THE PROTEIN DATA BANK

NEWSLETTER

Number 6

May 1978

Brookhaven, Cambridge, Melbourne, Tokyo

With the acquisition of our first coordinate sets for a protein which has not been studied crystallographically (Relaxin) the Protein Data Bank opens a new category of coordinate entries. We hope to obtain an increased number of representatives of this category, of hypothetical structures, because we feel that not only is the information of real utility but it represents the beginnings of a new phase of structural studies. The increasing availability of good graphics devices coupled to powerful computers allows intelligent, interpretive and "synthetic" use of the rapidly increasing body of knowledge of macromolecular structures. We expect that this beginning will presage extensive development in this area.

A second new category recently opened is that of 'repeating' linear polymers. Many important biological molecules are of this type (e.g. DNA, mRNA, structural proteins, polysaccharides) and the availability of coordinates for some representatives should be useful to both researchers and educators. The coordinate entry currently available is for a polysaccharide (Hyaluronic acid) and was derived from fiber-diffraction data. We expect that this entry will soon be joined by other depositions of experimentally-based coordinate sets. In addition, we plan to generate coordinates for some model structures and to make these available as well.

As indicated in the holdings list (Tables 1 and 2) a total of 18 new or replacement atomic coordinate entries has been generated since the last newsletter. This represents an acquisition rate of better than one entry every two weeks and brings our total number of distributable coordinate entries to 96. We plan to award a small prize to the depositor of the 100th coordinate entry (winner to be announced in the next newsletter!).

We are aware that there are some known structures not represented in the Bank, and we are attempting to make our coverage more comprehensive by actively soliciting depositions from laboratories thought to have coordinates available. We also are asking journal editors to suggest to authors of papers describing crystallographic studies of biological macromolecules, that the results of these studies be made available through the Protein Data Bank. The Journal of Biological Chemistry currently carries the sentence, "Authors of papers describing detailed (high resolution) structures are strongly encouraged to deposit an accompanying list of atomic coordinates in the Protein Data Bank, or as a JBC Document." in its Instructions to Authors, and we hope other journals may be persuaded to follow suit.

Our paper which describes the Bank (J. Mol. Biol. 112, 535 (1977)) has been reprinted in Eur. J. Biochem. 80, 319 (1977) and in Arch. Biochem. Biophys. 185, 584 (1978). This paper will also be reprinted in the new

edition of the IUPAC-IUB compendium of Recommendations from the Commission on Biochemical Nomenclature. Copies of the paper are available.

Two programs which operate on the atomic coordinate entries are now available for distribution. Both programs conform to our rule of having complete documentation in computer-readable form. Program PHIPS1 calculates main-chain torsion angles and produces a tabular print file and a sequential file suitable for further analysis. The TOTALS program examines each record in a Data Bank entry for a valid tagword and accumulates a count of each type of record. This program can therefore be used as an initial screen for the existence of (for example) non-standard components or secondary structure specifications in any or all entries of the Bank. These programs are listed in Table 3.

A list of substantive corrections which have been applied to the atomic coordinate entries since the last newsletter is given here as Table 4. In addition to these, one full entry (2PGK) has been reordered and several other minor changes made. This complete set of corrections is available on microfiche from Brookhaven. Also available on microfiche from Brookhaven are the output files of the program PHIPSI when run against the complete data base.

To request data or information from the Bank please complete the request form, given as the last sheet of this newsletter, and send it to the appropriate center.

AREA	ADDRESS OF CENTER	NAMES
The Americas	Chemistry Department Brookhaven National Laboratory Upton, New York 11973 USA	F.C.Bernstein (tel. 516-345-4382) T.F.Koetzle (tel. 516-345-4384) G.J.B.Williams (tel. 516-345-4383)
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, England	O. Kennard (tel. (0223)66499)
Australia	C.S.I.R.O. Division of Applied Organic Chemistry Box 4331 G.P.O. Melbourne, Victoria 3001 Australia	B. J. Poppleton
Japan	Department of Chemistry Faculty of Science The University of Tokyo Bunkyo-ku, Tokyo, Japan	M. Tasumi

