BROOKHAVEN NATIONAL LABORATORY

PROTEIN DATA BANK

NEWSLETTER

Number 4 May, 1977

A number of important developments have occurred since we distributed our last newsletter six months ago. All atomic coordinate entries in the Data Bank have now been converted to the 80-character format, and henceforth only 80-character entries will be distributed. This will make distribution tapes more compact, and generally should simplify processing for recipients. The size of the Data Bank has continued to increase, and we now have available for distribution a total of 77 coordinate entries for 47 different macromolecules. A current list of atomic coordinate holdings, with identification codes to be used in requesting data, is shown in Table 1. In addition, certain non-standard entries, containing structure factor-phase information and torsion angles, are available. These are shown in Table 2.

We have combined our mailing lists, and beginning with this issue, Brookhaven will mail newsletters directly to all users worldwide. Data distribution is divided geographically as follows: Brookhaven will handle the Americas, the University of Tokyo will handle Japan, and Cambridge University will distribute within Europe and worldwide. The request form included with this newsletter has been preaddressed to the center that handles your area. Please use this form to request data or copies of documentation. Data requests directed to Brookhaven should include a check or purchase order for U.S. $34.30, made to the order of Brookhaven National Laboratory, to cover postage and handling. This charge is subject to increases in the future. Requests should be accompanied by a new 2400' reel of magnetic tape. In the event it is not possible for the user to supply a tape, Brookhaven can do so at a total cost of $47.00. Cambridge and Tokyo presently distribute data free of charge.

Errors occasionally are found in data deposited with the Bank, and corrections and revisions are submitted by depositors or approved by them. We have compiled a list of corrections and revisions of the master file applied since June 1976, and this list is attached as Table 3.

As the size of the Data Bank increases, possibilities for interactive access become more attractive. Brookhaven recently has agreed to make portions of the file available through the NIH/EPA Chemical Information System (CIS). The CIS presently includes the Cambridge Bibliographic and Structural Data Files for organic and organometallic compounds. These data may be accessed within the U.S. via CYPHERNET, a commercial timesharing network. Initially, we plan to make available through CIS the Protein Data Bank bibliographic and sequence information, together with identification codes for the various entries, index citations to AMSOM (R. J. Feldmann, Atlas of Macromolecular Structure on Microfiche, Tracor Jitco Inc., Rockville MD, 1976, ISBN 0-917934-01-6), and certain other descriptive material. This interactive capability should be implemented before the end of 1977.

TABLE 1. PROTEIN DATA BANK ATOMIC COORDINATE HOLDINGS

10-MAY-77

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ STATUS
2ADK	ADENYLATE KINASE	G. SCHULZ	3/77 R
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I. BRANDEN	8/76
2ADH	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	K. KANNAN	6/76
1CAC	CARBONIC ANHYDRASE C	K. KANNAN	5/76
1CPA	CARBOXYPEPTIDASE A	W. LIPSCOMB	2/73
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	3/75
2CNA	CONCANAVALIN A	REEKE, BECKER, EDELMAN	4/75
3CNA	CONCANAVALIN A	K. HARDMAN	9/76 R
1B5C	CYTOCHROME B5	F. S. MATHEWS	8/72
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	8/76
1EST	ELASTASE	H. WATSON	5/76
1FDX	FERREDOXIN	L. JENSEN	8/76
1FXN	FLAVODOXIN (CLOSTRIDIUM MP)	M. LUDWIG	11/74
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M. ROSSMANN	7/75
2HHB	HEMOGLOBIN (HORSE, AQUO MET)	LADNER, HEIDNER, PERUTZ	2/77 R
1DHB	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
1HKX	HEXOKINASE (YEAST) BIII	T. STEITZ	9/76 B
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75
1FAB	IMMUNOGLOBULIN FAB' (NEW)	R. POLJAK	8/76
1REI	IMMUNOGLOBULIN B-J FRAGMENT REI	U. EPP, R. HUBER	3/76
4LDH	LACTATE DEHYDROGENASE	W. EVENTOFF, M. ROSSMANN	4/77 R
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	11/74 D
1LZM	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS	3/77
1LYZ	LYSOZYME (HEN EGG-WHITE, SET W2)	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 P
1MDH	MALATE DEHYDROGENASE	L. BANASZAK	6/76 A
1MBN	MYOGLOBIN (SPERM WHALE)	H. WATSON	4/73
2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	9/76
3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	9/76
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
1PGK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON	5/76 A
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, D. PHILLIPS	9/76 B
1PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, D. PHILLIPS	8/76
1RNS	RIBONUCLEASE S	H. WYCKOFF	4/73
2RXN	RUBREDOXIN	L. JENSEN	1/75 D
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	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 D
3TNA	TRANSFER RNA (YEAST, PHE)	JACK, LADNER, KLUG	2/77 N
1TIM	TRIOSE PHOSPHATE ISOMERASE	I. WILSON, D. PHILLIPS	9/76
1PTN	TRYPSIN (NATIVE, PH8)	FEHLHAMMER, BODE, SCHWAGER	1/77
2PTB	TRYPSIN(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHWAGER	1/77 R
1PTC	TRYPSIN TRYPSIN INHIBITOR COMPLEX	BODE ET AL.	11/76
3PTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER	11/76 R
1PTP	TRYPSIN (DIP INHIBITED)	J. CHAMBERS, R. STROUD	3/77

