THE PROTEIN DATA BANK

NEWSLETTER

Number 13 July 1980

We continue to be very busy: in 1979 we distributed 75 data tapes to 55 laboratories and during the first six months of this year 40 data tapes were sent to 34 laboratories. These figures do not include data sets distributed by the centers in England, Japan and Australia. Our holdings continue to grow and we are presently making an extra effort in soliciting structure factors and phase information from our depositors. We feel it is very important that these primary crystallographic data be widely available and that they be preserved for future use. With the release of our Builder's Kit (BLDKIT) program, we are expanding our services. We can run this program to individuals' specifications, thereby making it possible for users who have no convenient access to a computer to generate coordinate lists, scaled and oriented for use with any one of the commercially available Model Building Kits. Those interested in availing themselves of this service should get in touch with our center at Brookhaven National Laboratory.

In the future the Protein Data Bank's holdings will be augmented to include bibliographic entries on macromolecular structures for which the Data Bank does not currently carry atomic coordinates. Work has already started to generate these entries, which initially will be limited to medium- and high-resolution structures where atomic coordinates appear to be available but none have as yet been deposited with us. We hope subsequently to extend this file to include references to preliminary crystallization reports and low-resolution analyses. We will announce in a future newsletter when the bibliographic entries will be ready for distribution.

Frances Bernstein will be attending the ACA meeting at Calgary on August 17-22. We are planning to have a poster on display during the entire meeting, and Frances will be available to answer questions and receive suggestions from our users. To answer some questions about the Protein Data Bank, we are including a general overview of our services in this newsletter. A more detailed description can be found in J. Mol. Biol. 112, 532-42 (1977).

Data Input: The Protein Data Bank collects and stores two classes of information: atomic coordinates and structure factor-phase data. Also available are a number of computer programs that operate on the atomic coordinate entries. All data should be sent to Brookhaven in machine-readable form, preferably magnetic tape. Contributed computer programs of general interest will be accepted for distribution, provided adequate machine-readable documentation accompanies the source code.

Atomic coordinate data are processed into the standard Data Bank format, and returned to depositors for checking and approval before entries are released for public distribution. Corrections are applied when errors become known and are documented in remarks carried at the head of each entry. Of course, the contents of an entire entry may be replaced by newer, more accurate data at any time. Early deposition is valuable: a number of fairly preliminary sets of C^{α} coordinates have been contributed, and user demand for these has been quite high. The C^{α} data sets generally are replaced by complete atomic coordinate information, when it becomes available.

For mutual convenience, we have prepared a deposition form that we will gladly supply to all potential depositors. The Bank can also provide a magnetic tape for data transcription. In cases where depositors of atomic coordinate information have provided their own tapes, these are returned containing copies of the processed data entries.

Data Distribution: Worldwide distribution for the Protein Data Bank is handled through four centers, as listed below. The request form included with this Newsletter may be used to order data from Brookhaven or Cambridge; users in Japan or Australia should contact their centers for detailed information. From Brookhaven, data normally are distributed on magnetic tape or microfiche, as indicated in Tables 1 and 2 below. Requests for the standard data tape (DATAPRTP) usually are filled within a day or so unless new data are being added or corrections applied. It is simpler for us to send all current atomic coordinate entries and programs than to select a few entries, and the cost to the user is the same in any case. The other items in Tables 1 and 2 are requested less frequently and are generated as needed; this can cause a delay of up to one week.

A partial list of substantive corrections which have been applied to the atomic coordinate entries since January 1980 is given in Table 6. The complete list of corrections is available on microfiche free of charge. All new requests are automatically filled with the latest data including all corrections.

It is expected that the Protein Data Bank be acknowledged in publications which result from work making use of the Bank's services. In citing the Protein Data Bank in print, we suggest that a reference be included to F. C. Bernstein, T. F. Koetzle, G. J. B. Williams, E. F. Meyer, Jr., M. D. Brice, J. R. Rodgers, O. Kennard, T. Shimanouchi, and M. Tasumi, J. Mol. Biol. 112, 535-42 (1977). We would appreciate receiving reprints.

