

THE PROTEIN DATA BANK

NEWSLETTER

Number 11

January 1980

We are pleased to announce that Professor Harold Scheraga of Cornell University has agreed to serve on the Protein Data Bank Advisory Board for a three-year term. Also continuing on the Board are Dr. David Davies (NIH) and Professor Michael Rossmann (Purdue). At this time we would like to express our deepest appreciation to Professor Ken Neet of Case Western Reserve University for having served on the Board since its inception in 1975. The Advisory Board was formed to oversee the Data Bank and continues to provide advice, support and perspective for our activities.

Thomas Koetzle will be attending the Alabama ACA Meeting March 17-21, and Enrique Abola will be at the West Coast Protein Workshop at Asilomar March 16-19. We will be delighted to discuss the Data Bank with users, contributors and anyone who may be interested. We are especially eager to receive suggestions for improvements and new services which we may offer.

We have just finished analyzing the returns of the questionnaire sent out last year to data recipients. The survey was designed to aid us in planning for future activities, and the replies have helped us to understand the makeup of our present user community and suggest additional types of services we could offer that might be found generally beneficial. Out of 91 questionnaires mailed, 38 were returned. Interestingly, half of those responding are crystallographers and half belong to other disciplines. More than three-quarters of the replies indicated interest in our plans to develop new computer programs which operate on the atomic coordinate data. Only about a quarter of the responses indicated use of the Data Bank in teaching, and we are currently exploring possibilities whereby the Bank can have a greater impact in this area (e.g. in courses on molecular structure/function relationships). The comments from the questionnaire were generally favorable and encouraging, and we intend to incorporate several of the specific suggestions as part of our future plans.

Up-to-date holdings information is given in Tables 1-5. The Bank continues to grow, and a total of 126 atomic coordinate entries are now available for distribution. The deposition by Professor Rossmann of coordinates for the coat protein of southern bean mosaic virus has added yet another dimension to our holdings. We are optimistic that in the very near future, coordinates from other viruses will become available.

A list of substantive corrections which have been applied to the coordinate entries since the last Newsletter is given in Table 6. The complete set of corrections is available on microfiche from Brookhaven 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.

Charges

A revised schedule of charges for requests to Brookhaven is given in the request form. The data preparation charge for distributions on magnetic tape has risen slightly (from \$55.20 to \$63.80 per tape). To ensure proper payment and prompt distribution, please use this current form for requests to Brookhaven or Cambridge; users in Australia and Japan should contact their centers for ordering information.

Area	Address of Center	Name	Telephone
The Americas	Protein Data Bank	E. Abola	516-345-4383
	Chemistry Department	F. C. Bernstein	516-345-4382
	Brookhaven National Laboratory Upton, New York 11973 USA	T. F. Koetzle	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
31-JAN-80

CODE	ITEM
DATAPRTP	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3.4)
NONSTDFI	ALL STRUCTURE FACTOR HOLDINGS (TABLE 5)
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS
CONNECTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS
DGPLOTPP	DIAGONAL PLOTS (LINE PRINTER)
DSTNCEP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES
FISITLTP	PHI/PSI PLOTS (LINE PRINTER)
PHIPSIIP	LISTS OF PHI/PSI/OMEGA VALUES

* NEW OR REPLACEMENT ENTRY SINCE OCT-79 NEWSLETTER

ITEM DSTNCEP REQUIRES TWO TAPES AT 800CPI. OTHER ITEMS COMPRISE ONE TAPE EACH

TABLE 2. PROTEIN DATA BANK. INFORMATION AVAILABLE ON MICROFICHE
31-JAN-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
CORRDSFI	*LIST OF CORRECTIONS NO. 5 (AUG/79-JAN/80)	1	FREE
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	2	\$66.66
CONNECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	12	\$80.96
DGPLOIFI	DIAGONAL PLOTS (LINE PRINTER)	5	\$70.95
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	24	\$98.12
FISITLFI	PHI/PSI PLOTS (LINE PRINTER)	1	\$65.23
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	5	\$70.95