STATUS CODES

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

TABLE 2. PROTEIN DATA BANK NON-STANDARD ENTRIES

10-MAY-77

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
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
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	4/76 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	6/76 SF
RDEMYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76 SF
RRUBY02	RUBREDOXIN	L. JENSEN	3/74 SF
TOKSNA01	TORSION ANGLES (11 PROTEINS)	T. WU, E. KABAT	5/73 TA

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. CORRECTIONS AND REVISIONS OF ATOMIC COORDINATE DATA

21-APR-77

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*IDENT,1MBNA
*DELETE,1MBN.3
HEADER    OXYGEN STORAGE                          05-APR-73    1MBN

*IDENT,1ADKA
*DELETE,1ADK.3
HEADER    TRANSFERASE(PHOSPHO)PHOSPHORYL ACCEPTOR 11-JUN-76    1ADK
*DELETE,1ADK.6
AUTHOR    G.E. SCHULZ, M. ELZINGA, F. MARX AND R.H. SCHIRMER
*DELETE,1ADK.8
REMARK   1 REFERENCE 1. G.E. SCHULZ, M. ELZINGA, F. MARX AND R.H.
*DELETE,1ADK.9
REMARK   1 SCHIRMER, THREE-DIMENSIONAL STRUCTURE OF ADENYLATE KINASE.
*DELETE,1ADK.12
REMARK   1 COMPARISON OF ADENYLATE KINASE WITH OTHER PROTEINS, NATURE,
*DELETE,1ADK.14
REMARK   1 REFERENCE 3. G.E. SCHULZ, C.D. BARRY, J. FRIEDMAN, P.Y.CHOU
*DELETE,1ADK.18
REMARK   1 SECONDARY STRUCTURE OF ADENLYATE KINASE, NATURE, VOL. 250,
*INSERT,1ADK.27
REMARK    5
REMARK    5 RESIDUE ASP 65 CHANGED TO GLN 65 AND SEVERAL TYPOGRAPHICAL
REMARK    5 ERRORS CORRECTED. *NOTE* THE RESIDUE CHANGE MEANS THAT 1
REMARK    5 SHOULD BE ADDED TO ALL ATOM SERIAL NUMBERS PAST RESIDUE
REMARK    5 65.  THIS WILL BE CORRECTED WHEN THE FULL STRUCTURE
REMARK    5 BECOMES AVAILABLE.  12-JUL-76
REMARK    5
*DELETE,1ADK.32
SEQRES    5    194  ARG GLY LYS MET LEU SER GLU ILE MET GLU LYS GLY GLN
*DELETE,1ADK.111
ATOM    480  CA  GLN    65      26.000  21.900  36.000  1.00  0.00

*IDENT,1ADKB
*DELETE,1ADK.242
MASTER       28    0    0    0    0    0    0    3  194    1    0   15

*IDENT,1MBNB
*INSERT,1MBN.32
REMARK    6
REMARK    6 CORRECTION. THE CONECT 1219 RECORD WAS WRONG.  THE 736
REMARK    6 SHOULD HAVE BEEN, AND IS NOW, 740. 20-SEP-76
*DELETE,1MBN.1334
CONECT 1219  740 1220 1225 1236
*DELETE,1MBN.1379
MASTER       27    8    1    8    0    3    2    6 1260    1   46   12

*IDENT,1CYCA
*INSERT,1CYC.21
REMARK    5
REMARK    5 CORRECTION MADE 25-OCT-76. THE SECOND CONECT RECORD FOR
REMARK    5 ATOM 803 SHOULD HAVE 827  835 (NOT 819  835).
*DELETE,1CYC.894
CONECT  803  827  835
*DELETE,1CYC.937
MASTER       18    0    1    5    0    3    0    9  839    1   48    8

*IDENT,3CHAA
*INSERT,3CHA.44
REMARK    6
REMARK    6 CORRECTED 04-DEC-76. THE CONECT RECORDS WERE INCORRECT. FCB
*DELETE,3CHA.1824,1828
CONECT    6    5  893
CONECT  302  301  418
CONECT  418  417  302
CONECT  893  892    6
CONECT  986  985 1445
CONECT 1218 1217 1334
CONECT 1334 1218 1333
CONECT 1383 1382 1584
CONECT 1445  986 1444
CONECT 1584 1383 1583
*DELETE,3CHA.1829
MASTER       40    0    0    1   14    0    0    9 1733    2    5   19

*IDENT,3CHAB
*DELETE,3CHAA.2
REMARK    6 CORRECTION. THE CONECT RECORDS WERE INCORRECT. 04-DEC-76
REMARK    7
REMARK    7 COPPECTION. CORRECT MASTER RECORD. 03-JAN-77
*DELETE,3CHAA.13
MASTER       42    0    0    1   14    0    0    9 1733    2   10   19