TABLE 1. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

17-MAY-78

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ STATUS
1ACT	ACTINIDIN	E. BAKER	7/77
2ADK	ADENYLATE KINASE (PORCINE MUSCLE).	G. SCHULZ	3/77 R
1WGA	*AGGLUTININ (WHEAT GERM)	C. S. WRIGHT	2/78 A
1AOH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I. BRANDEN	8/76
2AOH	ALCOHOL DEHYDROGENASE (ORTHOPHEN)	C.-I. BRANDEN	8/76
1BCL	BACTERIOCHLOROPHYLL A-PROTEIN(CORE ONLY)	B. MATTHEWS	3/77
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74
3CPV	CALCIUM-BINDING PARVALBUMIN SET 61	R. KRETSINGER	8/74
1CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	8/76
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76
1CPA	CARBOXYPEPTIDASE A (BOVINE)	H. LIPSCOMB	2/73
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M.SCHMID, J.HERRIOTT	9/76 A
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/75 R
3CHA	ALPHA-CHYMOTRYPSIN	A. TULINSKY	8/76
1GCH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	2/77
1CHG	CHYMOTRYPSINOGEN	J. KRAUT, J. BIRKTOFT	3/75
2CNA	CONCANAVALIN A	REEKE, BECKER, EDELMAN	4/75
3CNA	CONCANAVALIN A	K. HARDMAN	9/76 R
2B5C	*CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77 R
1CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	R. DICKERSON	9/76
2CYT	CYTOCHROME C (ALBACORE, REDUCED)	R. DICKERSON	9/76
1CYC	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	8/76
1C2C	CYTOCHROME C2	J. KRAUT	3/73
155C	CYTOCHROME C550	R. TIMKOVICH	8/78
1EST	ELASTASE (PORCINE,TOSYL)	H. WATSON	5/76
1FDX	FERREDOXIN	ADMAN, SIEKER, JENSEN	8/78
3FXN	*FLAVODOXIN (CLOSTRIDIUM MP,OXIDIZED)	M. LUDWIG	12/77 R
4FXN	*FLAVODOXIN (CLOSTRIDIUM MP,SEMIQUINONE)	M. LUDWIG	12/77
1GCN	GLUCAGON	T. BLUNDELL	10/77
1PGI	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M. ROSSMANN	7/75
1HRB	*HEMERYTHRIN B	W. HENDRICKSON	6/76 AP
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	LADNER, HEIDNER, PERUTZ	2/77 R
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73
1HHB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	4/75
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	8/76
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	3/73
2YHX	*HEXOKINASE (YEAST) FORM B(1)	T. STEITZ	9/76 RN
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75
1HYA	*HYALURONIC ACID	S. ARNOTT	11/77
1FAB	IMMUNOGLOBULIN FAB' (NEW)	R. POLJAK	8/76
1MCG	*IMMUNOGLOBULIN B-J FRAGMENT MCG	SCHIFFER,EDMUNDSON ET AL.	5/78 AP
1REI	IMMUNOGLOBULIN B-J FRAGMENT REI	O. EPP, R. HUBER	3/76
1RHE	*IMMUNOGLOBULIN B-J FRAGMENT RHE	WANG, YOD, SAX	12/77 A
4LDH	LACTATE DEHYDROGENASE	W. EVENTOFF, M. ROSSMANN	4/77 R
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	11/74
1LZM	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS	3/77
1LYZ	LYSOZYME (HEN EGG-WHITE, SET H2)	R. DIAMOND, D. PHILLIPS	2/75
2LYZ	LYSOZYME (HEN EGG-WHITE, SET RS5D)	R. DIAMOND, D. PHILLIPS	2/75
3LYZ	LYSOZYME (HEN EGG-WHITE, SET RS6A)	R. DIAMOND, D. PHILLIPS	2/75
4LYZ	LYSOZYME (HEN EGG-WHITE, SET RS9A)	R. DIAMOND, D. PHILLIPS	2/75
5LYZ	LYSOZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND, D. PHILLIPS	2/75
6LYZ	LYSOZYME (HEN EGG-WHITE, SET RS16)	R. DIAMOND, D. PHILLIPS	2/75
7LYZ	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	A. YONATH	5/77
8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY	9/77
1MDH	MALATE DEHYDROGENASE	L. BANASZAK	8/76 A
1MBN	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON	1/73
2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	9/76
3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	9/76
1MBR	*MYOHEMERYTHRIN	W. HENDRICKSON	6/76 AP
8PAP	PAPAIN (NATIVE)	J. DRENTH	11/76 R
1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)	J. DRENTH	11/76 R
2PAD	PAPAIN (CYS DERIV OF CYS-25)	J. DRENTH	11/76 R
3PAD	PAPAIN (OXIDIZED CYS-25)	J. DRENTH	11/76 R
4PAD	PAPAIN (TOS-LYS, CYS-25)	J. DRENTH	11/76 R
5PAD	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH	11/76 R
6PAD	PAPAIN (BZOXY-PHE-ALA, CYS-25)	J. DRENTH	11/76 R
1PGX	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON	5/76 A
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE	9/76 B
1PGM	*PHOSPHOGLYCERATE MUTASE	CAMPBELL,WATSON,HODGSON	8/75 A
2PAB	PREALBUMIN (HUMAN, PLASMA)	S. OAILEY, C. BLAKE	9/77 R
1RLX	*RELAXIN(MODEL,CONFORMATION A,UNREFINED)	A. EVANS, A.C.T. NORTH	3/78 N
2RLX	*RELAXIN(MODEL,CONFORMATION B,UNREFINED)	A. EVANS, A.C.T. NORTH	3/78 N
3RLX	*RELAXIN(MODEL,CONFORMATION B,REFINED)	A. EVANS, A.C.T. NORTH	3/78 N
4RLX	*RELAXIN(MODEL,CONFORMATION B,REFINED)	A. EVANS, A.C.T. NORTH	3/78 N
1RHD	*RHODANESE	W. HOL	12/77
1RNS	RIBONUCLEASE S	H. HYCKOFF, F. RICHARDS	4/73
2RXN	RUBREDOXIN	L. JENSEN	1/75
1SNS	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	4/73
1SGB	STREPTOMYCES GRISEUS PROTEINASE B	M. JAMES	5/76 A
1SBT	SUBTILISIN BPN'	J. KRAUT	8/72
2SBT	SUBTILISIN NOVO	J. DRENTH	9/76
1SOD	SUPEROXIDE DISMUTASE	J. AND D. RICHARDSON	8/75 A
1TLN	THERMOLYSIN (UNREFINED)	B. MATTHEWS	4/75
2TLN	THERMOLYSIN (REFINED)	B. MATTHEWS	4/75
1SRX	THIOREDOXIN (OXIDIZED)	B.-O. SODERBERG	5/76 A
1TNA	TRANSFER RNA (YEAST, PHE)	J. SUSSMAN, S.-H. KIM	12/75
2TNA	TRANSFER RNA (YEAST, PHE)	M. SUNDARALINGAM	5/76
4TNA	*TRANSFER RNA (YEAST, PHE)	JACK, LADNER, KLUG	4/78 R
1TIM	TRIOSE PHOSPHATE ISOMERASE	I. WILSON, D. PHILLIPS	9/76
1PTN	TRYPSIN (NATIVE, PH8)	FEHLHAMMER, BODE, SCHNAGER	1/77
2PTB	TRYPSIN(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHNAGER	1/77 R
1PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R. HUBER, W. BODE	11/76
3PTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	11/76 R
3PTP	*TRYPSIN (DIP INHIBITED)	J. CHAMBERS, R. STROUD	12/77 R

* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER (NOV/77)

STATUS CODES

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

TABLE 2. PROTEIN DATA BANK, NON-STANDARD ENTRIES

18-MAY-78

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R1ACTSF	ACTINIDIN	E. BAKER	7/77 SF
CHYMOF	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	4/73 SF
RCARP04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCARP05	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCYTB502	CYTOCHROME B5	F. S. MATHEWS	5/73 TA
R2B5CSF	*CYTOCHROME B5	F. S. MATHEWS	12/77 SF
RTUNOX201	CYTOCHROME C (ALBACORE, OXIDIZED)	R. DICKERSON	5/76 SF
RTUNRD201	CYTOCHROME C (ALBACORE, REDUCED)	R. DICKERSON	5/76 SF
RCYC5501	CYTOCHROME C550	R. TIMKOVICH	4/78 SF
RGPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M. ROSSMANN	8/75 SF
RHUMDEH02	HEMOGLOBIN (HUMAN,DEOXY)	M. PERUTZ, G. FERMI	5/75 SF
LAMPRY1	HEMOGLOBIN (LAMPREY)	HENDRICKSON,LOVE,KARLE	5/73 SF
RLDH06	LACTATE DEHYDROGENASE	M. ROSSMANN	8/75 SF
RLDH07	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	8/75 SF
RMETMYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/78 SF
RDEMYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	8/76 SF
RRUBY02	RUBREDOXIN	L. JENSEN	3/74 SF
TORSNA01	TORSION ANGLES (11 PROTEINS)	T. WU, E. KABAT	5/73 TA

* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER (NOV/77)

CODES

SF	STRUCTURE FACTORS
TA	TORSION ANGLES

NOTE IN SOME CASES, MORE RECENT TORSION ANGLES THAN THOSE CONTAINED IN THE ABOVE ENTRIES MAY BE CALCULATED FROM THE APPROPRIATE ATOMIC COORDINATE ENTRIES LISTED IN TABLE 1.