* NEW OR REPLACEMENT ENTRY SINCE OCT-79 NEWSLETTER

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

TABLE 2. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

31-JAN-80

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/STATUS
1APF	*ACID PROTEINASE (ENDOTHIA PARASITICA)	T. BLUMHILL	10/79
1APY	*ACID PROTEINASE (PENICILLIUM ANTHRALINUM)	N. JAMES, I. HSU	12/79 H
1APZ	*ACID PROTEINASE (RHIZOPUS CHINESIS)	D. BAYLES	8/79
2ACF	*ACTINIDIN	E. BAKER	11/79 N
2AKK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77 R
1AGA	AGAROSE	S. ARNOTT	5/78 N
1AGA	AGGLUTININ (WHEAT GERM)	C. MRIGHT	2/78 A
1ADH	ALCOHOL DEHYDROGENASE (GDP-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
1ATC	ASPARTATE CARBOXYL TRANSFERASE	CRAWFORD, DONACO, LIPSCOMB	8/79
2BCL	BACTERIOCHLOROPHYLL A-PROTEIN	B. MATTHEWS	1/79 PA
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6B	R. KRETSINGER	8/74
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	8/74
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI 141)	S. ARNOTT	5/78 H
1CAG	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	6/76
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76
1CPA	CARBOXYPEPTIDASE A (BOVINE)	M. LIPSCOMB	2/73
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M. SCHMID, J. HEPIOTT	9/76 A
1CAR	CARRAGEENAN	S. ARNOTT	5/78 H
1C4S	CHONDROITIN-4-SULFATE	S. ARNOTT	5/78 H
2C4S	CHONDROITIN-4-SULFATE (CA SALT)	S. ARNOTT	5/78 H
2C1A	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/75 R
3C1A	ALPHA-CHYMOTRYPSIN	A. TULINSKY	8/76
1GCH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	2/77
1C1G	CHYMOTRYPSINOGEN	J. KRAUT, J. BIRKHOFF	3/75
2C1A	CALCAREALIN A	G. REEKE, J. BECKER, G. EDELMAN	4/75
3C1A	CALCAREALIN B	K. HORNMAN	9/76 R
2C5C	CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77 R
156B	CYTOCHROME B562 (E. COLI, OXIDIZED)	BETHGE, CZEPWINSKI, MATHEWS	8/79
1C5T	CYTOCHROME C (CALBACORE, OXIDIZED)	R. TICKERSON	9/76
2C5T	CYTOCHROME C (CALBACORE, REDUCED)	R. TICKERSON	9/76
1C5L	CYTOCHROME C (Rabbit, HEART)	M. KAMUDO	8/76
1C2C	CYTOCHROME C2	J. KRAUT	3/73
155C	CYTOCHROME C550	R. TIKHOVICH	8/76