*IDENT,1CHGA
*INSERT,1CHG.43
REMARK    5
REMARK    5 CORRECTION. IN RESIDUES TYR 94, TYR 171, AND TYR 228,
REMARK    5  ATOM OH WAS MISNAMED AS O, WHICH NAME THEREFORE OCCURRED
REMARK    5  TWICE. IT HAS BEEN RENAMED AND RESTORED TO ITS CORRECT
REMARK    5  POSITION AFTER CZ. THUS NECESSITATING RENUMBERING OF THE
REMARK    5  INTERVENING ATOMS CB THROUGH CZ. (OH FORMERLY HAD SERIAL
REMARK    5  NUMBERS 699, 1269, 1661 AND NOW HAS 706, 1276, 1668
REMARK    5  RESPECTIVELY IN THE THREE TYROSINE RESIDUES.) 03-JAN-77.
*DELETE,1CHG.720,727
ATOM    699  CB  TYR    94      22.522  15.085   6.574  1.00  0.00
ATOM    700  CG  TYR    94      22.612  15.072   8.174  1.00  0.00
ATOM    701  CD1 TYR    94      22.888  16.371   8.687  1.00  0.00
ATOM    702  CD2 TYR    94      22.232  13.962   8.963  1.00  0.00
ATOM    703  CE1 TYR    94      22.882  16.460   9.988  1.00  0.00
ATOM    704  CE2 TYR    94      22.418  14.151  10.366  1.00  0.00
ATOM    705  CZ  TYR    94      22.597  15.449  10.877  1.00  0.00
ATOM    706  OH  TYR    94      22.492  15.535  12.378  1.00  0.00
*DELETE,1CHG,1205,1212
ATOM   1269  CB  TYR   171      30.355  33.165  18.662  1.00  0.00
ATOM   1270  CG  TYR   171      30.046  34.557  19.272  1.00  0.00
ATOM   1271  CD1 TYR   171      30.040  34.545  20.672  1.00  0.00
ATOM   1272  CD2 TYR   171      29.552  35.658  18.580  1.00  0.00
ATOM   1273  CE1 TYR   171      29.830  35.737  21.301  1.00  0.00
ATOM   1274  CE2 TYR   171      29.342  36.850  19.209  1.00  0.00
ATOM   1275  CZ  TYR   171      29.432  36.939  20.690  1.00  0.00
ATOM   1276  OH  TYR   171      29.026  38.229  21.399  1.00  0.00
*DELETE,1CHG,1597,1604
ATOM   1661  CB  TYR   228      19.924  28.607  12.779  1.00  0.00
ATOM   1662  CG  TYR   228      19.523  29.191  14.082  1.00  0.00
ATOM   1663  CD1 TYR   228      20.485  29.896  14.792  1.00  0.00
ATOM   1664  CD2 TYR   228      18.259  28.974  14.674  1.00  0.00
ATOM   1665  CE1 TYR   228      20.182  30.482  16.095  1.00  0.00
ATOM   1666  CE2 TYR   228      18.053  29.561  15.879  1.00  0.00
ATOM   1667  CZ  TYR   228      18.918  30.264  16.588  1.00  0.00
ATOM   1668  OH  TYR   228      18.712  30.852  17.792  1.00  0.00
*DELETE,1CHG,1740
MASTER       44    0    0    2   14    0    0    6 1643    1   10   19

*IDENT,1CPAA
*INSERT,1CPA.26
REMARK    5
REMARK    5 CORRECTION. INSERT MISSING CONECT RECORD. 03-JAN-77
*INSERT,1CPA,2567
CONECT 1277 1119 1276
*DELETE,1CPA,2570
MASTER       20    2    1    8    8   32    0    6 2453    2    6   25

