Protein Data Bank

Quarterly Newsletter

Number 61 July 1992

July Update

The July 1992 PDB release includes 54 new atomic coordinate entries (Table 3). The total number of atomic coordinate entries is now 957, representing approximately a 40 percent increase compared to the number available a year ago. In addition to these 957 entries, 189 pre-release entries from the pending list (Table 8) are included in DATAPRTP. The size of DATAPRTP (the atomic coordinate and bibliographic entry database) is now 270 Mbytes.

All pre-release entries are available from the PDB anonymous FTP server as well as from the affiliated centers listed on page 8. Additional entries will be loaded as soon as they are ready. Due to the preliminary nature of pre-release entries it is suggested that those using them check with the PDB anonymous FTP server for update notices which will be posted regularly. Pre-release entries carry 5-character IDENT CODEs, which begin with the letter 'P' in column 62 for easy identification.

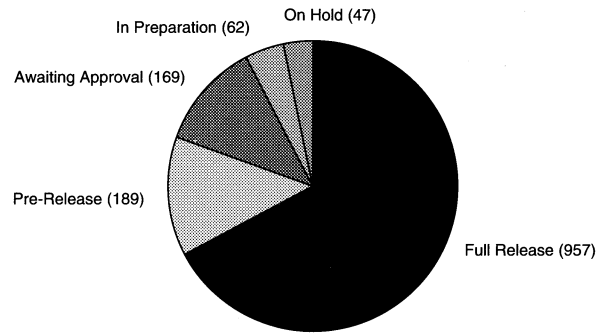
Beginning with the October 1992 release, the PDB will be available on CD ROM (ISO 9660 format). The cost of a CD ROM, which will include all available structure factor entries as well as the atomic coordinate and bibliographic entries, is expected to be approximately $200-250. More information on the CD ROM will be included in the October PDB Newsletter.

The PDB Newsletter is available in text and PostScript formats from the PDB anonymous FTP and e-mail server.

Data preprocessing requires approximately three weeks, after which time depositors will be notified of their entry IDENT CODE(s), or apprised of any questions or problems related to their data. Please allow adequate time for this!

Data will not be accepted for preprocessing until the coordinates, deposition form, and preprints/reprints have been received.

Status of Atomic Coordinate Entries



The PDB has printed a User Guide, which is intended as a handy description of the database. To order a copy of the User Guide, which is available free of charge, please use the Brookhaven Order Form at the back of this Newsletter.

Accessing PDB via WAIS

In June 1992 the PDB began operating a WAIS server. The purpose of this server is to facilitate the quick identification and acquisition of information from the PDB. Full details are available in the PDB User Guide.

Following is network access information needed to connect to the WAIS PDB source.

Internet address:	130.199.144.8
Internet name:	irisc2.pdb.bnl.gov
TCP port:	210
Database-name:	protein-data-bank

Table of Contents

A number of tables in this July 1992 Newsletter are abbreviated and contain only new or updated information. Full versions of all tables are available from the PDB anonymous FTP and e-mail server or by normal mail upon request.

PDB Staff

Enrique E. Abola
Frances C. Bernstein
Judy A. Callaway
Joseph J. Christian
Betty R. Deroski
Pamela A. Esposito (ed.)
Arthur Forman
Thomas F. Koetzle
Patricia A. Langdon
John E. McCarthy
Regina K. Shea
John G. Skora
Karen E. Smith (Bailey)

To Contact the PDB

Protein Data Bank
Chemistry Department, Building 555
Brookhaven National Laboratory
Upton, NY 11973 USA

Telephone: +1 516-282-3629
Facsimile: +1 516-282-5751
e-mail: pdb@bnlchm.bitnet
pdb@chm.chm.bnl.gov

Please include your telephone number, facsimile number, mailing address, and e-mail address in all correspondence.

Statement of Support

The PDB is supported by a combination of Federal Government Agency funds (work supported by the U.S. National Science Foundation; the U.S. Public Health Service, National Institutes of Health, National Center for Research Resources, National Institute of General Medical Sciences, and National Library of Medicine; and the U.S. Department of Energy under contract DE-AC02-76CH00016) and user fees.

File Server and Anonymous FTP

At Brookhaven, the PDB has an e-mail file server available for your use. This server provides PDB general information and documentation files. For more information, send an e-mail message to fileserv@pb1.pdb.bnl.gov and include the following text:

send info your_e-mail_address.

The PDB also has an anonymous FTP account available on the system pdb.pdb.bnl.gov with Internet address 130.199.144.1. It is possible to transfer files to and from this system using "anonymous" as the FTP user name and your real user name as the password. PDB general information and documentation files, as well as pre-release atomic coordinate entries and full-release entries approved for distribution since the last tape release, are available for downloading. You also can upload any files that you may wish to send to the PDB. Those using VMS may need to place quotes around file names.

Anyone experiencing problems or having questions related to the above network service should send an e-mail message to skora@bnl.gov.

Anonymous FTP for the Beginner

Frances Bernstein

Above, we provide some general information about accessing Protein Data Bank material via anonymous FTP. Based on telephone calls, we realize that there are people who are not familiar with the FTP program and this is intended as an introduction covering only the simplest commands.

FTP stands for 'file transfer protocol' and it is a package that allows you to log into another computer. Using FTP, you can transfer files between your own computer and the PDB machine.

You make the initial connection by typing

ftp pdb.pdb.bnl.gov

on your own computer. It is preferable to address a computer by name but if this fails you can try

ftp 130.199.144.1

A prompt should appear. At this point you have to log in by typing

login anonymous (use lower case)

When the computer says Password: please type your name. You should immediately see some general messages from the PDB followed by a prompt.

The material that we offer is organized into several subdirectories. You can get into subdirectory pub (for example) by typing

cd pub

and you can return to the directory one level higher by typing

cd ..

When you are in a (sub)directory you can list the files included in it by typing

ls

but you should be aware that we do not allow users to list the contents of the directory which is used by depositors to deposit new data.

To transfer single files between computers there are two commands - get and put. Get will copy a file from the PDB computer into your computer; put will copy a file from your computer into the PDB computer. Each of these commands takes two arguments which are file names. The first is the existing file that is to be transferred and the second is the name of the new file that is to be created.

You can terminate a session by typing quit.

Guidelines for Depositing Data in the PDB

The PDB accepts depositions of atomic coordinate parameters and other related experimental data resulting from structural studies on biological macromolecules. Included are results of studies of proteins, RNA, DNA, viruses and carbohydrates. The normal PDB deposition will include atomic coordinates and structure factors for diffraction studies or a listing of NOE restraints in the case of NMR studies. Data deposited with the PDB are converted to a standard format for coordinate entries, archived and redistributed world-wide.

Data Depositions

A PDB data deposition has three essential components, all of which must be received at Brookhaven before we can proceed to process a submission. These are:

Deposition Form. A PDB data deposition form must be completed. If you prefer, you may enter the relevant information in your computer and e-mail or FTP it to us. A current version of the deposition form is available *via* the PDB e-mail server or anonymous FTP. Please let us know if you would like us to mail you a printed copy of the data deposition form.

Reprints and Preprints. In order to complete our file on your structure, we must have copies of all relevant papers that are to be cited in your PDB entry. We realize that this means a bit of extra work for you, but it allows us to achieve significant time savings in processing your data.

Data Files. Data files should be in PDB format and may be sent *via* FTP or e-mail, floppy disk, or tape as described in the data deposition form. If you FTP the data, instructions are provided when you carry out the remote FTP. If you e-mail to

pdb@bnlchm.bitnet or
pdb@chm.chm.bnl.gov

Please send each file twice, so that we can detect transmission errors, which occasionally do occur. The program PDBCON, available through the FTP and e-mail server, can be used to convert coordinate data files into standard PDB format (see detailed description of ATOM records given on pages 5-6).

Items to be mailed should be addressed to:

Protein Data Bank Depositions
Chemistry Department, Building 555
Brookhaven National Laboratory
Upton, NY 11973 USA

Items Essential for Data Submission

Contact Names. On the deposition form, provide the following information for both a primary and secondary contact person who can answer questions on the deposition:

Name
Address
Telephone Number
Facsimile Number
E-mail address

Compound Name. Provide a complete name for the macromolecule including well-known synonyms. Genetic and chemical modifications should be clearly explained. Additional experimental and/or other conditions that differentiate the deposition from others concerning the same macromolecule should also be enumerated.

Biological Source. Provide the species, organ, tissue and mutant from which the macromolecule has been obtained. If the molecule was obtained *via* recombinant preparation, please provide the source of the genetic sequence and give a brief description of the expression system used.

Key References. Provide us with preprints or reprints of all papers that you wish to include as references in the PDB entry.

Experiment Used in the Study. Indicate if the structure was obtained *via* X-ray diffraction, NMR or other experimental means, or by theoretical computation techniques, if the latter is the case.

Model Refinement. Provide us with a complete description of the method used to refine the structure. Enumerate names of the programs used with authors, final R-value, rms deviation from ideality for all parameters used as restraints in the analysis, and number of reflections and nominal resolution of the data set included in the refinement.

Replacement Entries. Provide us with the PDB IDENT code(s) and molecule name(s) for previous entry(ies) to be superseded by the current deposition.

Chemical Sequence. Provide us with the complete amino acid, nucleotide, or saccharide sequence of the molecule. Indicate any known differences between the sequence of the submitted entry and those given in the sequence databases. Residues modeled as two or more different constituents because of microheterogeneity should be specified. Any sequence numbering scheme other than one that is strictly ordinal should be fully explained.