Area	Address of Center	Name	Telephone
The Americas	Protein Data Bank Chemistry Department Brookhaven National Laboratory Upton, New York 11973 USA	E. Abola F. C. Bernstein T. F. Koetzle	516-345-4383 516-345-4382 516-345-4384
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, England	O. Kennard S. Bellard	0223-66499
Australia	CSIRO Div. of Chemical Physics P. O. Box 160 Clayton, Victoria 31368 Australia	B. J. Poppleton	
Japan	Institute for Protein Research Osaka University 5311, Yamada-Kami, Suita Osaka, Japan	M. Kakudo	(06) 877-5111 ext. 3836

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

09-JUL-80

CODE	ITEM
DATAPRTP	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3,4)
NONSTDTP	ALL STRUCTURE FACTOR HOLDINGS (TABLE 5)
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS
BLDKITTP	*MODEL BUILDER*S KIT
CONECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS
DGPLOTTP	DIAGONAL PLOTS (LINE PRINTER)
DIHDRLTP	COMPLETE TORSION ANGLES
DSTNCETP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES

* NEW OR REPLACEMENT ENTRY SINCE APR-80 NEWSLETTER

ITEM DSTNCETP REQUIRES TWO TAPES AT 800CPI, OTHER ITEMS COMPRISE ONE TAPE EACH

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

09-JUL-80

CODE	ITEM	NO. OF FICHE	PRICE
DATAPRFI	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3,4)	14	$83.82
NONSTDFI	ALL STRUCTURE FACTOR HOLDINGS (TABLE 5)	12	$80.96
CORR06FI	*LIST OF CORRECTIONS NO. 6 (JAN/80-JUL/80)	1	FREE
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	2	$66.66
BLDKITFI	*MODEL BUILDER*S KIT	PLEASE	INQUIRE
CONECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	12	$80.96
DGPLOTFI	DIAGONAL PLOTS (LINE PRINTER)	5	$70.95
DIHDRLFI	COMPLETE TORSION ANGLES	7	$73.81
DSTNCEFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	24	$98.12
FISIPLFI	PHI/PSI PLOTS (LINE PRINTER)	1	$65.23
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	5	$70.95

* NEW OR REPLACEMENT ENTRY SINCE APR-80 NEWSLETTER

PRICES QUOTED ARE IN U.S. DOLLARS FOR DISTRIBUTIONS FROM BROOKHAVEN. REQUESTORS FROM OTHER CENTERS SHOULD INQUIRE FOR AVAILABILITY AND PRICES.