TABLE 3. PROTEIN DATA BANK, AVAILABLE PROGRAMS

18-MAY-78

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
PHIPSI	*MAIN-CHAIN TORSION ANGLES	ANDREWS,BERNSTEIN,WILLIAMS	5/78 YES
TOTALS	*VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	5/78 YES

* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER (NOV/77)

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

TABLE 4. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES

18-MAY-78

```
*IDENT,1SRXC
*INSERT,1SRXB.35
REMARK   9
REMARK   9 CORRECTION.  CORRECT ALPHA ON CRYST1 RECORD.  09-NOV-77.
*DELETE,1SRX.54
CRYST1   89.700   51.100   60.300  90.00 113.50  90.00 C 2          8
*DELETE,1SRXB.35
MASTER      50    0    0    4    5    5    1    3  108    1    0    9
*IDENT,1FABD
*INSERT,1FABC.39
REMARK   8
REMARK   8 CORRECTION. INSERT JRNL REFERENCE. 15-FEB-78.
*INSERT,1FABC.4
JRNL        AUTH   F.A.SAUL,L.M.AMZEL,R.J.POLJAK
JRNL        TITL   PRELIMINARY REFINEMENT AND STRUCTURAL ANALYSIS OF
JRNL        TITL 2 THE FAB FRAGMENT FROM HUMAN IMMUNOGLOBULIN NEW AT
JRNL        TITL 3 2.0 ANGSTROMS RESOLUTION
JRNL        REF    J.BIOL.CHEM.                  V. 253   585 1978
JRNL        REFN   ASTM JBCHA3  US ISSN 0021-9258                  071
*DELETE,1FABC.45
MASTER      54    0    0    3   33    0    0    6 3187    2   10   33
*IDENT,1CPVC
*INSERT,1CPVB.98
REMARK   7
REMARK   7 CORRECTION. CORRECT NAMING AND ORDERING OF THE THREE ATOMS
REMARK   7  OF ACE 0.  20-MAR-78.
*DELETE,1CPV.85,87
ATOM      1  C   ACE     0      11.044  33.325  18.267  1.00  9.00
ATOM      2  O   ACE     0       9.893  33.758  18.108  1.00  9.00
ATOM      3  CH3 ACE     0      11.285  31.889  18.737  1.00  9.00
*DELETE,1CPVB.101
MASTER     102    0    2    6    0    0    0    6  837    1   18    9
*IDENT,2CPVC
*INSERT,2CPVB.98
REMARK   7
REMARK   7 CORRECTION. CORRECT NAMING AND ORDERING OF THE THREE ATOMS
REMARK   7  OF ACE 0.  20-MAR-78.
*DELETE,2CPV.85,87
ATOM      1  C   ACE     0      11.193  33.318  18.254  1.00 33.70
ATOM      2  O   ACE     0       9.870  33.899  18.312  1.00 42.30
ATOM      3  CH3 ACE     0      11.409  32.063  18.606  1.00 48.90
*DELETE,2CPVB.101
MASTER     102    0    2    6    0    0    0    6  837    1   18    9
*IDENT,3CPVC
*INSERT,3CPVB.98
REMARK   7
REMARK   7 CORRECTION. CORRECT NAMING AND ORDERING OF THE THREE ATOMS
REMARK   7  OF ACE 0.  20-MAR-78.
*DELETE,3CPV.85,87
ATOM      1  C   ACE     0      11.193  33.318  18.254  1.00 33.70
ATOM      2  O   ACE     0       9.870  33.899  18.312  1.00 42.30
ATOM      3  CH3 ACE     0      11.409  32.063  18.606  1.00 48.90
*DELETE,3CPVB.101
MASTER     102    0    2    6    0    0    0    6  950    1   18    9
*IDENT,1PTCB
*INSERT,1PTCA.85
REMARK   6
REMARK   6 CORRECTION. ATOM OXT GLY I 57 IS RENAMED N ALA I 58.  ATOM
REMARK   6  SERIAL NUMBERS 2083 THROUGH 2087 ARE RESERVED FOR THE
REMARK   6  MISSING ATOMS OF ALA I 58.  ALL WATER MOLECULES WERE
REMARK   6  RENUMBERED.  NO COORDINATES WERE CHANGED. 25-APR-78.
*DELETE,1PTC.2163,2353
ATOM   2082  N   ALA I  58      13.124 101.757   -.052  1.00  0.00    1
TER    2088      ALA I  58
HETATM 2089  O   HOH   400      14.487  79.513  18.006  1.00  0.00
HETATM 2090  O   HOH   401      11.773  64.780  15.479  1.00  0.00
  ...
  ... (185 WATER MOLECULES OMITTED FROM THIS LISTING)
  ...
HETATM 2276  O   HOH   603        .604  80.577  12.143  1.00  0.00
HETATM 2277  O   HOH   604      11.290  55.390   8.020  1.00  0.00    1
*DELETE,1PTCA.96
