Protein Data Bank

Quarterly Newsletter

Number 63 January 1993

State of the PDB

The Protein Data Bank (PDB) is very much a resource in transition. In fulfilling its mission to provide the international scientific and technological community with access to information and knowledge on 3-D structures of biological macromolecules, PDB is reorganizing its staff, while developing increasingly automated procedures for data submission and validation. New procedures for data distribution and user access, and for maintenance of the PDB archive at Brookhaven, also are being developed. PDB is actively planning to expand its role as a center for coordination and development of the new database management, manipulation and analysis tools that will be required in the future if the rapidly growing mass of 3-D structural information is to be effectively utilized. At the same time PDB plans to develop a research program strongly coupled to the database, involving application of the data for forefront studies in structural biology.

An important milestone reached with this release brings PDB's coverage completely up-to-date on prerelease. All prerelease entries have been checked using PDB's structure validation software, but annotation is limited to bibliographic citations, primary sequence data, and other essential information. PDB plans to complete full annotation of all structures in time for the August 1993 Beijing International Union of Crystallography (IUCr) Congress when a total of 2,300 entries is expected. Current trends suggest that the number of depositions in PDB is growing exponentially and, if this is indeed the case, a total of more than 10,000 entries can be expected by the end of 1998.

The entire PDB collection of prerelease and full-release entries is now available from Brookhaven free of charge over Internet. Distribution *via* Internet is expected to continue to increase in importance in the future. For details on how to access the PDB e-mail server and anonymous FTP, see page 5. If you wish to purchase PDB data from Brookhaven on CD ROM or magnetic tape, please use the Brookhaven Order Form on pp. 13-14. The database is also available from the PDB Affiliated Centers listed on page 15.

Important new developments presently underway at PDB include the following:

- PDB has officially adopted the IUCr's Crystallographic Information File (CIF) standard as its future data interchange format. The ASN.1 interchange standard used

continued on p. 2

January 1993 PDB Release

1055 fully annotated atomic coordinate entries
(53 new full-release entries)

- 944 proteins, enzymes and viruses
- 90 DNA's
- 2 RNA's
- 9 tRNA's
- 10 carbohydrates

437 prerelease atomic coordinate entries
270 structure factor entries
23 NMR experimental entries

The total size of the atomic coordinate entry database is 375 Mbytes, uncompressed.

Table of Contents

in a number of molecular biology databases also will be supported. Support of the traditional PDB fixed field-length format will continue in parallel with CIF and ASN.1 for several years.

- Data entry will, as much as possible, be performed by the depositors. PDB will set standards for an open, extensible PDB-AUTHORIN data entry software system and a validation suite incorporating PDB and community-supplied modules. PDB will maintain the AUTHORIN and validation suite software products through regular public releases.

- An on-line PDB database will be developed which will support intelligent interactive queries and analysis from Brookhaven over Internet. This will provide the primary access mechanism for the PDB of the future. Initial implementation will be as PDB-SYBASE (relational database management system). In the future, the use of object-oriented database technology will be considered as well.

In fulfilling its goals and objectives, PDB is relying on an extensive network of collaborations with members of the community. These collaborations are central to all three areas of development highlighted above and are expected to assume greater importance in the future.

Thomas F. Koetzle
Head, PDB

Issuing Idcodes

New procedures giving depositors direct access to PDB processing and checking programs *via* Internet will be available for depositor testing starting in March 1993. Depositors using these new procedures can expect to receive confirmation of their deposition along with their entry idcode within three days of deposition. Further details and login instructions will be available shortly on the PDB anonymous FTP account.

Several options will be available to speed up the deposition procedure:

- Files that are in standard PDB format will be processed for prerelease directly with minimal staff intervention. This new procedure will require files to be fully annotated and to conform to standard PDB data representation.

- Depositors can enter annotation directly into PDB-SYBASE deposition tables using an interface developed at Brookhaven. Atomic coordinate data must be submitted in PDB format.

- A new PDB deposition form is being formulated. This new form is expected to facilitate transcription of information directly into PDB-SYBASE tables.

PDB Data Interchange Format

The PDB has adopted the IUCr's Crystallographic Information File (CIF) as its future data interchange format. Based on the Self-Defining Text Archive and Retrieval (STAR) procedure [1], the CIF is a general free-format text archive file. A comprehensive CIF dictionary of crystallographic data items for reporting results emanating from structural studies of small organic and inorganic molecules already has been adopted by the IUCr [2]. Union journals now accept for publication manuscripts and data written in CIF format.

A Working Group on Macromolecular CIF Definitions of the IUCr Commission on Crystallographic Data and the IUCr Commission on Journals, headed by Dr. P. M. D. Fitzgerald, is working at extending the CIF dictionary to represent results from structural studies of biological macromolecules. The Working Group is presenting the macromolecular extensions to the core dictionary to the IUCr for formal approval at the XVIth Congress and General Assembly of the IUCr to be held in Beijing, China in August 1993. The Working Group actively is seeking input from the community concerning the macromolecular CIF dictionary. A presentation of the dictionary will be made at the Annual Meeting of the American Crystallographic Association (ACA) to be held in Albuquerque, NM on May 23-28, 1993. The draft will be available for public comment and suggestions after the ACA meeting.

All CIF data items are defined in a dictionary,itself also written in CIF. As an example, given below are the CIF Core Dictionary (Core Version 1991 [2]) items corresponding to the data items in a PDB CRYST1 record and a PDB CRYST1 record in a CIF representation.

```
data_cell_angle_
      loop_ _name                '_cell_angle_alpha'
                                 '_cell_angle_beta'
                                 '_cell_angle_gamma'
      _type                      numb
      _enumeration_range         0.0:180.0
      _enumeration_default       90.0
      _esd                       yes
      _esd_default               0.0
      _definition

;

      Unit-cell angles in degrees of the reported structure.The
      values of _refln_index_h, *_k, *_l must correspond to
      the cell defined by these values and _cell_length_a, *_b
      and *_c. The values of _diffrn_refln_index_h, *_k, *_l
```

[1] S. R. Hall (1991). "The STAR File: A New Format for Electronic Data Transfer and Archiving". *J. Chem. Inf. Comput. Sci.* **31**, 326-333.

[2] S. R. Hall, F. H. Allen and I. D. Brown (1991). "The Crystallographic Information File (CIF): A New Standard Archive File for Crystallography". *Acta Cryst.* **A47**, 655-685.

may not correspond to these values if a cell transformation took place following the measurement of diffraction intensities. See also _diffrn_refIns_transf_matrix_.
;

```
data_cell_formula_units_Z
      _name                  '_cell_formula_units_Z'
      _type                  numb
      _enumeration_range     1:
      _definition
;

      The number of the formula units in the unit cell as specified
      by _chemical_formula_structural, _chemical_formula_moiety
      or _chemical_formula_sum.
;

data_cell_length_
      loop_ _name            '_cell_length_a'
                             '_cell_length_b'
                             '_cell_length_c'
      _type                  numb
      _enumeration_range     0.0:
      _esd                   yes
      _esd_default           0.0
      loop_ _units_extension
            _units_description
            _units_conversion  ' '    'Angstroms'   *1.0
                               '_pm'  'picometres'  /100.
                               '_nm'  'nanometres'  *10.
      _definition
;

      Unit-cell lengths corresponding to the structure
      reported. The values of _refIn_index_h, *_k, *_l
      must correspond to the cell defined by these
      values and _cell_angle_ values. The values of
      _diffrn_refIn_index_h, *_k, *_l may not correspond
      to these values if a cell transformation took place
      following the measurement of diffraction inten-
      sities. See also _diffrn_refIns_transf_matrix_.
;

data_symmetry_space_group_name_H-M
      _name                  '_symmetry_space_group_name_H-M'
      _type                  char
      loop_ _example         'P 21 21 21'
                             'P 2/n 2/n 2/n (origin at -1)'
                             'R -3 2/m'
      _definition
;

      Hermann-Mauguin space-group symbol. Note that the
      H-M symbol does not necessarily contain complete
      information about the symmetry and the space-group
      origin. If used always supply the FULL symbol from
      International Tables for Crystallography, Vol. A (1987)
      and indicate the origin and the setting if it is not implicit.
      If there is any doubt that the equivalent positions can
      be uniquely deduced from this symbol specify the
      _symmetry_equiv_pos_as_xyz or *_Hall data items as
      well. Leave spaces between symbols referring to differ-
      ent axes.
;
```