TABLE 3. PROTEIN DATA BANK, ATOM93 COORDINATE 80LDIN7S

09-JUL-80

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/ STATUS
1APE	ACID PROTEINASE(ENDOTHIA PARASITICA)	T.BLUNDELL	10/79
1APP	ACID PROTEINASE(PENICILLIUMJANTHINELLUM)	M.JAMES,I.HSU	12/79
1APR	ACID PROTEINASE(RHIZOPUS CHINENSIS)	D.DAVIES	8/79
2ACT	ACTINIDIN	E.BAKER	11/79 R
2ADK	ADENYLATE KINASE (PORCINE MUSCLE)	G.SCHULZ	3/77 R
1AGA	AGAROSE	S.ARNOTT	5/78
2WGA	*AGGLUTININ (WHEAT GERM)	C.WRIGHT	5/80 R
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I.BRANDEN	8/76
2ADH	ALCOHOL DEHYDROGENASE (ORTHOPHEN)	C.-I.BRANDEN	8/76
4ADH	ALCOHOL DEHYDROGENASE (APO)	C.-I.BRANDEN	8/79
1ALP	ALPHA LYTIC PROTEASE	BRAYER,DELBAERE,JAMES	6/79
1ABP	*L-ARABINOSE-BINDING PROTEIN	F.QUIOCHO,G.GILLILAND	5/80 P
1ATC	ASPARTATE CARBAMOYLTRANSFERASE	CRAWFORD,MONACO,LIPSCOMB	8/79 A
2BCL	BACTERIOCHLOROPHYLL A-PROTEIN	B.MATTHEWS	1/79 RA
1ABX	ALPHA-BUNGAROTOXIN	D.AGARD,S.SPENCER,R.STROUD	4/80 A
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
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	S.ARNOTT	5/78
1CAB	CARBONIC ANHYDRASE B (HUMAN)	K.KANNAN	6/76
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K.KANNAN	5/76
1CPA	CARBOXYPEPTIDASE A (BOVINE)	W.LIPSCOMB	2/73
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M.SCHMID,J.HERRIOTT	9/76 A
1CAR	CARRAGEENAN	S.ARNOTT	5/78
1C4S	CHONDROITIN-4-SULFATE	S.ARNOTT	5/78
2C4S	CHONDROITIN-4-SULFATE (CA SALT)	S.ARNOTT	5/78
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D.BLOW	1/75 R
3CHA	ALPHA-CHYMOTRYPSIN	A.TULINSKY	8/76
2GCH	*GAMMA-CHYMOTRYPSIN	COHEN,DAVIES,SILVERTON	5/80 R
1CHG	CHYMOTRYPSINOGEN	J.KRAUT,J.BIRKTOFT	3/75
2CNA	CONCANAVALIN A	G.REEKE,J.BECKER,G.EDELMAN	9/75
3CNA	CONCANAVALIN A	K.HARDMAN	9/76 R
2B5C	CYTOCHROME B5 (OXIDIZED)	F.S.MATHEWS	12/77 R
156B	CYTOCHROME B562 (E.COLI,OXIDIZED)	BETHGE,CZERWINSKI,MATHEWS	8/79
3CYT	*CYTOCHROME C (ALBACORE, OXIDIZED)	T.TAKANO,R.DICKERSON	7/80 RP
4CYT	*CYTOCHROME C (ALBACORE, REDUCED)	T.TAKANO,R.DICKERSON	7/80 RP
1CYC	CYTOCHROME C (BONITO, HEART)	M.KAKUDO	8/76
1C2C	CYTOCHROME C2	J.KRAUT	3/73
155C	CYTOCHROME C550	R.TIMKOVICH	8/76
251C	CYTOCHROME C551	R.DICKERSON	8/78 R
1DFR	DIHYDROFOLATE REDUCTASE (L.CASEI)	J.BOLIN,D.MATTHEWS,J.KRAUT	3/80
2DFR	DIHYDROFOLATE REDUCTASE (E. COLI)	J.BOLIN,D.MATTHEWS,J.KRAUT	3/80
1EST	ELASTASE (PORCINE, TOSYL)	H.WATSON	5/76
1EBX	*ERABUTOXIN B	B.LOW	7/79 N
1ECD	ERYTHROCRUORIN (REDUCED, DEOXY)	W.STEIGEMANN,E.WEBER	3/79
1ECO	ERYTHROCRUORIN (CARBONMONOXY)	W.STEIGEMANN,E.WEBER	3/79
1ECA	ERYTHROCRUORIN (AQUO, MET)	W.STEIGEMANN,E.WEBER	3/79
1ECN	ERYTHROCRUORIN (CYANO, MET)	W.STEIGEMANN,E.WEBER	3/79
1FDX	FERREDOXIN (PEPTOCOCCUS AEROGENES)	E.ADMAN,L.SIEKER,L.JENSEN	8/76
1FXC	FERREDOXIN (SPIRULINA PLATENSIS)	M.KAKUDO	8/79
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
2GPD	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M.ROSSMANN	12/79
1HRB	HEMERYTHRIN B	W.HENDRICKSON	6/76 A
1HMN	HEMERYTHRIN (MET, AQUO)	R.STENKAMP ET AL.	1/79 A
1HDS	HEMOGLOBIN (DEER, SICKLE CELL)	E.AMMA,R.GIRLING	10/79
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	R.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
1HCO	HEMOGLOBIN(HUMAN,CARBONMONOXY)	J.BALDWIN	8/79
2HCO	HEMOGLOBIN(HUMAN,CARBONMONOXY,NRG REFND)	J.BALDWIN	8/79
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J.FRIER	8/76
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON,LOVE,KARLE	3/73
2YHX	HEXOKINASE (YEAST) FORM BIII	STEITZ,ANDERSON,STENKAMP	3/78 R