*IDENT,1C2CA
*INSERT,1C2C.28
REMARK    4
REMARK    4 CORRECTION. IN RESIDUES TYR 46, TYR 48, TYR 52, TYR 70
REMARK    4  AND TYR 107, ATOM OH WAS MISNAMED AS O, WHICH NAME
REMARK    4  THEREFORE OCCURRED TWICE. IT HAS BEEN RENAMED AND
REMARK    4  RESTORED TO ITS CORRECT POSITION AFTER CZ. THUS
REMARK    4  NECESSITATING RENUMBERING OF THE INTERVENING ATOMS O
REMARK    4  THROUGH CZ. (OH FORMERLY HAD SERIAL NUMBERS 329, 346,
REMARK    4  379, 518, 811 AND NOW HAS 337, 354, 387, 526, 819 IN
REMARK    4  THE FIVE TYROSINE RESIDUES.) 03-JAN-77.
*DELETE,1C2C,384,392
ATOM    329  O   TYR    46      34.163  14.954  35.637  1.00 12.00
ATOM    330  CB  TYR    46      33.869  12.468  37.615  1.00 12.00
ATOM    331  CG  TYR    46      35.305  11.930  37.554  1.00 12.00
ATOM    332  CD1 TYR    46      36.177  11.548  36.332  1.00 12.00
ATOM    333  CD2 TYR    46      35.769  11.273  38.651  1.00 12.00
ATOM    334  CE1 TYR    46      37.553  11.159  36.401  1.00 12.00
ATOM    335  CE2 TYR    46      37.156  11.172  38.821  1.00 12.00
ATOM    336  CZ  TYR    46      38.021  10.823  37.672  1.00 12.00
ATOM    337  OH  TYR    46      39.341  10.278  37.803  1.00 12.00
*DELETE,1C2C,401,409
ATOM    346  O   TYR    48      37.961  14.496  31.832  1.00 13.00
ATOM    347  CB  TYR    48      35.422  12.358  32.003  1.00 13.00
ATOM    348  CG  TYR    48      34.558  11.302  32.752  1.00 13.00
ATOM    349  CD1 TYR    48      35.067  10.095  32.807  1.00 13.00
ATOM    350  CD2 TYR    48      33.942  11.539  33.976  1.00 13.00
ATOM    351  CE1 TYR    48      34.487   9.084  33.545  1.00 13.00
ATOM    352  CE2 TYR    48      33.070  10.614  34.448  1.00 13.00
ATOM    353  CZ  TYR    48      33.392   9.321  34.161  1.00 13.00
ATOM    354  OH  TYR    48      32.636   8.290  34.603  1.00 13.00
*DELETE,1C2C,434,442
ATOM    379  O   TYR    52      33.398  10.279  26.862  1.00 13.00
ATOM    380  CB  TYR    52      35.960  10.197  29.039  1.00 13.00
ATOM    381  CG  TYR    52      36.957   8.967  29.250  1.00 13.00
ATOM    382  CD1 TYR    52      36.301   7.714  29.514  1.00 13.00
ATOM    383  CD2 TYR    52      38.510   9.144  29.189  1.00 13.00
ATOM    384  CE1 TYR    52      37.092   6.615  29.860  1.00 13.00
ATOM    385  CE2 TYR    52      39.308   7.911  29.386  1.00 13.00
ATOM    386  CZ  TYR    52      38.603   6.742  29.934  1.00 13.00
ATOM    387  OH  TYR    52      39.410   5.650  30.564  1.00 13.00
*DELETE,1C2C,573,581
ATOM    518  O   TYR    70      40.160   -.951  28.287  1.00 16.00
ATOM    519  CB  TYR    70      36.948   -.435  27.636  1.00 16.00
ATOM    520  CG  TYR    70      37.333    .715  28.547  1.00 16.00
ATOM    521  CD1 TYR    70      38.098   1.591  28.170  1.00 16.00
ATOM    522  CD2 TYR    70      37.501    .394  29.868  1.00 16.00
ATOM    523  CE1 TYR    70      38.716   2.407  29.177  1.00 16.00
ATOM    524  CE2 TYR    70      37.809   1.305  30.923  1.00 16.00
ATOM    525  CZ  TYR    70      38.408   2.418  30.557  1.00 16.00
ATOM    526  OH  TYR    70      38.687   3.519  31.423  1.00 16.00
*DELETE,1C2C,866,874
ATOM    811  O   TYR   107      26.540  -5.038  36.793  1.00 12.00
ATOM    812  CB  TYR   107      29.256  -3.802  37.951  1.00 12.00
ATOM    813  CG  TYR   107      30.497  -3.825  36.915  1.00 12.00
ATOM    814  CD1 TYR   107      30.150  -3.821  35.544  1.00 12.00
ATOM    815  CD2 TYR   107      31.659  -3.038  37.371  1.00 12.00
ATOM    816  CE1 TYR   107      31.051  -3.268  34.638  1.00 12.00
ATOM    817  CE2 TYR   107      32.604  -2.936  36.393  1.00 12.00
ATOM    818  CZ  TYR   107      32.350  -3.429  35.153  1.00 12.00
ATOM    819  OH  TYR   107      33.447  -3.512  34.258  1.00 12.00
*DELETE,1C2C,1009
MASTER       30    0    1    6    0    4    0    6  904    1   48    9
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TABLE 3. CORRECTIONS AND REVISIONS OF ATOMIC COORDINATE DATA (CONT.)

