Protein Data Bank

Quarterly Newsletter

Release #69 July 1994

July 1994 PDB Release

2684 full-release atomic coordinate entries (249 new additions)

2478	proteins, enzymes and viruses
177	DNA's
10	RNA's
9	tRNA's
10	carbohydrates

357 structure factor entries
31 NMR experimental entries

The total size of the atomic coordinate entry database is 826 Mbytes uncompressed.

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The latest version of the Electronic Deposition Form should be obtained from the FTP /**pub** directory before depositing data.

What's New at the PDB

In an effort to provide better service to users and depositors, PDB has implemented several new procedures in the past few months. These include a new Electronic Deposition Form, the addition of multicolor images of structures on the PDB Gopher and World Wide Web (WWW) servers, and the introduction of an entry tracking system.

The new Electronic Deposition Form is now available from FTP. We encourage all depositors to use it. For information on how to retrieve a copy, please see the article entitled "New Electronic Deposition Form" on page 7.

A series of 474 multicolor images of PDB structures has been added to the PDB Gopher and WWW servers. Dr. Manuel Peitsch of The Glaxo Institute for Molecular Biology in Geneva prepared the images, designing them so that each one depicts the most important aspects of the entry or experiment that it represents. Users may access these images from the FTP (also Gopher or WWW *via* "The PDB's Anonymous FTP") directory /**images**.

Because the PDB cannot issue an ident code until an entry is processed, a tracking number uniquely defining each submission is issued at the time of initial deposit. This number enables users, journals and the PDB to follow the progress of every entry through the entire screening process *via* our Gopher system. Additional information on this tracking system may be found in the article below.

We encourage you to take advantage of the new tools offered by PDB. We are very excited about them and hope that you will find them to be useful additions. As always, your comments are welcome at pdb@bnl.gov.

Thank you.

— *Joel L. Sussman*

New Entry Tracking System

Many depositors, users and journals that refer to PDB have asked us to provide a mechanism for checking the status of entries from depositor's initial contact with PDB to the time when the work is published. This is now possible due to the establishment of tracking codes, one of which is given to each depositor upon deposition of an entry. This code can be used by depositors, users and journals to track an entry's progress until full release.

Upon receipt of coordinates for an entry, PDB issues a tracking number and sends a letter to the primary and secondary contacts that includes this number. The format of the tracking number is a number preceded by the letter T (*e.g.,* T9999).

PDB issues the PDB ident code, required by most journals, only after running some preliminary checking programs and receiving all required documentation, including (p)reprints.

The tracking number is published, for every entry that is currently being processed by PDB, in the file /**pub**/**pending_waiting.list** which is available from FTP. If you use Gopher to access PDB, this file is indexed by tracking number, author and compound name in order to speed searches.

Status for each pending and waiting entry is issued from the following list:

INCOMPLETE	-	if PDB is waiting for additional materials or information from depositor to make a complete deposition
PROCESSING	-	if PDB is checking and verifying entry
DEPOSITOR	-	if entry is with depositor for approval
REVIEW	-	if entry is undergoing final review
REL	-	if entry is in current release
HLD	-	if entry is on hold at present time

This number is not to be construed as an ident code. Its purpose is to speed up our searches, make our responses to inquiries faster and more accurate, and allow depositors to track the progress of their entries.

CIF and the PDB

Most of you have undoubtedly heard something about CIF (The Crystallographic Information File); many of you have asked for more information about CIF and how it will affect PDB users. There will be a series of Newsletter articles pertaining to CIF. This first article describes CIF from a computer user's point of view and deals with the nuts and bolts issues of using CIF on a computer. Articles in future Newsletters will discuss dictionaries and CIF from a crystallographer's point of view.

One of the most frequently asked questions is, "Why have a new file format at all?" The answer will become clearer over the course of this article and articles to follow in future Newsletters. The main issue is that PDB format is simply too inflexible to deal with the ever-expanding types of data that it is asked to contain. At the time PDB format was first conceived, 40 characters seemed adequate to store a molecule's "Functional Classification", 99,999 atoms in a chain seemed perfectly adequate, and one only needed a good memory to locate the interesting structures, not a computer. None of these conditions is true today, and we can foresee the need to adapt at a faster pace over the next several years. Therefore, some changes in format were inevitable and CIF seemed to be a possible candidate.

CIF is a direct descendent of the STAR (Self-defining Text Archive and Retrieval) file created by Sydney Hall in 1990 [S. R. Hall, The STAR File: A New Format for Electronic Data Transfer and Archiving. *J. Chem. Inf. Compt. Sci.* **31**, 326-333 (1992)]. Hall, with Frank Allen and David Brown, put some limitations on the STAR definition to arrive at CIF [S. R. Hall, F. H. Allen and I. D. Brown, The Crystallographic Information File (CIF): A New Standard Archive File for Crystallography. *Acta Cryst.* **A47**, 655 (1991)]. The stated goals of STAR (and CIF) were to have a format that would be able to store all kinds of data, be machine independent, be simple to read and access, and be flexible to future change. It was also a goal that the format not be tied to any one database model. How well STAR and CIF succeed at reaching each of these goals is open to discussion, but most people would agree that CIF is capable of storing a wide range of ASCII data, is mostly machine independent, is easily machine readable and, perhaps most importantly, is flexible.

So in the end, what is a CIF? It is a text file consisting of the printable ASCII characters from space to "~" and with some sort of new line character. The line lengths are limited to 80 characters.

A CIF is divided into a number of data blocks, each of which has a name. A block is introduced by a character string of the form:

data_*code*

where code may be up to 32 characters in length. A block is terminated by either the beginning of another block or the end-of-file. The block name cannot be duplicated in a CIF.

Each block consists of a sequence of data items which comes in two forms. The first and simplest gives the name of the item and its value. The names of all data items start with an "_", are limited to 32 characters, and must also be unique. All data items should simply be seen as text strings (we will delve deeper into this in a future article) which are delimited by spaces. The text strings can be quoted by either single or double quotes if they contain spaces. In addition, very long (more than 80 character) strings can be represented by starting a line with a semicolon and ending the data value with a subsequent line starting with a semicolon. Then, the string of characters from the first non-blank character following the first semicolon to the last non-blank character preceding the second semicolon is considered to be the value of the data item. End-of-line characters are discarded and multiple spaces are replaced with one space. (These last two restrictions are not part of the specification, but are needed for practical purposes.)

The second form is used to represent lists. It starts with the keyword "loop_" and is followed by a sequence of N data names, then a sequence of K*N data values. The names and values conform to the restrictions mentioned in the previous paragraph.

An example will make this clearer. The following CIF consists of two data blocks (address and papers) and demonstrates the various methods of data representation. The second data block contains a simple loop.

```
data_address
          _name          "Sydney R. Hall"
          _department    "Crystallography Centre"
          _organization  'University of Western Australia'
          _city          Nedlands
          _code          6009
          _country       Australia

data_papers
          loop_ _title _date
;
The Crystallographic Information File (CIF): a New Standard
 Archive File for Crystallography
;
1991
;
The STAR File: A New Format for Electronic Data Transfer and
 Archiving
;
1990
```

It is important that one understands that the data in a CIF are constrained neither in the order in which they appear, nor in their format. For example, the following CIF conveys the same information as that in the preceding column, *albeit* in a less (humanly) readable form.

```
data_address
          _name
;Sydney R. Hall
; _city         Nedlands
          _code          6009
          _country       Australia
          _department    'Crystallography Centre'
          _organization
;
University of Western Australia
;
data_papers
          loop_
_date _title
1991
;
The Crystallographic Information File (CIF): a New Standard
 Archive File for Crystallography
;
1990
;
The STAR File: A New Format for Electronic Data Transfer and
 Archiving
;
```

To those people accustomed to PDB format this is viewed as a major disadvantage, as some of the UNIX user's favorite tools (diff and grep) fail miserably with this format. Where CIF has an advantage over PDB format is in dealing with the question, "What do you mean by a data item?" In PDB format, one must look back at a document written in English that describes what is really meant by the data field of interest. If the definition is present at all (do we all understand and agree with the meaning of insertion code?) this can be interpreted in many ways due to the ambiguity inherent in all natural languages (*e.g.,* are Au and Australia both acceptable country names and are they equivalent?). In contrast each CIF has associated with it one or more dictionaries (also stored in a CIF), describing the attributes and in some cases acceptable values of every data item stored in the CIF. This allows for the possibility of automatically validating a CIF as being "correct" relative to a dictionary. If the people who write the dictionaries are careful, then it should be possible to provide air-tight definitions of each and every data item stored in a CIF. To an organization (like PDB) that must automate all of its operations, this is a huge advantage.

While there are some drawbacks to CIF as it currently exists, the community hopes to address many of these in the coming months *via* various working committees. The free format makes using familiar tools such as grep and awk difficult, therefore requiring new tools in order to access all of the data in the file. The limitation on line and word lengths are a bit archaic, and the failure to specify clearly the acceptable character set and escapes will cause some difficulty if not addressed (*e.g.,* storage of binary files and other CIFs within a CIF is not currently possible). Also, CIF does not address the issue of building more complex data types (*e.g.,* records or structs) as most data representation schemes do. Still, one must remember that CIF has been used in the small molecule field, and we look forward to similar success.

You are encouraged to look at two dictionaries that will be of greatest concern to macromolecular crystallographers over the next several years — the Core Dictionary and the mmCIF Dictionary — both of which are available on the PDB file server in the directory /**pub**/**Cif**. The Core Dictionary is an IUCr standard and the mmCIF dictionary has been published for comments after an enormous effort by Paula Fitzgerald, Helen Berman, Phil Bourne and Keith Watenpaugh, with contributions and suggestions from many other scientists. The mmCIF dictionary has been designed to be capable of representing the results of an experiment. In the next Newsletter, the issue of CIF dictionaries and DDLs (data definition languages) will be discussed in much greater detail.

The success or failure of CIF will depend to a large degree on the number and quality of software tools available to users. To begin with, a small library of C and FORTRAN callable functions which provide primitive access to the contents of a CIF has been placed on the PDB file server. These functions do not (at this time!) use any dictionaries to validate CIF files, but simply provide access. The primitive functions are:

```
int CifRead1(char* filename)
```

Reads an entire CIF into memory. Returns 0 if successful, non-zero if failed. A diagnostic is written to the stderr.

```
int CifLoopCount1(char* block, char* name)
```

Returns the number of values associated with the data item named "name" in the data block named "block". A return value of 0 implies that the named data item does not exist.

```
int CifExists1(char* block, char* name, int index)
```

Returns a non-zero value if the item named "name" in the block called "block" has index values associated with it. (The first occurrence has an index of 0!)

```
char* CifGet1(char* block, char* name, int index)
```

Returns a pointer to a character string giving the values of the specified data item.

With these functions, if the above examples of CIF are in the file hall.cif, the following code will read and output all of the titles of the papers stored in the CIF:

```
#include <stdio.h>

main()
{
            int nPapers;
            int iPaper;

            if (CifRead1("hall.cif")) {
                fprintf(stderr,
                   "could not read the file hall.cif\n");
                exit(1);
            }

            nPapers = CifCount1("papers","_title");
            for (iPaper=0; iPaper < nPapers; iPaper++) {
                printf("%s\n",
                   CifGet1("papers","_title",iPaper));
            }
}
```

These functions should be considered to be beta-versions and are subject to having bugs and being less than optimal, though they are constantly being improved. Your input is gratefully accepted. In the next Newsletter, an article will discuss those CIF dictionaries which are standards and those which are experimental. Some additional CIF tools will also be discussed. More sophisticated tools are available on the network; the anonymous FTP server at cuhhca.hhmi.columbia.edu is an excellent place to start searching.

Finally, it is important for the user community to understand that PDB's interest in CIF will not adversely impact your day to day operations. PDB's plans with respect to CIF are perfectly clear in one respect. We never will suddenly change the format of every entry held by PDB. Our plans call for:

- Making sure that current entries are complete in PDB format and contain as much information as possible so that converting a PDB entry to a CIF entry can be automated.

- Providing a tool that will take a CIF description of a PDB entry and render it in PDB format on a best effort basis. All existing files will be available in PDB format. All new entries submitted in PDB format will also be available in that form. All new entries submitted in CIF will probably have some limitations in their ability to be converted to PDB format (due to the greater information content of CIF), but for the time being, the two formats should be regarded as interchangeable.

- Supporting the community in accepting and archiving data which is simply not representable in PDB format.

- Working with the major distributors of codes and applications that have produced and used PDB format in the past to help them make the conversion to CIF-based representation.

We look forward to your opinions. Please feel free to contact Dave Stampf (drs@bnl.gov).

Improve Descriptions of Sequence Information

PDB plans to include new record types to improve descriptions of sequence information now given in the SEQRES records. The new records will provide annotation mechanisms to correlate information stored in PDB entries with that found in the various sequence databases (*e.g.,* PIR, SWISS-PROT).

The following is a summary description for the new record types.

Record Type	-	Purpose
DBREF	-	To provide cross-reference links between PDB sequences and corresponding sequence database entries.
SEQADV	-	To identify conflicts in sequence information between PDB sequences and sequence database entries.
MODRES	-	To provide descriptions of modifications (*e.g.,* chemical or post-translational) to protein and nucleic residues. Included will be a mapping between residue names given in a PDB entry and the standard 20 protein and 5 nucleic acid residues.

A number of recently-released PDB entries contain REMARK records that already give this information. PDB now wishes to standardize the format and representation for these data. In addition, these record types will help facilitate conversion of PDB entries into CIF format.

In general, PIR and SWISS-PROT entries contain information on the wild-type molecule. Each entry normally contains the sequence for one gene product, and some entries include the complete precursor sequence. Annotation is provided to describe residue modifications. In both databases, the residue names used are limited to the 20 standard amino acids.