A PDB file in CIF will present the CRYST1 information as follows:

```
_cell_length_a                    72.3
_cell_length_b                    72.3
_cell_length_c                    185.9
_cell_angle_alpha                 90.0
_cell_angle_beta                  90.0
_cell_angle_gamma                 120.0
_symmetry_space_group_name_H-M    'P 31 2 1'
_cell_formula_units_Z             6
```

New PDB Record Types

PDB is proposing new record types designed to represent relationships between components of structures such as symmetry-related domains. The new records can, for example, be used to generate biologically functional aggregates from atomic coordinates provided in PDB entries. We would like your comments and suggestions on these proposed new records. An explanation of existing PDB records can be found in the PDB Atomic Coordinate and Bibliographic Entry Format Description, which is available upon request.

SYMDES Cols. 1 – 6 SYMDES
8 – 10 Serial number
12 – 70 Description of crystallographic symmetry operator

FORMAT (6A1,1X,I3,1X,59A1)

Note: SYMDES records contain text fields that describe crystallographic symmetry operators given as matrix operators in PDB record type SYMOP (see below). Columns 12 -70 normally will contain a description of the operator in symbolic form. For example, in the space group P 2 the two-fold operator will be described as "-x,y,-z".

The serial number links SYMDES with SYMOP records. SYMOP records are described by SYMDES records of the same serial number.

SYMOP	Cols. 1-6	8-10	11-20	21-30	31-40	46-55
	SYMOP1	Ser. no.(i)	S_{11}	S_{12}	S_{13}	T_1
	SYMOP2	Ser. no.(i)	S_{21}	S_{22}	S_{23}	T_2
	SYMOP3	Ser. no.(i)	S_{31}	S_{32}	S_{33}	T_3

FORMAT (6A1,1X,I3,3F10.6,5X,F10.5)

Note: (i) One trio of SYMOP records with a constant serial number is given for each crystallographic symmetry operator described in SYMDES. SYMOP and MTRIX records that are included in an entry must be assigned distinct serial numbers.

(ii) The SYMOP transformations operate on the stored coordinates to yield crystallographically-equivalent representations of the structure in the same space.

MTXDES Cols. 1 – 6 MTXDES
8 – 10 Serial number
12 – 70 Description of non-crystallographic symmetry operator

FORMAT(6A1,1X,I3,1X,59A1)

Note: MTXDES records contain text fields that describe non-crystallographic symmetry operators given as matrix operators in MTRIX records.

The serial number links MTXDES with MTRIX records. MTRIX records are described by MTXDES records with the same serial number. SYMOP and MTRIX records that are included in an entry must be assigned distinct serial numbers.

CMPDES Cols. 1 – 6 CMPDES
8 – 10 Serial number
12 – 70 Description of component

FORMAT(6A1,1X,I3,1X,59A1)

Note: CMPDES records contain text describing structure components defined by COMPNT records. A CMPDES record must be supplied for each CMPONT record.

CMPONT Cols. 1 – 6 CMPONT
8 – 10 Serial number
12 – 14 Starting residue name
16 Starting residue chain identifier
18 – 21 Starting residue sequence number
22 Starting residue insertion code
24 – 26 Ending residue name
28 Ending residue chain identifier
30 – 33 Ending residue sequence number
34 Ending residue insertion code

FORMAT(6A1,1X,A3,1X,I3,1X,A1,1X,I4,A1,1X,A3,1X,I1,1X,I4,A1)

Note: CMPONT is used to describe structure components. Each component is delineated by a serial number and is defined by giving starting and ending residue information. CMPONT serial numbers are assigned beginning with 1. Components represented by a set of SEQRES records are numbered first, and then those representing HET groups are assigned successive numbers.

HET groups that are covalently linked to atoms in a chain represented by a set of SEQRES records (e.g., atoms that modify sidechains), have component numbers the same as those of the chain. See also the explanation of FORMUL records in the Atomic Coordinate and Bibliographic Entry Format Description.

Several CMPONT records with the same CMPONT serial number may be required to define a single structure unit which is not contiguous in the ATOM/HETATM record list (e.g., to include side chain modifications where the HET groups are listed following the chain in question).

Components can be assigned to any structure unit such as those generated by applying SYMOP or MTRIX symmetry operators to deposited coordinates. In such cases generated coordinates will be assigned new chain identifiers to differentiate them from deposited coordinates.

TRNSFM Cols. 1 – 6 TRNSFM
8 – 10 CMPONT serial number of transformed structure
12 – 14 SYMOP or MTRIX serial number
16 – 18 CMPONT serial number to which symmetry operator is to be applied

FORMAT(6A1,3(1X,I3))

Note: TRNSFM records are used to define operations to generate components related by SYMOP and MTRIX coordinate transformation records. Components specified in TRNSFM (cols. 8-10 and 16-18) must be described by CMPDES and CMPONT records.

Let (X,Y,Z) be coordinates of atoms in the component specified in columns 16-18.

Let the matrix

$$\begin{matrix} S_{11} & S_{12} & S_{13} & T_1 \\ S_{21} & S_{22} & S_{23} & T_2 \\ S_{31} & S_{32} & S_{33} & T_3 \end{matrix}$$

describe the SYMOP or MTRIX transformation operator specified in columns 12-14.

Then (X',Y',Z') are coordinates of atoms in the component specified by the serial number in columns 8-10.

$$\begin{matrix} X' \\ Y' \\ Z' \end{matrix} = \begin{matrix} S_{11}*X + & S_{12}*Y + & S_{13}*Z + & T_1 \\ S_{21}*X + & S_{22}*Y + & S_{23}*Z + & T_2 \\ S_{31}*X + & S_{32}*Y + & S_{33}*Z + & T_3 \end{matrix}$$

AGRDES Cols. 1 – 6 AGRDES
8 – 10 Serial number
12 – 70 Description of structure aggregate

FORMAT(6A1,1X,I3,1X,59A1)

Note: AGRDES records contain text describing structure aggregates defined by AGGRGT records. An AGRDES record must be supplied for each AGGRGT record.

AGGRGT	Cols. 1 – 6	AGGRGT
	8 – 10	Serial number
	12 – 14	Number of components in the structure aggregate
	16 – 18	CMPONT serial numbers included in the structure aggregate
	20 – 22	
	24 – 26	
	•	
	•	
	•	
	68 – 70	

FORMAT(6A1,16(1X,I3))

Note: AGGRGT records define structure aggregates as a combination of components specified in CMPONT records (e.g., a tetrameric molecule is defined in terms of 4-fold related monomers). AGRDES records provide text describing the aggregates.

Accessing PDB via Gopher

PDB is now accessible through the Internet Gopher. Gopher allows the user to easily access various types of data residing on multiple hosts. The user is the "client" who makes queries to a "server" residing on another host on the Internet network. This system has been set up so that the users do not need to know the location of servers: Gopher transparently handles the connections. The PDB Internet Gopher server allows access, search, and downloading of the same information and coordinate files as does anonymous FTP, but through a window environment. Merely choose "Protein Data Bank FTP Site" after opening Gopher. "Full-text search of PDB" allows one to search the PDB using either an idcode, author name, compound name, or any other term.