Non-standard Residues (Heterogens). A chemical structure drawing showing atomic nomenclature, bond type and connectivity should be provided for all HET groups. In these diagrams, hydrogen atoms should be shown where they are present in the coordinate set. Please provide us with the Chemical Abstracts (CAS) registry number for the HET group if this is available.

Chemical Modifications. Please describe any chemical modifications to main chain or side chain atoms.

Multimeric Molecules. The following should be provided:

a) Description of the crystallographic asymmetric unit.

b) Matrices which describe operations necessary to generate the complete molecule. Please include both non-crystallographic and crystallographic operators.

Space Group. The Hermann-Maugin symbol should be given. For non-standard settings, please include the full set of crystallographic symmetry operators.

Atomic Coordinates for:

Diffraction Studies. Please submit coordinates *in fractional* coordinates using the axial system of the crystallographic unit cell. Non-standard settings must be fully described and transformation operators that relate the deposition to the standard setting must be provided (see also above under Space Group).

NMR Studies. Multiple models in NMR structures should have a common orientation.

Solvent Molecules. Please provide us with a complete description of how solvent was modeled during refinement. Indicate the number of solvent molecules provided in the entry and the number used during refinement. Carefully inspect your data file before submission to ensure that all solvent molecules belong to the same asymmetric unit as the macromolecule.

Data Processing Protocol

Once all required information is in hand, each atomic coordinate submission undergoes preliminary checking to prepare the entry for pre-release. Any questions or problems encountered at this stage are relayed to the depositor at once. A response from the

depositor must be received before the PDB will issue an entry IDENT CODE. This response may take the form of corrections, explanations, or simply a statement that the depositor is opting to clear the data for pre-release in its present form.

To expedite the issuance of IDENT CODEs, the depositors may wish to review their entries prior to submission. The following is a list of items checked for possible errors at this stage of the data processing:

- Bond lengths and angles
- Chirality of atomic centers
- Comparison of the amino acid, nucleotide, or saccharide sequence with the reported chemical sequence
- Conformance to IUPAC-IUB nomenclature rules for atom names
- Crystal packing
- Deviations of the peptide groups from "trans" conformation
- Planarity of relevant groups
- Matthew's coefficient to verify the composition of the asymmetric unit
- Ramachandran plot
- Submitted coordinates, especially solvent molecules, to verify that they lie within the same asymmetric unit
- Thermal parameters

We anticipate adding other items to this list in the near future, *e.g.*, to check submitted entries for consistency with the expected stereochemical parameters described by Thornton and co-workers, *cf.* table 1 opposite.

We are requesting that all depositors submit their data to the PDB far enough in advance to ensure that publications are not delayed while waiting for their entry IDENT CODEs. For our part, we will make every effort to complete the preliminary checking process as soon as possible, normally within three weeks of receipt. In unusual circumstances, for example when a rapid publication is involved, please alert us so that we can expedite our processing.

Complete annotation and further checks are performed on submitted entries before they are ready for final and full release. At this latter stage of the process a careful examination of references submitted by the depositor is done to ensure that the full-release entry is consistent with the publications. Discrepancies are brought to the attention of the depositors.

Table 1: Summary of Expected Values for Stereochemical Parameters in Well-resolved Protein Structures [1]

Stereochemical Parameters	Expected Values
% of residues in CORE ϕ,ψ region	> 90%
χ_1 (gauche +)	-66.7 +/- 15.0°
χ_2 (gauche +)	+64.1 +/- 15.7°
χ_1 (trans)	183.6 +/- 16.8°
esd of pooled χ_1	15.7°
χ_3 (S-S bridge)	
Left handed	-85.8 +/- 10.7°
Right handed	96.8 +/- 14.8°
ϕ (Proline)	-65.4 +/- 11.2°
Helix angle	
ϕ	-65.3 +/- 11.9°
ψ	-39.4 +/- 11.3°
hydrogen bond energy	-2.03 +/- 0.75 kcal/mol
trans ω	179.6 +/- 4.7°
C^{α}--N--C--C^{β} torsion	33.9 +/- 3.5°

[1] A. L. Morris, M. W. MacArthur, E. G. Hutchinson and J. Thornton, "Stereochemical Quality of Protein Structure Coordinates", Proteins: Structure, Function and Genetics, 12: 345-364 (1992).

Description of PDB ATOM Records

The following ATOM record specification has been adapted from the PDB document "Atomic Coordinate and Bibliographic Entry Format Description". This document is available from the PDB anonymous FTP server or by mail if requested. The program PDBCON can be used to convert coordinate data files into this format.

ATOM Atomic coordinate records for "standard" groups

HETATM Atomic coordinate records for "non-standard" groups

Cols. 1-4 ATOM

or 1-6 HETATM

7-11 Atom serial number(i)

13-16 Atom name(ii)

17 Alternate location indicator(iii)

18-20 Residue name(iv,v)

22 Chain identifier, *e.g.,* A for hemoglobin a chain

23-26 Residue sequence number

27 Code for insertions of residues, *e.g.,* 66A, 66B, *etc.*

31-38 X
39-46 Y
47-54 Z
} Orthogonal Å coordinates

55-60 Occupancy

61-66 Temperature factor(vi)

68-70 Footnote number

FORMAT(6A1,I5,1X,A4,A1,A3,1X,A1,I4,A1,3X,3F8.3,2F6.2, 1X,I3)

Notes:

(i) Residues occur in order of their sequence numbers which always increase starting from the N-terminal residue for proteins and the 5'-terminal residue for nucleic acids. Within each residue the atoms are ordered as indicated in note (ii) below.

(ii) Amino Acids. The atom names follow the IUPAC-IUB rules[1] except:

a) Greek letter remoteness codes are transliterated as follows: α-A, β-B, γ-G, δ-D, ε-E, ζ- Z, η-H.

b) Atoms for which some ambiguity exists in the crystallographic results are designated A. This will usually apply only to the terminal atoms of asparagine and glutamine and to the ring atoms of histidine.

Within each residue the atoms occur in the order specified by the superscripts found in the figure "Atom Names, Remoteness Codes, and Order Indicators for the Common Amino Acids" in Appendix B of the document "Atomic Coordinate and Bibliographic Entry Format Description".

The extra oxygen atom of the carboxy terminal amino acid is designated OXT.

Four characters are reserved for these atom names. They are assigned as follows:

1-2 Chemical symbol - right justified
3 Remoteness indicator (alphabetic)
4 Branch designator (numeric)

c) For protein coordinate sets containing hydrogen atoms, the IUPAC-IUB rules[1] have been followed. Recommendation rule number 4.4 has been modified as follows: When more than one hydrogen atom is bonded to a single atom, the hydrogen atom number designation is given as the first character of the atom name rather than as the last character (e.g. $H^{\beta 1}$ is denoted as 1HB). Exceptions to these rules may occur in certain data sets at the depositors' request. Any such exceptions will be delineated clearly in FTNOTE and REMARK records.

Nucleic Acids. Atom names employed for polynucleotides generally follow the precedents set for mononucleotides. The following points are worthy of note.

a) The prime character (') commonly used to denote atoms of the ribose originally was avoided because of non-uniformity of its external representation. An asterisk (*) therefore was used in its place in entries released through January 1992.

Within each residue the atoms occur in the order specified by the superscripts in the figure "Atom Names and Order Indicators for the Common Ribonucleotides" in Appendix B of the document "Atomic Coordinate and Bibliographic Entry Format Description".

b) Of the four characters reserved for atom names, the leftmost two are reserved for the chemical symbol (right justified) and the remaining two denote the atom's position.

c) Atoms exocyclic to the ring systems have the same position identifier as the atom to which they are bonded except if this would result in identical atom names. In this case an alphabetic character is used to avoid ambiguity.

d) The ring-oxygen atom of the ribose is denoted O4 rather than O1.

e) The extra oxygen atom at the free 5'- phosphate terminus is designated OXT. This atom will be placed first in the coordinate set.

For nucleotides which are simple derivatives (*e.g.*, methyl or acetyl) of the parent nucleotide, the modifying atoms or groups occur immediately after the atom to which they are bonded. In the case of an acetyl modifier, the three atoms are ordered carbonyl carbon, carbonyl oxygen, methyl carbon.

(iii) Alternate locations for atoms may be denoted here by A, B, C, *etc.*

[1] IUPAC-IUB Commission on Biochemical Nomenclature. "Abbreviations and Symbols for the Description of the Conformation of Polypeptide Chains. Tentative Rules (1969)", J. Biol. Chem. 245, 6489 (1970).

The 1974 recommendations on the "Nomenclature of α–Amino Acids" (Biochemistry, 14, 449 (1975)) provides a scheme based on normal rules for organic compounds, but this scheme will not be used here.

(iv) Standard residue names are given in Appendix C of the document "Atomic Coordinate and Bibliographic Entry Format Description"; other components are defined in HET records.

(v) HETATM records are used for water molecules and atoms contained in HET groups.

(vi) Normally, the isotropic B value appears in this field. However, if anisotropic temperature factors have been provided, the temperature factor field of the corresponding ATOM or HETATM record will contain the equivalent U-isotropic [U(eq)] which is calculated by

$$U(eq) = 1/3[U(1,1) + U(2,2) + U(3,3)] \times 10^{-4}$$

where the integers U(i,j) stored on the corresponding ANISOU record are $U_{ij} \times 10^4$.