1HIP	HIGH POTENTIAL IRON PROTEIN	J.KRAUT	4/75
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S.ARNOTT	11/77
2HYA	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S.ARNOTT	5/78
3HYA	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S.ARNOTT	5/78
4HYA	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S.ARNOTT	5/78
2FAB	IMMUNOGLOBULIN FAB* NEW	R.POLJAK	6/79
1MCG	IMMUNOGLOBULIN B-J INTACT MCG	SCHIFFER,EDMUNDSON ET AL.	5/78 A
1REI	IMMUNOGLOBULIN B-J FRAGMENT(V-DIMER)	REI O.EPP,R.HUBER	3/76
1RHE	IMMUNOGLOBULIN B-J FRAGMENT(V-MNMER)	RHE B.WANG,C.YOO,M.SAX	12/77 A
1INS	*INSULIN(PORCINE,2-ZINC)	G.DODSON,D.HODGKIN	7/80 P
1KGA	KDPG ALDOLASE	A.TULINSKY	8/78 A
1KES	KERATAN SULFATE	S.ARNOTT	5/78
4LDH	LACTATE DEHYDROGENASE	W.EVENTOFF,M.ROSSMANN	4/77 R
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M.ROSSMANN	11/74
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)	W.MUSICK,M.ROSSMANN	9/78
1MBL	LEGHEMOGLOGIN	VAINSHTEIN,HARUTYUNYAN	11/78
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
8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S.OATLEY	9/77
9LYZ	LYSOZYME(HEN,NAM-NAG-NAM SUBSTRATE ONLY)	J.KELLY,M.JAMES	12/79
1MDH	MALATE DEHYDROGENASE	L.BANASZAK	6/76 A
1MLP	MUREIN LIPOPROTEIN (HYPOTHETICAL)	A.MCLACHLAN	8/78
1MBN	MYOGLOBIN (SPERM WHALE, MET)	H.WATSON	4/73
2MBN	MYOGLOBIN (SPERM WHALE, MET)	T.TAKANO	9/76
3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T.TAKANO	9/76
1MBS	MYOGLOBIN (SEAL, MET)	H.SCOULOUDI	3/79
1MHR	MYOHEMERYTHRIN	W.HENDRICKSON	6/76 A
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
1PEP	PEPSIN (PORCINE)	N.ANDREEVA ET AL.	7/78 A
1PGK	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.OATLEY,C.BLAKE	9/77 R
1PYK	PYRUVATE KINASE (CAT)	H.MUIRHEAD	1/80 A
1RLX	RELAXIN(MODEL,CONFORMATION A,UNREFINED)	A.EVANS,A.NORTH	3/78
2RLX	RELAXIN(MODEL,CONFORMATION B,UNREFINED)	A.EVANS,A.NORTH	3/78
3RLX	RELAXIN(MODEL,CONFORMATION A,REFINED)	A.EVANS,A.NORTH	3/78
4RLX	RELAXIN(MODEL,CONFORMATION B,REFINED)	A.EVANS,A.NORTH	3/78
1RHD	RHODANESE	W.HOL	12/77
2RSA	RIBONUCLEASE A	A.WLODAWER	6/79
1RNS	RIBONUCLEASE S	H.WYCKOFF,F.RICHARDS	4/73
2RXN	RUBREDOXIN	L.JENSEN	1/75
1SNS	STAPHYLOCOCCAL NUCLEASE	F.A.COTTON,E.HAZEN	4/73
1SGA	STREPTOMYCES GRISEUS PROTEINASE A	BRAYER,DELBAERE,JAMES	6/78
2SGB	STREPTOMYCES GRISEUS PROTEINASE B	DELBAERE,BRAYER,JAMES	6/79 R
2SSI	SUBTILISIN INHIBITOR (STREPTOMYCES)	Y.MITSUI ET AL.	4/80 R
1SBT	SUBTILISIN BPN'	J.KRAUT	8/72
2SBT	SUBTILISIN NOVO	J.DRENTH	9/76
2SOD	SUPEROXIDE DISMUTASE	J.RICHARDSON,D.RICHARDSON	3/80 R
1TLN	THERMOLYSIN (UNREFINED)	B.MATTHEWS	4/75
2TLN	THERMOLYSIN (REFINED)	B.MATTHEWS	4/75
1SRX	THIOREDOXIN (E. COLI, OXIDIZED)	B.-O.SODERBERG	5/76 A
4TNA	TRANSFER RNA (YEAST, PHE)	A.JACK,J.LADNER,A.KLUG	4/78 R
6TNA	TRANSFER RNA (YEAST, PHE)	S.-H.KIM ET AL.	11/78 R
8TNA	TRANSFER RNA (YEAST, PHE)	M.SUNDARALINGAM	2/79 R
1TIM	TRIOSE PHOSPHATE ISOMERASE	I.WILSON,D.PHILLIPS	9/76
1PTN	TRYPSIN (NATIVE, PHB)	FEHLHAMMER,BODE,SCHWAGER	1/77
2PTB	TRYPSIN(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER,BODE,SCHWAGER	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
1TGP	TRYPSINOGEN/TRYPSIN INHIBITOR	W.BODE,P.SCHWAGER,R.HUBER	3/79
1TPI	TRYPSINOGEN/TRYPSIN INHIBITOR/ILE-VAL	W.BODE,P.SCHWAGER,R.HUBER	3/79
1TGA	TRYPSINOGEN (MGSO4, WITHOUT CA)	BODE,FEHLHAMMER,HUBER	3/79
1TGB	TRYPSINOGEN (WITH CA, FROM PEG)	BODE,FEHLHAMMER,HUBER	3/79
1TGN	TRYPSINOGEN	A.KOSSIAKOFF,R.STROUD	9/79
1SBV	VIRUS COAT PROTEIN(SOUTHERN BEAN MOSAIC)	M.ROSSMANN	12/79 BN