21-APR-77

```
*IDENT,1ESTA
*DELETE,1EST,34
REMARK   6
REMARK   6 CORRECTION. INSERT MISSING CONECT RECORDS. 03-JAN-77
*INSERT,1EST,1946
CONECT  352  231  351
*INSERT,1EST,1948
CONECT 1341 1223 1340
*INSERT,1EST,1950
CONECT 1466  980 1465
CONECT 1613 1400 1612
*DELETE,1EST,1961
MASTER       23    4    2    2   17    0    1    6 1858    1   19   19

*IDENT,1FABA
*INSERT,1FAB,31
REMARK   5
REMARK   5 CORRECTION. INSERT MISSING CONECT RECORDS. 03-JAN-77
*INSERT,1FAB,3297
CONECT  608  152  607
*INSERT,1FAB,3298
CONECT 1415  963 1414
*INSERT,1FAB,3300
CONECT 2297 1716 2296
*INSERT,1FAB,3301
CONECT 3039 2625 3038
CONECT 3197 1547 3196
*DELETE,1FAB,3302
MASTER       26    0    0    3   33    0    0    6 3187    2   10   33

*IDENT,1FDXA
*INSERT,1FDX,27
REMARK   6
REMARK   6 CORRECTION. THE SG ATOMS OF CYSTEINES 11, 14, 18, 35, 38,
REMARK   6  41, 45 HAD INCORRECT Y AND Z COORDINATES. (WHEN THE VALUE
REMARK   6  WAS GREATER THAN 9.999 THE HIGH-ORDER DIGIT WAS LOST.)
REMARK   6  03-JAN-77.
*DELETE,1FDX,120
ATOM     79  SG  CYS    11      33.270  10.970  14.503  1.00  0.00
*DELETE,1FDX,135
ATOM     94  SG  CYS    14      30.364   5.564  15.917  1.00  0.00
*DELETE,1FDX,166
ATOM    125  SG  CYS    18      27.166    .502  21.043  1.00  0.00
*DELETE,1FDX,289
ATOM    248  SG  CYS    35      21.379   -.585  18.201  1.00  0.00
*DELETE,1FDX,311
ATOM    270  SG  CYS    38      22.448   3.239  23.185  1.00  0.00
*DELETE,1FDX,337
ATOM    286  SG  CYS    41      24.135   5.093  17.630  1.00  0.00
*DELETE,1FDX,351
ATOM    310  SG  CYS    45      27.795  11.065  13.311  1.00  0.00
*DELETE,1FDX,456
MASTER       18    0    2    0    0    0    0    6  389    1   24    5

*IDENT,1H1PA
*INSERT,1H1P,40
REMARK   6
REMARK   6 CORRECTION. IN RESIDUE TYR 19, ATOM OH WAS MISNAMED AS O,
REMARK   6  WHICH NAME THEREFORE OCCURRED TWICE. IT HAS BEEN RENAMED
REMARK   6  AND RESTORED TO ITS CORRECT POSITION AFTER CZ. THUS
REMARK   6  NECESSITATING RENUMBERING OF THE INTERVENING ATOMS O
REMARK   6  THROUGH CZ. (OH FORMERLY HAD SERIAL NUMBER 120 AND NOW
REMARK   6  HAS 128.) BNL 03-JAN-77.
*DELETE,1H1P,177,185
ATOM    120  O   TYR    19      22.870  10.840  13.970  1.00  0.00
ATOM    121  CB  TYR    19      19.860  11.020  12.910  1.00  0.00
ATOM    122  CG  TYR    19      19.450  11.400  14.340  1.00  0.00
ATOM    123  CD1 TYR    19      18.640  12.540  14.520  1.00  0.00
ATOM    124  CD2 TYR    19      19.920  10.710  15.430  1.00  0.00
ATOM    125  CE1 TYR    19      18.260  12.910  15.800  1.00  0.00
ATOM    126  CE2 TYR    19      19.550  11.070  16.770  1.00  0.00
ATOM    127  CZ  TYR    19      18.750  12.210  16.920  1.00  0.00
ATOM    128  OH  TYR    19      18.410  12.580  18.210  1.00  0.00
*DELETE,1H1P,774
MASTER       36    0    1    2    3    0    0    6  700    1   12    7

*IDENT,1PEIA
*INSERT,1PEI,53
REMARK   8
REMARK   8 CORRECTION. INSERT MISSING CONECT RECORDS. 03-JAN-77
*INSERT,1PEI,1840
CONECT  671  164  670
*INSERT,1PEI,1841
CONECT 1499  992 1498
*DELETE,1PEI,1842
MASTER       47    8    0    0   18   18    5    9 1707    2    4   18

*IDENT,1ADHA
*INSERT,1ADH,57
REMARK   5
REMARK   5 CORRECTION. MOVE THE HET CARDS TO THEIR PROPER POSITION.
REMARK   5  ALSO CORRECT THE SHIFT FOR Z IN REMARK 4. 28-MAR-77.
*DELETE,1ADH,57
REMARK   4      0.0       0.0      -1.0            90.85
*DELETE,1ADH,58,60
*INSERT,1ADH,89
HET    ZN1       1       1     CATALYTIC ZINC(II) ION
HET    ZN2       2       1     SECOND ZINC(II) ION
HET    APP       4      35     ADP-RIBOSE (PSEUDO COFACTOR)
*DELETE,1ADH,3014
MASTER       52    0    3   10   22   17    0    6 2822    1   45   29
```

```
*IDENT,2ADHA
*DELETE,2ADH,46
REMARK   4 THE CRYSTALLOGRAPHIC ASYMMETRIC UNIT OF THIS STRUCTURE
REMARK   4  CONTAINS ONE POLYPEPTIDE CHAIN WHICH IS COMPRISED OF TWO
REMARK   4  DOMAINS. TO GENERATE COORDINATES FOR THE OTHER CHAIN WHICH