Information for setting up an Internet Gopher client including source files for different machines is available via anonymous ftp to boombox.micro.umn.edu (134.84.132.2) under the directory /pub/gopher. Those now running a Gopher client can access the PDB server by including the following link:

Name = Protein Data Bank FTP site
Type = 1
Host = pdb.pdb.bnl.gov
Port = 70
Path = 1/

For more information or help in accessing the PDB via Gopher, send e-mail to oeder@bnl.gov.

File Server and Anonymous FTP

The PDB e-mail file server and anonymous FTP are available for all users. In addition to the atomic coordinate entry files, it is possible to access and download PDB general information and documentation. For more information about the e-mail server, send a 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**. Files may be transferred to and from this system using **anonymous** as the FTP user name and your real user name as the password. Besides downloading data files and documentation, it is possible to upload any files you may wish to send to the PDB. Please note that those using VMS may need to place quotes around file names.

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

Anonymous FTP for the Beginner

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. The following is intended as an introduction covering only the simplest commands.

FTP stands for 'File Transfer Program' and 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 may 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.

CD ROM Information

PDB releases are now available on CD ROM in *ISO 9660* format. To avoid confusion, the layout of the files on the CD ROM mirrors that of the tape distribution. The entry files themselves are in ASCII format and should be readable by any software able to read text files. The structure factor files will be compressed using the standard UNIX compress command.

The CD ROM now includes the MAGE and PERKIN structure display and manipulation software by Richardson and Richardson [1], in both PC and Macintosh versions.

VAX/VMS systems currently do not directly support access to *ISO 9660* formatted CD ROMs. The PDB CD ROM may be accessed on VAX/VMS systems by two approaches:

1. There is an *ISO 9660* compliant device driver available from Digital Equipment Corporation (DEC) that allows direct access to the CD ROM (driver part number YT-GS001-01). Please contact your DEC sales representative for further information.

2. There is a public utility for accessing *ISO 9660* CD ROMs, called CD_ACCESS, written by Peter Stockwell, University of Otago, New Zealand, that will allow all the files on the CD ROM to be copied to a magnetic disk drive. This utility can be obtained from the EMBL e-mail server (for further information you may contact DataLib@EMBL-Heidelberg.DE). When copying files using CD_ACCESS, be sure to use the /BINARY qualifier to the copy command.

[1] D. C. Richardson and J. S. Richardson (1992). "The Kinemage: A Tool for Scientific Communication". *Protein Science* 1, 3-9.

Newly Released Entries

IDCODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
2P07	ALPHA-LYTIC PROTEASE MUTANT(M192A)	R.BONE,D.AGARD	10/90
1P11	ALPHA-LYTIC PROTEASE/PHOSPHONATE ESTER (STRUCTURE 1)	R.BONE,D.AGARD	10/90
1P12	ALPHA-LYTIC PROTEASE/PHOSPHONATE ESTER (STRUCTURE 2)	R.BONE,D.AGARD	10/90
1LPR	ALPHA-LYTIC PROTEASE MUTANT(M192A)/ METHOXYSUCCINYL-A-A-P-ALANINE BORONIC ACID	R.BONE,D.AGARD	8/91
2LPR	ALPHA-LYTIC PROTEASE MUTANT(M192A)/ METHOXYSUCCINYL-A-A-P-VALINE BORONIC ACID	R.BONE,D.AGARD	8/91
3LPR	ALPHA-LYTIC PROTEASE MUTANT(M192A)/ METHOXYSUCCINYL-A-A-P-NORLEUCINE BORONIC ACID	R.BONE,D.AGARD	8/91
4LPR	ALPHA-LYTIC PROTEASE MUTANT(M192A)/ METHOXYSUCCINYL-A-A-P-LEUCINE BORONIC ACID	R.BONE,D.AGARD	8/91
5LPR	ALPHA-LYTIC PROTEASE MUTANT(M213A)/ METHOXYSUCCINYL-A-A-P-ALANINE BORONIC ACID	A.FUJISHIGE,R.BONE,D.AGARD	8/91
6LPR	ALPHA-LYTIC PROTEASE MUTANT(M213A)/ METHOXYSUCCINYL-A-A-P-NORLEUCINE BORONIC ACID	R.BONE,D.AGARD	8/91
7LPR	ALPHA-LYTIC PROTEASE MUTANT(M213A)/ METHOXYSUCCINYL-A-A-P-LEUCINE BORONIC ACID	A.FUJISHIGE,R.BONE,D.AGARD	8/91
8LPR	ALPHA-LYTIC PROTEASE MUTANT(M213A)/ METHOXYSUCCINYL-A-A-P-PHE BORONIC ACID	A.FUJISHIGE,R.BONE,D.AGARD	8/91
9LPR	ALPHA-LYTIC PROTEASE/METHOXYSUCCINYL-A-A-P-LEUCINE BORONIC ACID	R.BONE,D.AGARD	8/91
3CHY	CHE Y(ESCHERICHIA COLI)	K.VOLZ,P.MATSUMURA	4/91
1CP4	CYTOCHROME P450CAM(PHENYL RADICAL)	R.RAAG,T.POULOS	6/91
2CP4	CYTOCHROME P450CAM MUTANT(T252A)	R.RAAG,T.POULOS	6/91
3CP4	CYTOCHROME P450CAM(11 WEEK ADAMANTANE)	R.RAAG,T.POULOS	6/91
4CP4	CYTOCHROME P450CAM(RECOMBINANT)	R.RAAG,T.POULOS	6/91
1D75	DNA(CGCGAATT(O8A)GCG)	G.A.LEONARD,A.GUY,T.BROWN, R.TEOULE,W.N.HUNTER	5/92
6EBX	ERABUTOXIN B(LATICAUDA SEMIFASCIATA)	T.PRANGE,P.SALUDJIAN	5/91
2HAD	HALOALKANE DEHALOGENASE	K.H.G.VERSCHUEREN,S.M.FRANKEN, B.W.DIJKSTRA	8/92
6FAB	FAB 36-71(MURINE ANTI-PHENYLARSONATE)	R.STRONG ET AL.	1/91
1APH	INSULIN(BOVINE,CUBIC,PH7)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
1BPH	INSULIN(BOVINE,CUBIC,PH9)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
1CPH	INSULIN(BOVINE,CUBIC,PH10)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
1DPH	INSULIN(BOVINE,CUBIC,PH11)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
2RIG	INTERFERON-GAMMA	C.T.SAMUDZI,L.E.BURTON,J.R.RUBIN	1/93
2CPK	C-AMP-DEPENDENT PROTEIN KINASE(CATALYTIC SUBUNIT)	D.R.KNIGHTON,J.ZHENG,L.F.TEN EYCK, V.A.ASHFORD,N.-H.XUONG,S.S.TAYLOR, J.M.SOWADSKI	10/92
4BLM	BETA-LACTAMASE(BACILLUS LICHENIFORMIS)	J.KNOX,P.MOEWS	5/91
1LAA	LYSOZYME(HUMAN) MUTANT (D53E)	K.HARATA,M.MURAKI,Y.JIGAMI	6/92
1TAY	LYSOZYME(HUMAN) MUTANT(Y63A)	K.HARATA,M.MURAKI,Y.JIGAMI	8/92
1TBY	LYSOZYME(HUMAN) MUTANT(Y63L)	K.HARATA,M.MURAKI,Y.JIGAMI	8/92
1TCY	LYSOZYME(HUMAN) MUTANT(Y63F)	K.HARATA,M.MURAKI,Y.JIGAMI	8/92
1TDY	LYSOZYME(HUMAN) MUTANT(Y63W)	K.HARATA,M.MURAKI,Y.JIGAMI	8/92
2MCM	MACROMOMYCIN(STREPTOMYCES MACROMOMYCETICUS)	P.VAN ROEY	5/91
2MM1	MYOGLOBIN(HUMAN) MUTANT(K45R,C110A)(HUMAN)	S.HUBBARD,W.HENDRICKSON, D.LAMBRIGHT,S.BOXER	2/91

Newly Released Entries (cont.)

IDCODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
3OVO	OVOMUCOID 3RD DOMAIN CLEAVED(JAPANSE QUAIL)	D.MUSIL,W.BODE	5/91
4OVO	OVOMUCOID 3RD DOMAIN CLEAVED(SILVER PHEASANT)	D.MUSIL,W.BODE	5/91
3PSG	PEPSINOGEN(PORCINE)	HARTSUCK,KOELSCH,REMINGTON	9/91
2HPR	HISTIDINE-CONTAINING PHOSPHOCARRIER PROTEIN MUTANT(M51V,S83C)	O.HERZBERG	9/92
1CPC	C-PHYCOCYANIN(FREMYELLA DIPLOSIPHON)	M.DUERRING,G.B.SCHMIDT,R.HUBER	10/90
1ULA	PURINE NUCLEOSIDE PHOSPHORYLASE	S.E.EALICK ET AL.	11/91
1ULB	PURINE NUCLEOSIDE PHOSPHORYLASE/GUANINE	S.E.EALICK ET AL.	11/91
5RNT	RIBONUCLEASE T1/GUANOSINE-3',5'-BISPHOSPHATE	W.SAENGER,U.HEINEMANN,A.LENZ	4/91
6RNT	RIBONUCLEASE T1/2'-AMP	W.SAENGER ET AL.	8/91
7RNT	RIBONUCLEASE T1 MUTANT(Y45W)/2'-AMP	W.SAENGER ET AL.	8/91
8RNT	RIBONUCLEASE T1/ZN++	DING,CHOE,GRANZIN,SAENGER	9/91
9RNT	RIBONUCLEASE T1/CA++	J.MARTINEZ-OYANEDEL,U.HEINEMANN, W.SAENGER	9/91
1RN4	RIBONUCLEASE T1 MUTANT(H92A)	W.SAENGER ET AL.	11/91
1RGK	RIBONUCLEASE T1 MUTANT(E46Q)/2'-AMP	J.GRANZIN,R.PURAS-LUTZKE,O.LANDT, H.-P.GRUNERT,U.HEINEMANN	2/92
1RGL	RIBONUCLEASE T1 MUTANT(E46Q)/2'-GMP	J.GRANZIN,R.PURAS-LUTZKE,O.LANDT, H.-P.GRUNERT,U.HEINEMANN,W.SAENGER, U.HAHN	2/92
9RUB	RUBISCO(R.RUBRUM)/RIBULOSE-1,5-BISPHOSPHATE	T.LUNDQVIST,G.SCHNEIDER	11/90
2SNM	STAPH NUCLEASE MUTANT(V66K)	W.STITES,A.GITTIS,E.LATTMAN,D.SHORTLE	4/91
1BPT	BOVINE PANCREATIC TRYPSIN INHIBITOR MUTANT(Y23A)	D.HOUSSET,A.WLODAWER,F.TAO, J.FUCHS,C.WOODWARD	12/91
R3CHYSF	CHE Y(ESCHERICHIA COLI)	K.VOLZ,P.MATSUMURA	4/91
R6EBXSF	ERABUTOXIN B(LATICAUDA SEMIFASCIATA)	T.PRANGE,P.SALUDJIAN	8/91
R1APHSF	INSULIN(BOVINE,CUBIC,PH7)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
R1BPHSF	INSULIN(BOVINE,CUBIC,PH9)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
R1CPHSF	INSULIN(BOVINE,CUBIC,PH10)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
R1DPHSF	INSULIN(BOVINE,CUBIC,PH11)	O.GURSKY,J.BADGER,Y.LI,D.L.D.CASPAR	10/92
R4BLMSF	BETA-LACTAMASE(BACILLUS LICHENIFORMIS)	J.KNOX,P.MOEWS	5/91
R2MM1SF	MYOGLOBIN MUTANT(K45R,C110A)(HUMAN)	S.HUBBARD,W.HENDRICKSON, D.LAMBRIGT,S.BOXER	3/90
R1ULASF	PURINE NUCLEOSIDE PHOSPHORYLASE	S.E.EALICK ET AL.	11/91
R1ULBSF	PURINE NUCLEOSIDE PHOSPHORYLASE/GUANINE	S.E.EALICK ET AL.	11/91
R5RNTSF	RIBONUCLEASE T1/GUANOSINE-3',5'-BISPHOSPHATE	W.SAENGER,U.HEINEMANN,A.LENZ	4/91
R8RNTSF	RIBONUCLEASE T1/ZN++	J.DING,H.-W.CHOE,J.GRANZIN,W.SAENGER	11/91
R9RNTSF	RIBONUCLEASE T1/CA++	J.MARTINEZ-OYANEDEL,U.HEINEMANN, W.SAENGER	9/91
R1RGKSF	RIBONUCLEASE T1 MUTANT(E46Q)/2'-AMP	J.GRANZIN,R.PURAS-LUTZKE,O.LANDT, H.-P.GRUNERT,U.HEINEMANN, W.SAENGER,U.HAHN	2/92
R1RGLSF	RIBONUCLEASE T1 MUTANT(E46Q)/2'-GMP	J.GRANZIN,R.PURAS-LUTZKE,O.LANDT, H.-P.GRUNERT,U.HEINEMANN, W.SAENGER,U.HAHN	2/92
R2SNMSF	STAPH NUCLEASE MUTANT(V66K)	W.STITES,A.GITTIS,E.LATTMAN,D.SHORTLE	4/91