* NEW OR REPLACEMENT ENTRY SINCE APR-80 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	REPLACES AN OUT-OF-DATE PARAMETER SET

TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

09-JUL-80

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	1/79 YES
BLDKIT	*MODEL BUILDER*S KIT	E.ABOLA	7/80 YES
CHIRAL	CHECK CHIRALITY	E.ABOLA	3/80 YES
CONECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	4/79 YES
CONTCT	INTERMOLECULAR CONTACTS	L.ANDREWS	10/79 NO
DGPLOT	DIAGONAL PLOTS ON PRINTER	E.SWANSON,F.BERNSTEIN	3/79 YES
DIHDRL	COMPLETE TORSION ANGLES	E.ABOLA	3/80 YES
DSTNCE	CALC DISTANCES FROM CONECT RECORDS	F.BERNSTEIN	3/79 YES
FISIPL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79 YES
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78 NO
PHIPSI	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	2/79 YES
STEREO	EXTRACT X,Y,Z FROM STEREO DIAGRAMS	M.ROSSMANN	6/79 NO
TAPDIR	PRINT DIRECTORY OF TAPE CONTENTS	H.BERNSTEIN,F.BERNSTEIN	12/79 YES
TORSRU	COMPLETE TORSION ANGLES	G.REEKE	10/79 NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	5/78 YES

* NEW OR REPLACEMENT ENTRY SINCE APR-80 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

09-JUL-80

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
R2B5CSF	CYTOCHROME B5	F.S.MATHEWS	12/77 SF
R3CYTSF	*CYTOCHROME C (ALBACORE, OXIDIZED)	T.TAKANO,R.DICKERSON	7/80 SF
R4CYTSF	*CYTOCHROME C (ALBACORE, REDUCED)	T.TAKANO,R.DICKERSON	7/80 SF
RCYC5501	CYTOCHROME C550	R.TIMKOVICH	4/76 SF
R151CSF	CYTOCHROME C551	R.DICKERSON	8/78 SF
RGPDO4	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M.ROSSMANN	8/75 SF
R2GPDSF	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M.ROSSMANN	12/79 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