MASTER      95    9    0    4    2    0    0    6 2256    2   18   23
*IDENT,1TNAD
*INSERT,1TNAC.4
REMARK  10
REMARK  10 CORRECTION.  CORRECT H,O COUNTS ON FORMUL RECORD FOR
REMARK  10  RESIDUE YG.  27-APR-78.
*DELETE,1TNAC.12
FORMUL   1   YG    C21 H26 N5 O11 P1
*DELETE,1TNAC.1666
MASTER      59    0    1    0    0    0    0    6 1652    1   41    6
*IDENT,2TNAC
*INSERT,2TNAB.5
REMARK  10
REMARK  10 CORRECTION.  CORRECT H,O COUNTS ON FORMUL RECORD FOR
REMARK  10  RESIDUE YG.  27-APR-78.
*DELETE,2TNAB.13
FORMUL   1   YG    C21 H26 N5 O11 P1
*DELETE,2TNAB.1687
MASTER      73    0    1    0    0    0    0    6 1652    1   41    6
*IDENT,3TNAC
*INSERT,3TNAB.4
REMARK  11
REMARK  11 CORRECTION.  CORRECT H,O COUNTS ON FORMUL RECORD FOR
REMARK  11  RESIDUE YG.  27-APR-78.
*DELETE,3TNAB.12
FORMUL   1   YG    C21 H26 N5 O11 P1
*DELETE,3TNAB.1658
MASTER      63    0    1    0    0    0    0    6 1644    1   33    6
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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 ATOMIC COORDINATE 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.

REQUEST FORM

1. Name: _____ Date: _____

   Address: _____ Telephone: _____

   _____

   _____

2. Send the following information (please check):

   ( ) all current coordinate entries and programs on tape

   ( ) all current coordinate entries and programs on microfiche

   ( ) parameter sets listed (complete 3. below)

   ( ) description of file record formats

   ( ) list of revisions on microfiche

   ( ) torsion angles on microfiche

3. Parameter sets requested (by ident code please):

   _____ _____ _____ _____ _____ _____ _____

   _____ _____ _____ _____ _____ _____ _____

   _____ _____ _____ _____ _____ _____ _____

4. Tape: I am sending a new 2400 foot reel of magnetic tape ( ) yes ( ) no.

5. Tape format desired:

( ) 7 track	( ) 556 cpi	( ) BCD - 7 track only	( ) Unlabelled (preferred)
( ) 9 track	( ) 800 cpi	( ) ASCII - 9 track only	( ) Labelled-user's label
	( ) 1600 cpi	( ) EBCDIC - 9 track only	_____ retained

Tape copies are normally blocked since otherwise the entire contents will not fit on a 2400 foot reel of tape. Indicate the maximum block size allowed if blocks of 5120 characters (bytes) cannot be handled, _____.

Please complete reverse side.

REQUEST FORM

6. Charge (Brookhaven requests only) Enter Amount

A. Data preparation (unit charge per magnetic tape) $ _____

Employee of U. S. Department of Energy	$40.25	( )	
Employee of other U. S. Federal Agency	$47.45	( )	
All others	$51.00	( )	

B. Magnetic tape $ 8.59 ( ) $ _____
(please check if answer to 4. above was NO)

C. Postage (for magnetic tapes only) $ _____

U. S. and Canada	$ 2.00	( )	
Air Mail to other countries	$17.00	( )	

D. All coordinate entries on microfiche $37.50 ( ) $ _____

E. Torsion angles on microfiche $30.30 ( ) $ _____

F. Total charge (A + B + C + D + E) $ _____

G. Payment to the order of Brookhaven National Laboratory

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

Brookhaven requires that either a check or actual purchase order be received before data is shipped.

Mail this completed form to the appropriate center (Brookhaven, Cambridge, Melbourne or Tokyo) at the address listed in the body of the Newsletter.

It is expected that the Protein Data Bank be acknowledged in publications which result from work making use of the Bank's services. We would appreciate receiving reprints of any such publications.