

Even a quick look at our holdings lists will show that data continue to arrive at an astounding rate. In the last three months we have received as much new data as we used to get in a typical year. Some delays in processing will occur of necessity -- it is important that we continue to check data carefully.

Of particular interest in our new arrivals are two data sets based on neutron studies: carbonmonoxy sperm whale myoglobin and ribonuclease A. The latter set is the result of a joint refinement employing x-ray and neutron data. Both sets will be processed after we have modified our programs to accept hydrogen and deuterium atoms.

The information provided by our contributors on data deposition forms greatly expedites the processing of new data sets. If you are planning to send new coordinates to the Bank but do not have deposition forms, these may be ordered by checking the appropriate box on the request form at the back of the newsletter.

Inquiries and suggestions are welcomed and may be addressed to any of the persons listed below.

Area	Address of Center	Name	
The Americas	Protein Data Bank	E. Abola	516-282-4383
	Chemistry Department	F. C. Bernstein	516-282-4382
	Brookhaven National Laboratory	T. F. Koetzle	516-282-4384
	Upton, New York 11973 USA		
Europe and Worldwide	University Chemical Laboratory	O. Kennard	0223-66499
	Lensfield Road Cambridge CB2 1EW, England	S. Bellard	
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002 Australia	C. Garrow	03-419-1333
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2, Suita, 565 Japan	N. Yasuoka	(06) 877-5111 ext. 3912

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

CODE	ITEM	13-JUL-82		AVAILABILITY			
		NO. TAPES 800 1600		US	UK	JA	AUS
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	2	1	X	X	X	X
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	2	1	X	X	X	
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	2	1	X	X	X	
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	X			
BLDKITTP	MODEL BUILDER'S KIT						
CONNECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	X			
DGPLOTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	X			
DIHDLRTP	COMPLETE TORSION ANGLES	2	1	X			
DSTNCETP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	X			
FIS1PLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	X			
PHIPS1TP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	X			

* NEW OR REPLACEMENT ENTRY SINCE APR-82 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	13-JUL-82			
		US	UK	JA	AUS
DATAPRFI	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	X	X	X	
NONSTIFI	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	X	X	X	
NONST2FI	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	X	X	X	
CORROBFI	LIST OF CORRECTIONS NO. 10 (JAN/82 - JUL/82)	X	X	X	X
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X			
BLDKITFI	MODEL BUILDER'S KIT				
CONNECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS				
DGPFOTFI	DIAGONAL PLOTS (LINE PRINTER)	X			
DIHDLRFI	COMPLETE TORSION ANGLES	X			
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X			
FIS1PLFI	PHI/PSI PLOTS (LINE PRINTER)	X			
PHIPS1FI	LISTS OF PHI/PSI/OMEGA VALUES	X			

* NEW OR REPLACEMENT ENTRY SINCE APR-82 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

13-JUL-82

Table with columns: IDENT, MOLECULE, DEPOSITOR(S), DATE/STATUS, and a list of protein entries with their respective coordinates and depositories.

* NEW OR REPLACEMENT ENTRY SINCE APR-82 NEWSLETTER

STATUS CODES

- BLANK STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A ALPHA CARBON ATOMS ONLY
B BACKBONE ONLY
N NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
P IN PREPARATION
R REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

Table with 4 columns: NAME, PURPOSE, AUTHOR(S), REV DATE/SUPPORTED. Lists various programs like BENDER, BLDKIT, CHIRAL, etc.

* NEW OR REPLACEMENT ENTRY SINCE APR-82 NEWSLETTER

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

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 1, SEE ALSO TABLE 6)

Table with 4 columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/CODE. Lists structure factor holdings for molecules like ACTININ, RCARP04, etc.

CODES SF STRUCTURE FACTORS

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

Table with 4 columns: IDENT CODE, MOLECULE, DEPOSITOR, DATE/CODE. Continuation of structure factor holdings for molecules like R351CSF, R451CSF, etc.

* NEW OR REPLACEMENT ENTRY SINCE APR-82 NEWSLETTER

CODES SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

Table with 2 columns: IDENT CODE, TITLE. Lists bibliographic entries for proteins like OEAP, OADC, OMAA, etc.

