

The Protein Data Bank is extremely pleased that the number of new structures being deposited is increasing significantly, as can be seen in the list of coordinate and structure factor entries in preparation (Table 9 on page 4). We are attempting to prepare these entries for release as quickly as possible, and we ask for your patience as we do this work.

Recently there has been no demand for data distribution on 800 cpi density magnetic tape, so that we are considering discontinuing this option. Any user who would be seriously inconvenienced by not being able to obtain 800 cpi tapes should contact Brookhaven as soon as possible.

Tom Koetzle will be attending the XIV IUCr Congress in Perth, Australia, August 12-20. Tom will present a poster on the Protein Data Bank, as part of a demonstration of crystallographic databases coordinated by the Data Commission of the IUCr. Tom plans to be in Perth for the entire Congress, and he will be happy to receive comments and suggestions from Data Bank users and contributors.

Inquiries may be addressed to any of the persons listed below. The order form on pages 7-8 of this newsletter may be used to order data from Brookhaven. Please note that this form 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>Name</u>	<u>Phone</u>
Worldwide except Australia and Japan	Protein Data Bank Chemistry Department Brookhaven National Laboratory Upton, New York 11973, USA (BITNET address: ABOLA@BNLDAG)	Data Bank Inquiries E. E. Abola F. C. Bernstein S. H. Bryant T. F. Koetzle J. C. Weng	516-282-4382 516-282-4383 516-282-4382 516-282-4375 516-282-4384 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 K. Yoshida	(06) 877-5111 ext. 3912

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TABLE 1. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MAGNETIC TAPE

Table with columns: CODE, ITEM, AVAILABILITY USA JAP AUS. Includes entries for DATAPRTP, YEAR86TP, PART87TP, PDBPGMTP, NONST1TP, NONST2TP, NONST3TP, NONST4TP, BENDR1P, BLDKITTP, CONECTTP, DGPLOTTP, DIHRLTTP, DSTNCTTP, FISIPLTP, PHIPS1TP.

* NEW OR REPLACEMENT ENTRY SINCE APR-87 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

Table with columns: CODE, ITEM, AVAILABILITY USA JAP AUS. Includes entries for DATAPRF1, YEAR86F1, PART87F1, CORR20F1, NONST1F1, NONST2F1, NONST3F1, NONST4F1, BENDR1F1, BLDKITF1, CONECTF1, DGPLOTF1, DIHRLTF1, DSTNCF1, FISIPLF1, PHIPS1F1.

* NEW OR REPLACEMENT ENTRY SINCE APR-87 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, COMPUTER PROGRAMS AND MISCELLANEOUS FILES

Table with columns: NAME, PURPOSE, AUTHOR(S), REV DATE/SUPPORTED. Divided into PART A and PART B. Includes programs like BENDER, BLDKIT, BRUKTP, CONECT, CONCT, DGPLOT, DIHRL, DRCTY, DSTNCE, FISIPL, LSH, NAMOD, PHIPS1, REFHTE, STEREO, TAPDIR, THEOD, TORSRU, TOTALS, ALB, CRYSTAL.

* NEW OR REPLACEMENT ENTRY SINCE APR-87 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 (PART 1, SEE ALSO TABLES 5,6,7)

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/CODE. Lists structure factor holdings for various proteins like ACTINIDIN, ALPHACHYMOTRYPSIN, CALCIUM-BINDING PARVALBUMIN, etc.

SF STRUCTURE FACTORS

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 2, SEE ALSO TABLES 4,6,7)

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/CODE. Lists structure factor holdings for various proteins like CYTOCHROME C, CYTOCHROME C551, CYTOCHROME C551 (REDUCED), etc.

SF STRUCTURE FACTORS

TABLE 6. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 3, SEE ALSO TABLES 4,5,7)

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/CODE. Lists structure factor holdings for various proteins like CATALASE (BEEF LIVER), ALPHACHYMOTRYPSIN (BOVINE), GAMMA-CHYMOTRYPSIN, etc.

SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 4, SEE ALSO TABLES 4,5,6)

Table with columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/CODE. Lists structure factor holdings for various proteins like RIZAPPSF, R23ASF, R2AZASF, R31CBSP, etc.