Citing the PDB

Frances Bernstein

Any researcher making use of information from the PDB should reference the data as follows:

1. The original authors and publication should be cited. Each entry has one or more AUTHOR records with the official author list for the PDB entry. If there is a paper describing the coordinates deposited with the PDB, it is presented on JRNL records. If there are no JRNL records the entry may be cited as a "private communication".

2. The PDB should be cited. The appropriate references are F. C. Bernstein, T. F. Koetzle, G. J. B. Williams, E. F. Meyer, Jr., M.D. Brice, J. R. Rodgers, O. Kennard, T. Shimanouchi, and M. Tasumi, "The Protein Data Bank: A Computer-based Archival File for Macromolecular Structures", J. Mol. Biol., 112, 535-542 (1977) and E. Abola, F. C. Bernstein, S. H. Bryant, T. F. Koetzle, and J. Weng, "Protein Data Bank" in Crystallographic Databases - Information Content, Software Systems, Scientific Applications, eds. F. H. Allen, G. Bergerhoff, and R. Sievers, Data Commission of the International Union of Crystallography, Bonn/Cambridge/Chester, 1987, pp. 107-132.

SAMPLE CITATION:

We used coordinates[1] for molecule x[2] obtained from the Protein Data Bank[3] at Brookhaven National Laboratory.

[1] Entry 1ABC, version of July 1987

[2] J. Smith, S. Doe, journal reference

[3] (a) F. C. Bernstein, ...
(b) E. E. Abola, ...

We would appreciate receiving reprints of all publications making use of data from the PDB. Please send them to Ms. Frances C. Bernstein, Protein Data Bank, Chemistry Department, Building 555, Brookhaven National Laboratory, Upton, NY 11973 USA.

Affiliated Centers

Eleven affiliated centers offer DATAPRTP for distribution. These centers, listed immediately below, are members of the Protein Data Bank Service Association (PDBSA). Centers designated with an asterisk(*) distribute DATAPRTP on magnetic media; those without an asterisk are on-line DATAPRTP distributors.

CAN/SND
Canadian Scientific Numeric Data Base Service
Ottawa, Ontario, Canada
Roger Gough
613-993-3294
cansnd@vm.nrc.ca

CAOS/CAMM
Dutch National Facility for Computer Assisted Chemistry
Nijmegen, The Netherlands
Jan Noordik
31-80-653386
noordik@caos.caos.kun.nl

CINECA
NE Italy Interuniversity Computing Center
Caselecchio di Reno (BO), Italy
Salvatore Rago
39-51-598411
argo@icineca.bitnet

EMBL
European Molecular Biology Laboratory
Heidelberg, Germany
Peter Rice
49-6221-387-247
peter.rice@embl-heidelberg.de

*JAICI
Japan Association for International Chemical Information
Tokyo, Japan
Hideaki Chihara
81-3-816-3389

NCSA
National Center for Supercomputing Applications
University of Illinois at Urbana-Champaign
Champaign, Illinois
Marcia Miller
217-244-2756
mmiller@ncsa.uiuc.edu

*Osaka University
Institute for Protein Research
Osaka, Japan
Yukiteru Katsube
81-6-877-5111 ext 3912

Pittsburgh Supercomputing Center
Pittsburgh, Pennsylvania
Hugh Nicholas
412-268-4960
nicholas@cpwpsca.bitnet

Prophet
BBN Systems and Technologies Corporation
Cambridge, Massachusetts
Wayne Rindone
617-873-2669
prophet-help@bbn.com

SDSC
San Diego Supercomputer Center
San Diego, CA
Lynn Ten Eyck
619-534-8189
teneyckl@sdsc.bitnet

SEQNET
Daresbury Laboratory
Warrington, United Kingdom
User Interface Group
44-925-603351
uig@daresbury.ac.uk

TABLE 1 - INFORMATION AVAILABLE ON MAGNETIC TAPE - JULY 1992

CODE	ITEM
DATAPRTP	ALL AVAILABLE COORDINATE ENTRIES (TABLE 3), BIBLIOGRAPHIC ENTRIES (TABLE 4 - NO COORDINATES IN BIB ENTRIES), AND SOME COMPUTER PROGRAMS (TABLE 2, PART A)
PDBPGMTP	ALL COMPUTER PROGRAMS AND MISCELLANEOUS FILES (TABLE 2, PARTS A AND B)
NONST1TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 1)
NONST2TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 2)
NONST3TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 3)
NONST4TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 4)
NONST5TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 5)
NONST6TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 6)
NONST7TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 7)
NONST8TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 8)
NONST9TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 9)
NONST10TP	STRUCTURE FACTOR ENTRIES (TABLE 5 - PART 10)
NMRRS1TP	NMR EXPERIMENTAL DATA ENTRIES (TABLE 6)

TABLE 2 - COMPUTER PROGRAMS AND MISCELLANEOUS FILES - JULY 1992

NAME	PURPOSE	AUTHOR(S)	REV. DATE	SUPPORTED
PART A - AVAILABLE ON **DATAPRTP, PDBPGMTP**				
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	4/82	YES
BLDKIT	MODEL BUILDER'S KIT	E.ABOLA	2/84	YES
BRUKTP	MAKE VAX/VMS FILES FROM PDB TAPE	H.BOSSHARD	8/85	NO
CONECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	7/89	YES
CONTNT	GENERATE PDB CONTENTS LIST	H.NICHOLAS JR.	4/91	NO
CONTCT	INTERMOLECULAR CONTACTS	L.ANDREWS	5/83	NO
DGPLOT	DIAGONAL PLOTS ON PRINTER	E.SWANSON,F.BERNSTEIN	1/83	YES
DIHDRL	COMPLETE TORSION ANGLES	E.ABOLA	3/80	YES
DRCTRY	DIRECTORY OF PDB DISTRIBUTION TAPE	E.ABOLA	7/86	YES
DSTNCE	CALC DISTANCES FROM CONECT RECORDS	F.BERNSTEIN	8/82	YES
FISIPL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79	YES
LSM	COLOR-CODED ALPHA-CARBON MODELS	R.MATELA,R.FLETTERICK	3/82	NO
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	4/89	NO
PHIPSI	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	2/79	YES
REFMTE	REFORMAT DATA FOR SUPERTAB,SUPERB	L.RELLICK,J.DUANE	12/83	NO
STEREO	EXTRACT X,Y,Z FROM STEREO DIAGRAMS	M.ROSSMANN	6/79	NO
TAPDIR	PRINT DIRECTORY OF TAPE CONTENTS	H.BERNSTEIN,F.BERNSTEIN	11/79	YES
THEOD	MEASURE COORDINATES WITH THEODOLITE	L.LEBIODA	1/82	NO
TORSRU	COMPLETE TORSION ANGLES	G.REEKE	10/79	NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	3/82	YES
PART B - AVAILABLE ON PDBPGMTP ONLY				
ALB	SECONDARY STRUCT. CALC.,PREDICTION	A.FINKELSTEIN,O.PTITSYN	10/85	NO
CRYSTAL	DATA BASE-PROTEIN CRYSTALLIZATION	G.GILLILAND	12/84	NO
NDB	NUCLEIC ACID DATA BASE + PROGRAMS	H.BERMAN ET AL.	9/89	NO
NEWHEL92	DNA HELIX ANALYSIS	R.DICKERSON ET AL.	2/92	NO
NUPARM	NUCLEIC ACID PARAMETER DETERMINATN	M.BANSAL,D.BHATTACHARYYA	5/90	NO
SEARCHDB	SEQUENCE SEARCH OF PDB ENTRIES	D.BLOCH	6/88	NO
TABLES	DISPLAY SPACE-GROUP SYMMETRY IN 3D	C.ABAD-ZAPATERO,T.O'DONNELL	12/87	NO