251C	CYTOCHROME C551	R. TICKERSON	8/78 R
1E5T	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76
1E5D	ERYTHROCRUORIN (REDUCED, DEOXY)	M. STEIGEMANN, E. WEBER	3/79
1E5C	ERYTHROCRUORIN (CARBOHYMOXY)	M. STEIGEMANN, E. WEBER	3/79
1E5A	ERYTHROCRUORIN (AQUO, MET)	M. STEIGEMANN, E. WEBER	3/79
1E5H	ERYTHROCRUORIN (CYANO, MET)	M. STEIGEMANN, E. WEBER	3/79
1E5X	FERRIDOXIN (PEPTOCOCCUS AERGENES)	E. ANHAN, L. STEFER, L. JENSEN	8/76
1E5Y	FERRIDOXIN (SPIRULINA PLATENSIS)	H. KAMUDO	8/79
1E5Z	FERRIDOXIN (CLUSTRIUM NP, OXIDIZED)	N. LUDWIG	12/77 R
4E5I	FERRIDOXIN (CLUSTRIUM NP, SERRAVALONE)	N. LUDWIG	12/77
1G5H	GLUCAGON	T. BLUMHILL	10/77
1PG1	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MURHEAD	7/77
1GGP	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	H. ROSSMANN	7/75
2GGD	*GDP-GLYCERALDEHYDE-3-P-DEHYDROGENASE	H. ROSSMANN	12/79 H
1H1B	HEMPYRININ B	D. HERRICKSON	6/76 A
1H1A	HEMPYRININ (MET, AQUO)	P. STENKAMP ET AL.	1/79 A
1H1S	HEMOGLOBIN (HEK, STEPLE CELL)	E. ANHAN, R. STALING	10/79
2H1B	HEMOGLOBIN (HORSE, AQUO, MET)	R. LADNER, H. JINER, PEPUTZ	2/77 R
2H1G	HEMOGLOBIN (HORSE, DEOXY)	H. PERUTZ, G. FERRE	11/73
1H1R	HEMOGLOBIN (HUMAN, DEOXY)	H. PERUTZ, G. FERRE	1/75
1H1C	HEMOGLOBIN (HUMAN, CARBOHYMOXY)	J. BALDWIN	8/79
2H1D	HEMOGLOBIN (HUMAN, CARBOHYMOXY, NRG REFIND)	J. FRIER	8/76
1H1H	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	HENDRICKSON, LOVE, KARLE	3/73
1H1B	HEMOGLOBIN (LADFREY)	STELTZ, ANDERSON, STENKAMP	3/78 R
2H1X	HEMOGLOBIN (YEAST) FORM B11	J. KRAUT	4/75
1H1P	HIGH POTENTIAL IRON PROTEIN	S. ARNOTT	11/77
1H1A	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78 N
2H1A	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S. ARNOTT	5/78 N
3H1A	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S. ARNOTT	5/78 N
4H1A	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78 N
2H1A	HUMANOGLOBIN IN FAB*	R. POLJAK	6/79
1H1G	HUMANOGLOBIN B-J INTACT HCG	SCHIFFER, EDMUNDSON ET AL.	5/78 A
1H1F	HUMANOGLOBIN B-J FRAGMENT (Y-DIMER) REI	O. EPP, R. HUBER	3/76
1H1E	HUMANOGLOBIN B-J FRAGMENT (Y-DIMER) PHE	B. MANS, C. YOO, H. SAX	12/77 A