New Depositions*

IDCODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
Atomic Coordinate Entries			
1DTC	ACETYL-DELTA-TOXIN(NMR,12 STRUCTURES)	C.M.BLADON,P.BLADON,J.A.PARKINSON	10/92
1ACA	ACYL-COENZYME A BINDING PROTEIN/PALMITOYL-COENZYME A	B.B.KRAGELUND,K.V.ANDERSEN,J.C.MADSEN,J.KNUDSEN	11/92
1ALB	ADIPOCYTE LIPID-BINDING PROTEIN	Z.XU,L.J.BANASZAK	9/92
1ADS	ALDOSE REDUCTASE WITH BOUND NADPH	D.K.WILSON,F.A.QUIOCHO	7/92
6TAA	ALPHA AMYLASE	H.J.SWIFT,L.BRADY,Z.S.DEREWENDA,E.J.DODSON, J.P.TURKENBURG,A.J.WILKINSON	8/92
1NEA	ALPHA TOXIN	S.ZINN-JUSTIN,C.ROUMESTAND,B.GILQUIN, F.BONTEMS,A.MENEZ,F.TOMA	9/92
1AAN	AMICYANIN	L.CHEN,R.C.E.DURLEY,L.W.LIM,F.S.MATHEWS	4/92
1AAJ	APOAMICYANIN	R.C.E.DURLEY,L.CHEN,L.W.LIM,F.S.MATHEWS	4/92
1AVH	ANNEXIN V (HEXAGONAL)	R.HUBER,R.BERENDES,A.BURGER,M.SCHNEIDER,A.KARSHIKOV, H.LUECKE,J.ROEMISCH,E.PAQUES	10/91
1AVR	ANNEXIN V (RHOMBOHEDRAL)	R.HUBER,R.BERENDES,A.BURGER,M.SCHNEIDER,A.KARSHIKOV, H.LUECKE,J.ROEMISCH,E.PAQUES	10/91
1ABE	L-ARABINOSE-BINDING PROTEIN/L-ARABINOSE	F.A.QUIOCHO,N.K.VYAS	4/92
1ABF	L-ARABINOSE-BINDING PROTEIN/D-FUCOSE	D.K.WILSON,F.A.QUIOCHO	4/92
1RAA	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 1)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAB	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 2)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAC	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 3)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAD	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 4)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAE	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 5)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAF	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 6)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAG	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 7)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAH	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 8)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1RAI	ASPARTATE TRANSCARBAMOYLASE(T STATE)/CTP (REFINEMENT 9)	R.P.KOSMAN,J.E.GOUAUX,W.N.LIPSCOMB	8/92
1AZB	AZURIN(COPPER-REMOVED)	E.BAKER,W.SHEPARD	12/92
1AZC	AZURIN(APO FORM)	E.BAKER,W.SHEPARD,R.KINGSTON	12/92
1BAA	BARLEY ENDOCHITINASE(26 KD)	P.J.HART,A.F.MONZINGO,M.P.READY,S.R.ERNST,J.D.ROBERTUS	11/92
2BPA	BACTERIOPHAGE PHIX174 CAPSID PROTEINS GPF,GPG,GPJ AND FOUR NUCLEOTIDES	M.G.ROSSMANN	10/92
1BAC	BACTERIORHODOPSIN(7-HELIX BUNDLE,ALL-TRANS RETINAL)	K.C.CHOU,L.GARLACCI,G.M.MAGGIORA,L.A.PARODI,M.W.SCHULZ	7/92
1BAD	BACTERIORHODOPSIN(7-HELIX BUNDLE,13-CIS RETINAL)	K.C.CHOU,L.GARLACCI,G.M.MAGGIORA,L.A.PARODI,M.W.SCHULZ	7/92
1BW3	BARWIN(NMR,20 STRUCTURES)(NOE,DIHEDRAL RESTRAINTS)	F.M.POULSEN	7/92
1BW4	BARWIN(NMR,20 STRUCTURES)(NOE,DIHEDRAL,HYDROGEN BOND RESTRAINTS)	F.M.POULSEN	7/92
1BBM	CALMODULIN BINDING DOMAIN(NMR,24 MODELS)	G.M.CLORE,A.BAX,M.IKURA,A.M.GRONENBORN	5/92
1CLL	CALMODULIN(VERTEBRATE RECOMBINANT)	R.CHATTOPADHYAYA,F.A.QUIOCHO	9/92
1CRA	CARBONIC ANHYDRASE(HUMAN)/1,2,4-TRIAZOLE	S.MANGANI,A.LILJAS	10/92
1BIC	CARBONIC ANHYDRASE MUTANT(T200H)/BICARBONATE	Y.XUE,J.VIDGREN,L.A.SVENSSON,A.LILJAS,B.H.JONSSON,S.LINDSKOG	9/92
1CAI	CARBONIC ANHYDRASE II MUTANT(E106A)	Y.XUE,A.LILJAS,B.H.JONSSON,S.LINDSKOG	9/92
1CAJ	CARBONIC ANHYDRASE II MUTANT(E106D)	Y.XUE,A.LILJAS,B.H.JONSSON,S.LINDSKOG	9/92
1CAK	CARBONIC ANHYDRASE II MUTANT(E106Q)	Y.XUE,A.LILJAS,B.H.JONSSON,S.LINDSKOG	9/92
1HVA	CARBONIC ANHYDRASE II MUTANT(H94C)	R.S.ALEXANDER,D.W.CHRISTIANSON	10/92
1CAL	CARBONIC ANHYDRASE II MUTANT(T199A)	Y.XUE,A.LILJAS,B.H.JONSSON,S.LINDSKOG	9/92
1CAM	CARBONIC ANHYDRASE II MUTANT(T199A)/BICARBONATE	Y.XUE,A.LILJAS,B.H.JONSSON,S.LINDSKOG	9/92
3SC2	SERINE CARBOXYPEPTIDASE II	D.I.LIAO,S.J.REMINGTON	7/92
1CCX	CARDIOTOXIN CTX IIB(NMR,20 MODELS)	J.O'CONNELL,K.WUTHRICH	11/92
1CRD	CHARYBDOTOXIN(NMR,12 STRUCTURES)	F.BONTEMS,C.ROUMESTAND,B.GILQUIN,A.MENEZ,F.TOMA	6/92
2BB2	BETA-B2 CRYSTALLIN	B.BAX ET AL.	9/92
4GCR	GAMMA-B CRYSTALLIN	C.SLINGSBY,S.NAJMUDIN,V.NALINI,H.DRIESSEN,T.BLUNDELL,D.MOSS,P.LINDLEY	4/92
2DTB	DELTA-TOXIN(NMR,9 MODELS)	C.M.BLADON,P.BLADON,J.A.PARKINSON	9/92
3DNI	DEOXYRIBONUCLEASE I	C.OEFNER,D.SUCK	8/92
2DNJ	DEOXYRIBONUCLEASE I/DNA(GCGATCGC)	A.LAHM,D.SUCK	8/92
1DNK	DEOXYRIBONUCLEASE I/DNA(GGTATACC)	S.WESTON,A.LAHM,D.SUCK	8/92
3DRC	DIHYDRFOLATE REDUCTASE	S.J.OATLEY,J.KRAUT	9/92
2PDD	DIHYDROLIPOAMIDE ACETYLTRANSFERASE(BINDING DOMAIN)(NMR)	Y.N.KALIA ET AL.	11/92
1PDE	DIHYDROLIPOAMIDE ACETYLTRANSFERASE(BINDING DOMAIN,SYNTH) (NMR,MINIMIZED STRUCT.)	Y.N.KALIA,S.M.BROCKLEHURST,D.S.HIPPS,E.APPELLA, A.SAKAGUCHI,R.N.PERHAM	5/92
1D83	DNA(AAGGCCTT,SYNTHETIC)/CHROMYCIN A_3(NMR)	X.GAO,P.MIRAU,D.J.PATEL	7/92
1D60	DNA(CCAACITTGG,SYNTHETIC,TRIGONAL)	A.A.LIPANOV,M.L.KOPKA,M.KACZOR-GRZESKOWIAK,R.E.DICKERSON	2/92
1D61	DNA(CCAACITTGG,SYNTHETIC,MONOCLINIC)	A.A.LIPANOV,M.L.KOPKA,M.KACZOR-GRZESKOWIAK,R.E.DICKERSON	2/92
1D62	DNA(B,CCAACITTGG,SYNTHETIC)	A.A.LIPANOV,M.L.KOPKA,M.KACZOR-GRZESKOWIAK,J.QUINTANA,R.E.DICKERSON	3/92
1D70	DNA(5'-GTATAATG-3',5'-CATTATAC-3')(NMR,3 MODELS,SYNTHETIC)	U.SCHMITZ,T.L.JAMES	4/92
1DA3	DNA(B,CGATC-GPM^{6}ATCG,SYNTHETIC)	I.BAIKALOV,K.GRZESKOWIAK,K.YANAGI,J.QUINTANA,R.E.DICKERSON	11/92
3EGF	EPIDERMAL GROWTH FACTOR(MOUSE)(NMR,16 MODELS)	G.T.MONTELIONE,K.WUTHRICH,A.W.BURGESS,E.C.NICE, G.WAGNER,K.D.GIBSON,H.A.SCHERAGA	8/92
1FAS	FASCICULIN 1	M.H.LE DU,P.MARCHOT,P.E.BOUGIS,J.C.FONTECILLA-CAMPS	8/92
2HMB	FATTY ACID BINDING PROTEIN(HOLO FORM)	G.ZANOTTI,G.SCAPIN,P.SPADON,J.H.VEERKAMP,J.C.SACCHETTINI	9/92
1FER	FERREDOXIN I(PH 6.5)	E.A.MERRITT,G.H.STOUT,S.TURLEY,L.C.SIEKER,L.H.JENSEN,W.H.ORME-JOHNSON	9/92