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TABLE 8. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

13-JUL-82

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,TOTALS2
 *INSERT,TOTALS1.14
 C
 C CORRECTION. COMPARE THE COMPUTED TOTALS TO THOSE ON MASTER
 C RECORD. PRINT ERROR MESSAGE FOR DISCREPANCY. 26-MAR-82.
 C

*DELETE,TOTALS1.4
 C
 C LAST REVISION. 4/82

*INSERT,TOTALS.38
 DIMENSION ITOTSF(12),LIN(8)
 *INSERT,TOTALS.42
 DATA IDISCR(0)
 *DELETE,TOTALS.97
 IF (IDENT(LINE,IMASTE,4).NE.0) GO TO 55
 WRITE (6,220) LINE
 ENCODE (80,200,LIN) LINE
 DECODE (80,250,LIN) ITOTSF

*INSERT,TOTALS.103
 55 CONTINUE
 DO 56 I=1,12
 IF (ITOTSF(I).NE.ITOTSF(1)) IDISCR=IDISCR+1
 56 CONTINUE
 IF (IDISCR.NE.0) WRITE (6,260) IDISCR

*INSERT,TOTALS.104
 IDISCR=0
 *INSERT,TOTALS.155
 250 FORMAT (10X,12I5)
 260 FORMAT(100X,12H DISCREPANCY,15)

*COMPILE,BLDKIT
 *IDENT,BLDKIT1
 *INSERT,BLDKIT1.30
 C
 C CORRECTION. DELETE TWO DUPLICATE RECORDS. 05-MAY-82.
 C

*DELETE,BLDKIT.6
 C
 C LAST REVISION. 5/82

*IDENT,BENDER3
 *INSERT,BENDER2.13
 C
 C CORRECTION. ENDFILE JOUT BETWEEN DATA ENTRIES. 26-APR-82.
 C

*DELETE,BENDER2.4
 C
 C LAST REVISION. 4/82

*INSERT,BENDER.492
 ENDFILE JOUT
 *IDENT,ISRXJ
 *INSERT,ISRX1.5
 REMARK 17
 REMARK 17 CORRECTION. DELETE DUPLICATE TER RECORD. 01-MAR-82.
 *DELETE,ISRX1.115
 *DELETE,ISRX1.116
 MASTER 76 0 0 4 5 5 1 3 108 1 0 9

*IDENT,ITGBD
 *INSERT,ITGBC.3
 REMARK 10
 REMARK 10 CORRECTION. CHANGE RESIDUES 70 AND 80 TO GLU UPON
 REMARK 10 DEPOSITOR'S INSTRUCTIONS. 02-MAR-82.
 *DELETE,ITGB.65,68
 SEQRES 5 229 GLN VAL ARG LEU GLY GLU ASP ASN ILE ASN VAL VAL GLU
 SEQRES 6 229 GLY ASN GLU GLN PHE ILE SER ALA SER LYS SER ILE VAL
 *DELETE,ITGB.478,486
 ATOM 425 N GLU 70 49.400 11.692 32.754 .64 1.22
 ATOM 426 CA GLU 70 50.609 12.356 33.239 .58 1.30
 ATOM 427 C GLU 70 51.377 11.511 34.252 .58 1.29
 ATOM 428 O GLU 70 50.775 10.810 35.071 .58 1.20
 ATOM 429 CB GLU 70 50.217 13.671 33.846 .64 1.19
 ATOM 430 CG GLU 70 49.858 14.680 32.851 .64 1.25
 ATOM 431 CD GLU 70 51.044 15.355 32.158 .64 1.26
 ATOM 432 OE1 GLU 70 52.185 14.880 32.349 .64 1.27
 ATOM 433 OE2 GLU 70 50.820 16.405 31.473 .64 1.29
 *DELETE,ITGB.554,562
 ATOM 501 N GLU 80 50.453 11.154 27.437 .56 1.58
 ATOM 502 CA GLU 80 49.461 12.174 27.744 .61 1.53
 ATOM 503 C GLU 80 48.370 12.349 26.707 .61 1.29
 ATOM 504 O GLU 80 48.597 12.154 25.515 .61 1.24
 ATOM 505 CB GLU 80 50.148 13.446 27.926 .56 1.29
 ATOM 506 CG GLU 80 51.136 13.418 29.002 .56 1.29
 ATOM 507 CD GLU 80 52.599 13.346 28.539 .56 1.19
 ATOM 508 OE1 GLU 80 52.830 12.996 27.360 .56 1.22
 ATOM 509 OE2 GLU 80 53.513 13.577 29.396 .56 1.17
 *DELETE,ITGBC.4
 MASTER 65 4 1 3 0 0 0 6 1750 1 12 18