TABLE 3 - ATOMIC COORDINATE ENTRIES (AVAILABLE) - JULY 1992

new or replacement data only

IDENT CODE		MOLECULE	DEPOSITOR(S)	DATE	STATUS
1APS	*	ACYLPHOSPHATASE(NMR,5 STRUCTURES)	V.SAUDEK ET AL.	2/91	
1ACM	*	ATCASE(R(A)54A,R(C)54A)(R STATE)/PALA	STEVENS,KANTROWTZ,LIPSCOMB	7/92	
1RNB	*	BARNASE/D(GPC) (BAC. AMYLOLIQUEFACIENS)	J.JANIN,S.BAUDET	3/91	
4CLN	*	CALMODULIN(DROSOPHILA MELANOGASTER)	J.SACK	6/91	
6CA2	*	CARBONIC ANHYDRASE II MUTANT(V143F)	R.ALEXANDER,D.CHRISTIANSON	7/91	
7CA2	*	CARBONIC ANHYDRASE II MUTANT(V143G)	S.NAIR,D.CHRISTIANSON	7/91	
8CA2	*	CARBONIC ANHYDRASE II MUTANT(V143H)	R.ALEXANDER,D.CHRISTIANSON	7/91	
9CA2	*	CARBONIC ANHYDRASE II MUTANT(V143Y)	R.ALEXANDER,D.CHRISTIANSON	7/91	
1COL	*	COLICIN(C-TERMINAL DOMAIN)(E.COLI)	M.PARKER ET AL.	7/91	
4CNA	*	CONCANAVALIN A/ALPHA-METHYL-MANNOSIDE	Z.DEREWENDA ET AL.	10/90	
2YCC	*	CYTOCHROME C(YEAST,ISO-1,OXIDIZED)	A.BERGHUIS,G.BRAYER	1/91	
1DFN	*	DEFENSIN HNP-3(HUMAN)	HILL,YEE,SELSTED,EISENBERG	1/91	
1ATN	*	DEOXYRIBONUCLEASE I/ACTIN	W.KABSCH ET AL.	3/91	
1D56	*	DNA(CGATATATCG)/CALCIUM	YUAN,QUINTANA,DICKERSON	2/92	
1D57	*	DNA(CGATATATCG)/MAGNESIUM	YUAN,QUINTANA,DICKERSON	2/92	
1D76	*	DNA(CGU+ACG)	SCHNEIDER,BERMAN ET AL.	5/92	
1FXA	*	FERREDOXIN(ANABAENA 7120)	H.HOLDEN	1/91	
1FHA	*	FERRITIN(HUMAN,H CHAIN)	P.ARTYMIUK,P.HARRISON	12/90	
4FBP	*	FRUCTOSE-1,6-BISPHOSPHATASE/AMP	KE,LIANG,ZHANG,LIPSCOMB	2/91	
5FBP	*	FRUCTOSE-1,6-BISPHOSPHATASE/F6P	KE,ZHANG,LIANG,LIPSCOMB	2/91	
1HBG	*	HEMOGLOBIN(GLYCERA DIBRANCHIATA,CO)	ARENTS,BRADEN,PADLAN,LOVE	2/91	
2HBG	*	HEMOGLOBIN(GLYCERA DIBRANCHIATA,DEOXY)	G.ARENTS,W.LOVE	2/91	
2HIP	*	HIPIP(ECTOTHIORHODOSPIRA HALOPHILA)	H.HOLDEN ET AL.	6/91	
8I1B	*	INTERLEUKIN 1B(MOUSE)	DUPONT PROTEIN CRYSTLLGRPY	1/91	
4LZM	*	LYSOZYME(T4)(HIGH SALT)	B.MATTHEWS ET AL.	1/91	
5LZM	*	LYSOZYME(T4)(MEDIUM SALT)	B.MATTHEWS ET AL.	1/91	
6LZM	*	LYSOZYME(T4)(LOW SALT)	B.MATTHEWS ET AL.	1/91	
7LZM	*	LYSOZYME(T4)(DITHIOTHREITOL)	B.MATTHEWS ET AL.	1/91	
1MBP	*	D-MALTODEXTRIN-BINDING PROTEIN/D-MALTOSE	J.SPURLINO,F.QUIOCHO	12/90	A
5MBA	*	MET MYOGLOBIN(A.LIMACINA)/AZIDE PH 7.0	M.BOLOGNESI ET AL.	1/91	R
1NN2	*	NEURAMINIDASE N2(A/TOKYO/3/67)	J.VARGHESE,P.COLMAN	3/91	
2NN9	*	NEURAMINIDASE N9 MUTANT(S370L)	P.COLMAN ET AL.	3/91	
3NN9	*	NEURAMINIDASE N9 MUTANT(N329D)	P.COLMAN ET AL.	3/91	
4NN9	*	NEURAMINIDASE N9 MUTANT(I368R)	P.COLMAN ET AL.	3/91	
5NN9	*	NEURAMINIDASE N9 MUTANT(A369D)	P.COLMAN ET AL.	3/91	
6NN9	*	NEURAMINIDASE N9 MUTANT(K432N)	P.COLMAN ET AL.	3/91	
1Q21	*	C-H-RAS P21 PROTEIN/GDP	S.-H.KIM	9/91	R
2Q21	*	C-H-RAS P21 PROTEIN MUTANT(G12V)/GDP	S.-H.KIM	9/91	R
4Q21	*	C-H-RAS P21 PROTEIN(RESIDUES 1-188)/GDP	S.-H.KIM	9/91	
6Q21	*	C-H-RAS P21 PROTEIN/GDPCP	S.-H.KIM	7/92	
1PGX	*	PROTEIN G(B2 DOMAIN)	WHITLOW,ACHARI,HOWARD	4/92	
1RMS	*	RIBONUCLEASE MS/3'-GUANYLIC ACID	NONAKA,MITSUI,NAKAMURA	12/91	
1ROP	*	ROP(COL E1)	M.KOKKINIDIS ET AL.	4/91	
8RUB	*	RUBISCO(SPINACH)/CABP	KNIGHT,ANDERSSON,BRANDEN	11/90	
1TPK	*	TISSUE PLASMINOGEN ACTIVATOR(KRINGLE2)	A.DE VOS ET AL.	9/91	
1TIE	*	TRYPSIN INHIBITOR(ERYTHRINA CAFFRA)	S.ONESTI,P.BRICK,D.BLOW	2/91	
2TLD	*	TRYPSIN/SSI MUTANT(M70G,M73K)	Y.MITSUI ET AL.	9/91	
2DPV	*	PARVOVIRUS(CANINE,MONOCLINIC)	M.ROSSMANN ET AL.	7/92	
1XIS	*	D-XYLOSE ISOMERASE(S.RUBIGINOSUS)/MNCL2	M.WHITLOW,A.HOWARD	3/91	
2XIS	*	D-XYLOSE ISOMERASE(S.RUB.)/XYLITOL	M.WHITLOW,A.HOWARD	3/91	
3XIS	*	D-XYLOSE ISOMERASE(S.RUB.)/XYLOSE	M.WHITLOW,A.HOWARD	3/91	

TABLE 3 - ATOMIC COORDINATE ENTRIES (AVAILABLE) - JULY 1992

new or replacement data only

IDENT CODE		*MOLECULE*	*DEPOSITOR(S)*	*DATE*	*STATUS*
4XIS	*	D-XYLOSE ISOMERASE(S.RUB.)/XYLOSE/MNCL2	M.WHITLOW,A.HOWARD	3/91	
2IGE	*	IMMUNOGLOBULIN E(FC FRAGMENT) MODEL	E.PADLAN,B.HELM	10/90	
5TRA	*	TRANSFER RNA(YEAST,SER) MODEL	A.DOCK-BREGEON	2/90	

* New or replacement entry since April 1992 Newsletter

Status Codes:

Blank	Standard entry available for distribution
A	Alpha carbon atoms only
B	Backbone atoms only
R	Replacement

TABLE 4 - BIBLIOGRAPHIC ENTRIES (NO COORDINATES) - JULY 1992

Unchanged. All full tables are available from the PDB anonymous FTP and e-mail server or by regular mail upon request.

TABLE 5 - STRUCTURE FACTOR ENTRIES (AVAILABLE) - PART 10 - JULY 1992

new data only (parts 1-9 unchanged)

IDENT CODE		MOLECULE	DEPOSITOR(S)	DATE	STATUS
R2YCCSF	*	CYTOCHROME C(YEAST,ISO-1,OXIDIZED)	A.BERGHUIS,G.BRAYER	1/91	S
R1DFNSF	*	DEFENSIN HNP-3(HUMAN)	D.EISENBERG ET AL.	1/91	S
R1D56SF	*	DNA(CGATATATCG)/CALCIUM	YUAN,QUNTANA,DICKERSON	2/92	S
R1D57SF	*	DNA(CGATATATCG)/MAGNESIUM	YUAN,QUNTANA,DICKERSON	2/92	S
R1D76SF	*	DNA(CGU+ACG)	SCHNEIDER,BERMAN ET AL	5/92	S
R1HBGSF	*	HEMOGLOBIN(GLYCERA DIBRANCHIATA,CO)	W.LOVE ET AL.	2/91	S
R2HBGSF	*	HEMOGLOBIN(GLYCERA DIBRANCHIATA,DEOXY)	W.LOVE ET AL.	2/91	S
R5MBASF	*	MET MYOGLOBIN(A.LIMACINA)/AZIDE PH 7.0	M.BOLOGNESI ET AL.	1/91	S
R1NN2SF	*	NEURAMINIDASE N2(A/TOKYO/3/67)	J.VARGHESE,P.COLMAN	3/91	S
R2NN9SF	*	NEURAMINIDASE N9 MUTANT(S370L)	P.COLMAN ET AL.	3/91	S
R3NN9SF	*	NEURAMINIDASE N9 MUTANT(N329D)	P.COLMAN ET AL.	3/91	S
R4NN9SF	*	NEURAMINIDASE N9 MUTANT(I368R)	P.COLMAN ET AL.	3/91	S
R5NN9SF	*	NEURAMINIDASE N9 MUTANT(A369D)	P.COLMAN ET AL.	3/91	S
R6NN9SF	*	NEURAMINIDASE N9 MUTANT(K432N)	P.COLMAN ET AL.	3/91	S

* New or replacement entry since April 1992 Newsletter

Status Codes:

S Structure factors

TABLE 6 - NMR EXPERIMENTAL DATA ENTRIES (AVAILABLE) - JULY 1992

new data only

IDENT CODE		MOLECULE	DEPOSITOR(S)	DATE	STATUS
R1APSMR	*	ACYLPHOSPHATASE(NMR)	V.SAUDEK ET AL.	2/91	M

* New or replacement entry since April 1992 Newsletter

Status Codes:

M NMR restraints and other NMR experimental data

TABLE 7 - CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS - JULY 1992

REVDAT	10	15-JUL-92	1GPDI	1	COMPND
REVDAT	9	15-JUL-92	1RNSH	1	COMPND
REVDAT	4	15-JUL-92	1C4SC	1	FORMUL
REVDAT	4	15-JUL-92	2C4SC	1	FORMUL
REVDAT	6	15-JUL-92	1FC1E	3	HETATM
REVDAT	6	15-JUL-92	1FC2E	3	HETATM
REVDAT	5	15-JUL-92	1HYAD	3	HETATM
REVDAT	4	15-JUL-92	2HYAC	3	HETATM
REVDAT	4	15-JUL-92	3HYAC	3	FORMUL HETATM
REVDAT	5	15-JUL-92	4HYAD	1	FORMUL
REVDAT	9	15-JUL-92	2YHXH	1	FORMUL
REVDAT	6	15-JUL-92	2ATCE	1	SHEET
REVDAT	6	15-JUL-92	4CATE	1	REMARK
REVDAT	9	15-JUL-92	4DFRH	1	FORMUL
REVDAT	2	15-JUL-92	1IGEA	3	EXPDTA HETATM
REVDAT	4	15-JUL-92	2MCPC	1	HET
REVDAT	5	15-JUL-92	7ADHD	1	COMPND
REVDAT	3	15-JUL-92	1CMSB	1	AUTHOR JRNL
REVDAT	4	15-JUL-92	1DNEC	1	AUTHOR
REVDAT	2	15-JUL-92	1PAZA	1	SHEET
REVDAT	2	15-JUL-92	1RBBA	1	COMPND
REVDAT	3	15-JUL-92	2DCGB	1	REMARK
REVDAT	2	15-JUL-92	2GLSA	1	JRNL
REVDAT	3	15-JUL-92	2MEVB	1	JRNL
REVDAT	3	15-JUL-92	2WRPB	1	JRNL
REVDAT	7	15-JUL-92	3ESTF	1	FTNOTE
REVDAT	2	15-JUL-92	4I1BA	1	AUTHOR
REVDAT	3	15-JUL-92	2MBAB	3	OBSLTE
REVDAT	5	15-JUL-92	2P21D	3	OBSLTE
REVDAT	3	15-JUL-92	3P21B	3	OBSLTE
REVDAT	2	15-JUL-92	1BDNA	1	FORMUL
REVDAT	2	15-JUL-92	1CLAA	1	FORMUL
REVDAT	2	15-JUL-90	1D10A	2	CONECT
REVDAT	2	15-JUL-92	1D11A	2	CONECT
REVDAT	2	15-JUL-92	1D12A	2	CONECT
REVDAT	2	15-JUL-92	1D13A	1	REMARK
REVDAT	2	15-JUL-92	1D14A	1	REMARK
REVDAT	2	15-JUL-92	1D15A	3	HET FORMUL HETATM CONECT
REVDAT	3	15-JUL-92	1DHFB	2	CONECT
REVDAT	3	15-JUL-92	1DNFB	1	AUTHOR
REVDAT	3	15-JUL-92	1FCBB	1	JRNL
REVDAT	3	15-JUL-92	1MHUB	1	HET
REVDAT	4	15-JUL-92	1MRBC	1	HET
REVDAT	3	15-JUL-92	1MRTB	1	HET
REVDAT	2	15-JUL-92	1OMDA	1	FORMUL
REVDAT	2	15-JUL-92	1SRNA	1	COMPND
REVDAT	2	15-JUL-92	1TPTA	1	FORMUL
REVDAT	2	15-JUL-92	256BA	1	COMPND
REVDAT	2	15-JUL-92	2MCGA	1	SPRSDE
REVDAT	3	15-JUL-92	2MHUB	1	HET
REVDAT	2	15-JUL-92	2MLTA	1	SPRSDE
REVDAT	5	15-JUL-92	2MRBD	1	HET
REVDAT	3	15-JUL-92	2MRTB	1	HET
REVDAT	2	15-JUL-92	3CLAA	1	FORMUL
REVDAT	2	15-JUL-92	3ER5A	1	AUTHOR

TABLE 7 - CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS - JULY 1992

REVDAT	3	15-JUL-92	3ICDB	1	SHEET
REVDAT	3	15-JUL-92	4ICDB	1	SHEET
REVDAT	3	15-JUL-92	7DFRB	2	CONECT
REVDAT	2	15-JUL-92	1AK3A	1	REMARK
REVDAT	2	15-JUL-92	1BJLA	1	REMARK
REVDAT	2	15-JUL-92	1D26A	1	HET
REVDAT	2	15-JUL-92	1D27A	1	HET
REVDAT	2	15-JUL-92	1D40A	1	COMPND
REVDAT	2	15-JUL-92	1D41A	1	COMPND
REVDAT	2	15-JUL-92	1DRFA	2	CONECT
REVDAT	2	15-JUL-92	1HMDA	1	REMARK
REVDAT	2	15-JUL-92	1HMOA	1	REMARK
REVDAT	2	15-JUL-92	1NDNA	1	FORMUL
REVDAT	2	15-JUL-92	1OVAA	1	FORMUL
REVDAT	2	15-JUL-92	1PCDA	1	FORMUL
REVDAT	2	15-JUL-92	1TABA	1	FORMUL
REVDAT	2	15-JUL-92	2BJLA	1	JRNL
REVDAT	2	15-JUL-92	2D47A	1	AUTHOR JRNL
REVDAT	2	15-JUL-92	2ZNFA	1	FORMUL
REVDAT	2	15-JUL-92	41BIA	1	REMARK
REVDAT	2	15-JUL-92	4CLAA	1	FORMUL
REVDAT	2	15-JUL-92	4ESTA	1	FORMUL
REVDAT	2	15-JUL-92	4P2PA	1	HET
REVDAT	2	15-JUL-92	5P2PA	1	FORMUL
REVDAT	2	15-JUL-92	6ICDA	1	SHEET
REVDAT	2	15-JUL-92	6XIAA	1	SHEET
REVDAT	2	15-JUL-92	9HVPA	1	FORMUL
REVDAT	2	15-JUL-92	9XIAA	3	HET FORMUL HETATM

THE FOLLOWING DATA SETS HAVE BEEN REPLACED

OBSLTE	15-JUL-92	2MBA	5MBA
OBSLTE	15-JUL-92	2P21	1Q21
OBSLTE	15-JUL-92	3P21	2Q21

TABLE 8 - ATOMIC COORDINATE, STRUCTURE FACTOR, AND NMR EXPERIMENTAL DATA ENTRIES (IN PREPARATION) - JULY 1992

new data only

IDENT CODE		MOLECULE	DEPOSITOR(S)	DATE	STATUS
1APT	*	ACID PROTEINASE(PENICILLIUM JANTHINELLUM)	A.R.SIELECKI,M.N.G.JAMES	12/91	P
1APU	*	ACID PROTEINASE(PENICILLIUM JANTHINELLUM)	A.R.SIELECKI,M.N.G.JAMES	12/91	P
1APV	*	ACID PROTEINASE(PENICILLIUM JANTHINELLUM)	A.R.SIELECKI,M.N.G.JAMES	12/91	P
1APW	*	ACID PROTEINASE(PENICILLIUM JANTHINELLUM)	A.R.SIELECKI,M.N.G.JAMES	12/91	P
1PPL	*	ACID PROTEINASE(PENICILLIUM JANTHINELLUM)-WITH BOUND PHOSPHONATE INHIBITOR	M.FRASER,M.JAMES	6/92	P
1PPM	*	ACID PROTEINASE(PENICILLIUM JANTHINELLUM)-WITH BOUND PHOSPHONATE INHIBITOR	M.FRASER,M.JAMES	6/92	P
1ABD	*	ACYL COENZYME A BINDING PROTEIN(NMR,20)	K.ANDERSEN,F.POULSEN	3/92	P
1BBA	*	BOVINE PANCREATIC POLYPEPTIDE(NMR)	C.DOBSON ET AL.	3/92	P
1BBM	*	CALMODULIN BINDING DOMAIN	G.M.CLORE,A.BAX,M.IKURA, A.M.GRONENBORN	5/92	P
12CA	*	CARBONIC ANHYDRASE II MUTANT(V121A)	S.NAIR,D.CHRISTIANSON	10/91	P
1CA3	*	CARBONIC ANHYDRASE II(PH 5.7)	S.NAIR,D.CHRISTIANSON	11/91	P
5CAC	*	CARBONIC ANHYDRASE C/SO3	A.LILJAS ET AL.	3/92	P
2CBA	*	CARBONIC ANHYDRASE	K.HEKANSSON,M.CARLSSON, L.A.SVENSSON,A.LILJAS	3/92	P
2CBB	*	CARBONIC ANHYDRASE(PH 6.0)	A.LILJAS ET AL.	6/92	P
2CBC	*	CARBONIC ANHYDRASE	K.HEKANSSON,M.CARLSSON, L.A.SVENSSON,A.LILJAS	3/92	P
2CBD	*	CARBONIC ANHYDRASE/BISULFITE	A.LILJAS ET AL.	6/92	P
2CBE	*	CARBONIC ANHYDRASE	K.HEKANSSON,M.CARLSSON, L.A.SVENSSON,A.LILJAS	3/92	P
1CBN	*	CRAMBIN	M.M.TEETER,S.M.ROE,N.H.HEO	10/91	P
1BBH	*	CYTOCHROME C'	Z.REN,D.E.MCREE	5/92	P
1DRA	*	DIHYDROFOLATE REDUCTASE MUTANT(D27E)	S.OATLEY,J.KRAUT	11/91	P
1DRB	*	DIHYDROFOLATE REDUCTASE MUTANT(D27C)	C.DAVID,J.KRAUT	11/91	P
1DR1	*	DHFR(CHICKEN LIVER)/NADP+/BIOPTERIN	M.MCTIGUE,J.KRAUT ET AL.	3/92	P
1DR2	*	DHFR(CHICKEN LIVER)/THIO-NADP+	M.MCTIGUE,J.KRAUT ET AL.	3/92	P
1DR3	*	DHFR(CHICKEN LIVER)/THIO-NADP+/BIOPTERIN	M.MCTIGUE,J.KRAUT ET AL.	3/92	P
1DR4	*	DHFR(CHICKEN LIVER)/CYS 11 HGCH3/NADP+	M.MCTIGUE,J.KRAUT ET AL.	3/92	P
1DR5	*	DHFR(CHICKEN)/C11 HGCH3/NADP+/BIOPTERIN	M.MCTIGUE,J.KRAUT ET AL.	3/92	P
1DR6	*	DHFR(CHICKEN)/MERCURIBNZ/NADP+/BIOPTERIN	M.MCTIGUE,J.KRAUT ET AL.	3/92	P
1DR7	*	DHFR(CHICKEN)/C11 MERCURIBENZOATE/NADP	M.MCTIGUE,J.KRAUT ET AL.	3/92	P
1D52	*	DNA (CCCCCGCGGGGG)	N.VERDAGUER,J.AYMAMI,I.FITA, M.COLL,J.A.SUBIRANA	9/91	P
1D58	*	DNA (TGATCA)-4' EPIADRIAMYCIN	B.L.D'ESTAINTOT,B.GALLOIS,T.BROWN, W.N.HUNTER	2/92	P
1D68	*	DNA(GCGTATACGC)(NMR)	CHENG,CHOU,SALAZAR,REID	4/92	P
1D69	*	DNA(ATGAGGAATA)(NMR)	CHOU,CHENG,REID	4/92	P
1D75	*	DNA (CGCGAATT(O8A)GCG)	G.A.LEONARD,A.GUY,T.BROWN, R.TEOULE,W.N.HUNTER	5/92	P
1D78	*	DNA (GTGTACAC) A-CONFORMATION	N.THOTA,X.H.LI,C.BINGMAN, M.SUNDARALINGAM	6/92	P
1D79	*	DNA (GTGTACAC) A-CONFORMATION	N.THOTA,X.H.LI,C.BINGMAN, M.SUNDARALINGAM	6/92	P
1BBL	*	E3-BINDING DOMAIN (NMR)	G.M.CLORE,M.A.ROBIEN, A.M.GRONENBORN	2/92	P
1PPF	*	ELASTASE(HUMAN)/OVOMUCOID THIRD DOMAIN	W.BODE,A.WEI	10/91	P
1PPG	*	ELASTASE/MEO-SMC-AAPV-CHLOROMETHYLKETONE	W.BODE,A.WEI	10/91	P
1FKR	*	FKBP(FK506-, RAPAMYCIN-RECEPTOR)(NMR,20)	S.MICHNICK ET AL.	3/92	P
1FKS	*	FKBP(FK506-, RAPAMYCIN-RECEPTOR)(NMR,AV)	S.MICHNICK ET AL.	3/92	P