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New Depositions (cont.)*

IDCODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
Atomic Coordinate Entries (cont.)			
1TEN	FIBRONECTIN TYPE III	D.J.LEAHY,W.A.HENDRICKSON,I.AUKHIL,H.P.ERICKSON	8/92
1BAR	FIBROBLAST GROWTH FACTOR(ACIDIC,BOVINE) MUTANT(C47A,H93G)	X.ZHU,H.KOMIYA,A.CHIRINO,S.FAHAM,G.M.FOX,T.ARAKAWA,B.T.HSU,D.C.REES	9/92
1BAS	FIBROBLAST GROWTH FACTOR(BASIC,HUMAN) MUTANT(C70S,C88S)	A.J.CHIRINO,D.C.REES	9/92
1FBC	FRUCTOSE-1,6-BISPHOSPHATASE/2,5-ANHYDROMANNITOL-1,6-BISPHOSPHATE/ MAGNESIUM	Y.ZHANG,J.-Y.LIANG,S.HUANG,H.KE,W.N.LIPSCOMB	10/92
1FBD	FRUCTOSE-1,6-BISPHOSPHATASE/2,5-ANHYDROGLUCITOL-1,6-BISPHOSPHATE/ MANGANESE	Y.ZHANG,J.-Y.LIANG,S.HUANG,H.KE,W.N.LIPSCOMB	10/92
1FBE	FRUCTOSE-1,6-BISPHOSPHATASE/2,5-ANHYDROGLUCITOL-1,6-BISPHOSPHATE/ ZINC	Y.ZHANG,J.-Y.LIANG,S.HUANG,H.KE,W.N.LIPSCOMB	10/92
1FBF	FRUCTOSE-1,6-BISPHOSPHATASE/2,5-ANHYDROGLUCITOL-1,6-BISPHOSPHATE/ MAGNESIUM	Y.ZHANG,J.-Y.LIANG,S.HUANG,H.KE,W.N.LIPSCOMB	10/92
1FBG	FRUCTOSE-1,6-BISPHOSPHATASE/2,5-ANHYDROMANNITOL-1,6-BISPHOSPHATE/ MANGANESE	Y.ZHANG, J.-Y.LIANG,S.HUANG,H.KE,W.N.LIPSCOMB	10/92
1FBH	FRUCTOSE-1,6-BISPHOSPHATASE/FRUCTOSE-1,6-BISPHOSPHATE	Y.ZHANG,J.-Y.LIANG,S.HUANG,H.KE,W.N.LIPSCOMB	10/92
1FVC	FV FRAGMENT OF HUMANIZED ANTIBODY 4D5(VERSION 8)	C.EIGENBROT,M.RANDAL,A.A.KOSSIAKOFF	10/92
1FVD	FV FRAGMENT OF HUMANIZED ANTIBODY 4D5(VERSION 4)	C.EIGENBROT,M.RANDAL,A.A.KOSSIAKOFF	10/92
1FVE	FV FRAGMENT OF HUMANIZED ANTIBODY 4D5(VERSION 7)	C.EIGENBROT,M.RANDAL,A.A.KOSSIAKOFF	10/92
1GPT	GAMMA-1-H THIONIN(NMR,8 MODELS)	M.BRUIX,M.A.JIMENEZ,J.SANTORO,C.GONZALEZ,F.J.COLILLA,E.MENDEZ,M.RICO	7/92
1GPS	GAMMA-1-P THIONIN(NMR,8 MODELS)	M.BRUIX,M.A.JIMENEZ,J.SANTORO,C.GONZALEZ,F.J.COLILLA,E.MENDEZ,M.RICO	7/92
1GAL	GLUCOSE OXIDASE	H.J.HECHT,K.KALISZ,J.HENDLE,R.D.SCHMID,D.SCHOMBURG	8/92
1GSS	GLUTATHIONE S-TRANSFERASE(HUMAN PLACENTA)	P.REINEMER,H.W.DIRR,R.LADENSTEIN,M.LO BELLO,G.FEDERICI, R.HUBER,M.W.PARKER	5/92
1GLA	GLYCEROL KINASE/GLYCEROL/ESCHERICHIA COLI GLUCOSE-SPECIFIC FACTOR III	J.HURLEY,D.WORTHYLAKE,H.FABER,N.MEADOW, S.ROSEMAN,D.PETTIGREW,S.REMINGTON	10/92
1GLB	GLYCEROL KINASE/GLYCEROL/ADP/ESCHERICHIA COLI GLUCOSE-SPECIFIC FACTOR III	J.HURLEY,D.WORTHYLAKE,H.FABER,N.MEADOW, S.ROSEMAN,D.PETTIGREW,S.REMINGTON	10/92
1ABB	GLYCOGEN PHOSPHORYLASE	D.D.LEONIDAS,N.G.OIKONOMAKOS,A.C.PAPAGEORGIOU, K.R.ACHARYA,D.BARFORD,L.N.JOHNSON	4/92
1LLA	HEMOCYANIN SUBUNIT II(LIMULUS POLYPHEMUS)	B.HAZES,W.G.J.HOL	9/92
1BBB	HEMOGLOBIN A(HUMAN,CARBONMONOXY)	A.ARNONE,M.M.SILVA	4/92
1BAB	HEMOGLOBIN(HUMAN,THIONVILLE)	J.S.KAVANAUGH,A.ARNONE	5/92
1HGC	HEMOGLOBIN(T STATE,ALPHA-OXY)	R.LIDDINGTON,Z.DEREWENDA,E.DODSON,R.HUBBARD,G.DODSON	10/91
1HGB	HEMOGLOBIN(T STATE,AQUOMET)	R.LIDDINGTON,Z.DEREWENDA,E.DODSON,R.HUBBARD,G.DODSON	10/91
1HGA	HEMOGLOBIN(T STATE,DEOXYGENATED)	R.LIDDINGTON,Z.DEREWENDA,E.DODSON,R.HUBBARD,G.DODSON	10/91
1CMY	HEMOGLOBIN YPSILANTI(HUMAN,CARBON MONOXY)	F.R.SMITH,E.E.LATTMAN,C.W.CARTER JR.	9/92
1ISU	HIGH-POTENTIAL IRON-SULFUR PROTEIN(HIPIP)	H.M.HOLDEN	9/92
1HIC	HIRUDIN VARIANT 1(NMR,20 MODELS)	T.SZYPERSKI,P.GUNTERT,S.R.STONE,K.WUTHRICH	4/92
1HEF	HIV 1 PROTEASE/SKF 108738(HEG)	H.M.MURTHY,E.L.WINBORNE,M.D.MINNICH,J.S.CULP,C.DEBOUCK	9/92
1HEG	HIV 1 PROTEASE/SKF 107457(HEG)	H.M.MURTHY,E.L.WINBORNE,M.D.MINNICH,J.S.CULP,C.DEBOUCK	9/92
1BBD	FAB FRAGMENT FROM 8F5 ANTIBODY AGAINST HRV2	J.TORMO,D.BLAAS,I.FITA	5/92
2HHR	HUMAN GROWTH HORMONE/RECEPTOR(EXTRACELLULAR DOMAIN)	A.H.DE VOS,M.U.ULTSCH,A.A.KOSSIAKOFF	10/92
1DBA	IGG1 FAB'(KAPPA 1,SUBGROUP 2A) OF THE DB3 MONOCLONAL ANTIBODY	J.H.AREVALO,I.A.WILSON	11/92
2HHM	INOSITOL MONOPHOSPHATASE DIMER/GADOLINIUM/SULFATE	R.BONE	10/92
1IZA	INSULIN(PORCINE)(2.5 ANGSTROMS)	B.XIAO,G.G.DODSON	10/92
1IZB	INSULIN(PORCINE)(2.0 ANGSTROMS)	B.XIAO,G.G.DODSON	10/92
3INK	INTERLEUKIN 2 MUTANT(C125A)	D.B.MCKAY,B.J.BRANDHUBER	8/92
1RCB	INTERLEUKIN 4(HUMAN,RECOMBINANT)	A.WLODAWER,A.PAVLOVSKY,A.GUSTCHINA	8/92
1MBL	BETA-LACTAMASE MUTANT(E166A,B.LICHENIFORMIS)	J.R.KNOX,P.C.MOEWS	8/92
1LPF	LIPOAMIDE DEHYDROGENASE(PSEUDOMONAS FLOURESCENS)	A.MATTEVI,W.HOL	10/92
1HWA	LYSOZYME(HEN)(NMR,1 MODEL)	L.J.SMITH,M.J.SUTCLIFFE,C.REDFIELD,C.M.DOBSON	8/92
101L	LYSOZYME(T4) MUTANT(INS K48-HP)	D.W.HEINZ,B.W.MATTHEWS	9/92
102L	LYSOZYME(T4) MUTANT(INS N40-A)	D.W.HEINZ,B.W.MATTHEWS	9/92
103L	LYSOZYME(T4) MUTANT(INS N40-SLD)	D.W.HEINZ,B.W.MATTHEWS	9/92
104L	LYSOZYME(T4) MUTANT(INS S44-AA)	D.W.HEINZ,B.W.MATTHEWS	9/92
105L	LYSOZYME(T4) MUTANT(INS S44-AAA)	D.W.HEINZ,B.W.MATTHEWS	9/92
2CMD	MALATE DEHYDROGENASE	M.D.HALL,L.J.BANASZAK	9/92
1OMP	D-MALTODEXTRIN-BINDING PROTEIN	A.J.SHARFF,F.A.QUIOCHO	9/92
2MBP	D-MALTODEXTRIN-BINDING PROTEIN/D-MALTOSE	J.C.SPURLINO,G.-Y.LU,F.A.QUIOCHO	9/92
1MRM	MANDELATE RACEMASE(PSEUDOMONAS PUTIDA)	D.J.NEIDHART,G.A.PETSKO	6/91
1MEA	METHIONYL-TRNA SYNTHETASE ZINC-BINDING DOMAIN	D.FOURMY,F.DARDEL	11/92
1CMB	MET APOREPRESSOR	J.B.RAFFERTY,K.PHILLIPS,S.E.V.PHILLIPS	8/92
1CMC	MET REPRESSOR/COREPRESSOR(TRIGONAL)	W.S.SOMERS,S.E.V.PHILLIPS	8/92
1CMA	MET REPRESSOR/OPERATOR	W.S.SOMERS,S.E.V.PHILLIPS	8/92
3MON	MONELLIN(SERENDIPITY BERRY)	F.JIANG,L.TONG,S.-H.KIM	8/92
1MYP	MYELOPEROXIDASE	R.E.FENNA,J.ZENG	4/92
2NPX	NADH PEROXIDASE	T.STEHLE,A.CLAIBORNE,G.E.SCHULZ	5/92
2BAT	NEURAMINIDASE N2/SIALIC ACID	J.N.VARGHESE,P.M.COLMAN	8/92

