

Altogether, 30 new atomic coordinate entries have been added to the Protein Data Bank since the previous release in January, thus bringing the current number of holdings to more than 350 atomic coordinate entries, as listed in Table 5. Table 6 lists 59 additional entries that we are in the process of preparing for inclusion in future releases.

The Protein Data Bank will be represented at the annual American Crystallographic Association meeting, Philadelphia, PA, June 26 - July 1, and at the Gordon Conference on Computational Chemistry, Plymouth College, NH, July 4 - 8.

We are extremely pleased to announce the inauguration of service by two centers which will be providing on-line access to the Protein Data Bank atomic coordinate and bibliographic entries. Starting with the current release, on-line service will be provided by the Canadian Scientific Numeric Database Service (CAN/SND) operated by the Canada Institute for Scientific and Technical Information (CISTI), (contact Dr. Roger S. Gough, CISTI, National Research Council of Canada, Ottawa, Ontario K1A 0S2, Canada, Telephone 613-993-3294, Electronic Mail, CANSND@NRCVM01), and by the Pittsburgh Supercomputing Center (contact Dr. Hugh B. Nicholas, Pittsburgh Supercomputing Center, 4400 Fifth Avenue, Pittsburgh, PA 15213, Telephone 412-268-4960, Electronic Mail, NICHOLAS@CPWPSCA). The CISTI and Pittsburgh on-line services will provide users with a convenient path to download selected Protein Data Bank entries to their own computers. The data base will be updated quarterly by CISTI and Pittsburgh, corresponding to each release from Brookhaven.

The established Protein Data Bank centers will continue to provide their full range of services as before. Inquiries may be addressed as shown below. The order form on pages 5-6 of this newsletter may be used to order data from Brookhaven. It is possible to place a standing order for each quarterly DATAPRTP release; anyone interested in placing such a standing order should contact F. C. Bernstein. Please note that the order form on pages 5-6 should be used only for Brookhaven orders; users in Japan or Australia should contact their centers for detailed information.

<u>Area</u>	<u>Address of Center</u>	<u>BITNET (BNL Only)</u>	<u>Name</u>	<u>Phone</u>
Worldwide except Australia and Japan	Protein Data Bank	PDB@BNLCHM	Inquiries	516-282-4382
	Chemistry Department	ABOLA@BNLCHM	E. E. Abola	516-282-4383
	Brookhaven National	BERNSTEIN@BNLCHM	F. C. Bernstein	516-282-4382
	Laboratory	BRYANT@BNLCHM	S. H. Bryant	516-282-4375
	Upton, NY 11973	KOETZLE@BNLCHM	T. F. Koetzle	516-282-4384
USA	WENG@BNLCHM	J. C. Weng	516-282-4382	
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002, Australia		T. Graddon	03-418-7266
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2 Suita, Osaka 565, Japan		Y. Katsube	(06) 877-5111 ext. 3912

TABLE 1. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MAGNETIC TAPE 16-APR-88

Table with columns: CODE, ITEM, AVAILABILITY USA JAP AUS. Includes entries like DATAPRTP, YEAR87TP, PART88TP, PDBPGMTP, NONST1TP, etc.

* NEW OR REPLACEMENT ENTRY SINCE JAN-88 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE 16-APR-88

Table with columns: CODE, ITEM, AVAILABILITY USA JAP AUS. Includes entries like DATAPRFI, YEAR87FI, PART88FI, CORR21FI, etc.

* NEW OR REPLACEMENT ENTRY SINCE JAN-88 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, COMPUTER PROGRAMS AND MISCELLANEOUS FILES 16-APR-88

Table with columns: NAME, PURPOSE, AUTHOR(S), REV DATE/SUPPORTED. Includes entries like PART A - AVAILABLE ON DATAPRTP, BENDERP, BLDKIT, etc.

* NEW OR REPLACEMENT ENTRY SINCE JAN-88 NEWSLETTER

SUPPORTED PROGRAMS ARE THOSE FOR WHICH STAFF OF THE PROTEIN DATA BANK WILL PROVIDE CORRECTIONS FOR DEMONSTRATED ERRORS.

TABLE 4. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS 16-APR-88

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/ CODE. Includes entries like PART 1 - AVAILABLE ON NONST1TP, RIAC2SF, etc.

PART 2 - AVAILABLE ON NONST2TP, NONST2FI

Table with columns: R1NANP2, R2BNAS, R3BNAS, R4BNAS, R5BNAS, etc. Lists various protein entries and their depositories.

PART 3 - AVAILABLE ON NONST3TP, NONST3FI

Table with columns: R1CATSF, R4CHASF, R2CCHSF, R3CC2SF, R3C2CSF, etc. Lists various protein entries and their depositories.

PART 4 - AVAILABLE ON NONST4TP, NONST4FI

Table with columns: R2APRSF, R1MBSF, R1L7TSF, R2MRSF, R1R2SF, etc. Lists various protein entries and their depositories.

PART 5 - AVAILABLE ON NONST5TP, NONST5FI

Table with columns: R1MEVSF, MENGO VIRUS, M.ROSSMANN, 2/87 SF

PART 6 - AVAILABLE ON NONST6TP, NONST6FI

Table with columns: R3APRSF, R4RVSFA, R4RVSFB, R4RVSFC. Lists various protein entries and their depositories.

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Table with columns: CODES, SF STRUCTURE FACTORS. Lists various protein entries and their depositories.

TABLE 5. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS 16-APR-88

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR(S), DATE/ STATUS. Includes entries like 4APE, 2APP, 2APR, etc.