SF STRUCTURE FACTORS

SF STRUCTURE FACTORS

TABLE 11. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS
16-JUL-87

THE CORRECTIONS IN THIS TABLE ARE GIVEN IN THE FORM OF 'UPDATE' MODIFICATIONS, AND CONSIST OF 'UPDATE' DIRECTIVES PLUS NEW DATA RECORDS THAT ARE TO BE INSERTED OR THAT REPLACE ERRONEOUS RECORDS IN CERTAIN DATA BANK ENTRIES. 'UPDATE' IS THE CDC LIBRARY-FILE MANAGEMENT SYSTEM UNDER WHICH THE MASTER PROTEIN DATA BANK FILE IS MAINTAINED. FOR A DESCRIPTION OF 'UPDATE' USERS ARE REFERRED TO THE 'UPDATE REFERENCE MANUAL' PUBLICATION NUMBER 60342500, CONTROL DATA CORPORATION, ARDEN HILLS, MN, 1974. BRIEFLY, EACH DATA ENTRY IS GIVEN AN IDENTIFICATION CODE WHICH ALSO SERVES AS THE UPDATE 'DECK' NAME. EACH RECORD IN THE FILE IS IDENTIFIED WITH TWO TAGS. THE FIRST TAG IS SIMPLY THE 'DECK' NAME (OR AN 'IDENT' NAME -SEE BELOW) AND THE SECOND IS A SEQUENCE NUMBER WITHIN THE 'DECK' (OR 'IDENT'). THESE TAGS ARE INCLUDED IN CHARACTERS 73-80 OF THE RECORDS IN EACH DATA ENTRY AS DISTRIBUTED.