In contrast, PDB entries contain multichain molecules with sequences that may be wild type, variant, or synthetic. Sequences may also have been modified through site-directed mutagenesis experiments (engineered). A number of PDB entries report structures of domains cleaved from larger molecules.

The DBREF record was designed to account for these differences by providing explicit correlations between contiguous segments of sequences as given in PDB ATOM records and PIR or SWISS-PROT entries. Several cases are easily represented by means of pointers between the databases using DBREF. PDB entries containing heteropolymers will be linked to different sequence database entries. In some cases, such as those PDB entries containing immunoglobulin Fab fragments, each chain will be linked to two different PIR and/or SWISS-PROT entries. This facility is needed, because these databases represent sequences for the various immunoglobulin domains as separate entries. DBREF should also be able to represent molecules engineered by altering the gene (fusing genes, altering sequences, creating chimeras, or circularly permuting sequences). This design has one additional advantage, *i.e.*, it will be possible to construct pointers to other databases such as those describing sequence motifs (*e.g.,* PROSITE, BLOCKS).

Selection of the appropriate sequence database entry or entries to be linked to a PDB entry will be done on the basis of molecule name and source. Questions on entry assignment that may arise will be resolved by consultation with PIR and SWISS-PROT staff.

In a number of cases, conflicts between the sequences found in PDB entries and in PIR or SWISS-PROT entries have been noted. There are several possible reasons for these conflicts: PDB may contain variant sequences or engineered sequences (mutants), polymorphic sequences, or ambiguous or conflicting experimental results. These discrepancies, which were previously described in REMARK records, will now be reported in SEQADV records.

Finally, residues modified post-translationally or by design will be described in MODRES records. In those cases where PDB has opted to use a non-standard residue name for the residue, MODRES will also provide a mapping to the precursor standard residue name.

There remain a number of unresolved issues related to the SEQRES records. Most significant is the need to represent sequences for the multiply-branched polysaccharides. PDB plans to address this in the future.

PDB wishes to solicit your input regarding these new records. Please send comments and suggestions to Enrique Abola (abola1@bnl.gov).

– *Record Descriptions*

Record Name: *DBREF*

Cols.	Contents and Description
01 - 05	DBREF
07 - 10	PDB ident code
12	Chain name
14 - 17	Initial sequence number of PDB sequence segment
18	Initial insertion code of PDB sequence segment
20 - 23	Ending sequence number of PDB sequence segment
24	Ending insertion code of PDB sequence segment
26 - 31	Sequence database name (PIR,SWS,GDB, BLOCKS, PROSIT)
33 - 40	Sequence database accession code
42 - 53	Sequence database identification code
55 - 60	Initial sequence number in the sequence database
62 - 66	Ending sequence number in the sequence database

DBREF records have been developed identifying sequence correlations between PDB ATOM records and corresponding PIR or SWISS-PROT entries. PDB entries containing chains for which residues are missing primarily due to disorder will contain several DBREF records, each linking an observed sequence segment to a sequence database entry.

Examples:

```
DBREF 1ABC A  1A 100 SWS  P10725  ALR_BACSU 15 114
DBREF 1ABC A  1A 100 PIR  JS0443            15 114
```

Record Name: *SEQADV*

Cols.	Contents and Description
01 - 06	SEQADV
08 - 11	PDB ident code
13 - 15	PDB residue name
17	PDB chain name
19 - 22	PDB sequence number
23	PDB insertion code
25 - 30	Sequence database name (PIR, SWS, PROSIT)
32 - 39	Sequence database accession number
40 - 42	Sequence database residue name
44 - 47	Sequence database sequence number
50 - 70	Conflict comment

SEQADV describes conflicts between residue sequences given by PDB ATOM records and those in the appropriate sequence database entry, such as residues missing due to disorder.

Example of possible conflict comments:

Cloning artifact
Engineered
Disordered
Variant
Insertion
Deletion

When conflicts arise which are not classifiable by these terms then a reference to either a published paper, a PDB entry, or a REMARK within the entry will be given. References will be given in the form YY-VOL-PAGE-CSDCODEN where YY is year of publication, VOL is the journal volume number, PAGE is the starting page and CSDCODEN is the 4-digit code assigned to journals by PDB and the Cambridge Structural Database (CSD). When reference is made to a PDB entry, then the form is PDB: 1ABC, where 1ABC is the relevant entry ident code. Finally, the comment “SEE REMARK XXX” will be included, where XXX is the remark number within the entry in which the primary explanation to the discrepancy is given.

Examples:

```
SEQADV 1ABC ASN A 100A SWS P10725 ASP 100  1994-300-1200-0070
SEQADV 2ABC ASN A 100A SWS P10725 ASP 100  PDB: 1ABC
SEQADV 1ABC MET A  -1  SWS P10725          CLONING ARTIFACT
SEQADV 1ABC GLY A  50  SWS P10725 VAL  50  ENGINEERED
```

Record Name: *MODRES*

Cols.	Contents and Description
01 - 06	MODRES
08 - 11	PDB ident code
13 - 15	Residue name
17	Chain name
19 - 22	Sequence number
23	Insertion code
25 - 27	Standard residue name
30 - 70	Modification description

Examples of modification descriptions:

Glycosylation site
Post-translational modification
Designed chemical modification
Phosphorylation site
Blocked N-terminus
Aminated C-terminus

Examples:

```
MODRES  1ABC ASN  A  22A ASN  GLYCOSYLATION SITE
MODRES  1ABC TTQ  A  50A TRP  POST-TRANSLATIONAL MODIFICATION
```

PDB User Group

A User Group has been instituted for PDB, headed by Jane Richardson of Duke University. There is a Coordinating Committee to represent the diverse spectrum of users: so far the members of this committee are Mike Summers (University of Maryland) who represents the NMR community and Judy Voet (Swarthmore College) who represents those who use the PDB in teaching. At the broad level, of course, everyone interested is by definition a member of the User Group.

The User Group aims to facilitate communication in both directions between PDB and all categories of its users, improving knowledge of what is already available or in progress, collecting user feedback, diagnosing problems quickly, and collectively arriving at the best ideas and innovations for the future. Thus far the User Group's main activities, based on user input, have been:

- Initiating the setup of an on-line, user-queriable directory that gives the status of all entries between deposition and release. A query is carried out by reaching PDB *via* Gopher (gopher.pdb.bnl.gov), choosing the indexed search "*NEW* check the status of a pending entry by ident code, tracking, author, *etc*.", and supplying the desired search word. Alternatively, the file /**pub**/**pending_waiting.list** can be retrieved from FTP, Gopher or WWW and searched for the desired entry. Please see additional information in the article entitled "New Entry Tracking System" on page 1.

- Initiating efforts by PDB to provide a definition of the functioning biological unit for entries and a procedure by which this may be generated. On an experimental basis, the full coordinates generated for these biological units will be made available from FTP. Please see the article below for additional information.

- Establishing an on-line directory known as "/**user_group**" in which the User Group will have available various subsets and annotations of PDB entries, for such purposes as teaching and structural analysis. This will be available from FTP.

Your input is solicited. Please let us know what type of user you are and what you consider priorities for the future. Respond by e-mail to: PDBusrgp@suna.biochem.duke.edu or by postal mail to: Jane Richardson, PDB User Group, Box 3711 DUMC, Durham, NC 27710, USA.

The Biological Molecule

PDB plans to distribute new files that contain the coordinates for complete multimeric molecules. These files are to be called bio1abc.xyz where 1abc is the PDB ident code for the entry from which the multimer is generated. Multimers will be generated when it is determined that the physiologically active molecule (or biologically relevant molecule) includes subunits for which coordinates are currently not given in the entry. These multimers are described in PDB entries explicitly by non-crystallographic operators (MTRIX records) or implicitly *via* the crystallographic space group operators. Thus, unlike regular PDB entries, these files may include coordinates for crystallographically-related subunits.

This work is being carried out in response to Jane Richardson's request to have these files available. In an informal survey carried out as part of her efforts to organize the new PDB User Group, Jane found that availability of these files was desired by a large number of users.

Several steps have already been taken by PDB to ensure that the complete description of the biologically active molecules is available. Most significant is the inclusion of questions in PDB's new Electronic Deposition Form requesting information on the subunit composition of the molecule. For those entries in the current release of the PDB, subunit compositions are generated using information available from the corresponding SWISS-PROT (sequence database) entry.

Loading of these files on the PDB anonymous server will start shortly and is expected to be completed (current with the release) late this fall. Please send comments and suggestions on the contents of these files directly to PDB or to the User Group.

Getentry

If you use C shell on a UNIX system, a script for easily locating and transferring PDB files is now available. Named getentry, this script, written by J. P. Rose, E. E. Abola and M. D. Libeson, allows straightforward searches, based on compound, author name, source and resolution, as well as retrieval of coordinate entries and some other files. To obtain the script, retrieve the file /**pub**/**getentry** from FTP. Installation instructions are found at the top of the file. Searches can make use of UNIX regular expressions, allowing flexibility.

Options allow searching certain of the index files from FTP, retrieving the new Electronic Deposition Form, retrieving the file /**pub**/**pending_waiting.list,** and obtaining addresses of crystallographers from the electronic list maintained by Dr. Martha M. Teeter, Department of Chemistry, Boston College, Chestnut Hill, MA. Other options may be added in the future.

Deposition of Data

– New Electronic Deposition Form

A new Electronic Deposition Form is now available. Our goal in designing the Form was to create a document that would be easy for depositors to fill out and also for PDB staff to process electronically, minimizing errors and increasing efficiency. The Form has provisions for depositors to include information necessary in a complete entry, *i.e.*, refinement details and sequence information, especially regarding any differences between the full protein sequence and the sequence of residues for which there are actual atomic coordinates. The Form also requests information for the cross-referencing of sequence information to the protein sequence databases (PIR, SWISS-PROT), making it easier to use information stored in PDB for homology model building. In addition, the Form clearly distinguishes between NMR and X-ray data.

The Electronic Deposition Form begins with a description of the standard structure of a PDB coordinate file and provides guidelines for preparing data for deposition. These guidelines should be studied and followed carefully for the most efficient processing of your data. Additional information not included in PDB's old form is now requested. These data items will significantly help our staff to prepare an entry for distribution. The Form leads you through the needed material, from depositor information to the description of the experiment, bibliographic references, crystallographic data, het group description, *etc.* Finally, secondary structure information is now being prepared by PDB using the Kabsch and Sander algorithm [Dictionary of Protein Secondary Structure: Pattern Recognition of Hydrogen-bonded and Geometrical Features. *Biopolymers* **22**, 2577-637 (1983)], as implemented in the program Procheck, making submission of HELIX, SHEET and TURN records optional. However, we will gladly also include your secondary structure specifications if you wish.

The most current version of the Electronic Deposition Form should be used when preparing your deposition. You may use FTP (ftp.pdb.bnl.gov), Gopher (gopher.pdb.bnl.gov) or WWW (www.pdb.bnl.gov) to retrieve the file /**pub**/**dep_form.txt**. You may request the Form by sending e-mail to pdb@bnl.gov. Please read and follow the instructions carefully.

PDB will be happy to receive your comments on the design and ease of use of the Electronic Deposition Form. For help in filling out the form or to give us your comments, send e-mail to pdb@bnl.gov.

– Guidelines for Deposition

PDB accepts depositions of biological macromolecule structures and the corresponding crystallographic structure factors or NMR experimental data. Types of structures accepted include proteins, carbohydrates, viruses, DNA and RNA. We convert deposited data to standard PDB format, run verification, checking and quality control programs on the data, and archive and distribute the data worldwide. A deposition has three essential components, all of which must be received by PDB before we can begin processing an entry: the completed Electronic Deposition Form, (p)reprints of all referenced papers, and the atom coordinates formatted as PDB ATOM and HETATOM records. The Electronic Deposition Form and coordinates must be submitted in machine readable form *via* one of the following:

e-mail:	pdb@bnl.gov
FTP:	connect to ftp.pdb.bnl.gov using anonymous FTP cd to the /new_uploads directory upload your files
postal mail:	Protein Data Bank Depositions Chemistry Department, Building 555 Brookhaven National Laboratory P.O. Box 5000 Upton, NY 11973-5000 USA

The paper (p)reprints must be sent *via* facsimile (516-282-5751) or air mail.

Please obtain the latest version of the new Electronic Deposition Form from the FTP directory /**pub** each time that you make a deposit; edit and return the completed Form to us electronically.

Be sure to include identifying information, including your name, postal mailing address, e-mail address, facsimile number and telephone number, in the header of all items submitted.

– Deposition Contact Persons

PDB requires the names of two contact persons — a primary and a secondary contact — on the Electronic Deposition Form, for each new structure.

The primary contact is the person who has the authority to grant approval for release of the completed PDB entry. Both contacts should be able to help in preparing the entry if we need any answers or clarification. The secondary contact should be able to help locate the primary contact if this becomes necessary. The prepared PDB entry and request for release approval will be sent to the primary contact. A note will be sent to the secondary contact stating that these files have been sent to the primary contact.

Discontinuation of Tape Distribution

Due to the small number of tapes being ordered, PDB is contemplating discontinuation of the distribution on these media. Information will be forthcoming on the status and time frame involved. Anyone who anticipates a continuing need for tapes should speak up now.

Help PDB to Identify JRNL Records from Years Ago

Over the years, a number of PDB entries have been entered into the database before their respective journal articles appeared in print. Consequently, instead of their JRNL records giving full proper references, all that appears is “TO BE PUBLISHED” or “IN PRESS”. Unfortunately, in many cases, these records were never updated, so that entries from years ago still read this way.