* NEW OR REPLACEMENT ENTRY SINCE APR-80 NEWSLETTER

CODES

SF	STRUCTURE FACTORS

TABLE 6. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

09-JUL-80

THE NOMENCLATURE FOR VALINES AND LEUCINES WAS STANDARDIZED TO FOLLOW IUPAC-IUB SPECIFICATIONS. THIS REQUIRED INTERCHANGING CG1 AND CG2 OR CD1 AND CD2 IN MANY DATA ENTRIES.

```
*IDENT,1HYAA
*INSERT,1HYA.51
REMARK   6
REMARK   6 CORRECTION. STANDARDIZE COMPND, REMARK 3, HET, HETATMS 127-
REMARK   6  129, CONECT 111 TO CONFORM TO OTHER POLYSACCHARIDE
REMARK   6  ENTRIES.  CORRECT GCU AND NAG FORMUL RECORDS.  28-MAR-80.
REMARK   7
REMARK   7 THE GLUCURONIC ACID-GLUCOSAMINE LINKAGE IS BETA(1,3) AND
REMARK   7 THE GLUCOSAMINE-GLUCURONIC ACID LINKAGE IS BETA(1,4).
*DELETE,1HYA.4,7
COMPND    HYALURONIC ACID
COMPND   2 (POLY D-GLUCURONIC ACID-N-ACETYL-D-GLUCOSAMINE)
COMPND   3 SODIUM SALT, TRIGONAL FORM.
*DELETE,1HYA.35,36
REMARK   3 REFINEMENT. BY A LINKED-ATOM LEAST-SQUARES MODEL-BUILDING
REMARK   3  PROCEDURE.  SEE REFERENCE 1 ABOVE.
*DELETE,1HYA.53,63
HET    GCU   -999      17     D-GLUCURONIC ACID
HET    NAG   -999      25     N-ACETYL-D-GLUCOSAMINE
HET     NA   -999       1     SODIUM +1 COUNTER ION
FORMUL   1  GCU    3(C6 H10 O7)
FORMUL   1  NAG    3(C8 H15 N1 O6)
*DELETE,1HYA.198,200
HETATM  127 NA     NA      1       2.912   1.524   1.596  1.00  0.00
HETATM  128 NA     NA      2       5.714   6.849  11.096  1.00  0.00
HETATM  129 NA     NA      3       8.924   1.760  20.596  1.00  0.00
*DELETE,1HYA.323
CONECT  111   -1  104
*DELETE,1HYA.339
MASTER       43    0    3    0    0    0    0    6  141    0  126    1

*IDENT,1SGAC
*INSERT,1SGAB.2
REMARK   8
REMARK   8 CORRECTION. CORRECT TYPOGRAPHICAL ERROR ON SEQRES 8 RECORD.
REMARK   8 FOLLOWING DEPOSITOR,S INSTRUCTIONS, CHANGE RESIDUE 115
REMARK   8 FROM ASN TO ASP AND INSERT SALT BRIDGE BETWEEN ATOMS 476
REMARK   8 AND 491.  07-APR-80.
*DELETE,1SGA.71
SEQRES   6   181  ALA ALA ASP GLY ARG VAL TYR LEU TYR ASN GLY SER TYR
*DELETE,1SGA.73
SEQRES   8   181  ALA VAL GLN ARG SER GLY SER THR THR GLY LEU ARG SER
*DELETE,1SGA.556,563
ATOM    470  N   ASP   115      -.762   4.374  24.559  1.00  0.00
ATOM    471  CA  ASP   115     -1.376   3.492  23.558  1C00  0C00
ATOM    472  C   ASP   115     -1.595   3.938  22.112  1.00  0.00
ATOM    473  O   ASP   115     -2.296   4.925  21.850  1.00  0.00
ATOM    474  CB  ASP   115     -2.777   3.056  24.036  1.00  0.00
ATOM    475  CG  ASP   115     -2.962   1.567  23.909  1.00  0.00
ATOM    476  OD1 ASP   115     -3.113    .971  22.856  1.00  0.00
ATOM    477  OD2 ASP   115     -2.881    .851  25.096  1.00  0.00
*INSERT,1SGA.1352
CONECT  476  475                           491
CONECT  491  490                                               476
*DELETE,1SGAB.4
MASTER       60    0    0    0    0    0    0    6 1265    1    2   14

*IDENT,1S6BB
*INSERT,1S6BA.4
REMARK   7
REMARK   7 CORRECTION. DELETE SPURIOUS ATOM 346 AND RENUMBER ALL
REMARK   7  FOLLOWING ATOMS.  07-APR-80.
*DELETE,1S6B.409,910
ATOM    346  N   LYS    50      -1.318   5.280 -12.647  1.00  0.00
ATOM    347  CA  LYS    50      -2.071   4.097 -13.078  1.00  0.00
ATOM    348  C   LYS    50      -3.301   4.520 -13.908  1.00  0.00
ATOM    349  O   LYS    50      -3.176   5.005 -15.048  1.00  0.00
ATOM    350  CB  LYS    50      -2.546   3.293 -11.872  1.00  0.00
.
. CARDS OMITTED HERE
.
HETATM  848  O1D HEM     1       3.507   7.247  -6.630  1.00  0.00
HETATM  849  O2D HEM     1       3.428   9.414  -6.212  1.00  0.00
*DELETE,1S6BA.5
MASTER       35    2    1    4    0    2    0    9  845    1   46    8

*IDENT,1CACF
*INSERT,1CACE.3
REMARK  13
REMARK  13 CORRECTION. CORRECT SCALE MATRIX.  07-APR-80.
*DELETE,1CAC.117,119
SCALE1      -.024173   .001163  -.000098        -.445661
SCALE2      -.001155  -.023935   .000919        -.819958
SCALE3       .003561  -.001187   .013833         .184571
*DELETE,1CACE.4
MASTER       88   10    1    8   10   10    0    6 2059    0    4   20

*IDENT,1CHGE
*INSERT,1CHGD.5
REMARK   9
REMARK   9 CORRECTION. STANDARDIZE NOMENCLATURE TO FOLLOW IUPAC-IUB