REMARK   4  COMPLETES THE BIOLOGICALLY ACTIVE DIMER THE OPERATION
REMARK   4  GIVEN BELOW MUST BE APPLIED. NOTE THAT THIS IS A TRUE
REMARK   4  CRYSTALLOGRAPHIC DIAD SYMMETRY ELEMENT.
REMARK   4      -1.0       0.0       0.0             0.0
REMARK   4       0.0       1.0       0.0             0.0
REMARK   4       0.0       0.0      -1.0            90.85
REMARK   5
REMARK   5 CORRECTION. MOVE THE HET CARDS TO THEIR PROPER POSITION.
REMARK   5  ALSO INSERT MISSING REMARK 4. 28-MAR-77.
*DELETE,2ADH,47,49
*INSERT,2ADH,78
HET    ZN1       1       1     CATALYTIC ZINC(II) ION
HET    ZN2       2       1     SECOND ZINC(II) ION
HET    OPH       4      14     ORTHOPHENANTHROLINE
*DELETE,2ADH,2962
MASTER       50    0    3   10   22   17    0    6 2801    1   25   29

*IDENT,1CABA
*INSERT,1CAB,28
REMARK   6
REMARK   6 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK   6  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1CAB,2126
MASTER       25   10    1    7   10   11    0    6 2024    1    5   21

*IDENT,1CACA
*INSERT,1CAC,53
REMARK   8
REMARK   8 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK   8  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1CAC,2183
MASTER       48   10    1    8   10   10    0    6 2059    0    4   20

*IDENT,2CHAA
*INSERT,2CHA,80
REMARK   7
REMARK   7 CORRECTION. FIX SOME CONECT RECORDS THAT WERE IN ERROR.
REMARK   7  28-MAR-77.
*DELETE,2CHA,1931,1938
CONECT    6    5  893
CONECT  302  301  418
CONECT  418  302  417
CONECT  893    6  892
CONECT  986  985 1445
CONECT 1218 1217 1334
CONECT 1334 1218 1333
CONECT 1383 1382 1584
*DELETE,2CHA,1940,1941
CONECT 1445  986 1444
CONECT 1584 1383 1583
*DELETE,2CHA,1952
MASTER       73    5    1    3   14    0    0    9 1796    2   21   19

*IDENT,3CHAC
*INSERT,3CHAB,3
REMARK   8
REMARK   8 CORRECTION. ORDER THE CONNECTIVITIES FOR SEVERAL ATOMS TO
REMARK   8  BE IN ASCENDING ORDER. 28-MAR-77.
*DELETE,3CHAA,5,6
CONECT  418  302  417
CONECT  893    6  892
*DELETE,3CHAB,4
MASTER       45    0    0    1   14    0    0    9 1733    2   10   19

*IDENT,1CYTA
*DELETE,1CYT,49,52
REMARK   6 OF THE OXIDIZED INNER MOLECULE IS GIVEN IN THE MTRIX
REMARK   6 RECORDS BELOW.
*INSERT,1CYT,55
REMARK   8
REMARK   8 CORRECTION. REMOVE NON-CRYSTALLOGRAPHIC TRANSFORMATION FROM
REMARK   8  REMARK 6 AND INSERT IT AS MTRIX 1 TRANSFORMATION BELOW.
REMARK   8  28-MAR-77.
*INSERT,1CYT,98
MTRIX1  1   .418450   .907990   .021520     -50.254000
MTRIX2  1   .908170  -.041860   .002080     -17.993000
MTRIX3  1   .011620   .018340  -.999760      34.745000
*DELETE,1CYT,1888
MASTER       46    0    0   10    0   10    0    9 1692    2   95   16

*IDENT,1DHBA
*INSERT,1DHB,38
REMARK   7
REMARK   7 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK   7  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1DHB,2480
MASTER       35    7    2   16    0    0    0    9 2289    2   92   23

*IDENT,1FXNA
*INSERT,1FXN,35
REMARK   6
REMARK   6 CORRECTION. USE * INSTEAD OF SPECIAL CHARACTER -PRIME-
REMARK   6  FOR ATOM NAMES IN THE RIBITOL PORTION OF THE FMN.
REMARK   6  28-MAR-77.
*DELETE,1FXN,1163,1171
HETATM 1093  C1* FMN     1      30.915   -.780  13.113  1.00  0.00
HETATM 1094  C2* FMN     1      31.136    .658  12.625  1.00  0.00
HETATM 1095  O2* FMN     1      31.852   1.598  13.431  1.00  0.00
HETATM 1096  C3* FMN     1      29.744   1.196  12.314  1.00  0.00
HETATM 1097  O3* FMN     1      29.398    .024  10.978  1.00  0.00
HETATM 1098  C4* FMN     1      29.651   2.711  12.440  1.00  0.00
HETATM 1099  O4* FMN     1      28.280   3.120  12.443  1.00  0.00
HETATM 1100  C5* FMN     1      30.375   3.323  11.246  1.00  0.00
HETATM 1101  O5* FMN     1      31.104   4.500  11.580  1.00  0.00
*DELETE,1FXN,1207
MASTER       23    0    1    4    5    7    0    6 1104    1   31   11
```