The PDB staff is therefore asking the scientific community, particularly the original depositors of these entries, to please inform us of the complete corrected JRNL references of such entries as soon as possible. Thank you very much.

Missing Data

PDB is now handling approximately 90 new coordinate depositions per month. Almost all coordinate data arrives electronically, as does the Electronic Deposition Form. The (p)reprints still generally arrive by postal mail.

The following should be obvious to all of us:

- Transmission errors occur occasionally. These are easy to resolve if the depositor still has a copy of the file sent.
- E-mail sometimes does not arrive at its destination. If this problem could be resolved everyone using the Internet would breathe a sigh of relief.
- Computers crash in unexpected ways.
- We try to be perfect in our operations but admit that mistakes can happen.

Each item that arrives (data, Electronic Deposition Form, (p)reprints, letters, *etc.*) must be identified and associated with one another and, after the data has arrived, logged into our entry tracking system.

We strongly recommend that depositors check the pending_waiting list on FTP (see additional information in article entitled “New Entry Tracking System” beginning on page 1) to make sure that their data has been logged. Allowing for our fluctuating work load, we suggest that you contact us if your data does not appear on this list within a month of your sending it to us.

Please keep copies of everything you send us.

Access to PDB

– FTP

PDB has an anonymous FTP account on the computer system **ftp.pdb.bnl.gov** (Internet address 130.199.144.1). Files may be transferred to and from this system using anonymous as the FTP user name and your e-mail address as the password. Besides downloading entries, data files and documentation, it is possible to upload any files that you may wish to send to PDB, only into the directory **/new_uploads**. Those using VMS may need to place quotes around file names.

– Gopher

PDB has a Gopher server on the system **gopher.pdb.bnl.gov** (130.199.144.1). This server is accessible using a Gopher client connecting to the following link:

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

As a Gopher client, you may navigate through a hierarchy of directories and documents or ask an index server to return a list of all documents that contain one or more specified words. For instance, you can choose “The PDB Anonymous FTP” after reaching PDB’s Gopher server in order to search and download the same information and coordinate files as through FTP. Alternatively, you can select “An (almost) full-text search of the PDB Bibliographic Headers” in order to search PDB using any keyword.

– World Wide Web (WWW)

PDB has a World Wide Web (WWW) server on the computer system **www.pdb.bnl.gov** (130.199.144.1). This server is accessible using the Document URL http://www.pdb.bnl.gov/.

Besides including links to the PDB FTP and Gopher servers, the WWW server includes links to many other useful databases and information servers.

– Listserv

PDB has a mailing list devoted to discussions concerning its operation, contents, and access procedures.

To subscribe, send e-mail to listserv@pdb.pdb.bnl.gov with the one-line message:

subscribe PDB-L Firstname Lastname

To find out what can be done with this mailing list, send e-mail to the same address (listserv@pdb.pdb.bnl.gov) with the one-line message of help.

To send a message to all PDB-L subscribers, e-mail the message to:

PDB-L@pdb.pdb.bnl.gov

Ident Codes

– Issuance Of

Each PDB entry is uniquely identified by a four-character ident code (also sometimes referred to as an accession code). Presently PDB practice is to issue ident codes without regard for the structure name. However, we recognize that many depositors would like to have ident codes that are related mnemonically to the names of their structures. Should you have a preference for a particular ident code, PDB requests that you inform us about this on your Electronic Deposition Form. All reasonable suggestions will be considered. Of course, if the ident code that you are suggesting has already been used for an existing entry, then an alternative code will have to be issued by PDB.

– Obtainment for a New Entry

PDB issues the ident code of a new entry only after receiving the complete deposition and verifying the correctness and integrity of the data. The prepared entry as well as a letter stating the ident code, describing any problems found in the entry and requesting approval for release is sent to the primary contact. A note will also be sent to the secondary contact stating that these files have been sent to the primary contact (for additional information see article entitled “Deposition Contact Persons” on page 7).

To facilitate issuance of the ident code, the Electronic Deposition Form should be filled out and returned electronically. It is important to pick up the latest version of the Electronic Deposition Form from FTP and fill it out completely and accurately. Coordinate data must be in PDB format (see the latest Format Description document) and (p)reprints of all journal articles referenced must be sent *via* facsimile (516-282-5751) or air mail.

– Location for an Existing Entry

A PDB ident code is helpful for retrieving the file for a particular macromolecular structure. Tables of all PDB entries with their ident codes can be obtained electronically from FTP, Gopher, WWW, the PDB Listserver or by postal mail upon request. Also, some published articles reporting results of structural analyses of biological macromolecules provide the PDB ident code.

If you are searching PDB using FTP (also Gopher or WWW *via* “The PDB’s Anonymous FTP”), there are two directories that are especially useful for locating ident codes. The first such directory is /**index**. This contains the following files which are updated continuously:

author.idx	- Ident code and author
cmpd_res.idx	- Ident code, resolution and compound name
compound.idx	- Ident code and full compound name from the COMPND records
crystal.idx	- Ident code, unit-cell dimensions, space group and Z value
entries.idx	- Ident code, classification, accession date, compound, source, author list, resolution and experiment type
molecule.idx	- Ident code, resolution and macromolecule name
resolu.idx	- Ident code and resolution
source.idx	- Ident code and biological source from the SOURCE records
src_simple.idx	- Ident code and biological source

Other index files may be added from time to time.

The second useful directory is /**newsletter/newsletterYYmon** (*e.g.,* /newsletter/newsletter94jan). This directory contains text (.txt) and PostScript (.ps) files of tables listing all currently available and pending entries. You may retrieve and peruse index files, tables and directory listings to determine whether or not a structure of interest is available and, if it is, locate its ident code. As entries are added to FTP between quarterly releases, they are placed in the directory /**newly_released**. Be sure to scan this directory for the latest PDB entries. The /**current_release** directory contains the entire up-to-date PDB collection, while the /**fullrelease** directory contains the last quarterly release.

Coordinate files are named pdb1abc.ent, structure factor files are named r1abcsf.ent and NMR experimental data files are named 1abc.mr, where 1abc is the PDB ident code.

UNIX-Based Filters and Browser

The response to our PC-based PDB-Shell has been so positive that a similar system, PDB-Browse, has been developed for PDB’s UNIX users.

The PDB-Browse system consists of three parts. The first of these builds indices (based on UNIX standard dbm files) of PDB entries as they exist on the user’s computer system. The requirements for running this part are PERL and 50 Mbytes of disk space (the disk requirement can be lowered by indexing fewer fields in the PDB file). Currently indexed are the AUTHOR, COMPND, CRYST1, JRNL, SOURCE, EXPDAT, HET, FORMUL and REMARK records, plus the accession date, functional classification (as it appears in the HEADER record) and resolution fields, as well as the file location as a function of ident code.

The second part of PDB-Browse consists of a number of PERL programs that act as filters and scan the above indices. The programs auth.pl, comp.pl, cryst.pl, expd.pl, jrnl.pl, rem.pl and sour.pl scan the appropriate records. For example,

```
expd.pl –a NMR
```

returns the ident codes of all (-a) entries for which NMR techniques were used to collect the data. (Adding a -v flag would report all non-nmr entries.) To find out which of these entries describe DNA, execute the command:

```
expd.pl -a NMR | comp.pl DNA
```

which will return the entries satisfying both conditions. To find out which of these have a SYNTHETIC source, execute

```
expd.pl -a NMR | comp.pl DNA | sour.pl SYNTHETIC
```

to produce the ident codes of those (currently 24 in number). On a Silicon Graphics workstation, with the indices residing on an NFS-mounted file system, the above query took less than 10 seconds.

A PERL program called loc.pl is also provided which, given an ident code, will provide the location of an entry. Combining loc.pl with the pipeline, one could view each of the above files with the command:

```
view `expd.pl -a NMR | comp.pl DNA | sour.pl SYNTHETIC | loc.pl`
```

PERL scripts are also provided to scan the accession date (before.pl and after.pl), functional classification (head.pl), and the resolution as it appears in remark 2 (resoluge.pl and resolule.p). In addition, full.pl searches the full file for a particular expression including wild cards, list.pl lists an entire index and lookup.pl extracts certain records or fields from a list of ident codes. For example, to find the authors (not ident codes) from the above set, one would execute:

```
expd.pl -a NMR | comp.pl DNA | sour.pl SYNTHETIC | lookup.pl auth
```

The third part of the PDB-Browse system, called browse, is a graphical user interface (GUI) front-end for all of these filters (as well as custom filters that may be written by the user). This front-end requires the user to install tcl and tk (Tool Command Language and Tool Kit, public domain utilities written by John Ousterhout of UC Berkeley and available *via* anonymous FTP from harbor.ecn.purdue.edu). It is also helpful, but not required, to have a graphical viewing program such as RASMOL (by Roger Sayle, available from ftp.dcs.ed.ac.uk) or MidasPlus (by Conrad Huang and Thomas Ferrin of UCSF).

All of the programs making up the PDB-Browse system are available in source form *via* each of PDB's distribution methods, in a directory named /**pub**/**pdbbrowse**. Before downloading, be sure to read the file ReadMeFirst in that directory. Please send all comments and suggestions for improvements to Dave Stampf (drs@bnl.gov).