TABLE 8 - ATOMIC COORDINATE, STRUCTURE FACTOR, AND NMR EXPERIMENTAL DATA ENTRIES (IN PREPARATION) - JULY 1992

new data only

IDENT CODE		*MOLECULE*	*DEPOSITOR(S)*	*DATE*	*STATUS*
1FKT	*	FKBP(FK506-, RAPAMYCIN-RECEPTOR)(NMR,AV)	S.MICHNICK ET AL.	3/92	P
1GST	*	GLUTATHIONE S-TRANSFERASE/GLUTATHIONE	GILLILAND,ARMSTRONG,JI	3/92	P
1AAQ	*	HIV-1 PROTEASE/HYDROXYETHYLENE ISOSTERE	M.LEWIS	4/92	P
1IMM	*	IMMUNOGLOBULIN VL DOMAIN MCPC603	B.STEIPE,R.HUBER	3/92	P
1IMN	*	IGG VL(MCPC603-CDR1 REPLACED BY MOPC167)	B.STEIPE,R.HUBER	3/92	P
1DFB	*	IGG1 K FAB FRAGMENT	HE,RUEKER,CASALE,CARTER	3/92	P
1LHH	*	LYSOZYME (HUMAN) MUTANT(V110P)	K.INAKA,M.MATSUSHIMA,T.HERNING, R.KUROKI,K.YUTANI,M.KIKUCHI	3/92	P
1LHI	*	LYSOZYME (HUMAN) MUTANT(P71G)	K.INAKA,M.MATSUSHIMA,T.HERNING, R.KUROKI,K.YUTANI,M.KIKUCHI	3/92	P
1LHJ	*	LYSOZYME (HUMAN) MUTANT(P103G)	K.INAKA,M.MATSUSHIMA,T.HERNING, R.KUROKI,K.YUTANI,M.KIKUCHI	3/92	P
1LHK	*	LYSOZYME (HUMAN) MUTANT(A47P)	K.INAKA,M.MATSUSHIMA,T.HERNING, R.KUROKI,K.YUTANI,M.KIKUCHI	3/92	P
1LHL	*	LYSOZYME (HUMAN) MUTANT(D91P)	K.INAKA,M.MATSUSHIMA,T.HERNING, R.KUROKI,K.YUTANI,M.KIKUCHI	3/92	P
1CMD	*	MALATE DEHYDROGENASE(E.COLI)/CITRATE	M.HALL,L.BANASZAK	3/92	P
1CME	*	MALATE DEHYDROGENASE(E.COLI)/MALATE/NAD	M.HALL,L.BANASZAK	3/92	P
1AAH	*	METHANOL DEHYDROGENASE	Z.XIA,F.S.MATHEWS	4/92	AP
1MAE	*	METHYLAMINE DEHYDROGENASE	E.G.HUIZINGA,F.M.D.VELLIEUX, W.G.J.HOL	5/92	P
1MAF	*	METHYLAMINE DEHYDROGENASE	E.G.HUIZINGA,F.M.D.VELLIEUX W.G.J.HOL	5/92	P
2PMG	*	PHOSPHOGLUCOMUTASE- PHOSPHOTRANSFERASE COMPLEX	W.J.RAY,J.-B.DAI,Y.LIU,M.KONNO	8/92	P
1CDE	*	PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE	R.J.ALMASSY	5/92	P
1PPA	*	PHOSPHOLIPASE A2 (LYS 49 VARIANT)	D.R.HOLLAND,K.D.WATENPAUGH	10/91	P
2POR	*	PORIN(RHODOBACTER CAPSULATUS)	M.WEISS,G.SCHULZ	4/92	P
1RBC	*	RIBONUCLEASE S MUTANT(M13A)	R.VARADARAJAN,F.M.RICHARDS	6/92	P
1RBD	*	RIBONUCLEASE S MUTANT(M13ANB)	R.VARADARAJAN,F.M.RICHARDS	6/92	P
1RBE	*	RIBONUCLEASE S MUTANT(M13F)	R.VARADARAJAN,F.M.RICHARDS	6/92	P
1RBF	*	RIBONUCLEASE S MUTANT(M13G)	R.VARADARAJAN,F.M.RICHARDS	6/92	P
1RBG	*	RIBONUCLEASE S MUTANT(M13I)	R.VARADARAJAN,F.M.RICHARDS	6/92	P
1RBH	*	RIBONUCLEASE S MUTANT(M13L)	R.VARADARAJAN,F.M.RICHARDS	6/92	P
1RBI	*	RIBONUCLEASE S MUTANT(M13V)	R.VARADARAJAN,F.M.RICHARDS	6/92	P
1AAI	*	RICIN(CASTOR PLANT)	J.ROBERTUS ET AL.	4/92	P
1STP	*	STREPTAVIDIN-BIOTIN COMPLEX	DUPONT PROTEIN CRYSTALLOGRAPHY	3/92	P
1SOS	*	SUPEROXIDE DISMUTASE	H.E.PARGE,R.A.HALLEWELL,J.A.TAINER	2/92	P
1BBQ	*	THYMIDYLATE SYNTHASE(E.COLI)/DUMP/CB3717	J.FINER-MOORE ET AL.	3/92	P
1THC	*	TRANSTHYRETIN/3',5'-DIBROMOAURONE	E.CISZAK,V.CODY,J.LUFT	4/92	P
1PPC	*	TRYPSIN(BOVINE)/NAPAP	W.BODE,D.TURK	10/91	P
1PPH	*	TRYPSIN(BOVINE)/3TAPAP	W.BODE,D.TURK	10/91	P
1PPE	*	TRYPSIN(BOVINE)/CMTI-I	W.BODE,R.HUBER	10/91	P
1AAL	*	TRYPSIN INHIBITOR MUTANT(C30V,C51A)	EIGENBROT,RANDAL,KOSSIAKFF	4/92	P
1HPT	*	PANCREATIC SECRETORY TRYPSIN INHIBITOR VARIANT 3	H.J.HECHT,M.SZARDENINGS, J.COLLINS,D.SCHOMBURG	3/92	P
1NRC	*	U1 SN RIBONUCLEOPROTEIN A(RNA-BNDG DOMN)	P.EVANS ET AL.	3/92	P
1AAR	*	DI-UBIQUITIN	W.J.COOK ET AL	4/92	P
1AAK	*	UBIQUITIN CONJUGATING ENZYME	W.J.COOK ET AL	4/92	P
1IFD	*	FD STRAIN OF INOVIRUS MAJOR COAT PROTEIN (FIBER)	D.A.MARVIN	2/92	P