Table listing protein entries with columns for accession number, protein name, source, and page number. Entries include ASPARTATE CARBOXYLTRANSFERASE, AZURIN, BACTERIOCHLOROPHYLL A, and many others.

Table with columns: ID, Name, Depositor, Date, Status. Includes entries like 1TP0 TRYP SIN (ORTHORHOMBIC), 3PTN TRYP SIN (TRIGONAL, 2.4M (NH4)2SO4), 3PTB TRYP SIN (BENZAMIDINE INHIBITED), etc.

MODEL STRUCTURES

Table with columns: ID, Name, Depositor, Date, Status. Includes entries like 1DN7 DNA (POLY (DG) -POLY (DC), SYNTHETIC) MODEL, 22NA DNA (Z-I, CGCGCG, SYNTHETIC) MODEL, etc.

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STATUS CODES

Table with columns: Code, Description. Includes entries like BLANK STANDARD ENTRY AVAILABLE FOR DISTRIBUTION, A ALPHA CARBON ATOMS ONLY, B BACKBONE ONLY, R RECENT (1986-1987) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 6. COORDINATE AND STRUCTURE FACTOR ENTRIES IN PREPARATION 16-APR-88

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR (S), DATE/, STATUS. Includes entries like 4WGA AGGLUTININ (WHEAT GERM, ISOLECTIN 2), 1AMT *ALAMETHICIN (TRICHODERMA VIRIDE), 1CEH ALPHA-CEMOVICID COMPLEX, etc.

Table with columns: ID, Name, Depositor, Date, Status. Includes entries like R7LDHSF LACTATE DEHYDROGENASE COMPLEXES, R6LDHSF APO-M4-LACTATE DEHYDROGENASE (DOGFISH), R1LDMSF LACTATE DEHYDROGENASE/NADH/OXAMATE (DOGFISH), etc.

* NEW OR REPLACEMENT ENTRY SINCE JAN-88 NEWSLETTER

STATUS CODES

Table with columns: Code, Description. Includes entries like A ALPHA CARBON ATOMS ONLY, B BACKBONE ONLY, C NEW ENTRY Awaiting APPROVAL BY DEPOSITOR, P IN PREPARATION, R REPLACEMENT FOR ENTRY IN TABLE 5, SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES (NO COORDINATES)

16-APR-88

Table with columns: ID, Name, Depositor, Date, Status. Includes entries like 0EAP ACID PROTEINASE (ENDOTHEIA PARASITICA), 0WGI AGGLUTININ (WHEAT GERM, ISOLECTIN 1), 0BOE ALPHA-AMYLASE INHIBITOR HOE-467A (STREPTOMYCES TENDEAE 4158), etc.

* NEW OR REPLACEMENT ENTRY SINCE JAN-88 NEWSLETTER

BROOKHAVEN ORDER FORM (Please include a self-addressed label)

1. Name _____ Date _____
 Address _____ Telephone _____
 _____ Electronic Mail _____

2. Documentation desired (no charge).

- Introduction to The Protein Data Bank (April 1988)
 Latest Newsletter
 Atomic Coordinate and Bibliographic Entry Format Description
 for DATAPRTP and DATAPRFI (January 1985)
 Current DATAPRTP Directory
 Sources of Visual Aids for Macromolecular Structure (February 1988)
 Non-Standard Entries (Structure Factors) Format Description
 Data Deposition Form

3. Please send the following magnetic tape items (from Table 1).

	6250 cpi	1600 cpi	TK50
DATAPRTP (coordinate tape)			
VAX/VMS BACKUP	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	<input type="checkbox"/> \$283
VAX/VMS COPY	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	<input type="checkbox"/> \$283
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$310	
PDBPGMTP			
VAX/VMS COPY	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	<input type="checkbox"/> \$283
NONST1TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST2TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST3TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST4TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST5TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
NONST6TP			
Unlabelled ASCII	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	
Unlabelled EBCDIC	<input type="checkbox"/> \$267	<input type="checkbox"/> \$267	

Cost: _____

Special order items (described in Table 1): Please inquire at Brookhaven for availability and price.

YEAR87TP	CONNECTP	DSTNCETP
PART88TP	DGPLOTTP	FISIPLTP
BENDERTP	DIHDRLTP	PHIPSITP

(Continued)

4. Foreign air mail postage for tape items listed in 3 above mailed from Brookhaven to destinations outside the U.S. and Canada. A postage surcharge of \$19 is required per item.

Number of items x \$19 = _____

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$292, postage included. Correction fiche are free.

Items: _____ Cost: _____

6. Please send the following printed listings. Each listing costs \$95, postage included.

Ident Code(s) (From Table 5): _____ Cost: _____

7. **Total charges - All prices are expected to be valid through September 30, 1988. After that date please confirm prices.**

Magnetic tape charges (3 above) _____
 Foreign air mail postage charges (4 above) _____
 Microfiche charges (5 above) _____
 Printed listing charges (6 above) _____
 Bank charge _____
 No charge for checks drawn in U.S. dollars on _____
 U.S. bank, otherwise \$10 _____

TOTAL COST : _____

Method of Payment:

Brookhaven requires that either a written purchase order or check payable to Brookhaven National Laboratory be received before service is provided. Order forms and purchase orders may be sent by facsimile to (United States) 516-282-3000. The original order forms and purchase orders should also be sent to Brookhaven by mail.

() check is () enclosed
 () purchase order number _____ () sent separately

Please return to

Ms. F. C. Bernstein
 Chemistry Department - Bldg. 555
 Brookhaven National Laboratory
 Upton, New York 11973 USA
 (516-282-4382)

It is advisable to send a photocopy of this order form directly to Brookhaven; experience shows that purchasing departments often do not forward this form with the order.