Newly Released Entries

IDENT CODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
1PPK	ACID PROTEINASE/ISOVALERYL (IVA)-VAL-VAL-STA(P)-O-ET (STATINE ANALOGUE)	N.C.J.STRYNADKA,M.N.G.JAMES	1/94
1AFG	ACIDIC FIBROBLAST GROWTH FACTOR (AFG)	M.BLABER,J.DISALVO,K.A.THOMAS,B.W.MATTHEWS	12/93
2BTF	BETA-ACTIN-PROFILIN COMPLEX	C.E.SCHUTT,J.C.MYSLIK,M.D.ROZYCKI,N.C.W.GOONESEKERE	1/94
1ANK	ADENYLATE KINASE (ADK)	M.B.BERRY,B.MEADOR,T.BILDERBACK,P.LIANG,M.GLASER, G.N.PHILLIPS,JUNIOR	2/94
2ACR	ALDOSE REDUCTASE WILD TYPE/NADP+/CACODYLATE	D.H.HARRISON,K.M.BOHREN,K.H.GABBAY,G.A.PETSKO,D.RINGE	4/94
2ACS	ALDOSE REDUCTASE WILD TYPE/NADP+/CITRATE	D.H.HARRISON,K.M.BOHREN,K.H.GABBAY,G.A.PETSKO,D.RINGE	4/94
2ACQ	ALDOSE REDUCTASE WILD TYPE/NADP+/GLUCOSE-6-PHOSPHATE	D.H.HARRISON,K.M.BOHREN,K.H.GABBAY,G.A.PETSKO,D.RINGE	4/94
2ACU	ALDOSE REDUCTASE MUTANT(Y48H)/NADP+/CITRATE	K.M.BOHREN,C.E.GRIMSHAW,C.-J.LAI,K.H.GABBAY,G.A.PETSKO, D.H.HARRISON,D.RINGE	4/94
1AHC	ALPHA-MOMORCHARIN (TYPE I RIBOSOME-INACTIVATING PROTEIN)	J.REN,Y.WANG,Y.DONG,D.I.STUART	1/94
1AHA	ALPHA-MOMORCHARIN/ADENINE	J.REN,Y.WANG,Y.DONG,D.I.STUART	1/94
1AHB	ALPHA-MOMORCHARIN/FORMYCIN 5'-MONOPHOSPHATE	J.REN,Y.WANG,Y.DONG,D.I.STUART	1/94
1BYA	BETA-AMYLASE	B.MIKAMI,M.DEGANO,E.J.HEHRE,J.C.SACCHETTINI	1/94
1BYB	BETA-AMYLASE REACTED WITH 200 MM MALTOSE /MALTOTETRAOSE	B.MIKAMI,M.DEGANO,E.J.HEHRE,J.C.SACCHETTINI	1/94
1BYC	BETA-AMYLASE REACTED WITH 8 MM MALTOSE/MALTOTETRAOSE	B.MIKAMI,M.DEGANO,E.J.HEHRE,J.C.SACCHETTINI	1/94
1BYD	BETA-AMYLASE REACTED WITH 100 MM MALTAL/ 2-DEOXYMALTOSE	B.MIKAMI,M.DEGANO,E.J.HEHRE,J.C.SACCHETTINI	1/94
1ATT	ANTITHROMBIN III (ATIII)	L.MOUREY,J.P.SAMAMA,M.DELARUE,D.MORAS	3/93
1HRS	APOFERRITIN CO-CRYSTALLIZED WITH SN-PROTOPORPHYRIN IX IN CADMIUM SULFATE	G.PRECIGOUX,J.YARIV,B.GALLOIS,A.DAUTANT,C.COURSEILLE, B.LANGLOISD'ESTAINTOT	11/93
1PAR	ARC REPRESSOR AND A 22-MER DNA CONTAINING THE SEQUENCE OF THE ARC OPERATOR	B.E.RAUMANN,M.A.ROULD,C.O.PABO,R.T.SAUER	3/94
1AKA	ASPARTATE AMINOTRANSFERASE MUTANT (K258H) (PLP-FORM)	V.N.MALASHKEVICH,J.N.JANSONIUS	2/94
1AKB	ASPARTATE AMINOTRANSFERASE MUTANT (K258H)/ N-(5'-PHOSPHOPYRIDOXYL)-L-ASPARTATE	V.N.MALASHKEVICH,J.N.JANSONIUS	2/94
1AKC	ASPARTATE AMINOTRANSFERASE MUTANT (K258H)/ N-(5'-PHOSPHOPYRIDOXYL)-L-GLUTAMATE	V.N.MALASHKEVICH,J.N.JANSONIUS	2/94
1AST	ASTACIN	W.BODE,F.X.GOMIS-RUETH,W.STOECKER	4/93
1BNS	BARNASE (G SPECIFIC ENDONUCLEASE) MUTANT (T26A)	Y.W.CHEN	4/94
1BRG	BARNASE (G SPECIFIC ENDONUCLEASE) MUTANT (F7L)	Y.W.CHEN,A.R.FERSHT,K.HENRICK	
1BRS	BARNASE (G SPECIFIC ENDONUCLEASE)/BARSTAR MUTANT (C40A,C82A)	A.M.BUCKLE,G.SCHREIBER,A.R.FERSHT	3/94
1BTA	BARSTAR (NMR, MINIMIZED AVERAGE STRUCTURE)	M.J.LUBIENSKI,M.BYCROFT,S.M.V.FREUND,A.R.FERSHT	5/94
1BTB	BARSTAR (NMR, 30 STRUCTURES)	M.J.LUBIENSKI,M.BYCROFT,S.M.V.FREUND,A.R.FERSHT	5/94
1DEG	CALMODULIN MUTANT (DEL E84)	S.RAGHUNATHAN,R.CHANDROSS,B.P.CHENG,A.PERSECHINI, S.E.SOBOTTK,R.H.KRETSINGER	6/93
1CMK	CAMP-DEPENDENT PROTEIN KINASE CATALYTIC SUBUNIT	J.ZHENG,D.R.KNIGHTON,N.-H.XUONG,S.S.TAYLOR,J.M.SOWADSKI, L.F.TENEYCK	11/93
1NBA	N-CARBAMOYLSARCOSINE AMIDOHYDROLASE	M.J.ROMAO,D.TURK,F.-Z.GOMIS-RUTH,R.HUBER,G.SCHUMACHER, H.MOLLERING,L.RUSSMANN	5/92
1WHS	SERINE CARBOXYPEPTIDASE II (NATIVE FORM)	T.L.BULLOCK,S.J.REMINGTON	3/94
1WHT	SERINE CARBOXYPEPTIDASE II/L-BENZYLSUCCINATE	T.L.BULLOCK,S.J.REMINGTON	3/94
1AAG	CARCINOGENIC EMBRYO ANTIGEN ANTIBODY (THEORETICAL MODEL)	M.T.MAS,K.C.SMITH,D.L.YARMUSH,K.AISAKA,R.M.FINE	4/92
1CRE	CARDIOTOXIN II (NMR,MINIMIZED AVERAGE STRUCTURE)	R.BHASKARAN,C.C.HUANG,K.D.CHANG,C.YU	3/94
1CRF	CARDIOTOXIN II (NMR,12 STRUCTURES)	R.BHASKARAN,C.C.HUANG,K.D.CHANG,C.YU	3/94
1CHN	CHEY/MG2+ IN THE ACTIVE SITE	L.BELLSOLELL,M.COLL	4/94
1COM	CHORISMATE MUTASE/PREPHENATE	Y.M.CHOOK,H.KE,W.N.LIPSCOMB	4/94
2CHS	CHORISMATE MUTASE	Y.M.CHOOK,H.KE,W.N.LIPSCOMB	4/94
2CHT	CHORISMATE MUTASE/AN ENDO-OXABICYCLIC TRANSITION STATE ANALOG	Y.M.CHOOK,H.KE,W.N.LIPSCOMB	4/94
1CRP	C-H-RAS P21 PROTEIN (CATALYTIC DOMAIN)/GDP AND MG (NMR,FIRST 20 STRUCTURES)	P.J.KRAULIS,P.J.DOMAILLE,S.L.CAMPBELL-BURK,T.VAN AKEN,E.D.LAUE	11/93
1CRQ	C-H-RAS P21 PROTEIN (CATALYTIC DOMAIN)/GDP AND MG (NMR,RESTRAINED MIN. AVE)	P.J.KRAULIS,P.J.DOMAILLE,S.L.CAMPBELL-BURK,T.VAN AKEN,E.D.LAUE	11/93
1CRR	C-H-RAS P21 PROTEIN (CATALYTIC DOMAIN)/GDP AND MG (NMR,FINAL 20 STRUCTURES)	P.J.KRAULIS,P.J.DOMAILLE,S.L.CAMPBELL-BURK,T.VAN AKEN,E.D.LAUE	11/93
1PLL	C-H-RAS P21 PROTEIN MUTANT(G12P)/GUANOSINE-DIPHOSPHATE	A.SCHEIDIG,A.SANCHEZ-LLORENTE,A.LAUTWEIN,E.F.PAI,J.E.T.CORRIE, G.P.REID,A.WITTINGHOFER,R.S.GOODY	3/94
1PLK	C-H-RAS P21 PROTEIN MUTANT(G12P)/ GUANOSINE-TRIPHOSPHATE	A.SCHEIDIG,A.SANCHEZ-LLORENTE,A.LAUTWEIN,E.F.PAI,J.E.T.CORRIE, G.P.REID,A.WITTINGHOFER,R.S.GOODY	3/94
1PLJ	C-H-RAS P21 PROTEIN MUTANT(G12P)/ NITROPHENYLETHYL-GUANOSINE(IMIDO)TRIPHOSPHATE	A.SCHEIDIG,A.SANCHEZ-LLORENTE,A.LAUTWEIN,E.F.PAI,J.E.T.CORRIE, G.P.REID,A.WITTINGHOFER,R.S.GOODY	3/94
1GHA	GAMMA CHYMOTRYPSIN IN 4% AQUEOUS SOLUTION OF ISOPROPANOL	H.P.YENNAWAR,N.H.YENNAWAR,G.K.FARBER	4/94
1GHB	GAMMA CHYMOTRYPSIN/N-ACETYL D-TRYPTOPHAN	H.P.YENNAWAR,N.H.YENNAWAR,G.K.FARBER	4/94
1GCD	GAMMA CHYMOTRYPSIN/DIETHYL PHOSPHORYL (PH 5.6, TEMPERATURE 90K)	M.HAREL,J.L.SUSSMAN,I.SILMAN	5/94
1CCF	COAGULATION FACTOR X (CALCIUM FORM) (NMR,15 STRUCTURES)	M.SELANDER-SUNNERHAGEN,M.ULLNER,M.PERSSON,O.TELEMAN, J.STENFLO,T.DRAKENBERG	5/93
1MJC	MAJOR COLD SHOCK PROTEIN 7.4 (CSPA (CS 7.4)) OF (ESCHERICHIA COLI)	H.SCHINDELIN,U.HEINEMANN	3/94

Newly Released Entries (cont.)

IDENT CODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
5CNA	CONCANAVALIN A/ALPHA-METHYL-D-MANNOPYRANOSIDE	J.H.NAISMITH,C.EMMERICH,J.HABASH,S.J.HARROP,J.R.HELLIWELL, W.N.HUNTER,J.RAFTERY,A.J.KALB(GILBOA),J.YARIV	2/94
1SCS	CONCANAVALIN A (COBALT SUBSTITUTED FOR MANGANESE)	C.EMMERICH,J.R.HELLIWELL,M.REDSHAW,J.H.NAISMITH,S.J.HARROP, J.RAFTERY,A.J.KALB,J.YARIV,Z.DAUTER,K.S.WILSON	12/93
1SCR	CONCANAVALIN A (NICKEL SUBSTITUTED FOR MANGANESE)	C.EMMERICH,J.R.HELLIWELL,M.REDSHAW,J.H.NAISMITH,S.J.HARROP, J.RAFTERY,A.J.KALB,J.YARIV,Z.DAUTER,K.S.WILSON	12/93
1CUS	CUTINASE	C.MARTINEZ,C.CAMBILLAU	4/94
1CLH	CYCLOPHILIN (NMR,12 STRUCTURES)	R.T.CLUBB,G.WAGNER	12/93
1FRC	CYTOCHROME C (REDUCED) (NMR, AVERAGE STRUCTURE)	P.X.QI,D.L.DISTEFANO,A.J.WAND	3/94
2BMH	CYTOCHROME P450 (BM-3) (HEMOPROTEIN DOMAIN)	H.LI,T.L.POULOS	5/94
1CTM	CYTOCHROME F (REDUCED)	S.E.MARTINEZ,D.HUANG,A.SZCZEPANIAK,W.A.CRAMER,J.L.SMITH	1/94
1CCE	CYTOCHROME C PEROXIDASE (CCP-MKT) MUTANT(H175G)	D.E.MCREE,G.M.JENSEN,M.M.FITZGERALD,H.A.SIEGEL,D.B.GOODIN	5/94
1CCG	CYTOCHROME C PEROXIDASE (CCP-MKT) MUTANT(H175G)/ IMIDAZOLE	D.E.MCREE,G.M.JENSEN,M.M.FITZGERALD,H.A.SIEGEL,D.B.GOODIN	5/94
1DEM	DENDROTOXIN I (NMR,MINIMIZED AVERAGE STRUCTURE)	J.-M.LANCELIN,M.-F.FORAY	3/94
1DEN	DENDROTOXIN I (NMR,29 STRUCTURES)	J.-M.LANCELIN,M.-F.FORAY	3/94
1DIR	DIHYDROPTERIDINE REDUCTASE (DHPR)	K.I.VARUGHESE,Y.SU,M.M.SKINNER,D.A.MATTHEWS,J.M.WHITELY,N.H.XUONG	4/94
1DDT	DIPHTHERIA TOXIN (DIMERIC)	M.J.BENNETT,D.EISENBERG	3/94
1MDT	MONOMERIC DIPHTHERIA TOXIN	M.J.BENNETT,D.EISENBERG	3/94
161D	DNA/RNA (5'-D(CPCPGPGPCP)-R(GP)-D(CPCPGPG)-3')	C.BAN,B.RAMAKRISHNAN,M.SUNDARALINGAM	2/94
118D	DNA (5'-D(GPTPGPCPGPCPAPC)-3')	C.BINGMAN,X.LI,G.ZON,M.SUNDARALINGAM	2/93
158D	DNA (5'-D(CP*CP*AP*AP*GP*CP*TP*TP*GP*G)-3')/CALCIUM	K.GRZESKOWIAK,D.S.GOODSELL,M.KACZOR-GRZESKOWIAK,D.CASCIO, R.E.DICKERSON	2/94
150D	DNA (5'-D(CP*GP*CP*GP*AP*AP*TP*TP*1,N==6==-ETHENO-AP* GP*CP*G)-3')	G.A.LEONARD,K.E.MC AULEY-HECHT,N.J.GIBSON,T.BROWN,W.P.WATSON, W.N.HUNTER	12/93
151D	DNA (5'-D(CP*GP*AP*TP*CP*G)-3')/ADRIAMYCIN (-160 C)	L.A.LIPSCOMB,M.E.PEEK,F.X.ZHOU,J.A.BERTRAND,D.VANDERVEER, L.D.WILLIAMS	12/93
152D	DNA (5'-D(CP*GP*AP*TP*CP*G)-3')/DAUNOMYCIN (-160 C)	L.A.LIPSCOMB,M.E.PEEK,F.X.ZHOU,J.A.BERTRAND,D.VANDERVEER, L.D.WILLIAMS	12/93
160D	DNA (5'-D(CPCPCPGPGPCPCPGPGPG)-3')	B.RAMAKRISHNAN,M.SUNDARALINGAM	2/94
1DGC	GCN4 LEUCINE ZIPPER/SPECIFIC ATF/CREB SITE DNA	T.J.RICHMOND	7/93
169D	DNA/RNA (5'-R(GPCPGP)-D(TPAPTPAPCPCPC)-3')/ (5'-D(GPGPGPTPAPTPAPCPGPC)-3')(NMR)	M.SALAZAR,O.Y.FEDOROFF,L.ZHU,B.R.REID	4/94
170D	DNA (5'-D(CPGPCPGPAPAPTPTP)-ARA(CP)-2 D(GPCPG)-3') (NMR,MINIMIZED AVE STRUCTURE)	B.I.SCHWEITZER,T.MIKITA,G.W.KELLOGG,K.H.GARDNER,G.P.BEARDSLEY	3/94
171D	DNA (5'-D(CPGPCPGPAPAPTPTPCPGPCPG)-3') SELF-COMPLEMENTARY DUPLEX(NMR,MIN. AVE)	B.I.SCHWEITZER,T.MIKITA,G.W.KELLOGG,K.H.GARDNER,G.P.BEARDSLEY	3/94
179D	DNA (5'-D(TPCPGPA)-3') (NMR, 6 STRUCTURES)	Y.WANG,D.J.PATEL	6/94
1BPB	DNA POLYMERASE BETA (BETA POLYMERASE) (APO, 31KD DOMAIN)	M.R.SAWAYA,H.PELLETIER,A.KUMAR,S.H.WILSON,J.KRAUT	4/94
1BPD	DNA POLYMERASE BETA (BETA POLYMERASE) (APO, FULL PROTEIN)	M.R.SAWAYA,H.PELLETIER,A.KUMAR,S.H.WILSON,J.KRAUT	4/94
1BPE	DNA POLYMERASE BETA (BETA POLYMERASE) FULL PROTEIN/DEOXY-ATP	M.R.SAWAYA,H.PELLETIER,A.KUMAR,S.H.WILSON,J.KRAUT	4/94
1KFD	DNA POLYMERASE I (KLENOW FRAGMENT)/DCTP	L.S.BEESE,J.M.FRIEDMAN,T.A.STEITZ	9/93
1ELB	ELASTASE/TRIFLUOROACETYL-L-LYSYL-L-LEUCYL-P- ISOPROPYLANILIDE	C.MATTOS,B.RASMUSSEN,X.DING,G.A.PETSKO,D.RINGE	12/93
1ELS	ENOLASE (2-PHOSPHO-D-GLYCERATE HYDROLASE)/ PHOSPHONOACETOHYDROXAMATE AND MN	E.ZHANG,M.HATADA,J.M.BREWER,L.LEBIODA	4/94
1EPA	EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN (B-FORM)	M.E.NEWCOMER	6/93
1EPB	EPIDIDYMAL RETINOIC ACID-BINDING PROTEIN (B-FORM)/ RETINOIC ACID	M.E.NEWCOMER	6/93
1ERA	ERABUTOXIN B (NMR, MINIMIZED AVERAGE STRUCTURE)	H.HATANAKA,D.KOHDA,F.INAGAKI	3/94
1FRA	ERABUTOXIN B (NMR, 14 STRUCTURES)	H.HATANAKA,D.KOHDA,F.INAGAKI	3/94
1FCT	FERREDOXIN CHLOROPLASTIC TRANSIT PEPTIDE (NMR, 27 STRUCTURES)	J.-M.LANCELIN,M.BLACKLEDGE	3/94
1FRD	HETEROCYST [2FE-2S] FERREDOXIN (OXIDIZED, RECOMBINANT FORM)	B.L.JACOBSON,Y.K.CHAE,J.L.MARKLEY,I.RAYMENT,H.M.HOLDEN	4/93
1HLB	HEMOGLOBIN (SEA CUCUMBER)	M.L.HACKERT,D.T.MITCHELL	3/94
1FTZ	FUSHI TARAZU PROTEIN (HOMEODOMAIN) (NMR,20 STRUCTURES)	Y.Q.QIAN,K.FURUKUBO-TOKUNAGA,D.RESENDEZ-PEREZ,M.MULLER, W.J.GEHRING,K.WUTHRICH	1/94
1GLG	GALACTOSE/GLUCOSE-BINDING PROTEIN/D-GALACTOSE	M.N.VYAS,N.K.VYAS,F.A.QUIOCHO	12/93
1YHB	GENE V PROTEIN MUTANT WITH TYR 41 REPLACED BY PHE (Y41F)	Y.GUAN,H.ZHANG,R.N.H.KONINGS,C.W.HILBERS,T.C.TERWILLIGER, A.H.-J.WANG	4/94
1YHA	GENE V PROTEIN MUTANT WITH TYR 41 REPLACED BY HIS (Y41H)	Y.GUAN,H.ZHANG,R.N.H.KONINGS,C.W.HILBERS,T.C.TERWILLIGER, A.H.-J.WANG	4/94
1CPM	CIRCULARLY PERMUTED (1-3,1-4)-BETA-D-GLUCAN 4-GLUCANOHY- DROLASE (CPA16M-59)	M.HAHN,U.HEINEMANN	3/94
1CPN	CIRCULARLY PERMUTED (1-3,1-4)-BETA-D-GLUCAN 4-GLUCANOHY- DROLASE (CPA16M-57)	M.HAHN,U.HEINEMANN	3/94
1GLM	GLUCOAMYLASE-471 (1,4-ALPHA-D-GLUCAN GLUCOHYDROLASE)	A.E.ALESHIN,C.HOFFMAN,L.M.FIRSOV,R.B.HONZATKO	4/94
2GDA	GLUCOCORTICOID RECEPTOR (DNA BINDING DOMAIN, GR-DBD) (NMR, 24 STRUCTURES)	H.BAUMANN,K.PAULSEN,H.KOVACS,H.BERGLUND,A.P.H.WRIGHT, J.-A.GUSTAFSSON,T.HARD	3/94
1GDC	GLUCOCORTICOID RECEPTOR (DNA BINDING DOMAIN) (NMR, MINIMIZED AVERAGE STRUCTURE)	H.BAUMANN,K.PAULSEN,H.KOVACS,H.BERGLUND,A.P.H.WRIGHT, J.-A.GUSTAFSSON,T.HARD	3/94