TABLE 8 - ATOMIC COORDINATE, STRUCTURE FACTOR, AND NMR EXPERIMENTAL DATA ENTRIES (IN PREPARATION) - JULY 1992

new data only

IDENT CODE		*MOLECULE*	*DEPOSITOR(S)*	*DATE*	*STATUS*
1VTM	*	VIRUS(TOBACCO MOSAIC, U2 STRAIN)	G.STUBBS,R.PATTANAYEK	3/92	P
1NCP	*	TWO ZINC BINDING DOMAIN (NMR)	G.M.CLORE,J.G.OMICHINSKI, A.M.GRONENBORN	11/91	P
2APD	*	APOLIPOPROTEIN D (MODEL)	M.C.PEITSCH,M.S.BOGUSKI	4/92	P
1BBE	*	COLLAGEN(3 CHAINS OF 4(G-P-P))(MODEL 1)	G.NEMETHY ET AL.	4/92	P
1BBF	*	COLLAGEN(3 CHAINS OF 4(G-P-P))(MODEL 2)	G.NEMETHY ET AL.	4/92	P
1D71	*	DNA(NODULE, DOUBLE TRIPLEX) MODEL	D.SPROUS,S.HARVEY	4/92	P
R1ABDMR	*	ACYL COENZYME A BINDING PROTEIN(NMR,20)	K.ANDERSEN,F.POULSEN	3/92	M
R1BBMMR	*	CALMODULIN BINDING DOMAIN	G.M.CLORE,A.BAX,M.IKURA, A.M.GRONENBORN	5/92	M
R1BBLMR	*	E3-BINDING DOMAIN (NMR)	G.M.CLORE,M.A.ROBIEN, A.M.GRONENBORN	2/92	M
R5CACSF	*	CARBONIC ANHYDRASE C/SO3	A.LILJAS ET AL.	9/91	S
R1D58SF	*	DNA (TGATCA)-4' EPIADRIAMYCIN	B.L.D'ESTAINTOT,B.GALLOIS,T.BROWN, W.N.HUNTER	2/92	S
R1D78SF	*	DNA (GTGTACAC) A-CONFORMATION	N.THOTA,X.H.LI,C.BINGMAN, M.SUNDARALINGAM	6/92	S
R1D79SF	*	DNA (GTGTACAC) A-CONFORMATION	N.THOTA,X.H.LI,C.BINGMAN, M.SUNDARALINGAM	6/92	S
R1MYGSF	*	MYOGLOBIN(PIG)	S.SMERDON ET AL.	2/92	S
R1MYHSF	*	MYOGLOBIN(PIG) MUTANT(K45R)	S.SMERDON ET AL.	2/92	S
R1MYISF	*	MYOGLOBIN(PIG) MUTANT(K45S)	S.SMERDON ET AL.	2/92	S
R1MYJSF	*	MYOGLOBIN(PIG) MUTANT(V68T)	S.SMERDON ET AL.	2/92	S
R1CDESF	*	PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE	R.J.ALMASSY	5/92	S
R2PORSF	*	PORIN(RHODOBACTER CAPSULATUS)	M.WEISS,G.SCHULZ	4/92	S
R1RBCSF	*	RIBONUCLEASE S MUTANT(M13A)	R.VARADARAJAN,F.M.RICHARDS	6/92	S
R1RBDSF	*	RIBONUCLEASE S MUTANT(M13ANB)	R.VARADARAJAN,F.M.RICHARDS	6/92	S
R1RBESF	*	RIBONUCLEASE S MUTANT(M13F)	R.VARADARAJAN,F.M.RICHARDS	6/92	S
R1RBFSF	*	RIBONUCLEASE S MUTANT(M13G)	R.VARADARAJAN,F.M.RICHARDS	6/92	S
R1RBGSF	*	RIBONUCLEASE S MUTANT(M13I)	R.VARADARAJAN,F.M.RICHARDS	6/92	S
R1RBHSF	*	RIBONUCLEASE S MUTANT(M13L)	R.VARADARAJAN,F.M.RICHARDS	6/92	S
R1RBISF	*	RIBONUCLEASE S MUTANT(M13V)	R.VARADARAJAN,F.M.RICHARDS	6/92	S
R1AALSF	*	TRYPSIN INHIBITOR MUTANT(C30V,C51A)	C.EIGENBROT ET AL.	4/92	S
R1HPTSF	*	PANCREATIC SECRETORY TRYPSIN INHIBITOR VARIANT 3	H.J.HECHT,M.SZARDENINGS,J.COLLIN, D.SCHOMBURG	3/92	S
R1AARSF	*	DI-UBIQUITIN	W.J.COOK ET AL	4/92	S
R1AAKSF	*	UBIQUITIN CONJUGATING ENZYME	W.J.COOK ET AL	4/92	S

* New or replacement entry since April 1992 Newsletter

Status Codes:

- A Alpha carbon atoms only
- B Backbone only
- M NMR restraints and other NMR experimental data
- N New entry awaiting approval by depositor
- P In preparation
- R Replacement for entry in Table 3
- S Structure factors

TABLE 9 - ATOMIC COORDINATE, STRUCTURE FACTOR, AND NMR EXPERIMENTAL DATA ENTRIES (ON HOLD) - JULY 1992

IDENT CODE		MOLECULE	DEPOSITOR(S)	DATE	HOLD EXPIRES	STATUS
1AEC		ACTINIDIN/E-64	K.VARUGHESE	2/92	2/93	H
1ACH		ALPHA1 ANTICHYMOTRYPSIN(HUMAN)	U.BAUMANN,R.HUBER ET AL.	1/91	1/93	H
1AOZ		ASCORBATE OXIDASE(ZUCCHINI)	A.MESSERSCHMIDT ET AL.	1/92	1/93	H
1AT2		ASPARTATE CARBAMOYLTRANSFERASE (B.SUBTLS)	STEVENS,REINISCH, LIPSCOMB	6/91	3/93	H
2AZU		AZURIN(P.AERUGINOSA) MUTANT(H35L)	NAR,MESSERSCHMIDT, HUBER	1/91	1/93	H
3AZU		AZURIN(P.AERUGINOSA) MUTANT(H35Q)	MESSERSCHMIDT,NAR, HUBER	1/91	1/93	H
4AZU		AZURIN(P.AERUGINOSA) (PH 5.5)	NAR,MESSERSCHMIDT, HUBER	6/91	6/93	H
5AZU		AZURIN(P.AERUGINOSA) (PH 9.0)	NAR,MESSERSCHMIDT, HUBER	6/91	6/93	H
1CPL		CYCLOPHILIN(HUMAN T CELL)	KE,ZYDOWSKY,LIU,WALSH	9/91	9/92	H
1DHR		DIHYDROPTERIDINE REDUCTASE(RAT LIVER)	K.VARUGHESE	3/92	3/93	H
1D55		DNA(GAAGCTTC)/ACTINOMYCIN D	S.KAMITORI,F.TAKUSAGAWA	2/92	2/93	H
1D77	*	DNA (CGCIAATTCGCG)	J.C.XUAN,I.T.WEBER	5/92	6/93	H
1DRI		D-RIBOSE-BINDING PROTEIN(E.COLI)	S.MOWBRAY,L.B.COLE	2/92	9/92	H
9EST		ELASTASE(PORCINE)/PEPTIDYL BENZOXALOSE	E.MEYER JR. ET AL.	1/91	1/93	H
1EPS		5-ENOL-PYRUVYL-3-PHOSPHATE SYNTHASE	W.STALLINGS	4/91	4/93	AH
1FPB		FRUCTOSE-1,6-BISPHOSPHATASE/FRU-2,6-P2	W.LIPSCOMB ET AL.	2/92	2/93	H
1CGP		CATABOLITE GENE ACTIVATOR PROTEIN/DNA	SCHULTZ,SHIELDS,STEITZ	8/91	8/92	H
1GPR		GLUCOSE PERMEASE(IIA DOMAIN)(B.SUBTILIS)	D.-I.LIAO,O.HERZBERG	9/91	9/92	H
1GGA		G-GLYCERALDEHYDE-PHOSPHATE DEHYDROGENASE	F.VELLIEUX,J.HAJDU,W.HOL	10/91	10/92	H
1HHR		GROWTH HORMONE/RECEPTOR EXTRACELLR DOMN	DE VOS,ULTSCH, KOSSIAKOFF	1/92	1/93	H
2HTC		HIRUDIN(VARIANT 2)/THROMBIN COMPLEX	A.TULINSKY ET AL.	4/91	4/93	H
1HGT		HIRUGEN/THROMBIN COMPLEX	A.TULINSKY ET AL.	6/91	6/93	H
2HGT		HIRULOG 1/THROMBIN COMPLEX	A.TULINSKY,V.CARPEROS	6/91	6/93	H
1HIO		HISTONE OCTAMER(CHICKEN)	G.ARENTS,E.MOUDRIANAKIS	9/91	9/93	H
1ITL		INTERLEUKIN 4(HUMAN)(NMR)	C.DOBSON ET AL.	2/92	2/93	H
1LAO		LYS-,ARG-,ORNITHINE-BINDING PROTEIN(LAO)	S.-H.KIM	10/91	1/93	H
1MYT		MYOGLOBIN(MET,YELLOWFIN TUNA)	BIRNBAUM,ROSE, PRZYBYLSKA	5/91	8/93	H
1NPX		NADH PEROXIDASE(NON-NATIVE,OXIDIZED)	G.SCHULZ ET AL.	8/91	7/92	H
1CDD	*	PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE	R.J.ALMASSY	5/92	5/93	H
1CPC		C-PHYCOCYANIN(FREMYELLA DIPLOSIPHON)	DUERRING,SCHMIDT,HUBER	10/90	10/92	H
1PF2		PROTHROMBIN CA-FRAGMENT 1	A.TULINSKY ET AL.	12/91	2/93	H
1HVT	*	REVERSE TRANSCRIPTASE	L.A.KOHLSTAEDT,J.WANG, J.M.FRIEDMAN,P.A.RICE, T.A.STEITZ	6/92	6/93	H
1RN1		RIBONUCLEASE T1(GLN 25)	R.ARNI ET AL.	11/91	11/92	H
1ST3		SUBTILISIN BL(BACILLUS LENTUS)	D.GODDETTE	11/91	6/93	H
1PPB	*	THROMBIN(HUMAN)/PPACK	W.BODE	10/91	12/92	H
3TGL		TRIACYLGLYCEROL ACYLHYDROLASE	Z.DEREWENDA	7/91	7/92	H
4TGL		TRIACYLGLYCEROL ACYLHYDROLASE COMPLEX	Z.DEREWENDA	7/91	7/92	H
4XIM	*	D-XYLOSE ISOMERASE CO COMPLEX	J.JANIN ET AL	3/92	4/93	H
5XIM	*	D-XYLOSE ISOMERASE SORBITOL-MG	J.JANIN ET AL	3/92	4/93	H
6XIM	*	D-XYLOSE ISOMERASE XYLOSE-MG	J.JANIN ET AL	3/92	4/93	H
7XIM	*	D-XYLOSE ISOMERASE DEMETALLIZED PH 5	J.JANIN ET AL	3/92	4/93	H
8XIM	*	D-XYLOSE ISOMERASE E186Q MUTANT XYLOSE-MG	J.JANIN ET AL	3/92	4/93	H