1KGA	KIPPS ALDOLASE	A. TULINSKY	8/78 H
1KES	KERATAN SULFATE	S. ARNOTT	5/78 H
4L1H	LACTATE DEHYDROGENASE	U. EVENTOFF, H. ROSSMANN	4/77 R
3L1H	LACTATE DEHYDROGENASE (HAD-PYRUVATE)	H. ROSSMANN	11/74
1L1Z	LACTATE DEHYDROGENASE (HOUSE TESTES)	U. HUSICK, H. ROSSMANN	9/78
1H1L	LEIGHENIOLIN	VAHISIKI, H. HARUYUKIYAN	11/78
1L2H	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS	3/77
1L1Z	LYSOZYME (HEN EGG-WHITE, SET W2)	R. DIAMOND, D. PHILLIPS	2/75
2L1Z	LYSOZYME (HEN EGG-WHITE, SET R55D)	R. DIAMOND, D. PHILLIPS	2/75
3L1Z	LYSOZYME (HEN EGG-WHITE, SET R56A)	R. DIAMOND, D. PHILLIPS	2/75
4L1Z	LYSOZYME (HEN EGG-WHITE, SET R59A)	R. DIAMOND, D. PHILLIPS	2/75
5L1Z	LYSOZYME (HEN EGG-WHITE, SET R512A)	R. DIAMOND, D. PHILLIPS	2/75
6L1Z	LYSOZYME (HEN EGG-WHITE, SET R516)	R. DIAMOND, D. PHILLIPS	2/75
7L1Z	LYSOZYME (HEN EGG-WHITE, TRICHLINIC)	A. YONATH	5/77
8L1Z	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY	9/77
9L1Z	*LYSOZYME (HEN, HAN-NAG-HAN SUBSTRATE ONLY)	J. KELLY, M. JAMES	12/79 H
1H1H	MALATE DEHYDROGENASE	L. BANASZAK	6/76 A
1H1P	MUREIN LIPOPROTEIN (HYPOTHETICAL)	A. MCLACHLAN	8/78
1H1B	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON	4/73
2H1B	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	9/76
3H1B	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	9/76
1H1S	MYOGLOBIN (SEAL, MET)	H. SAKOULOU DI	3/79
1H1R	NYOHENERYTHRIN	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 (BZOXI-GLY-PHE-GLY, CYS-25)	J. DRENTH	11/76 R
6PAD	PAPAIN (BZOXI-PHE-ALA, CYS-25)	J. DRENTH	11/76 R
1PEP	PEPSIN (PORCINE)	N. ANDREVA ET AL.	7/78 A
1PKK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON	5/76 A
2PKK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE	9/76 D
1PGH	PHOSPHOGLYCERATE MUTASE	CAMPBELL, WATSON, HODGSON	8/75 A
2PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, C. BLAKE	9/77 R
1PKY	*PYRUVATE KINASE (CAT)	H. MUIPHEAD	1/80 AN
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	RHODANASE	W. HOL	12/77
2PSA	RIBONUCLEASE A	A. M. ODAWER	6/79
1RHS	RIBONUCLEASE S	H. WICKOFF, F. RICHARDS	4/73
2RXN	RUBREDOXIN	L. JENSEN	1/75
1SHS	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	4/73
1SGH	STREPTOMYCES GRISEUS PROTEINASE A	BRAYER, DELBAERE, JAMES	6/78
2SGB	STREPTOMYCES GRISEUS PROTEINASE B	DELBAERE, BRAYER, JAMES	6/79 R
1SSI	SUBTILISIN INHIBITOR (STREPTOMYCES)	Y. HITSUI ET AL.	1/79 A
1SBT	SUBTILISIN 6PH*	J. KRAUT	8/72
2SBT	SUBTILISIN 10JO	J. DRENTH	9/76
1SOP	SUPEROXIDE DISMUTASE	J. RICHARDSON, D. RICHARDSON	8/75 A
11LN	THERMOLYSIN (UNREFINED)	B. MATTHEWS	4/75
21LN	THERMOLYSIN (REFINED)	B. MATTHEWS	4/75
1SRX	THIOREDOXIN (E. COLI, OXIDIZED)	B. - O. SODERBERG	5/76 A
4THA	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG	4/78 R
6THA	TRANSFER RNA (YEAST, PHE)	S. - H. KIM ET AL.	11/78 R
8THA	TRANSFER RNA (YEAST, PHE)	M. SUNDARLINGAM	2/79 R
1T1H	TRIOSE PHOSPHATE ISOMERASE	T. WILSON, D. PHILLIPS	9/76
1P1H	TRYPsin (NATIVE, PH8)	FEHLHÄNER, BODE, SCHWAGER	1/77
2P1B	TRYPsin (BENZAMIDINE INHIBITED, PH7)	FEHLHÄNER, BODE, SCHWAGER	1/77 R
1PTC	TRYPsin (TRYPsin INHIBITOR COMPLEX)	R. HUBER, W. BODE	11/76
3P1I	TRYPsin INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	11/76 R
3P1P	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 (TGS04, WITHOUT CA)	BODE, FEHLHÄNER, HUBER	3/79
1TGB	TRYPsinOGEN (WITH CA, FROM PEG)	BODE, FEHLHÄNER, HUBER	3/79
1TGH	TRYPsinOGEN	A. KOSSIAKOFF, R. STROUD	9/79
1SBV	*VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC)	H. ROSSMANN	12/79 BN