Newly Released Entries (cont.)

IDENT CODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
1GCG	GALACTOSE/GLUCOSE-BINDING PROTEIN (CLOSED, UNLIGANDED FORM)	M.M.FLOCCO,S.L.MOWBRAY	2/94
1GPH	GLUTAMINE PHOSPHORIBOSYLPYROPHOSPHATE AMIDOTRANSFERASE	J.L.SMITH	4/94
1GLP	GLUTATHIONE S-TRANSFERASE YFYF (CLASS PI)/ GLUTATHIONE SULFONIC ACID	I.GARCIA-SAEZ,M.COLL	3/94
1GLQ	GLUTATHIONE S-TRANSFERASE (YFYF,CLASS PI)/ S-(P-NITROBENZYL) GLUTATHIONE	I.GARCMA-SAEZ,M.COLL	3/94
2GLR	GLUTATHIONE S-TRANSFERASE YFYF (CLASS PI)/ S-HEXYL GLUTATHIONE	A.PARRAGA,I.GARCIA-SAEZ,M.COLL	5/94
1GLC	GLYCEROL KINASE/GLUCOSE-SPECIFIC FACTOR III/G3P/ ADP/MG(II)/ZN(II)	M.D.FEESE,N.D.MEADOW,S.ROSEMAN,D.W.PETTIGREW,S.J.REMINGTON	3/94
1GLD	GLYCEROL KINASE/GLUCOSE-SPECIFIC FACTOR III/G3P/ADP/MN(II)	M.D.FEESE,N.D.MEADOW,S.ROSEMAN,D.W.PETTIGREW,S.J.REMINGTON	3/94
1GLE	GLYCEROL KINASE/GLUCOSE-SPECIFIC FACTOR III/G3P/ADP/ZN(II)	M.D.FEESE,N.D.MEADOW,S.ROSEMAN,D.W.PETTIGREW,S.J.REMINGTON	3/94
1GNC	GRANULOCYTE COLONY STIMULATING FACTOR (RH-G-CSF)(NMR,10 STRUCTURES)	T.W.ZINK,A.ROSS,R.RUDOLPH,T.A.HOLAK	3/94
2DHC	HALOALKANE DEHALOGENASE/1,2-DICHLOROETHANE (SOAKED IN 10MM DCE,PH 5.0,4 DEG C)	K.H.G.VERSCHUEREN,B.W.DIJKSTRA	9/93
2DHD	HALOALKANE DEHALOGENASE/1,2-DICHLOROETHANE (SOAKED IN 10MM DCE,PH 5.0,RM TEMP.)	K.H.G.VERSCHUEREN,B.W.DIJKSTRA	9/93
1HDA	HEMOGLOBIN (DEOXY)	G.FERMI	5/93
1CBM	HEMOGLOBIN(BETA4,CARBONMONOXY) (R-LIKE QUATERNARY STATE)	G.E.O.BORGSTAHL,A.ARNONE	2/93
1CBL	HEMOGLOBIN(BETA4,DEOXY)(R-LIKE QUATERNARY STATE)	G.E.O.BORGSTAHL,A.ARNONE	2/93
1PGH	HEMOGLOBIN (AQUOMET)	D.S.KATZ,S.P.WHITE,W.HUANG,R.KUMAR,D.W.CHRISTIANSON	3/94
1FLP	HEMOGLOBIN I (MONOMERIC) (FERRIC)	M.RIZZI,J.B.WITTENBERG,P.ASCENZI,M.FASANO,A.CODA,M.BOLOGNESI	5/94
1HSL	HISTIDINE-BINDING PROTEIN/L-HISTIDINE	N.YAO,S.TRAKHANOV,F.A.QUIOCHO	1/94
1HDN	HISTIDINE-CONTAINING PHOSPHOCARRIER PROTEIN (HPR) (NMR, 30 STRUCTURES)	N.A.J.VAN NULAND,R.M.SCHEEK,G.T.ROBILLARD	2/94
1HME	HIGH MOBILITY GROUP PROTEIN FRAGMENT-B (BOX DOMAIN B, RAT HMG1)(NMR,1 STRUCTURE)	H.M.WEIR,P.J.KRAULIS,C.S.HILL,A.R.C.RAINE,E.D.LAUE,J.O.THOMAS	2/94
1HMF	HIGH MOBILITY GROUP PROTEIN FRAGMENT-B (BOX DOMAIN B,RAT HMG1)(NMR,30 STRUCTURES)	H.M.WEIR,P.J.KRAULIS,C.S.HILL,A.R.C.RAINE,E.D.LAUE,J.O.THOMAS	3/94
1HMA	HMG-D (HMG-BOX DOMAIN, RESIDUES 2 - 74) (NMR, 20 STRUCTURES)	D.N.M.JONES,M.A.SEARLES,G.L.SHAW,M.E.A.CHURCHILL,S.S.NER, J.KEELER,A.A.TRAVERS,D.NEUHAUS	5/94
1DLH	HUMAN CLASS II HISTOCOMPATIBILITY PROTEIN (EXTRACELLULAR DMN)/ANTIGENIC PEPTIDE	L.J.STERN	2/94
1HTE	HIV-1 PROTEASE/GR123976	H.JHOTI,A.WONACOTT,P.MURRAY-RUST	4/94
1HTF	HIV-1 PROTEASE/GR126045	H.JHOTI,A.WONACOTT,P.MURRAY-RUST	4/94
1HTG	HIV-1 PROTEASE/GR137615	H.JHOTI,A.WONACOTT,P.MURRAY-RUST	4/94
1HEF	HIV-1 PROTEASE/SKF 108738	K.MURTHY,E.L.WINBORNE,M.D.MINNICH,J.S.CULP,C.DEBOUCK	9/92
1HEG	HIV-1 PROTEASE/SKF 107457	K.MURTHY,E.L.WINBORNE,M.D.MINNICH,J.S.CULP,C.DEBOUCK	9/92
1RDH	HIV-1 REVERSE TRANSCRIPTASE (RIBONUCLEASE H DOMAIN)	B.C.FINZEL,D.CHATTOPADHYAY,H.M.EINSPAHR	3/93
1FIG	IMMUNOGLOBULIN G1 (KAPPA LIGHT CHAIN) FAB' FRAGMENT	M.R.HAYNES,E.A.STURA,D.HILVERT,I.A.WILSON	1/94
2CGR	IGG2B (KAPPA) FAB FRGMNT/N-(P-CYANOPHENYL)- DIPHENYLEMETHYL GUANIDINEACETIC ACID	L.W.GUDDAT,L.SHAN,A.B.EDMUNDSON	11/93
1CGS	IGG2B(KAPPA)FAB FRGMNT AGAINST CYANOPHENYL-DIPHENYLEMETHYL GUANIDINEACETIC ACID	L.W.GUDDAT,L.SHAN,A.B.EDMUNDSON	10/93
1VFA	FV FRAGMENT OF MOUSE MONOCLONAL ANTIBODY D1.3 (BALB/C,IGG1,K)	T.N.BHAT,R.J.POLJAK	12/93
1VFB	FV FRAGMENT OF MOUSE MONOCLONAL ANTIBODY D1.3/ HEN EGG LYSOZYME	T.N.BHAT,R.J.POLJAK	12/93
1ACY	IGG1 FAB FRAGMENT (59.1)/HIV-1 GP120 (MN ISOLATE) FRAGMENT (RESIDUES 308 - 332)	J.B.GHIARA,I.A.WILSON	2/94
1JEL	FAB JE142 MONOCLONAL ANTIBODY/HISTIDINE-CONTAINING PROTEIN (HPR)	L.PRASAD,L.T.J.DELBAERE,J.W.QUAIL,M.VANDONSELAAR	4/93
1FRG	IGG2A FAB FRAGMENT (FAB 26/9)/INFLUENZA HEMAGGLUTININ HA1 (STRAIN X47)	M.E.A.CHURCHILL,I.A.WILSON	1/94
1ITM	INTERLEUKIN 4 (IL-4) (NMR,MINIMIZED AVERAGE STRUCTURE)	C.REDFIELD,L.J.SMITH,J.BOYD,G.M.P.LAWRENCE,R.G.EDWARDS, C.J.GERSHATER,R.A.G.SMITH,C.M.DOBSON	2/94
1IKA	ISOCITRATE DEHYDROGENASE/ALPHA-KETOGLUTARATE	B.L.STODDARD,D.E.KOSHLAND JUNIOR	6/93
1IKB	ISOCITRATE DEHYDROGENASE/ISOCITRATE, NADP, AND CALCIUM	B.L.STODDARD,D.E.KOSHLAND JUNIOR	6/93
1CSK	C-SRC KINASE (SH3 DOMAIN)	M.MATHIEU,R.K.WIERENGA	3/94
1HPL	LIPASE (TRIACYLGLYCEROL HYDROLASE)	Y.BOURNE,C.CAMBILLAU	1/93
1LST	LYSINE-, ARGININE-, ORNITHINE-BINDING PROTEIN (LAO)/LYSINE	S.-H.KIM,B.-H.OH	2/93
2LAO	LYSINE-, ARGININE-, ORNITHINE-BINDING PROTEIN (LAO)	S.-H.KIM,B.-H.OH,C.-H.KANG	2/93
137L	LYSOZYME MUTANT(S44F,C54T, C97A)	M.BLABER,B.W.MATTHEWS	8/93
2EQL	LYSOZYME (APO FORM)	H.TSUGE,H.AGO,M.MIYANO	5/94
2IFF	IGG1 FAB FRAGMENT (HYHEL-5)/LYSOZYME MUTANT (R68K)	S.CHACKO,D.R.DAVIES	2/94
216L	LYSOZYME MUTANT(S44W,C54T,C97A)	M.BLABER,B.W.MATTHEWS	5/94
1BMD	MALATE DEHYDROGENASE (BACTERIAL)/NADH	C.A.KELLY,J.J.BIRKTOFT	11/92
1MOM	MOMORDIN	J.HUSAIN,I.J.TICKLE,S.P.WOOD	3/94
1MOL	MONELLIN (SINGLE-CHAIN, FUSED)	J.R.SOMOZA,S.-H.KIM	4/93
1BET	BETA-NERVE GROWTH FACTOR	N.Q.MC DONALD,R.LAPATTO,J.MURRAY-RUST,J.GUNNING,A.WLODAWER, T.L.BLUNDELL	4/93

Newly Released Entries (cont.)