*IDENT,ITGPD
 *INSERT,ITGPC.3
 REMARK 11
 REMARK 11 CORRECTION. CHANGE RESIDUES 70 AND 80 OF TRYPSINOGEN TO
 REMARK 11 GLU UPON DEPOSITOR'S INSTRUCTIONS. 02-MAR-82.
 *DELETE,ITGP.79,80
 SEQRES 5 2 229 GLN VAL ARG LEU GLY GLU ASP ASN ILE ASN VAL VAL GLU
 SEQRES 6 2 229 GLY ASN GLU GLN PHE ILE SER ALA SER LYS SER ILE VAL
 *DELETE,ITGP.506,514
 ATOM 425 N GLU Z 70 5.442 58.236 7.760 .96 1.45
 ATOM 426 CA GLU Z 70 6.504 58.697 6.853 .89 1.42
 ATOM 427 C GLU Z 70 7.810 57.977 7.195 .89 1.40
 ATOM 428 O GLU Z 70 8.199 57.889 8.364 .89 1.38
 ATOM 429 CB GLU Z 70 6.625 60.188 6.987 .96 1.45
 ATOM 430 CG GLU Z 70 5.402 60.906 6.608 .96 1.43
 ATOM 431 CD GLU Z 70 5.303 61.286 5.124 .96 1.40
 ATOM 432 OE1 GLU Z 70 5.883 60.547 4.374 .96 1.42
 ATOM 433 OE2 GLU Z 70 4.693 62.366 4.618 .96 1.41
 *DELETE,ITGP.582,590
 ATOM 501 N GLU Z 80 1.606 56.419 4.392 .76 1.48
 ATOM 502 CA GLU Z 80 1.108 57.703 4.910 .80 1.52
 ATOM 503 C GLU Z 80 -3.348 57.619 5.366 .80 1.50
 ATOM 504 O GLU Z 80 -1.183 57.067 4.658 .80 1.47
 ATOM 505 CB GLU Z 80 1.271 58.739 3.835 .76 1.52
 ATOM 506 CG GLU Z 80 2.645 59.234 3.705 .76 1.52
 ATOM 507 CD GLU Z 80 3.480 58.561 2.608 .76 1.49
 ATOM 508 OE1 GLU Z 80 2.984 57.566 2.002 .76 1.47
 ATOM 509 OE2 GLU Z 80 4.664 58.996 2.396 .76 1.50
 *DELETE,ITGPC.4
 MASTER 69 9 0 4 2 0 0 6 2246 1 18 23

*IDENT,ITPID
 *INSERT,ITPIC.3
 REMARK 11
 REMARK 11 CORRECTION. CHANGE RESIDUES 70 AND 80 OF TRYPSINOGEN TO
 REMARK 11 GLU UPON DEPOSITOR'S INSTRUCTIONS. 02-MAR-82.
 *DELETE,ITPI.79,80
 SEQRES 5 2 229 GLN VAL ARG LEU GLY GLU ASP ASN ILE ASN VAL VAL GLU
 SEQRES 6 2 229 GLY ASN GLU GLN PHE ILE SER ALA SER LYS SER ILE VAL
 *DELETE,ITPI.506,514
 ATOM 425 N GLU Z 70 5.415 57.879 7.861 .53 1.40
 ATOM 426 CA GLU Z 70 6.414 58.442 6.942 .55 1.49
 ATOM 427 C GLU Z 70 7.732 57.687 7.134 .55 1.47
 ATOM 428 O GLU Z 70 8.160 57.435 8.267 .55 1.60
 ATOM 429 CB GLU Z 70 6.546 59.908 7.222 .53 1.48
 ATOM 430 CG GLU Z 70 5.385 60.689 6.782 .53 1.56
 ATOM 431 CD GLU Z 70 5.127 60.876 5.268 .53 1.47
 ATOM 432 OE1 GLU Z 70 5.635 59.742 4.580 .53 1.94
 ATOM 433 OE2 GLU Z 70 4.464 61.644 4.760 .53 1.46
 *DELETE,ITPI.582,590
 ATOM 501 N GLU Z 80 1.309 55.927 4.289 .51 1.43
 ATOM 502 CA GLU Z 80 .963 57.198 4.945 .52 1.42
 ATOM 503 C GLU Z 80 -5.06 57.310 5.354 .52 1.29
 ATOM 504 O GLU Z 80 -1.391 56.882 4.614 .52 1.42
 ATOM 505 CB GLU Z 80 1.320 58.321 4.015 .51 1.64
 ATOM 506 CG GLU Z 80 2.765 58.477 3.816 .51 1.52
 ATOM 507 CD GLU Z 80 3.282 58.060 2.432 .51 1.48
 ATOM 508 OE1 GLU Z 80 2.626 57.193 1.784 .51 1.39
 ATOM 509 OE2 GLU Z 80 4.385 58.560 2.022 .51 1.55
 *DELETE,ITPIC.4
 MASTER 68 9 0 4 2 0 0 6 2256 1 18 23