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New Depositions (cont.)*

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Atomic Coordinate Entries (cont.)			
1NTX	ALPHA-NEUROTOXIN(NMR,20 STRUCTURES)	L.R.BROWN,K.WUTHRICH	4/92
1NIP	NITROGENASE IRON PROTEIN	H.KOMIYA,M.M.GEORGIADIS,P.CHAKRABARTI,D.WOO,J.J.KORNUC,D.C.REES	9/92
1RRO	ONCOMODULIN(RECOMBINANT RAT)	F.R.AHMED,D.R.ROSE,S.V.EVANS,M.E.PIPPY,R.TO	8/92
1OVB	OVOTRANSFERRIN(18KD FRAGMENT,DOMAIN II FROM N-TERMINAL LOBE)	P.KUSER,P.LINDLEY,R.SARRA	10/92
1MPP	PEPSIN(MUCOR PUSILLUS)	M.NEWMAN ET AL.	2/92
1ABH	PHOSPHATE-BINDING PROTEIN/PHOSPHATE	H.LEUCKE,F.A.QUIOCHO	4/92
3LYT	LYSOZYME(HEN,100 KELVIN)(R=0.203)	J.C.DEWAN,A.C.M.YOUNG,R.F.TILTON	3/92
4LYT	LYSOZYME(HEN,298 KELVIN)	J.C.DEWAN,A.C.M.YOUNG,R.F.TILTON	3/92
1HID	HISTIDINE-CONTAINING PHOSPHOCARRIER PROTEIN (NMR,MINIMIZED AVERAGE STRUCTURE)	M.WITTEKIND,P.RAJAGOPAL,B.R.BRANCHINI,J.REIZER, M.H.SAIER,JR.,R.E.KLEVIT	9/92
5LYT	LYSOZYME(HEN,100 KELVIN)(R=0.176)	J.C.DEWAN,A.C.M.YOUNG,R.F.TILTON	3/92
6LYT	LYSOZYME(HEN,298 KELVIN)	J.C.DEWAN,A.C.M.YOUNG,R.F.TILTON	3/92
1BBC	PHOSPHOLIPASE A2(HUMAN)	J.P.WERY ET AL.	5/92
2POL	BETA SUBUNIT OF POL III	X.-P.KONG,J.KURIYAN	11/92
1PIA	PHTHALATE DIOXYGENASE REDUCTASE	C.CORREL,C.BATIE,D.BALLOU,M.LUDWIG	11/92
1PAF	POKEWEED ANTIVIRAL PROTEIN	A.F.MONZINGO,E.J.COLLINS,S.R.ERNST,J.D.IRVIN,J.D.ROBERTUS	10/92
1PAG	POKEWEED ANTIVIRAL PROTEIN/FORMYCIN 5'-MONOPHOSPHATE	A.F.MONZINGO,E.J.COLLINS,S.R.ERNST,J.D.IRVIN,J.D.ROBERTUS	10/92
1PCA	PROCARBOXYPEPTIDASE A	A.GUASCH,M.COLL,R.HUBER	10/91
2IGG	PROTEIN G(SECOND IGG-BINDING DOMAIN)	L.Y.LIAN,J.P.DERRICK,M.J.SUTCLIFFE,J.C.YANG,G.C.K.ROBERTS	8/92
2IGH	PROTEIN G(THIRD IGG-BINDING DOMAIN)	L.Y.LIAN,J.P.DERRICK,M.J.SUTCLIFFE,J.C.YANG,G.C.K.ROBERTS	8/92
1GDP	C-H-RAS P21 PROTEIN CATALYTIC DOMAIN(RESIDUES 1 - 171)/GDP	D.C.DYKES,M.R.PINCUS	2/92
1LAB	PYRUVATE DEHYDROGENASE:LIPOAMIDE ACETYLTRANSFERASE SUB. (LIPOYLATED DOM.)(NMR,10 STRUCTURES)	F.DARDEL,A.L.DAVIS,E.D.LAUE,R.N.PERHAM	9/92
1LAC	PYRUVATE DEHYDROGENASE:LIPOAMIDE ACETYLTRANSFERASE SUB. (LIPOYLATED DOM.)(NMR,AVERAGED)	F.DARDEL,A.L.DAVIS,E.D.LAUE,R.N.PERHAM	9/92
1PYA	PYRUVOYL-DEPENDENT HISTIDINE DECARBOXYLASE	T. GALLAGHER,D.A.ROZWARSKI,S.R.ERNST,M.L.HACKERT	12/92
1BBS	RENIN(HUMAN)(GLYCOSYLATED,RECOMBINANT)	V.DHANARAJ,T.L.BLUNDELL	5/92
1AAU	RIBONUCLEASE A(BOVINE,NMR,8 MODELS)	J.SANTORO,C.GONZALEZ,M.BRUIX,J.L.NEIRA,J.L.NIETO,J.HERRANZ,M.RICO	3/92
1RTB	RIBONUCLEASE A(BOVINE,PANCREATIC)	D.L.BIRDSALL,A.MCPHERSON	8/92
1RTA	RIBONUCLEASE A/THYMIDYLIC ACID TETRAMER	D.L.BIRDSALL,A.MCPHERSON	8/92
1GMP	RIBONUCLEASE SA/2'-GUANOSINE MONOPHOSPHATE(EMBL DATA)	J. SEVCIK,C.HILL,Z.DAUTER,K.WILSON	10/92
1GMQ	RIBONUCLEASE SA	J.SEVCIK,C.HILL,Z.DAUTER,K.WILSON	10/92
1GMR	RIBONUCLEASE SA/2'-GUANOSINE MONOPHOSPHATE(UCLA DATA)	J.SEVCIK,C.HILL,Z.DAUTER,K.WILSON	10/92
2AAE	RIBONUCLEASE T1 MUTANT(H40K)/ISOZYME PHOSPHATE	I.ZEGERS,P.VERHELST,C.W.CHOE,J.STEYAERT, U.HEINEMANN,L.WYNS,W.SAENGER	9/92