REMARK   9  RECOMMENDATIONS.  INTERCHANGE CD1 AND CD2 FOR LEUCINES
REMARK   9  33, 46, 83.  INTERCHANGE CG1 AND CG2 FOR VALINES 23, 31,
REMARK   9  52, 53, 60, 65, 66, 67, 88, 200.  CORRECT SCALE MATRIX.
REMARK   9  07-APR-80.
*DELETE,1CHG.83,85
SCALE1       .000199  -.018701   .000082         .793122
SCALE2      -.015648  -.000157   .000133         .707859
SCALE3      -.000110  -.000055  -.012970         .467076
.
. CARDS OMITTED HERE
.
*DELETE,1CHGD.6
MASTER       86    0    0    2   14    0    0    6 1643    1   10   19

*IDENT,1CYCF
*INSERT,1CYCE.2
REMARK  10
REMARK  10 CORRECTION. STANDARDIZE NOMENCLATURE TO FOLLOW IUPAC-IUB
REMARK  10  RECOMMENDATIONS.  INTERCHANGE CD1 AND CD2 FOR LEUCINES
REMARK  10  68, 94.  INTERCHANGE CG1 AND CG2 FOR VALINES 20, 28, 58,
REMARK  10  95.  CORRECT SOURCE RECORD.  FOLLOWING DEPOSITOR,S
REMARK  10  INSTRUCTIONS, CHANGE GLN 44 TO GLU 44, LEU 57 TO ILE 57,
REMARK  10  GLN 61 TO GLU 61 AND CHANGE ATOM NAMES APPROPRIATELY.
REMARK  10  07-APR-80.
*DELETE,1CYC.5
SOURCE    BONITO (KATSUO) HEART
*DELETE,1CYC.25,26
SEQRES   4   103  THR GLY GLN ALA GLU GLY TYR SER TYR THR ASP ALA ASN
SEQRES   5   103  LYS SER LYS GLY ILE VAL TRP ASN GLU ASN THR LEU MET
.
. CARDS OMITTED HERE
.
*DELETE,1CYC.364,372
ATOM    322  N   GLU    44      -27.438   3.883  20.450  1.00  0.00
ATOM    323  CA  GLU    44      -28.131   2.497  20.261  1.00  0.00
ATOM    324  C   GLU    44      -27.060   1.615  20.891  1.00  0.00
ATOM    325  O   GLU    44      -26.556    .481  20.324  1.00  0.00
ATOM    326  CB  GLU    44      -28.635   2.371  18.749  1.00  0.00
ATOM    327  CG  GLU    44      -30.210    .993  18.749  1.00  0.00
ATOM    328  CD  GLU    44      -30.840   2.875  19.379  1.00  0.00
ATOM    329  OE1 GLU    44      -32.100   2.875  18.875  1.00  0.00
ATOM    330  OE2 GLU    44      -30.084   4.135  19.505  1.00  0.00
*DELETE,1CYC.463,470
ATOM    421  N   ILE    57      -20.130  17.113  23.285  1.00  0.00
ATOM    422  CA  ILE    57      -20.004  17.869  22.025  1.00  0.00
ATOM    423  C   ILE    57      -21.264  18.121  21.143  1.00  0.00
ATOM    424  O   ILE    57      -22.398  18.498  21.395  1.00  0.00
ATOM    425  CB  ILE    57      -18.996  17.491  21.395  1.00  0.00
ATOM    426  CG1 ILE    57      -19.374  16.357  20.513  1.00  0.00
ATOM    427  CG2 ILE    57      -17.862  17.050  22.025  1.00  0.00
ATOM    428  CD1 ILE    57      -19.122  16.609  19.127  1.00  0.00
.
. CARDS OMITTED HERE
.
*DELETE,1CYC.500,508
ATOM    458  N   GLU    61      -22.020  20.137  10.811  1.00  0.00
ATOM    459  CA  GLU    61      -21.138  20.263   9.425  1.00  0.00
ATOM    460  C   GLU    61      -19.626  20.389  10.181  1.00  0.00
ATOM    461  O   GLU    61      -18.744  19.507   9.803  1.00  0.00
ATOM    462  CB  GLU    61      -21.516  21.523   8.669  1.00  0.00
ATOM    463  CG  GLU    61      -22.020  21.523   7.409  1.00  0.00
ATOM    464  CD  GLU    61      -23.154  20.767   7.283  1.00  0.00
ATOM    465  OE1 GLU    61      -24.540  20.767   7.535  1.00  0.00
ATOM    466  OE2 GLU    61      -22.902  19.381   6.653  1.00  0.00
.
. CARDS OMITTED HERE
.
*DELETE,1CYCE.4
MASTER       54    0    1    5    0    3    0    9  839    1   48    8

*IDENT,1C2CD
*INSERT,1C2CC.2
REMARK   7
REMARK   7 CORRECTION. STANDARDIZE NOMENCLATURE TO FOLLOW IUPAC-IUB
REMARK   7  RECOMMENDATIONS.  INTERCHANGE CD1 AND CD2 FOR LEUCINES
REMARK   7  32, 57, 79, 95, 108.  INTERCHANGE CG1 AND CG2 FOR VALINES
REMARK   7  10, 78.  CORRECT SCALE MATRIX.  07-APR-80.
*DELETE,1C2C.54,55
SCALE2      0.000000   .026767  0.000000        0.000000
SCALE3      0.000000  0.000000   .011818        0.000000
.
. CARDS OMITTED HERE
.
*DELETE,1C2CC.5
MASTER       62    0    1    6    0    4    0    6  904    1   48    9

*IDENT,2ADHI
*INSERT,2ADHH.6
REMARK  13
REMARK  13 CORRECTION. FIX ERRORS ON ATOM 1384 WHICH WERE INTRODUCED
REMARK  13  BY BAD DUPLICATION ON 07-APR-80.  07-JUL-80.
*DELETE,2ADHH.30
ATOM   1384  CG2 VAL   186       3.300  19.950  35.450  1.00  0.00
*DELETE,2ADHH.61
MASTER      116    0    3   10   22   17    0    6 2801    1   25   29
```