IDENT CODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
1NDC	NUCLEOSIDE DIPHOSPHATE KINASE/2'-DEOXYTHYMIDINE DIPHOSPHATE	J.CHERFILS,S.MORERA,J.JANIN	4/94
1NLK	NUCLEOSIDE DIPHOSPHATE KINASE	R.L.WILLIAMS	3/94
1OLA	OLIGO-PEPTIDE BINDING PROTEIN (OPPA)/A FOUR-RESIDUE PEPTIDE	J.TAME,A.J.WILKINSON	4/94
1OLB	OLIGO-PEPTIDE BINDING PROTEIN (OPPA)/TRI-LYSINE	J.TAME,A.J.WILKINSON	4/94
2PAS	PARVALBUMIN (ALPHA LINEAGE, PI 5.0)/CALCIUM (NMR, 9 STRUCTURES)	A.PADILLA,A.CAVE,J.PARELLO,G.ETIENNE,C.BALDELLON	3/94
3PAT	PARVALBUMIN (ALPHA LINEAGE,PI 5.0)/CALCIUM (NMR, AVERAGE STRUCTURE)	A.PADILLA,A.CAVE,J.PARELLO,G.ETIENNE,C.BALDELLON	3/94
1PKT	PHOSPHATIDYLINOSITOL 3-KINASE (SH3 DOMAIN) (NMR,31 STRUCTURES)	S.KOYAMA,H.YU,D.C.DALGARNO,T.B.SHIN,L.D.ZYDOWSKY,S.L.SCHREIBER	3/94
1PKS	PHOSPHATIDYLINOSITOL 3-KINASE (SH3 DOMAIN) (NMR,MINIMIZED AVERAGE STRUCTURE)	S.KOYAMA,H.YU,D.C.DALGARNO,T.B.SHIN,L.D.ZYDOWSKY,S.L.SCHREIBER	3/94
1PHP	3-PHOSPHOGLYCERATE KINASE (PGK)	G.J.DAVIES,H.C.WATSON	4/94
1STO	OROTATE PHOSPHORIBOSYLTRANSFERASE (OPRTASE)	G.SCAPIN,C.GRUBMEYER,J.C.SACCHETTINI	12/93
1PPS	PHOTOSYSTEM I REACTION CENTER (TRIMERIC)	N.KRAUSS,W.HINRICHS,I.WITT,P.FROMME,W.PRIZKOW,Z.DAUTER,C.BETZEL, K.S.WILSON,H.T.WITT,W.SAENGER	1/93
1PMK	PLASMINOGEN KRINGLE 4	K.PADMANABHAN,A.TULINSKY	4/94
2PRF	PROFILIN IA (NMR,19 STRUCTURES)	S.J.ARCHER,V.K.VINSON,T.D.POLLARD,E.E.LATTMAN,D.A.TORCHIA	1/94
1RPA	PROSTATIC ACID PHOSPHATASE/TARTARIC ACID	Y.LINDQVIST,G.SCHNEIDER	7/93
1RPT	PROSTATIC ACID PHOSPHATASE/VANADATE	Y.LINDQVIST,G.SCHNEIDER	11/93
1MPT	M-PROTEASE (SUBTILISIN FAMILY)	T.YAMANE,T.KANI,T.HATANAKA,A.SUZUKI,T.ASHIDA,T.KOBAYASHI,S.ITO, O.YAMASHITA	4/94
2PCT	PROTEIN C (SERINE PROTEINASE DOMAIN)(THEORETICAL MODEL)	C.L.FISHER,J.S.GREENGARD,J.H.GRIFFIN	6/94
1PCU	PROTEIN C (SERINE PROTEINASE DOMAIN) (THEORETICAL MODEL)	C.L.FISHER,J.S.GREENGARD,J.H.GRIFFIN	12/93
2SPT	PROTHROMBIN FRAGMENT 1/STRONTIUM	A.TULINSKY	2/94
1PMY	PSEUDOAZURIN (CUPREDOXIN)	T.INOUE,Y.KAI,S.HARADA,N.KASAI,Y.OHSHIRO,S.SUZUKI,T.KOHZUMA,J.TOBARI	1/94
163D	REV RESPONSIVE ELEMENT(30 RIBONUCLEOTIDE FRGMT)/ HIV REV PROTEIN(FRAGMENT)(MODEL)	F.LECLERC,R.J.CEDERGREN,A.D.ELLINGTON	2/94
1DBP	D-RIBOSE-BINDING PROTEIN MUTANT (G72D)	S.L.MOWBRAY,A.J.JOAKIMBJORKMAN	1/94
1RBL	RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (RUBISCO)	J.NEWMAN,S.GUTTERIDGE,C.-I.BRAENDEN,T.A.JONES	5/93
157D	RNA (5'-R(CP*GP*CP*GP*AP*AP*UP*UP*AP*GP*CP*G)-3')	G.A.LEONARD,K.E.MC AULEY-HECHT,S.EBEL,D.M.LOUGH,T.BROWN, W.N.HUNTER	2/94
1YSC	SERINE CARBOXYPEPTIDASE (CPY, CPD-Y, OR PROTEINASE C)	J.A.ENDRIZZI,S.J.REMINGTON	3/94
1SAC	SERUM AMYLOID P COMPONENT (SAP)	H.E.WHITE,J.EMSLEY,B.P.O'HARA,G.OLIVIA,I.J.TICKLE,T.L.BLUNDELL, M.B.PEPYS,S.P.WOOD	1/94
1SET	SERYL-TRNA SYNTHETASE/5'-O-[N-(L-SERYL)-SULPHAMOYL] ADENOSINE	S.CUSACK,H.BELRHALI	2/94
1SES	SERYL-TRNA SYNTHETASE/SERYL-HYDROXAMATE-AMP	S.CUSACK,H.BELRHALI	2/94
1PCP	SPASMOLYTIC PROTEIN(PORCINE) (PSP)	M.D.CARR,C.J.BAUER,M.J.GRADWELL,J.FEENEY	2/94
2SPC	SPECTRIN (ONE REPEAT UNIT)	Y.YAN,E.WINOGRAD,A.VIEL,T.CRONIN,S.C.HARRISON,D.BRANTON	3/94
1SPR	SRC-SH2 (SRC HOMOLOGY (SH2) DOMAIN) (PEPTIDE-FREE FORM)	G.WAKSMAN,J.KURIYAN	3/93
1SRL	SRC TYROSINE KINASE TRANSFORMING PROTEIN (SH3 DOMAIN) (NMR,MINIMIZED AVERAGE)	H.YU,M.K.ROSEN,T.B.SHIN,C.SEIDEL-DUGAN,J.S.BRUGGE,S.L.SCHREIBER	3/94
1SRM	SRC TYROSINE KINASE TRANSFORMING PROTEIN (SH3 DOMAIN) (NMR,20 STRUCTURES)	H.YU,M.K.ROSEN,T.B.SHIN,C.SEIDEL-DUGAN,J.S.BRUGGE,S.L.SCHREIBER	3/94
1ENA	STAPHYLOCOCCAL NUCLEASE MUTANT (D21E)/CALCIUM ION	A.LIBSON,A.GITTIS,E.E.LATTMAN	2/94
1ENC	STAPHYLOCOCCAL NUCLEASE MUTANT (D21E)/ CALCIUM ION/THYMIDINE 3',5'-DIPHOSPHATE	A.LIBSON,A.GITTIS,E.E.LATTMAN	2/94
1SYB	STAPHYLOCOCCAL NUCLEASE MUTANT/DEOXY-DIPHOSPHOTHYMIDINE/CA	T.R.HYNES,R.A.KAUTZ,M.A.GOODMAN,J.F.GILL,R.O.FOX	1/94
2ENB	STAPHYLOCOCCAL NUCLEASE MUTANT (D21E)/THYMIDINE 3',5'-DIPHOSPHATE	A.LIBSON,A.GITTIS,E.E.LATTMAN	3/94
1STN	STAPHYLOCOCCAL NUCLEASE	T.R.HYNES,R.O.FOX	2/93
1STA	STAPHYLOCOCCAL NUCLEASE/CALCIUM AND THE INHIBITOR THYMIDINE 3',5'-DIPHOSPHATE	L.J.KEEFE,S.QUIRK,A.GITTIS,E.E.LATTMAN	1/94
1SYC	STAPHYLOCOCCAL NUCLEASE MUTANT(P117G)	T.R.HYNES,A.HODEL,R.O.FOX	1/94
1SYD	STAPHYLOCOCCAL NUCLEASE MUTANT(P117G)/ 2'-DEOXY-DIPHOSPHOTHYMIDINE/CA	T.R.HYNES,A.HODEL,R.O.FOX	1/94
1SYE	STAPHYLOCOCCAL NUCLEASE MUTANT(P117T)	T.R.HYNES,A.HODEL,R.O.FOX	1/94
1SYF	STAPHYLOCOCCAL NUCLEASE MUTANT(P117T)/ 2'-DEOXY-DIPHOSPHOTHYMIDINE/CA	T.R.HYNES,A.HODEL,R.O.FOX	1/94
1SYG	STAPHYLOCOCCAL NUCLEASE MUTANT(P117A)	T.R.HYNES,A.HODEL,R.O.FOX	1/94
1STB	STAPHYLOCOCCAL NUCLEASE INSERTION MUTANT(INS(L36-L))/ THYMIDINE DIPHOSPHATE/CA	S.QUIRK,A.GITTIS,L.J.KEEFE,E.E.LATTMAN	1/94
1HYT	THERMOLYSIN/BENZYLSUCCINIC ACID	A.C.HAUSRATH,B.W.MATTHEWS	5/94
1NRQ	ALPHA-THROMBIN/RECEPTOR BASED PEPTIDE D-FPR'S	A.TULINSKY,I.I.MATHEWS	1/94
1HUT	ALPHA-THROMBIN WITH CHLOROMETHYLKETONE REPLACED BY A METHYLENE GROUP	A.TULINSKY,K.PADMANABHAN	5/93
1NRP	ALPHA-THROMBIN/RECEPTOR BASED PEPTIDE NR'S	A.TULINSKY,I.I.MATHEWS	1/94
1NRO	ALPHA-THROMBIN/RECEPTOR BASED PEPTIDE NRP	A.TULINSKY,I.I.MATHEWS	1/94
1NRN	ALPHA-THROMBIN/RECEPTOR BASED PEPTIDE NRS	A.TULINSKY,I.I.MATHEWS	1/94

Newly Released Entries (cont.)