TABLE 3. CORRECTIONS AND REVISIONS OF ATOMIC COORDINATE DATA (CONT.)

21-APR-77

```
*IDENT,1MBNC
*INSERT,1MBNB,3
REMARK    7
REMARK    7 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK    7  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1MBNB,5
MASTER       30    6    1    8    0    3    2    6 1260    1   46   12

*IDENT,1MDHA
*DELETE,1MDH,24
REMARK    5
REMARK    5 CORRECTION. STANDARDIZE THE NAMING AND ORDERING OF THE
REMARK    5  ATOMS IN THE NAD CO-ENZYME. 28-MAR-77.
*DELETE,1MDH,355,442
HETATM  326 AP    NAD      1      43.400  31.080  17.680  1.00  0.00
HETATM  327 AO1   NAD      1      42.160  31.920  17.760  1.00  0.00
HETATM  328 AO2   NAD      1      44.500  31.280  18.640  1.00  0.00
HETATM  329 AO5*  NAD      1      43.980  31.300  16.100  1.00  0.00
HETATM  330 AC5*  NAD      1      45.160  30.580  15.680  1.00  0.00
HETATM  331 AC4*  NAD      1      45.140  30.320  14.180  1.00  0.00
HETATM  332 AO4*  NAD      1      46.160  29.400  13.860  1.00  0.00
HETATM  333 AC3*  NAD      1      45.440  31.560  13.340  1.00  0.00
HETATM  334 AO3*  NAD      1      44.220  32.280  13.140  1.00  0.00
HETATM  335 AC2*  NAD      1      45.980  30.960  12.040  1.00  0.00
HETATM  336 AO2*  NAD      1      44.860  30.520  11.240  1.00  0.00
HETATM  337 AC1*  NAD      1      46.780  29.780  12.560  1.00  0.00
HETATM  338 AN9   NAD      1      48.220  30.060  12.760  1.00  0.00
HETATM  339 AC8   NAD      1      48.940  30.580  13.760  1.00  0.00
HETATM  340 AN7   NAD      1      50.300  30.600  13.700  1.00  0.00
HETATM  341 AC5   NAD      1      50.460  29.760  12.560  1.00  0.00
HETATM  342 AC6   NAD      1      51.540  29.340  11.880  1.00  0.00
HETATM  343 AN6   NAD      1      52.720  29.660  12.320  1.00  0.00
HETATM  344 AN1   NAD      1      51.460  28.620  10.900  1.00  0.00
HETATM  345 AC2   NAD      1      50.240  28.320  10.400  1.00  0.00
HETATM  346 AN3   NAD      1      49.080  28.660  11.020  1.00  0.00
HETATM  347 AC4   NAD      1      49.220  29.400  12.000  1.00  0.00
HETATM  348  U3   NAD      1      42.920  29.600  17.540  1.00  0.00
HETATM  349 NP    NAD      1      42.700  28.480  18.720  1.00  0.00
HETATM  350 NO1   NAD      1      42.240  29.040  20.000  1.00  0.00
HETATM  351 NO2   NAD      1      41.880  27.260  18.120  1.00  0.00
HETATM  352 NO5*  NAD      1      44.200  27.900  18.860  1.00  0.00
HETATM  353 NC5*  NAD      1      44.420  26.600  19.480  1.00  0.00
HETATM  354 NC4*  NAD      1      45.780  26.540  20.180  1.00  0.00
HETATM  355 NO4*  NAD      1      46.020  25.240  20.820  1.00  0.00
HETATM  356 NC3*  NAD      1      45.960  27.560  21.320  1.00  0.00
HETATM  357 NO3*  NAD      1      47.340  28.000  21.320  1.00  0.00
HETATM  358 NC2*  NAD      1      45.560  26.800  22.560  1.00  0.00
HETATM  359 NO2*  NAD      1      46.280  27.400  23.680  1.00  0.00
HETATM  360 NC1*  NAD      1      46.120  25.420  22.230  1.00  0.00
HETATM  361 NN1   NAD      1      45.400  24.280  22.920  1.00  0.00
HETATM  362 NC2   NAD      1      46.160  23.300  23.560  1.00  0.00
HETATM  363 NC3   NAD      1      45.460  22.320  24.140  1.00  0.00
HETATM  364 NC7   NAD      1      46.060  21.380  24.760  1.00  0.00
HETATM  365 NO7   NAD      1      45.480  20.300  24.920  1.00  0.00
HETATM  366 NN7   NAD      1      47.260  21.600  25.200  1.00  0.00
HETATM  367 NC4   NAD      1      44.180  22.240  23.940  1.00  0.00
HETATM  368 NC5   NAD      1      43.500  23.280  23.280  1.00  0.00
HETATM  369 NC6   NAD      1      44.220  24.300  22.860  1.00  0.00
CONECT  326  327  328  329  348
CONECT  327  326
CONECT  328  326
CONECT  329  326  330
CONECT  330  329  331
CONECT  331  330  332  333
CONECT  332  331  337
CONECT  333  331  334  335
CONECT  334  333
CONECT  335  333  336  337
CONECT  336  335
CONECT  337  332  335  338
CONECT  338  337  339  347
CONECT  339  338  340
CONECT  340  339  341
CONECT  341  340  342  347
CONECT  342  341  343  344
CONECT  343  342
CONECT  344  342  345
CONECT  345  344  346
CONECT  346  345  347
CONECT  347  338  341  346
CONECT  348  326  349
CONECT  349  348  350  351  352
CONECT  350  349
CONECT  351  349
CONECT  352  349  353
CONECT  353  352  354
CONECT  354  353  355  356
CONECT  355  354  360
CONECT  356  354  357  358
CONECT  357  356
CONECT  358  356  359  360
CONECT  359  358
CONECT  360  355  358  361
CONECT  361  360  362  369
CONECT  362  361  363
CONECT  363  362  364  367
CONECT  364  363  365  366
CONECT  365  364
CONECT  366  364
CONECT  367  363  368
CONECT  368  367  369
CONECT  369  361  368
*DELETE,1MDH,443
MASTER       20    0    1    0    0    0    0    3 369    0   44    0
```

```
*IDENT,1MHBA
*INSERT,1MHB,39
REMARK    7
REMARK    7 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK    7  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1MHB,2481
MASTER       36    7    2   16    0    0    0    9 2289    2   92   23

*IDENT,1PABA
*INSERT,1PAB,44
REMARK    9
REMARK    9 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK    9  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1PAB,1842
MASTER       41    3    0    2   16    0    0    9 1766    0    0    0

*IDENT,2PTIA
*INSERT,2PTI,36
REMARK    4
REMARK    4 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK    4  FTNOTE RECORDS. 28-MAR-77.
*DELETE,2PTI,517
MASTER       32    4    0    1    2    0    0    6  454    1    6    5

*IDENT,3PTIA
*INSERT,3PTI,40
REMARK    5
REMARK    5 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK    5  FTNOTE RECORDS. 28-MAR-77.
*DELETE,3PTI,571
MASTER       36    4    0    1    2    0    0    6  504    1    6    5

*IDENT,1PTNA
*INSERT,1PTN,34
REMARK    5
REMARK    5 CORRECTION. REMOVE FOOTNOTE NUMBERS FROM THE ATOMS OF
REMARK    5  RESIDUE GLY 188A BECAUSE THERE IS NO FTNOTE 2. 28-MAR-77.
*DELETE,1PTN,1300,1303
ATOM   1233  N   GLY   188A     -9.465  10.433   8.499  1.00  0.00
ATOM   1234  CA  GLY   188A    -10.354   9.684   9.394  1.00  0.00
ATOM   1235  C   GLY   188A    -10.058   8.766  10.581  1.00  0.00
ATOM   1236  O   GLY   188A    -10.948   8.464  11.389  1.00  0.00
*DELETE,1PTN,1798
MASTER       31    4    1    3    0    0    0    6 1709    1   20   18

*IDENT,1RNSA
*INSERT,1RNS,45
REMARK    6
REMARK    6 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK    6  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1RNS,1047
MASTER       39    8    0    3    7    4    0    6  952    2    8   10

*IDENT,1SBTA
*INSERT,1SBT,52
REMARK    4
REMARK    4 CORRECTION. FIX MASTER RECORD TO SHOW CORRECT NUMBER OF
REMARK    4  FTNOTE RECORDS. 28-MAR-77.
*DELETE,1SBT,2057
MASTER       45    6    0    8    5    0    0    6 1955    1    0   22

*IDENT,1SRXA
*DELETE,1SRX,29
REMARK    7
REMARK    7 CORRECTION. CORRECT THE SHEET IDENTIFICATION FOR ALL
REMARK    7  STRANDS EXCEPT THE FIRST. 28-MAR-77.
*DELETE,1SRX,44,47
SHEET    2  B1 5 THR    54  LEU    58  1 N   ILE     4  0  VAL    55
SHEET    3  B1 5 ALA    22  TRP    28  1 N   ALA    56  0  LEU    24
SHEET    4  B1 5 THR    77  PHE    81 -1 N   VAL    25  0  LEU    79
SHEET    5  B1 5 ALA    88  LYS    90 -1 N   LEU    80  0  ALA    86
*DELETE,1SRX,167
MASTER       25    0    0    4    5    5    1    3  108    1    0    9

*IDENT,1TNAA
*INSERT,1TNA,37
REMARK    7
REMARK    7 CORRECTION. INSERT MISSING LINE IN REMARK 3. 18-APR-77.
*INSERT,1TNA,19
REMARK    3 FURTHER REFINEMENT HAS BEEN PERFORMED AND AN UPDATED
*DELETE,1TNA,1746
MASTER       31    0    1    0    0    0    0    6 1652    1   41    6
```