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.

REQUEST FORM

1. Name_____ Date_____

   Address_____ Telephone_____

   _____

   _____

   _____

2. Send the following information (please check):

   ( ) description of atomic coordinate entries (no charge, latest revision March 1979).

   ( ) the magnetic tape items listed below (from Table 1)

   _____ _____ _____ _____ _____

   (Item "DATAPRTP" comprises all atomic coordinate sets and programs)

   ( ) the microfiche items listed below (from Table 2)

   _____ _____ _____ _____ _____

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

4. 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

NOTE: All current coordinate entries and programs can be written to one 2400' reel of magnetic tape for one unit charge (see over) if some space economies are achieved by blocking the records. Please indicate here the maximum block size permitted if this is less than 5120 characters (bytes) _____.

(Please complete reverse side)

REQUEST FORM

5. Charges

(i) For requests to Brookhaven

A. Data preparation ($63.80 charge per magnetic tape) $ _____

B. Magnetic Tape (charge per tape) $ 8.85 $ _____
(please include if answer to 3 above was NO)

C. Postage (per magnetic tape) $ _____
U.S. and Canada $ 2.00 ( ) $ _____
Air Mail to Other Countries $17.00 ( )

D. Microfiche items (Price from Table 2) $ _____

E. Total Charge $ _____

F. 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 are shipped. Inclusion of check with order will expedite processing.

(ii) For requests to Cambridge

A. Data preparation and postage (per user-supplied tape) _____
Within United Kingdom £ 27.50 ( )
Elsewhere £ 35.00 ( )

B. Magnetic tape £ 8.00 ( )
(please check if NO was checked on 3 above) _____

C. Microfiche (please inquire for prices) _____

D. Total Charge _____

Please return to

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

or

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