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1NRS	ALPHA-THROMBIN/RECEPTOR BASED PEPTIDE NRP (FIRST FOUR RESIDUES ONLY)/HIRUGEN	A.TULINSKY,I.I.MATHEWS	1/94
1NRR	ALPHA-THROMBIN/RECEPTOR BASED PEPTIDE XA/PPACK	A.TULINSKY,I.I.MATHEWS	1/94
1TYS	THYMIDYLATE SYNTHASE MUTANT (C146S)	E.FAUMAN,E.RUTENBER,R.STROUD	5/93
1PML	TISSUE PLASMINOGEN ACTIVATOR KRINGLE 2	K.PADMANABHAN,A.TULINSKY	4/94
1TND	TRANSDUCIN (ALPHA SUBUNIT)/NONHYDROLYZABLE GTP ANALOGUE GTP GAMMA S	J.P.NOEL,H.E.HAMM,P.B.SIGLER	3/94
1TAH	TRIACYLGLYCEROL ACYL HYDROLASE	M.E.M.NOBLE,A.CLEASBY,L.N.JOHNSON,M.EGMOND,L.G.J.FRENKEN	12/93
1TCA	TRIACYLGLYCEROL HYDROLASE	J.UPPENBERG,T.A.JONES	2/94
1TCB	TRIACYLGLYCEROL HYDROLASE	J.UPPENBERG,T.A.JONES	2/94
1TCC	TRIACYLGLYCEROL HYDROLASE	J.UPPENBERG,T.A.JONES	2/94
1TMH	TRIOSEPHOSPHATE ISOMERASE MUTANT	K.V.RADHA KISHAN,J.PH.ZEELEN,R.K.WIERENGA	3/94
1TPD	TRIOSEPHOSPHATE ISOMERASE	M.E.M.NOBLE,J.PH.ZEELEN,R.K.WIERENGA	2/94
1TPE	TRIOSEPHOSPHATE ISOMERASE	M.E.M.NOBLE,K.V.RADHAKISHAN,J.PH.ZEELEN,R.K.WIERENGA	2/94
1TPF	TRIOSEPHOSPHATE ISOMERASE	K.V.RADHAKISHAN,J.PH.ZEELEN,R.K.WIERENGA	2/94
1TRI	TRIOSEPHOSPHATE ISOMERASE MUTANT WITH 15 RESIDUES (68-82) REPLACED BY 8 RESIDUES	R.K.WIERENGA	10/93
1TYT	TRYPANOTHIONE REDUCTASE (OXIDIZED FORM (E))	S.BAILEY,W.N.HUNTER	6/93
1SMF	TRYPSIN/BOWMAN-BIRK INHIBITOR	Q.HUANG,Y.LI,S.ZHANG,S.LIU,Y.TANG,C.QI	10/92
2LET	TRYPSIN INHIBITOR II MUTANT (I5L) (NMR,20 STRUCTURES)	K.J.NIELSEN,D.ALEWOOD,J.ANDREWS,S.B.H.KENT,D.J.CRAIK	1/94
1BRC	TRYPSIN VARIANT (D189G,G226D)/AMYLOID BETA-PROTEIN PRECURSOR(INHIBITOR DOMAIN)	J.J.PERONA,R.J.FLETTERICK	12/92
1BRB	TRYPSIN VARIANT (D189G, G226D)/BPTI VARIANT (C5A, C55A)	J.J.PERONA,R.J.FLETTERICK	12/92
1TNR	TUMOR NECROSIS FACTOR RECEPTOR P55(EXTRACELLULAR DMN)/TNF-BETA	D.W.BANNER	5/94
1BVH	TYROSINE PHOSPHATASE (NMR, 15 STRUCTURES)	T.M.LOGAN,M.-M.ZHOU,D.G.NETTESHEIM,R.P.MEADOWS,R.L.VAN ETTEN, S.W.FESIK	5/94
1UBI	UBIQUITIN	D.ALEXEEV,S.M.BURY,M.A.TURNER,O.M.OGUNJOBI,T.W.MUIR,R.RAMAGE, L.SAWYER	2/94
1IFD	INOVIRUS STRAIN FD MAJOR COAT PROTEIN ASSEMBLY (FIBER DIFFRACTION)	D.A.MARVIN	2/92
1IFI	INOVIRUS STRAIN FD MAJOR COAT PROTEIN ASSEMBLY, CANONICAL SYMMETRY (FIBER DIFF)	D.A.MARVIN	1/94
1IFJ	INOVIRUS STRAIN FD MAJOR COAT PROTEIN ASSEMBLY, DIAD SYMMETRY (FIBER DIFF)	D.A.MARVIN	1/94
1IFK	INOVIRUS STRAIN IF1 MAJOR COAT PROTEIN ASSEMBLY, CANONICAL SYMMETRY (FIBER DIFF)	D.A.MARVIN	1/94
1IFL	INOVIRUS STRAIN IKE MAJOR COAT PROTEIN ASSEMBLY, CANONICAL SYMMETRY (FIBER DIFF)	D.A.MARVIN	1/94
1IFM	INOVIRUS STRAIN PF1 MAJOR COAT PROTEIN ASSEMBLY, LOW-TEMP SYMMETRY (FIBER DIFF)	D.A.MARVIN	1/94
1IFN	INOVIRUS STRAIN PF1 MAJOR COAT PROTEIN ASSEMBLY, HIGH-TEMP SYMMETRY (FIBER DIFF)	D.A.MARVIN	1/94
1VTM	TOBACCO MOSAIC VIRUS, STRAIN U2 (FIBER DIFFRACTION)	G.STUBBS,R.PATTANAYEK	3/92
1VMO	VITELLINE MEMBRANE OUTER LAYER PROTEIN I	T.SHIMIZU,D.G.VASSYLYEV,S.KIDO,Y.DOI,K.MORIKAWA	1/94
1XYA	XYLOSE ISOMERASE	A.LAVIE,K.N.ALLEN,G.A.PETSKO,D.RINGE	1/94
1XYB	XYLOSE ISOMERASE/GLUCOSE	A.LAVIE,K.N.ALLEN,G.A.PETSKO,D.RINGE	1/94
1XYC	XYLOSE ISOMERASE/3-O-METHYLFRUCTOSE	A.LAVIE,K.N.ALLEN,G.A.PETSKO,D.RINGE	1/94
1XIB	D-XYLOSE ISOMERASE (PH 7.4)	H.L.CARRELL,J.P.GLUSKER	3/94
1XIC	D-XYLOSE ISOMERASE/D-XYLOSE (PH 9.0)	H.L.CARRELL,J.P.GLUSKER	3/94
1XID	D-XYLOSE ISOMERASE/L-ASCORBIC ACID, MN, AND MG (PH 7.4)	H.L.CARRELL,J.P.GLUSKER	3/94
1XIE	D-XYLOSE ISOMERASE/1,5-DIANHYDROSORBITOL (PH 7.4)	H.L.CARRELL,J.P.GLUSKER	3/94
1XIF	D-XYLOSE ISOMERASE/GLUCOSE, MN, AND MG (PH 8.0)	H.L.CARRELL,J.P.GLUSKER	3/94
1XIG	D-XYLOSE ISOMERASE/XYLITOL, MG, AND MN (PH 7.4)	H.L.CARRELL,J.P.GLUSKER	3/94
1XIH	D-XYLOSE ISOMERASE/D-SORBITOL AND NO ADDED MN (PH 9.0)	H.L.CARRELL,J.P.GLUSKER	3/94
1XII	D-XYLOSE ISOMERASE/300MM D-XYLULOSE AND MN (PH 8.0)	H.L.CARRELL,J.P.GLUSKER	3/94
1XIJ	D-XYLOSE ISOMERASE/THREONATE AND MN (PH 9.0)	H.L.CARRELL,J.P.GLUSKER	3/94
1XYL	XYLOSE ISOMERASE MUTANT (E(A 180)K,E(B 680)K)	K.N.ALLEN,A.LAVIE,G.A.PETSKO,D.RINGE	12/93
1XYM	XYLOSE ISOMERASE MUTANT (E(A 180)K,E(B 680)K)/GLUCOSE	K.N.ALLEN,A.LAVIE,G.A.PETSKO,D.RINGE	12/93
152L	LYSOZYME MUTANT (I3C,I9C,T21C,C54T,T142C,L164C)	M.MATSUMURA,L.H.WEAVER,B.W.MATTHEWS	1/94
1SPS	SRC-SH2 (SRC HOMOLOGY (SH2) DOMAIN)/PEPTIDE YEEI	G.WAKSMAN,J.KURIYAN	3/93

STRUCTURE FACTOR ENTRIES

R1APMSF	CAMP-DEPENDENT PROTEIN KINASE(CATALYTIC SUBUNIT)/PKI	D.R.KNIGHTON,S.M.BELL,J.ZHENG,L.F.TEN EYCK,N.XUONG,S.S.TAYLOR, J.M.SOWADSKI	1/93
R1ATPSF	CAMP-DEPENDENT PROTEIN KINASE/PKI/MNATP	J.ZHENG,E.A.TRAFNY,D.R.KNIGHTON,N.-H.XUONG,S.S.TAYLOR,L.F.TEN EYCK, J.M.SOWADSKI	3/93
R2MCMSF	MACROMOMYCIN(STREPTOMYCES MACROMOMYCETICUS)	P.VAN ROEY	5/91
R3SODSF	SUPEROXIDE DISMUTASE(CU,ZN) MUTANT(C6A)	J.TAINER ET AL.	6/90

NMR ENTRIES

NONE

Newly Deposited Entries (presently being processed - not yet released)

IDENT CODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
1IAG	ADAMALYSIN II(PROTEINASE II)	F.X.GOMIS-RUTH,W.STOCKER,W.BODE	5/94
1AGM	ALPHA-1->4-GLUCAN GLUCOHYDROLASE	A.E.ALESHIN,L.M.FIRSOV,R.B.HONZATKO	5/94
1AMP	AMINOPEPTIDASE(AEROMONAS PROTEOLYTICA)	B.CHEVRIER,C.SCHALK,H.D'ORCHIMONT,J.M.RONDEAU,D.MORAS,C.TARNUS	4/94
1AKP	APOKEDARCIDIN	K.L.CONSTANTINE,K.L.COLSON,M.WITTEKIND,M.S.FRIEDRICHS,N.ZEIN, J.TUTTLE,D.R.LANGLEY,J.E.LEET,D.R.SCHROEDER,K.S.LAM, B.T.FARMER II,W.J.METZLER,R.E.BRUCCOLERI,L.MUELLER	6/94
1ARS	ASPARTATE AMINOTRANSFERASE	A.OKAMOTO,T.HIGUCHI,K.HIROTSU	8/93
1ART	ASPARTATE AMINOTRANSFERASE	A.OKAMOTO,T.HIGUCHI,K.HIROTSU	8/93
1IAA	ASTACIN DIGESTIVE ZINC ENDOPEPTIDASE	F.X.GOMIS-RUTH,W.STOCKER,W.BODE	5/94
1IAB	ASTACIN DIGESTIVE ZINC ENDOPEPTIDASE	F.X.GOMIS-RUTH,W.STOCKER,W.BODE	5/94
1IAC	ASTACIN DIGESTIVE ZINC ENDOPEPTIDASE	F.X.GOMIS-RUTH,W.STOCKER,W.BODE	5/94
1IAD	ASTACIN DIGESTIVE ZINC ENDOPEPTIDASE	F.X.GOMIS-RUTH,W.STOCKER,W.BODE	5/94
1IAE	ASTACIN DIGESTIVE ZINC ENDOPEPTIDASE	F.X.GOMIS-RUTH,W.STOCKER,W.BODE	5/94
1BNC	BIOTIN CARBOXYLASE	G.WALDROP,I.RAYMENT,H.M.HOLDEN	4/94
1CDM	CALMODULIN BOUND TO A PEPTIDE ANALOGUE OF THE BRAIN CALMODULIN-DEPENDENT PROTEIN	W.E.MEADOR,F.A.QUIOCHO	10/93
1CDL	CALMODULIN (CAM)BOUND TO A PEPTIDE ANALOGUE OF THE CALMODULIN-BINDING PROTEIN	W.E.MEADOR,F.A.QUIOCHO	10/93
1GMT	GAMMA CHYMOTRYPSIN	K.KREUTTER,A.C.U.STEINMETZ,M.PROROK,R.ABELES,D.RINGE	5/94
172D	DNA D(GAAGCTTC)2	S.KAMITORI,F.TAKUSAGAWA	4/94
1DEC	DECORSIN	A.M.KREZEL,G.WAGNER,J.SEYMOUR-ULMER,R.A.LAZARUS	5/94
1DLC	DELTA-ENDOTOXIN CRYIIIA	J.LI	6/94
1DKA	2,2-DIALKYLGLYCINE DECARBOXYLASE (PYRUVATE)	M.D.TONEY,E.HOHENESTER,J.N.JANSONIUS	6/93
2DKB	2,2-DIALKYLGLYCINE DECARBOXYLASE (PYRUVATE)	M.D.TONEY,E.HOHENESTER,J.N.JANSONIUS	7/93
175D	DNA DUPLEX D(GCGAATGAGC)	S.H.CHOU,J.W.CHENG,O.Y.FEDOROFF,B.R.REID	4/94
2DRP	DNA/A TWO ZINC-FINGER PEPTIDE	L.FAIRALL,J.W.R.SCHWABE,L.CHAPMAN,J.T.FINCH,D.RHODES	6/94
174D	DNA (B, 5'-D(*CP*CP*AP*AP*CP*GP*TP*TP*GP*G)-3')/ANTHRAMYCIN	M.L.KOPKA,D.S.GOODSELL,R.E.DICKERSON	4/94
168D	DNA/OM-RNA	P.LUBINI,W.ZUERCHER,M.EGLI	4/94
178D	D(CGCAAATT(089)GCG)	K.E.MCAULEY-HECHT,G.A.LEONARD,N.J.GIBON,J.B.THOMSON,W.P.WATSON, W.N.HUNTER,T.BROWN	5/94
2BPF	DNA POLYMERASE-BETA	H.PELLETIER,M.R.SAWAYA,S.H.WILSON,J.KRAUT	5/94
2BPG	DNA POLYMERASE-BETA	H.PELLETER,M.R.SAWAYA,S.H.WILSON,J.KRAUT	5/94
177D	DNA	I.RADHAKRISHNAN,D.J.PATEL	5/94
1ENH	ENGRAILED HOMEODOMAIN	N.D.CLARKE,C.R.KISSINGER,J.DESJARLAIS,G.L.GILLILAND,C.O.PABO	5/94
1FDN	FERREDOXIN	E.DUEE,E.FANCHON,J.VICAT,L.C.SIEKER,J.MEYER,J-M.MOULIS	3/94
1HOB	HEMOGLOBIN	M.L.HACKERT,D.T.MITCHELL,ET AL.	2/94
1HNT	GAMMA-THROMBIN(HUMAN)	A.TULINSKY	5/94
1CEL	1,4-BETA-D-GLUCAN CELLOBIOHYDROLASE I	C.DIVNE,T.A.JONES	5/94
1GFC	GROWTH FACTOR RECEPTOR-BOUND PROTEIN	D.KOHDA,H.TERASAWA,H.HATANAKA,F.INAGAKI	6/94
1GFD	GROWTH FACTOR RECEPTOR-BOUND PROTEIN	D.KOHDA,H.TERASAWA,H.HATANAKA,F.INAGAKI	6/94
1NGI	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGJ	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGH	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(D10N)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGG	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(D10S)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGF	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(D199N)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGE	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(D199S)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGD	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(D206N)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGC	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(D206S)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGB	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(E175Q)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1NGA	HEAT-SHOCK COGNATE 70K PROTEIN (44K ATPASE FRAGMENT, N-TERMINAL) MUTANT(E175S)	K.M.FLAHERTY,S.M.WILBANKS,C.DELUCA-FLAHERTY,D.B.MCKAY	5/94
2HSC	HEAT-SHOCK COGNATE PROTEIN(44K ATPASE FRAGMENT, N-TERMINAL)	K.M.FLAHERTY,C.R.DELUCA-FLAHERTY,D.B.MCKAY	5/94
1HKT	HEAT SHOCK TRANSCRIPTION FACTOR	G.W.VUISTER,S.J.KIM,A.OROSZ,J.L.MARQUARDT,C.WU,A.BAX	6/94
1HCD	HISACTOPHILIN	J.HABAZETTL,D.GONDOL,R.WILTSCHECK,J.OTLEWSKI,M.SCHLEICHER, T.A.HOLAK	5/94
1GHC	HISTONE H1(GH1 GLOBULAR DOMAIN)(11L VARIANT)	C.CERF,G.LIPPENS,V.RAMAKRISHNAN,S.MUYLDERMANS,A.SEGERS,L.WYNS, S.J.WODAK,K.HALLENGA	5/94
1HVC	HIV-1 PROTEASE(TETHERED DIMER)/A76928 (S,S)	T.N.BHAT,E.T.BALDWIN,J.W.ERICKSON	6/94
2HSD	HYDROXYSTEROID DEHYDROGENASE	D.GHOSH,W.L.DUAX	3/94
1TYL	INSULIN (T3R3) COMPLEX	G.D.SMITH,E.CISZAK	6/94
1TYM	INSULIN (T3R3) COMPLEX	G.D.SMITH,E.CISZAK	6/94
1SLA	S-LECTIN(GALECIN-1)	Y.BOURNE,C.CAMBILLAU	5/94
1SLB	S-LECTIN(GALECIN-1)	Y.BOURNE,C.CAMBILLAU	5/94
1SLC	S-LECTIN(GALECIN-1)	Y.BOURNE,C.CAMBILLAU	5/94
1LEA	LEXA REPRESSOR(DNA BINDING DOMAIN)	R.H.FOGH,G.OTTLEBEN,H.RUETERJANS,M.SCHNARR,R.BOELENS,R.KAPTEIN	5/94

Newly Deposited Entries (cont.)

