S AT 6 ANGSTROM
REMARK   1  RESOLUTION, J. BIOL. CHEM., VOL. 242, P3749 (1967).
REMARK   2
REMARK   2 RESOLUTION. 2.0 ANGSTROMS.
REMARK   3
REMARK   3 REFINEMENT. BY A STEEPEST-DESCENTS PROCEDURE. REFER TO THE
REMARK   3  JRNL CITATION ABOVE.
REMARK   4
REMARK   4 THIS COORDINATE SET IS DESIGNATED 6D BY THE DEPOSITOR.
REMARK   5
REMARK   5 THE *S-PEPTIDE* (RESIDUES 1-20) WHICH FORMS A SEPARATE
REMARK   5 CHAIN FROM THE REMAINDER OF THE MOLECULE IS GIVEN THE
REMARK   5 CHAIN IDENTIFIER S.
SEQRES   1 S   20  LYS GLU THR ALA ALA ALA LYS PHE GLU ARG GLN HIS MET
SEQRES   2 S   20  ASP SER SER THR SER ALA ALA
SEQRES   1    104  SER SER SER ASN TYR CYS ASN GLN MET MET LYS SER ARG
SEQRES   2    104  ASN LEU THR LYS ASP ARG CYS LYS PRO VAL ASN THR PHE
SEQRES   3    104  VAL HIS GLU SER LEU ALA ASP VAL GLN ALA VAL CYS SER
SEQRES   4    104  GLN LYS ASN VAL ALA CYS LYS ASN GLY GLN THR ASN CYS
SEQRES   5    104  TYR GLN SER TYR SER THR MET SER ILE THR ASP CYS ARG
SEQRES   6    104  GLU THR GLY SER SER LYS TYR PRO ASN CYS ALA TYR LYS
SEQRES   7    104  THR THR GLN ALA ASN LYS HIS ILE ILE VAL ALA CYS GLU
SEQRES   8    104  GLY ASN PRO TYR VAL PRO VAL HIS PHE ASP ALA SER VAL
FTNOTE   1
FTNOTE   1 THE MAIN CHAIN AND MOST OF THE ASSOCIATED SIDE CHAINS ARE
FTNOTE   1 NOT WELL-DEFINED IN THE REGIONS OF RESIDUES 2, 65-72 AND
FTNOTE   1 119-123.
FTNOTE   2
FTNOTE   2 THE MAIN CHAIN IS VERY POORLY DEFINED OR NOT VISIBLE AT ALL
FTNOTE   2 IN THE ELECTRON DENSITY MAP IN THE REGIONS OF RESIDUES 1,
FTNOTE   2 18-20,21-23 AND  124.
HELIX    1  H1 THR S    3  MET S   13  1
HELIX    2  H2 ASN     24  ASN     34  1
```

TABLE 2—*continued*

```
HELIX    3  H3 SER      50  ALA      56  1
SHEET    1  S1 3 LYS     41  HIS      48  0
SHEET    2  S1 3 MFT     79  THR      87 -1  N  ASN     44   0  CYS     84
SHEET    3  S1 3 ALA     96  LYS     104 -1  N  ASP     83   0  THR    100
SHEET    1  S2 4 LYS     61  ALA      64  0
SHEET    2  S2 4 ASN     71  SER      75 -1  N  VAL     63   0  CYS     72
SHEET    3  S2 4 HIS    105  GLU     111 -1  N  TYR     73   0  VAL    108
SHEET    4  S2 4 VAL    116  VAL     124 -1  O  ALA    109   N  VAL    118
TURN     1  T1 VAL     54  VAL     57      PSEUDO 3/10 HELIX
TURN     2  T2 ALA     56  SER     59      PSEUDO 3/10 HELIX
TURN     3  T3 CYS     65  GLY     68      BETW STRNDS 1,2 OF SHEET S2
TURN     4  T4 THR     87  SER     90      END OF STRAND 2 OF SHEET S1
CRYST1   44.650    44.650    97.150  90.00  90.00 120.00 P 31 2 1      6
ORIGX1      1.000000  0.000000  0.000000        0.000000
ORIGX2      0.000000  1.000000  0.000000        0.000000
ORIGX3      0.000000  0.000000  1.000000        0.000000
SCALE1       .022396   .012931  0.000000        0.000000
SCALE2      0.000000   .025861  0.000000        0.000000
SCALE3      0.000000  0.000000   .010293        0.000000