1RTC	RICIN A CHAIN(CASTOR PLANT)	D.MLSNA,A.F.MONZINGO,B.J.KATZIN,S.ERNST,J.D.ROBERTUS	10/92
1CAA	RUBREDOXIN(PYROCOCCUS FURIOSUS)(OXIDIZED)	M.W.DAY,B.T.HSU,L.JOSHUA-TOR,J.B.PARK,Z.H.ZHOU,M.W.W.ADAMS,D.C.REES	5/92
1CAD	RUBREDOXIN(PYROCOCCUS FURIOSUS)(REDUCED)	M.W.DAY,B.T.HSU,L.JOSHUA-TOR,J.B.PARK,Z.H.ZHOU,M.W.W.ADAMS,D.C.REES	5/92
1ABM	MN SUPEROXIDE DISMUTASE(HUMAN KIDNEY)	G.E.O.BORGSTAHL,H.E.PARGE,J.A.TAINER	8/92
2MDS	MN SUPEROXIDE DISMUTASE(THERMUS THERMOPHILUS)	M.L.LUDWIG,A.L.METZGER,K.A.PATTRIDGE,W.C.STALLINGS	9/92
1DWB	THROMBIN(HUMAN)/BENZAMIDINE	D.W.BANNER,P.HADVARY	8/92
1DWC	THROMBIN(HUMAN)/MD-805	D.W.BANNER,P.HADVARY	8/92
1DWD	THROMBIN(HUMAN)/NAPAP	D.W.BANNER,P.HADVARY	8/92
1DWE	THROMBIN(HUMAN)/PPACK	D.W.BANNER,P.HADVARY	8/92
2BBQ	THYMIDYLATE SYNTHASE/DUMP/POLYGLUTAMYL CB3717	A.KAMB,J.FINER-MOORE,R.M.STROUD	9/92
1TFG	TRANSFORMING GROWTH FACTOR BETA2	M.GRUETTER,M.SCHLUNEGGER	11/92
1TTA	TRANSTHYRETIN	J.A.HAMILTON,L.K.STEINRAUF,B.C.BRADEN	11/92
1TTB	TRANSTHYRETIN MUTANT(A109T)	L.K.STEINRAUF,J.A.HAMILTON,B.C.BRADEN	11/92
1TTC	TRANSTHYRETIN MUTANT(V30M)	J.A.HAMILTON,L.K.STEINRAUF,B.C.BRADEN	11/92
1TRE	TRIOSEPHOSPHATE ISOMERASE(ESCHERICHIA COLI)	M.E.M.NOBLE,R.K.WIERENGA	10/92
1TRD	TRIOSEPHOSPHATE ISOMERASE 1(TRYPANOSOMA BRUCEI BRUCEI)	M.E.M.NOBLE,R.K.WIERENGA	10/92
7TIM	TRIOSE PHOSPHATE ISOMERASE/PHOSPHOGLYCOLOHYDROXAMATE	R.C.DAVENPORT,P.A.BASH,B.A.SEATON,M.KARPLUS,G.A.PETSKO,D.RINGE	4/91
1TBS	TRYPSIN(BENZAMIDINE INHIBITED,SALMO SALAR)	A.O.SMALAS	7/92
1PIT	TRYPSIN INHIBITOR(BOVINE,PANCREAS)(NMR,20 MODELS)	K.BERNDT,P.GUNTERT,L.P.M.ORBONS,K.WUTHRICH	4/92
1FAN	TRYPSIN INHIBITOR(BOVINE,PANCREAS) MUTANT(F45A)	A.T.DANISHEFSKY,A.WLODAWER,K.S.KIM,F.TAO,C.WOODWARD	8/92
1NAG	TRYPSIN INHIBITOR(BOVINE,PANCREAS) MUTANT(N43G)	A.T.DANISHEFSKY,A.WLODAWER,K.-S.KIM,F.TAO,C.WOODWARD	8/92
1MUP	MAJOR URINARY PROTEIN/2-(SEC-BUTYL)THIAZOLINE	Z.BOCSKEI,D.R.FLOWER,C.R.GROOM,S.E.V.PHILLIPS,A.C.T.NORTH	9/92
1BBT	FOOT AND MOUTH DISEASE VIRUS	K.R.ACHARYA,E.E.FRY,D.T.LOGAN,D.I.STUART	5/92
1HRI	RHINOVIRUS 14(HUMAN)/ANTIVIRAL AGENT SCH 38057	A.ZHANG,R.G.NANNI,E.ARNOLD	10/92
1SNW	SINDBIS VIRUS CAPSID PROTEIN(MONOCLINIC)	L.TONG,M.G.ROSSMANN	7/92
1XLA	D-XYLOSE ISOMERASE(APO FORM)	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91
1XLB	D-XYLOSE ISOMERASE/MAGNESIUM	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91
1XLC	D-XYLOSE ISOMERASE/D-XYLOSE/XYLULOSE/MAGNESIUM	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91
1XLD	D-XYLOSE ISOMERASE/D-XYLOSE/XYLULOSE/MANGANESE	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91
1XLE	D-XYLOSE ISOMERASE/XYLITOL/MANGANESE	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91
1XLF	D-XYLOSE ISOMERASE/GLUCONATE/MANGANESE	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91
1XLG	D-XYLOSE ISOMERASE/D-XYLOSE/XYLULOSE/MAGNESIUM/ALUMINUM	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91
1XLH	D-XYLOSE ISOMERASE/ALUMINUM	C.A.COLLYER,K.HENRICK,D.M.BLOW	10/91

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