CORRECTIONS MAY BE MADE USING 'UPDATE' DIRECTIVES TO 'INSERT' NEW RECORDS OR 'DELETE' OLD ONES. EACH CORRECTION SET BEGINS WITH A '*IDENT' DIRECTIVE. THIS IDENTIFIES THE CORRECTION SET, E.G. AS 'IMBNA' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK 'IMBN' FOR SPERM-WHALE MYOGLOBIN, 'IMBNB' FOR THE SECOND CORRECTION, ETC. '*DELETE' DIRECTIVES SPECIFY A RECORD OR INCLUSIVE RUN OF RECORDS TO BE DELETED. IF DATA RECORDS OCCUR IMMEDIATELY FOLLOWING '*DELETE', THESE ARE TO BE INSERTED IN PLACE OF THE RECORDS DELETED. '*INSERT' DIRECTIVES ARE USED TO SPECIFY A PARTICULAR RECORD AFTER WHICH INFORMATION IS TO BE INSERTED. THE RECORDS TO BE INSERTED FOLLOW IMMEDIATELY AFTER '*INSERT' IN THE CORRECTION SET. WITHIN EACH CORRECTION NEW RECORDS PLACED IN THE FILE ARE GIVEN THE 'IDENT' NAME AND NUMBERED SEQUENTIALLY.

```
*IDENT,2AZAA
*INSERT,2AZA.104
REMARK 13
REMARK 13 CORRECTION. MOVE ATOM RECORDS FOR THE B CONFORMATION TO BE
REMARK 13 IN THE CORRECT PLACES. THIS REQUIRES RENUMBERING MOST OF
REMARK 13 THE ATOMS IN THIS ENTRY. THE CORRECT RECORDS ARE NOT
REMARK 13 CHANGED BECAUSE THEY WERE BASED ON ATOMS APPEARING IN THE
REMARK 13 CORRECT ORDER WITH THE CORRECT NUMBERING. 06-MAR-87.
*INSERT,2AZA.6
REV DAT 2 06-MAR-87 2AZAA 3 ATOM HETATM TER
*DELETE,2AZA.417,2467
ATOM 215 CG BGLN A 28 -13.197 29.668 1.787 .20 18.82 2
ATOM 216 CD AGLN A 28 -14.346 30.203 3.457 .80 33.34 2
ATOM 217 CD BGLN A 28 -11.764 30.002 2.124 .20 27.48 2
.
.
HETATM 2264 O HOH B 274 24.432 11.998 28.821 1.00 81.76
HETATM 2265 O HOH B 275 9.137 -7.600 27.214 1.00 82.30
*DELETE,2AZA.2580
MASTER 102 6 5 4 18 26 4 9 2263 2 112 20
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*IDENT,1HKGF
*INSERT,1HKGF.3
REMARK 11
REMARK 11 CORRECTION. CORRECT ATOM ORDERING FOR ALL UNK RESIDUES.
REMARK 11 STANDARDIZE SOURCE RECORD. 16-APR-87.
*INSERT,1HKGF.6
REV DAT 7 16-APR-87 1HKGF 3 SOURCE ATOM
*DELETE,1HKGF.5
SOURCE YEAST (SACCHAROMYCES SCEREVISIAE)
*DELETE,1HKGF.112,117
ATOM 17 N UNK 5 49.409 -6.273 19.161 1.00 0.00 1
ATOM 18 CA UNK 5 49.233 -5.330 20.255 1.00 0.00 1
ATOM 19 C UNK 5 48.099 -4.517 19.988 1.00 0.00 1
ATOM 20 O UNK 5 47.425 -4.219 20.898 1.00 0.00 1
ATOM 21 CB UNK 5 50.344 -4.350 20.407 1.00 0.00 1
ATOM 22 CG UNK 5 49.845 -3.031 21.133 1.00 0.00 1
*DELETE,1HKGF.126,132
ATOM 31 N UNK 7 46.175 -5.438 17.268 1.00 0.00 2
ATOM 32 CA UNK 7 45.262 -6.418 16.982 1.00 0.00 2
.
.
ATOM 3286 CB UNK 456 -7.530 14.949 18.554 1.00 0.00 1
ATOM 3287 CG UNK 456 -7.317 16.254 19.329 1.00 0.00 1
*DELETE,1HKGF.3383,3388
ATOM 3288 N UNK 457 -11.114 15.391 17.507 1.00 0.00 1
ATOM 3289 CA UNK 457 -12.492 16.052 17.755 1.00 0.00 1
ATOM 3290 C UNK 457 -12.279 17.466 18.338 1.00 0.00 1
ATOM 3291 O UNK 457 -11.655 17.549 19.502 1.00 0.00 1
ATOM 3292 CB UNK 457 -13.299 15.134 18.812 1.00 0.00 1
ATOM 3293 CG UNK 457 -14.865 15.419 19.042 1.00 0.00 1
*DELETE,1HKGF.5
MASTER 62 6 0 0 0 0 0 6 3298 1 0 36
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*IDENT,1CCRD
*INSERT,1CCRD.5
REMARK 8
REMARK 8 CORRECTION. INTERCHANGE OCCUPANCY AND TEMPERATURE FACTOR
REMARK 8 FIELDS ON ALL ATOM AND HETATM RECORDS. 16-APR-87.
*INSERT,1CCRD.6
REV DAT 5 16-APR-87 1CCRD 3 ATOM HETATM
*DELETE,1CCRD.84,941
ATOM 1 C ACE 0 -4.251 25.565 42.602 1.00 14.18
ATOM 2 O ACE 0 -3.667 24.896 41.732 1.00 13.96
ATOM 3 CH3 ACE 0 -4.013 27.036 42.775 1.00 14.31
ATOM 4 N ALA 1 -5.115 24.987 43.439 1.00 13.99
.
.
ATOM 857 OG SER 111 -8.472 30.406 18.910 1.00 19.81
ATOM 858 OXT SER 111 -6.211 29.484 15.471 1.00 20.32
*DELETE,1CCRD.943,1037
HETATM 950 FE HEM 1 2.886 16.923 24.535 1.00 6.49
HETATM 861 CHA HEM 1 .478 14.744 23.614 1.00 6.28
HETATM 862 CHB HEM 1 .587 19.307 25.293 1.00 5.33
.
.
HETATM 953 O HOH 48 -6.073 31.642 34.628 1.00 17.69
HETATM 954 O HOH 49 -2.479 22.421 40.929 1.00 19.36
*DELETE,1CCRD.6
MASTER 49 4 3 5 0 8 0 6 953 1 56 9
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THE FOLLOWING DATA SETS HAVE BEEN REPLACED

	OLD ENTRY	NEW ENTRY
OBSLTE	16-JUL-87 1CPP	2CPP
OBSLTE	16-JUL-87 1APR	2APR

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

1. Name _____ Date _____
Address _____ Telephone _____

2. Documentation desired (no charge).

- Introduction to The Protein Data Bank (June 1986)
- 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 (September 1986)
- 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	800 cpi
DATAPRTP (coordinate tape)			
VAX/VMS BACKUP	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	
VAX/VMS COPY	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	
TK50 VAX/VMS BACKUP	<input type="checkbox"/> \$265		
TK50 VAX/VMS COPY	<input type="checkbox"/> \$265		
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	<input type="checkbox"/> \$326
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	<input type="checkbox"/> \$326
PDBPGMTP			
VAX/VMS COPY	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244
NONST1TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
NONST2TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
NONST3TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
NONST4TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285

Special order items:

Please inquire at Brookhaven for availability and price.
(Items are described in Table 1.)

YEAR86TP	CONECTTP	DSTNCETP
PART87TP	DGPLOTP	FISIPLTP
BENDERTP	DIHDRLTP	PHIPSITP

4. Please send the following microfiche items (from Table 2). Each microfiche item costs \$231, postage included. Correction fiche are free.

Items: _____ Total Cost: _____

5. Please send the following printed listings. Each listing costs \$84, postage included.

Ident Code(s) (From Table 7): _____ Total Cost: _____

6. Foreign air mail postage for tapes from Brookhaven to destinations outside the U. S. and Canada. A postage surcharge of \$19 is required per item.

Number of items x \$19.00 = _____

7. Total charges

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

Method of Payment:

Brookhaven requires that either a check or written purchase order 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
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.