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 '1MBNA' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK '1MBN' FOR SPERM-WHALE MYOGLOBIN, '1MBNB' 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 SEQUENCE OF RECORDS, 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.

Several new Data Bank services are planned, to start during the next six months. These include distribution of "model-builder's kits," to consist of compact hard-copy listings of atomic coordinates and torsion angles, intended as an aid in construction of models from standardized parts. In addition to these kits, we soon hope to have available for distribution computer programs for production of Ramachandran and diagonal plots. These programs will be written in simple standard FORTRAN and will operate directly on the atomic coordinate entries as distributed.

Currently, the majority of our budget is supplied by a grant to Brookhaven from the U.S. National Science Foundation, and we have received additional support from the National Institutes of Health. These funds are gratefully acknowledged. We also appreciate very much the support of our users; through distribution charges paid by you, we are now recovering some of our costs. Comments and suggestions on how service might be improved are always welcome. We want to thank all those who returned our recent questionnaire and hope to hear from more of you in the future.

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PROTEIN DATA BANK REQUEST

Name: _____

Adress: _____

_____

_____ Telephone: _____

Send the following information (please check):

( ) all current coordinate entries ( ) description of file record formats
( ) data entries listed below

I am supplying a NEW 2400' reel of magnetic tape which I would like written as follows:

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

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

To avoid delays, send all correspondence to the address given on the reverse side of this form.

A purchase order ( )/check ( ) is enclosed ( )/sent separately ( ). The charge is $34.30 per request or $47.00 if Brookhaven is to supply a tape.

Parameter sets requested (by code name please):

_____	_____	_____	_____	_____
_____	_____	_____	_____	_____
_____	_____	_____	_____	_____
_____	_____	_____	_____	_____
_____	_____	_____	_____	_____

Comments:

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

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