IDENT CODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
1LEB	LEXA REPRESSOR(DNA BINDING DOMAIN)	R.H.FOGH,G.OTTLEBEN,H.RUETERJANS,M.SCHNARR,R.BOELENS,R.KAPTEIN	5/94
1IAF	MEPRIN ALPHA CHAIN(CATALYTIC DOMAIN)	F.X.GOMIS-RUTH,W.STOCKER,W.BODE	5/94
146D	MITHRAMYCIN DIMER-D(TCGCGA)2 MG2+ COMPLEX	M.SASTRY,D.J.PATEL	11/93
1MDY	MYOD BASIC-HELIX-LOOP-HELIX REGION	P.C.M.MA,M.A.ROULD,H.WEINTRAUB,C.O.PABO	6/94
1MLU	MYOGLOBIN (CARBONMONOXY)	M.L.QUILLIN,G.N.PHILLIPS,JR.	6/94
1NMA	NEURAMINIDASE(N9)-NC10 FAB COMPLEX WILD TYPE	W.R.TULIP,J.N.VARGHESE,P.M.COLMAN	5/94
1ANS	NEUROTOXIN III (ATX III)(ANEMOINA SULCATA)	N.MANOLERAS,R.S.NORTON	6/94
1OCT	OCT-1 POU DOMAIN - OCTAMER COMPLEX	J.D.KLEMM,M.A.ROULD,R.AURORA,W.HERR,C.PABO	5/94
1TUR	OVOMUCOID INHIBITOR(THIRD DOMAIN)(TURKEY)	A.M.KREZEL,P.DARBA,A.D.ROBERTSON,J.FEJZO,S.MACURA,J.L.MARKEY	7/94
1TUS	OVOMUCOID INHIBITOR(TURKEY)(REACTIVE-SITE HYDROLYZED THIRD DOMAIN)	W.F.WALKENHORST,A.M.KREZEL,G.I.RHYU,J.L.MARKLEY	7/94
2HSP	PHOSPHOLIPASE C(SH3 DOMAIN)(NMR,11 STRUCTURES)	D.KOHDA,H.HATANAKA,M.ODAKA,F.INAGAKI	6/94
1HSQ	PHOSPHOLIPASE C(SH3 DOMAIN)(NMR,11 STRUCTURES)	D.KOHDA,H.HATANAKA,M.ODAKA,F.INAGAKI	6/94
1PLA	PLASTOCYANIN	S.BAGBY,P.C.DRISCOLL,T.S.HARVEY,H.A.O.HILL	5/94
1PLB	PLASTOCYANIN	S.BAGBY,P.C.DRISCOLL,T.S.HARVEY,H.A.O.HILL	5/94
1ACF	PROFILIN I	A.A.FEDOROV,K.A.MAGNUS,M.H.GRAUPE,E.E.LATTMAN,T.D.POLLARD, S.C.ALMO	7/94
1ACG	PROFILIN II	A.A.FEDOROV,K.A.MAGNUS,M.H.GRAUPE,E.E.LATTMAN,T.D.POLLARD, S.C.ALMO	7/94
1PRS	PROTEIN S	S.BAGBY,T.S.HARVEY,S.G.EAGLE,S.INOUYE,M.IKURA	3/94
2PCD	PROTOCATECHUATE 3,4-DIOXYGENASE	D.H.OHLENDORF,A.M.ORVILLE,J.D.LIPSCOMB	6/94
262D	REV BINDING ELEMENT/REV34-50 PEPTIDE (RBE-REV34-50)	F.LECLERC,R.J.CEDERGREN,A.D.ELLINGTON	4/94
1RCN	RIBONUCLEASE A	J.C.FONTECILLA-CAMPS	5/94
1RLS	RIBONUCLEASE T1	K.GOHDA,K.OKA,K.TOMITA,T.HAKOSHIMA	3/94
155D	RNA(PGGACUUCGGUCC)	S.R.HOLBROOK,J.YEH,S.H.KIM	12/93
165D	RNA(GCUUCGGC)-D[BR]U	T.PRANGE,P.SALUDJIAN,W.CRUSE,O.KENNARD	3/94
1SIP	SIV PROTEINASE (SIV MAC251-32H ISOLATE)	A.F.WILDERSPIN	4/94
1SRH	STREPTAVIDIN/3',5'-DIMETHOXY-HABA	DUPONT *PROTEIN *CRYSTALLOGRAPHY *GROUP	2/94
1SRI	STREPTAVIDIN/3',5'-DIMETHYL-HABA	DUPONT *PROTEIN *CRYSTALLOGRAPHY *GROUP	2/94
1SRG	STREPTAVIDIN/3'-METHYL-HABA	DUPONT *PROTEIN *CRYSTALLOGRAPHY *GROUP	2/94
1SRF	STREPTAVIDIN/3'-TERT-BUTYL-HABA	DUPONT *PROTEIN *CRYSTALLOGRAPHY *GROUP	2/94
1SRE	STREPTAVIDIN/HABA	DUPONT *PROTEIN *CRYSTALLOGRAPHY *GROUP	2/94
1SRJ	STREPTAVIDIN/NAPHTHYL-HABA	DUPONT *PROTEIN *CRYSTALLOGRAPHY *GROUP	2/94
1SUN	SUNY INTRON	L.JAEGER,E.WESTHOF,F.MICHEL	6/94
1TRF	TR1C FRAGMENT OF TURKEY SKELETAL MUSCLE TROPONIN C	W.A.FINDLAY,F.D.SOENNICHSEN,B.D.SYKES	12/93
1NDA	NADPH:OXIDIZED-TRYPANOTHIONE OXIDOREDUCTASE	C.B.LANTWIN,W.KABSCH,E.F.PAI,I.SCHLICHTING,R.L.KRAUTH-SIEGEL	7/93
1ATA	TRYPSIN INHIBITOR(ASCARIS)	G.M.CLORE,B.L.GRASBERGER,A.M.GRONENBORN	5/94
1ATB	TRYPSIN INHIBITOR(ASCARIS)	G.M.CLORE,B.L.GRASBERGER,A.M.GRONENBORN	5/94
1ATD	TRYPSIN INHIBITOR(ASCARIS)	G.M.CLORE,B.L.GRASBERGER,A.M.GRONENBORN	5/94
1ATE	TRYPSIN INHIBITOR(ASCARIS)	G.M.CLORE,B.L.GRASBERGER,A.M.GRONENBORN	5/94
1AYA	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	
1AYB	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	5/94
1AYC	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	5/94
1AYD	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	5/94

STRUCTURE FACTOR ENTRIES

R1BNSSF	BARNASE (G SPECIFIC ENDONUCLEASE) MUTANT (T26A)	Y.W.CHEN,A.R.FERSHT,K.HENRICK	4/94
R1BRGSF	BARNASE (G SPECIFIC ENDONUCLEASE) MUTANT (F7L)	Y.W.CHEN,A.R.FERSHT,K.HENRICK	3/94
R1MJCSF	MAJOR COLD SHOCK PROTEIN 7.4 (CSPA (CS 7.4)) OF (ESCHERICHIA COLI)	H.SCHINDELIN,U.HEINEMANN	3/94
R5CNASF	CONCANAVALIN A/ALPHA-METHYL-D-MANNOPYRANOSIDE	J.H.NAISMITH,C.EMMERICH,J.HABASH,S.J.HARROP,J.R.HELLIWELL, W.N.HUNTER,J.RAFTERY,A.J.KALB(GILBOA),J.YARIV	2/94
R1SCSSF	CONCANAVALIN A (COBALT SUBSTITUTED FOR MANGANESE)	C.EMMERICH,J.R.HELLIWELL,M.REDSHAW,J.H.NAISMITH,S.J.HARROP, J.RAFTERY,A.J.KALB,J.YARIV,Z.DAUTER,K.S.WILSON	12/93
R1SCRSF	CONCANAVALIN A (NICKEL SUBSTITUTED FOR MANGANESE)	C.EMMERICH,J.R.HELLIWELL,M.REDSHAW,J.H.NAISMITH,S.J.HARROP, J.RAFTERY,A.J.KALB,J.YARIV,Z.DAUTER,K.S.WILSON	12/93
R2BMHSF	CYTOCHROME P450 (BM-3) (HEMOPROTEIN DOMAIN)	H.LI,T.L.POULOS	5/94
R174DSF	DNA (B, 5'-D(*CP*CP*AP*AP*CP*GP*TP*TP*GP*G)-3')/ANTHRAMYCIN	M.L.KOPKA,D.S.GOODSELL,R.E.DICKERSON	4/94
R178DSF	D(CGCAAATT(089)GCG)	K.E.MCAULEY-HECHT,G.A.LEONARD,N.J.GIBON,J.B.THOMSON, W.P.WATSON, W.N.HUNTER,T.BROWN	5/94
R1FDNSF	FERREDOXIN	E.DUEE,E.FANCHON,J.VICAT,L.C.SIEKER,J.MEYER,J-M.MOULIS	3/94
R1HLBSF	HEMOGLOBIN (SEA CUCUMBER)	M.L.HACKERT,D.T.MITCHELL ET AL.	3/94
R1HOBSF	HEMOGLOBIN	M.L.HACKERT,D.T.MITCHELL,ET AL.	2/94
R1CPMSF	CIRCULARLY PERMUTED (1-3,1-4)-BETA-D-GLUCAN 4-GLUCANOHYDROLASE (CPA16M-59)	M.HAHN,U.HEINEMANN	3/94
R1CPNSF	CIRCULARLY PERMUTED (1-3,1-4)-BETA-D-GLUCAN 4-GLUCANOHYDROLASE (CPA16M-57)	M.HAHN,U.HEINEMANN	3/94
R1FLPSF	HEMOGLOBIN I (MONOMERIC) (FERRIC)	M.RIZZI,B.J.WITTENBERG,P.M.ASCENZI,P.FASANO,A.CODA,M.BOLOGNESI	5/94
R1ILRSF	INTERLEUKIN 1 RECEPTOR ANTAGONIST PROTEIN IL-1RA	H.A.SCHREUDER,J.M.RONDEAU,C.TARDIF	6/94
R1MLUSF	MYOGLOBIN (CARBONMONOXY)	M.L.QUILLIN,G.N.PHILLIPS,JR.	6/94
R1PHPSF	3-PHOSPHOGLYCERATE KINASE (PGK)	G.J.DAVIES,H.C.WATSON	4/94
R1MPTSF	M-PROTEASE (SUBTILISIN FAMILY)	T.YAMANE,T.KANI,T.HATANAKA,A.SUZUKI,T.ASHIDA,T.KOBAYASHI,S.ITO, O.YAMASHITA	4/94
R1TYTSF	TRYPANOTHIONE REDUCTASE (OXIDIZED FORM (E))	S.BAILEY,W.N.HUNTER	6/93
R1SMFSF	TRYPSIN/BOWMAN-BIRK INHIBITOR	Y.LI,Q.HUANG.S.ZHANG.S.LIU,Y.TANG.C.QI	10/92
R1AYASF	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	5/94

Newly Deposited Entries (cont.)

IDENT CODE	MOLECULE	DEPOSITOR(S)	ACCESSION DATE
R1AYBSF	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	5/94
R1AYCSF	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	5/94
R1AYDSF	PROTEIN TYROSINE PHOSPHATASE(N-TERMINAL SH2 DOMAIN)	C.H.LEE,J.KURIYAN	5/94
R1BBVSF	BLACK BEETLE VIRUS (BBV) CAPSID PROTEIN WITH DUPLEX RNA	M.V.HOSUR,J.P.WERY,V.S.REDDY,J.E.JOHNSON	12/93
NMR ENTRIES			
R1DECMR	DECORSIN	A.M.KREZEL,G.WAGNER,J.SEYMOUR-ULMER,R.A.LAZARUS	5/94
R1TURMR	OVOMUCOID INHIBITOR(THIRD DOMAIN)(TURKEY)	A.M.KREZEL,P.DARBA,A.D.ROBERTSON,J.FEJZO,S.MACURA,J.L.MARKEY	7/94
R1TUSMR	OVOMUCOID INHIBITOR(TURKEY)(REACTIVE-SITE HYDROLYZED THIRD DOMAIN)	W.F.WALKENHORST,A.M.KREZEL,G.I.RHYU,J.L.MARKLEY	7/94

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