* NEW OR REPLACEMENT ENTRY SINCE OCT-79 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

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
BEHNER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	1/79 YES
CONNECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	4/79 YES
CONTACT	*INTERMOLECULAR CONTACTS	L.ANDREWS	10/79 NO
DGDPLOT	DIAGONAL PLOTS ON PRINTER	E.SAMMONS,F.BERNSTEIN	3/79 YES
DISTNCE	CALC DISTANCES FROM CORRECT RECORDS	F.BERNSTEIN	3/79 YES
FISPLP	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79 YES
NAMOP	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78 NO
PHIPSI	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	2/79 YES
STERED	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 OCT-79 NEWSLETTER

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

TABLE 6. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

IDENT	DATE	REMARK	REV	DATE	SUPPORTED
*IDENT.2DHRD					
*INSERT.2DHRC.2					
REMARK 10					
REMARK 10 CORRECTION. CORRECT VALUE OF Z ON CRYST1 RECORD (SHOULD BE Z=0). 29-AUG-79.					
*DELETE.2DHR.87					
CRYST1	76.960	81.700	92.630	90.00	90.00 90.00 C 2 2 21 8
*DELETE.2DHRC.4					
MASTER	64	7	2	16	0 0 0 9 2269 2 92 23
*IDENT.1GCHB					
*INSERT.1GCHA.3					
REMARK 6					
REMARK 6 CORRECTION. FIX NAMING AND HENCE ORDERING OF TWO ATOMS.					
REMARK 6 22-OCT-79.					
*DELETE.1GCH.94.95					
ATOM	45	CE1	PHE	6	35.813 27.967 13.909 1.00 12.00
ATOM	46	CE2	PHE	6	37.306 29.328 15.177 1.00 12.00
*DELETE.1GCH.153.154					
ATOM	104	CE1	TYR	13	24.713 25.229 15.120 1.00 8.00
ATOM	105	CE2	TYR	13	25.108 26.342 13.035 1.00 8.00
*DELETE.1GCHA.5					
MASTER	30	2	0	1	0 0 0 6 246 1 0 3
*IDENT.1ECAA					
*INSERT.1ECA.65					
REMARK 6					
REMARK 6 CORRECTION. INSERT MISSING ALTERNATE LOCATION INDICATOR FOR ATOM OG OF SER 134. ALSO CORRECT OCCUPANCY AND REORDER					
REMARK 6 TO MEET SPECIFICATIONS. 12-DEC-79.					
*DELETE.1ECA.1131.1132					
ATOM	1031	OG	BSER	134	-4.732 19.389 36.529 .50 19.98
ATOM	1032	OG	BSER	134	-6.478 20.998 35.669 .50 23.76
*DELETE.1ELA.1336					
MASTER	58	5	1	9	0 0 0 6 1187 1 46 11

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLD

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
RIACTSF	ACTINIDIN	E.BAKER	7/77 SF
CH710F	ALPHA-CHYMOTRYPSIN (TOSYL)	D.BLOW	4/73 SF
RCARPO4	CALCIUM-BINDING PARVALBUMIN	R.KRETSINGER	2/74 SF
RCARPO5	CALCIUM-BINDING PARVALBUMIN	R.KRETSINGER	2/74 SF
R2B5CSF	CYTOCHROME B5	F.S.MATHEWS	12/77 SF
RTUHDZ01	CYTOCHROME C (ALBACORE, OXIDIZED)	R.DICKERSON	5/76 SF
RTUHDZ01	CYTOCHROME C (ALBACORE, REDUCED)	R.DICKERSON	5/76 SF
RCYC5501	CYTOCHROME C550	P.FILKOVICH	4/76 SF
R151CSF	CYTOCHROME C551	R.DICKERSON	8/78 SF
R6PD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	H.ROSSMANN	8/75 SF
R26PDSF	*APO-GLYCERALDEHYDE-3-P-HYDROGENASE	H.ROSSMANN	12/79 SF
RH0DHD02	HEMOGLOBIN (HUMAN, DEOXY)	H.HERPITZ,G.FERMI	5/75 SF
LAFRY1	HEMOGLOBIN (LAIPREY)	HERPITZ,LOVE,KARLE	5/73 SF
RLDH06	LACTATE DEHYDROGENASE	H.ROSSMANN	8/75 SF
RLDH07	LACTATE DEHYDROGENASE/MDP/PYRUVATE	H.ROSSMANN	8/75 SF
RNICHTY5F1	MYOGLOBIN (SPERM WHALE, MET)	T.TAKANO	6/76 SF
RDEHYSE1	MYOGLOBIN (SPERM WHALE, DEOXY)	T.TAKANO	6/76 SF
RRUBY02	RUBREDOXIN	L.JENSEN	3/74 SF

* NEW OR REPLACEMENT ENTRY SINCE OCT-79 NEWSLETTER

CODES
SF STRUCTURE FACTORS

THE CORRECTIONS IN THIS TABLE ARE GIVEN IN THE FORM OF 'UPDATE' INDICATORS 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 68342500. 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 '*IMHA' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK 'IMBH' FOR SPERM-WHALE MYOGLOBIN. '*IMHB' 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 SET 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)

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:

- | | | | |
|----------------------------------|-----------------------------------|--|--|
| <input type="checkbox"/> 7 track | <input type="checkbox"/> 556 cpi | <input type="checkbox"/> BCD-7 track only | <input type="checkbox"/> Unlabelled
(preferred) |
| <input type="checkbox"/> 9 track | <input type="checkbox"/> 800 cpi | <input type="checkbox"/> ASCII-9 track only | <input type="checkbox"/> Labelled, -
User's label |
| | <input type="checkbox"/> 1600 cpi | <input type="checkbox"/> 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

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.