TABLE 9 - ATOMIC COORDINATE, STRUCTURE FACTOR, AND NMR EXPERIMENTAL DATA ENTRIES (ON HOLD) - JULY 1992

IDENT CODE		MOLECULE	DEPOSITOR(S)	DATE	HOLD EXPIRES	STATUS
9XIM	*	D-XYLOSE ISOMERASE E186Q MUTANT XYLOSE-MN	J.JANIN ET AL	3/92	4/93	H
1XIN	*	D-XYLOSE ISOMERASE H220N MUTANT XYLOSE-MG	J.JANIN ET AL	4/92	4/93	H
2XIN	*	D-XYLOSE ISOMERASE H290N MUTANT SORBITOL-CO	J.JANIN ET AL	4/92	4/93	H
3XIN	*	D-XYLOSE ISOMERASE E181Q MUTANT	J.JANIN ET AL	4/92	4/93	H
5XIN	*	D-XYLOSE ISOMERASE D255A MUTANT XYLOSE-MG	J.JANIN ET AL	4/92	4/93	H
R1ITLMR		INTERLEUKIN 4(HUMAN)(NMR)	C.DOBSON ET AL.	2/92	2/93	MH
R1ACHSF		ALPHA1 ANTICHYMOTRYPSIN(HUMAN)	BAUMANN,HUBER ET AL.	1/91	1/93	SH
R1D55SF		DNA(GAAGCTTC)/ACTINOMYCIN D	KAMITORI,TAKUSAGAWA	2/92	2/93	SH
R1LAPSF		LEUCINE AMINOPEPTIDASE(BOVINE LENS)	W.LIPSCOMB ET AL.	8/90	10/94	SH
R1MADSF		METHYLAMINE DEHYDROGENASE	F.VELLIEUX,W.HOL	2/91	2/95	SH
R1MYTSF		MYOGLOBIN(MET,YELLOWFIN TUNA)	BIRNBAUM,ROSE,PRZBLSKA	5/91	8/93	SH
R1NPXSF		NADH PEROXIDASE(NON-NATIVE,OXIDIZED)	G.SCHULZ ET AL.	8/91	7/92	SH
R1CDDSF	*	PHOSPHORIBOSYLGLYCINAMIDE FORMYLTRANSFERASE	R.J.ALMASSY	5/92	5/93	SH
R2PNPSF		PURINE NUCLEOSIDE PHOSPHORYLASE(HUMAN)	S.EALICK ET AL.	11/89	1/94	SH
R1ST3SF		SUBTILISIN BL(BACILLUS LENTUS)	D.GODDETTE	11/91	6/93	SH
R3SODSF		SUPEROXIDE DISMUTASE(BOVINE)	J.TAINER ET AL.	6/90	6/94	SH

* New or replacement entry since April 1992 Newsletter

Status Codes:

- A Alpha carbon atoms only
- B Backbone only
- H Hold for delayed release as requested by depositor
- M NMR restraints and other NMR experimental data
- N New entry awaiting approval by depositor
- P In preparation
- R Replacement for entry in Table 3
- S Structure factors

Name of User _____ Date _____

Address _____ Phone _____

_____ E-mail _____

_____ Fax # _____

DATAPRTP

(all available coordinate entries, bibliographic entries, and some computer programs)

	6250cpi	1600cpi	TK50	1/4"	8mm	DAT
VAX/VMS *backup*	[ ] $413	[ ] $877	[ ] $560			
VAX/VMS *copy*	[ ] $413	[ ] $877	[ ] $560			
Unlabeled *ASCII*	[ ] $413	[ ] $877				
Unlabeled *EBCDIC*	[ ] $413	[ ] $877				
SGI/SUN/IBM/E&S UNIX *tar*	[ ] $348	[ ] $348	[ ] $348			

PDBPGMTP

(all computer programs and miscellaneous files)

	6250cpi	1600cpi	TK50	1/4"	8mm	DAT
VAX/VMS *copy*	[ ] $336	[ ] $336	[ ] $359			
SGI/SUN/IBM/E&S UNIX *tar*	[ ] $348	[ ] $348	[ ] $348			

STRUCTURE FACTOR ENTRIES

(experimental diffraction data)

Choose tape(s): [ ] NONST1TP [ ] NONST2TP [ ] NONST3TP [ ] NONST4TP
[ ] NONST5TP [ ] NONST6TP [ ] NONST7TP [ ] NONST8TP
[ ] NONST9TP [ ] NONST10TP

Choose one format for selection(s) shown above:

	6250cpi	1600cpi	TK50	1/4"	8mm	DAT
VAX/VMS *backup*	[ ] $336	[ ] $336	[ ] $359			
VAX/VMS *copy*	[ ] $336	[ ] $336	[ ] $359			
Unlabeled *ASCII*	[ ] $336	[ ] $336				
Unlabeled *EBCDIC*	[ ] $336	[ ] $336				
SGI/SUN/IBM/E&S UNIX *tar*	[ ] $348	[ ] $348	[ ] $348			

NMRRS1TP

(NMR experimental data entries)

	6250cpi	1600cpi	TK50	1/4"	8mm	DAT
VAX/VMS *backup*	[ ] $336	[ ] $336	[ ] $359			
VAX/VMS *copy*	[ ] $336	[ ] $336	[ ] $359			
Unlabeled *ASCII*	[ ] $336	[ ] $336				
Unlabeled *EBCDIC*	[ ] $336	[ ] $336				
SGI/SUN/IBM/E&S UNIX *tar*	[ ] $348	[ ] $348	[ ] $348			

PRINTED LISTINGS

Indicate IDENT Code(s) from list of available coordinate entries in Newsletter:

[ ] $102 (IDENT code _____) [ ] $102 (IDENT code _____)

TOTAL CHARGES

Magnetic tape charges ..... $ _____

Foreign air mail charges ($19 per tape item mailed outside U.S. and Canada) ..... $ 19.00 (if applicable)

Printed listing charges ..... $ _____

(Prices are valid until September 30, 1992) *TOTAL COST* ..... $ _____

PRINTED DOCUMENTATION (no charge)

[ ] Atomic Coordinate and Bibliographic Entry Format Description for DATAPRTP (Feb. 1992)
[ ] Complete List of Bibliographic Entries
[ ] Current DATAPRTP Directory
[ ] Data Deposition Form
[ ] Detailed Contents and Format Description for Each Structure Factor Entry
[ ] Latest Newsletter
[ ] Sources of Visual Aids for Macromolecular Structure (Feb. 1990)
[ ] User Guide (Summer 1992)

PLACING AN ORDER

(Prices are valid until September 30, 1992)

We must receive the following three items before service is provided:

1. completed order form
2. mailing label indicating exact shipping address
3. payment (use one of the methods listed below):

⇒ Check payable to Brookhaven National Laboratory in U.S. dollars and drawn on a U.S. bank. Foreign checks are not acceptable.

⇒ Original hardcopy of purchase order payable to Brookhaven National Laboratory. After your order is processed, our Fiscal Division will invoice you.

⇒ Wire transfer. In order to use wire transfer capabilities, we must ***first*** receive an original purchase order from you. After you receive our invoice, your bank should send a wire transfer to:

Bank name: Morgan Guarantee Trust Company of New York
Acct. name: Brookhaven National Laboratory
Cust. Acct. : 076-51-912

Please mail (facsimile is not recommended) all required items to:

Protein Data Bank Orders
Chemistry Department, Building 555
Brookhaven National Laboratory
Upton, NY 11973 USA

Protein Data Bank
Chemistry Department, Building 555
Brookhaven National Laboratory
Upton, NY 11973 USA

First Class