*IDENT,3CHAH
 *INSERT,3CHAG.5
 REMARK 13
 REMARK 13 CORRECTION. CORRECT MTRIX TRANSFORMATION. 24-MAY-82.
 *DELETE,3CHA.86,88
 MTRIX1 1 .913800 0.000000 .397300 -9.972000
 MTRIX2 4 0.000000 -1.000000 0.000000 39.110000
 MTRIX3 1 .397300 0.000000 -.913800 47.946000
 *DELETE,3CHAG.6
 MASTER 81 0 0 0 1 14 0 0 9 1733 2 10 19

REQUEST FORM

(Please include a self-addressed label)

1. Name _____ Date _____
 Address _____ Telephone _____

2. Documentation desired (no charge).

- () Latest Newsletter
 () Introduction to The Protein Data Bank (July 1982)
 () Sources of Visual Aids for Macromolecular Structure (May 1982)
 () Atomic Coordinate Entry Format Description for DATAPRTP and
 DATAPRFI (December 1981)
 () Non-Standard Entries (Structure Factors) format description for
 NONST1TP and NONST1FI (September 1981)
 () Non-Standard Entries (Structure Factors) format description for
 NONST2TP and NONST2FI (June 1982)
 () Data Deposition form

3. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs \$154 (£ 87); each 2-tape item costs \$188 (£ 106). Domestic postage is included.

<u>Item</u>	<u>Number of Tapes</u>	<u>Cost</u>
-------------	------------------------	-------------

Total _____

4. Tape format desired (all tapes are unlabelled)

	Availability	
	US	UK
() 9 track, 1600 cpi, EBCDIC	yes	yes
() 9 track, 800 cpi, EBCDIC	yes	yes
() 9 track, 1600 cpi, ASCII	yes	yes
() 9 track, 800 cpi, ASCII	yes	yes
() 7 track, 800 cpi, BCD	yes	please inquire

All tapes are distributed in blocked form with fixed record length and block size. Brookhaven normally uses a block size close to, but less than, 5120 characters. Please indicate here any difficulties this might cause.

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$92 (£ 52 from Cambridge), postage included. Correction fiche are free.

<u>Item</u>	<u>Cost</u>
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Total _____

6. Please send the following printed listings. Each listing costs \$58, (£ 33), postage included.

<u>Ident Code (From Table 3)</u>	<u>Cost</u>
----------------------------------	-------------

Total _____

7. Air mail postage from Brookhaven to destinations outside the U. S. and Canada or from Cambridge to destinations outside the United Kingdom. A postage surcharge of \$15 (£ 8) is required per magnetic tape (not per item).

Number of tapes x \$15.00 (£ 8) = _____

8. Total charges

Magnetic tape charges (3 above) _____

Microfiche charges (5 above) _____

Printed listing charges (6 above) _____

Air mail postage charges (7 above). _____

Total _____

For Brookhaven only:

Brookhaven requires that either a check or actual purchase order be received before data are shipped. Inclusion of check with order will expedite processing.

Payment to the order of Brookhaven National Laboratory

by () check _____ is () enclosed
 () purchase order number _____ () sent separately to the
 Protein Data Bank

Please return to

Ms. F. C. Bernstein
 Chemistry Department
 Brookhaven National Laboratory
 Upton, New York 11973 USA

or

Dr. S. Bellard
 University Chemical Laboratory
 Lensfield Road
 Cambridge CB2 1EW, England