ATOM       1  N   LYS S   1      -15.394   7.914  20.202  1.00  0.00     2
ATOM       2  CA  LYS S   1      -15.145   7.636  18.730  1.00  0.00     2
ATOM       3  C   LYS S   1      -14.982   6.107  18.763  1.00  0.00     2
ATOM       4  O   LYS S   1      -15.145   5.351  19.732  1.00  0.00     2
ATOM       5  CB  LYS S   1      -13.872   8.244  18.185  1.00  0.00     2
ATOM       6  CG  LYS S   1      -12.693   7.654  18.794  1.00  0.00     2

ATOM     927  N   ASP   121        -6.795  -9.247   7.034  1.00  0.00     1
ATOM     928  CA  ASP   121        -5.813  -9.425   5.935  1.00  0.00     1
ATOM     929  C   ASP   121        -6.217 -10.156   4.789  1.00  0.00     1
ATOM     930  O   ASP   121        -5.828  -9.850   3.652  1.00  0.00     1
ATOM     931  CB  ASP   121        -4.529 -10.015   6.648  1.00  0.00     1
ATOM     932  CG  ASP   121        -3.471  -9.503   5.687  1.00  0.00     1
ATOM     933  OD1 ASP   121        -3.320  -8.082   5.636  1.00  0.00     1
ATOM     934  OD2 ASP   121        -2.718 -10.333   4.799  1.00  0.00     1
ATOM     935  N   ALA   122        -7.049 -11.201   5.013  1.00  0.00     1
ATOM     936  CA  ALA   122        -7.865 -12.086   4.084  1.00  0.00     1
ATOM     937  C   ALA   122        -8.554 -13.331   4.724  1.00  0.00     1
ATOM     938  O   ALA   122        -8.495 -13.636   5.925  1.00  0.00     1
ATOM     939  CB  ALA   122        -6.991 -12.510   2.881  1.00  0.00     1
ATOM     940  N   SFR   123        -8.885 -13.915   3.717  1.00  0.00     1
ATOM     941  CA  SFP   123        -9.758 -15.155   3.627  1.00  0.00     1
ATOM     942  C   SFP   123        -8.915 -16.127   2.880  1.00  0.00     1
ATOM     943  O   SFR   123        -8.372 -15.812   1.810  1.00  0.00     1
ATOM     944  CB  SFP   123       -10.877 -14.659   2.597  1.00  0.00     1
ATOM     945  OG  SFR   123       -10.157 -14.035   1.530  1.00  0.00     1
ATOM     946  N   VAL   124        -8.845 -17.415   3.438  1.00  0.00     2
ATOM     947  CA  VAL   124        -8.591 -18.490   2.596  1.00  0.00     2
ATOM     948  C   VAL   124        -9.235 -18.381   1.209  1.00  0.00     2
ATOM     949  O   VAL   124        -8.580 -17.735    .377  1.00  0.00     2
ATOM     950  CB  VAL   124        -8.937 -19.929   3.162  1.00  0.00     2
ATOM     951  CG1 VAL   124        -9.135 -20.905   2.012  1.00  0.00     2
ATOM     952  CG2 VAL   124        -7.784 -20.573   4.226  1.00  0.00     2
ATOM     953  OXT VAL   124       -10.419 -19.165   1.046  1.00  0.00     2
TER      954      VAL   124
CONECT   196  195  644
CONECT   312  311  729
CONECT   448  447  844
CONECT   498  497  549
CONECT   549  498  548
CONECT   644  196  643
CONECT   729  312  728
CONECT   844  448  843
MASTER        36   10    0    3    7    4    0    6  952    2    8   10
END
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