Number 15 THE PROTEIN DATA BANK January 1981
NEWSLETTER

The XIIth Congress and General Assembly of the International Union of Crystallography will be held at Carleton University in Ottawa, Canada from 16-25 August 1981. We will be making a presentation about the Protein Data Bank and are looking forward to meeting users at the Congress. If anyone would like to visit Brookhaven before or after the congress please get in touch with us. We are about 70 miles (110 km) east of New York City; please contact us in advance for information regarding transportation and accommodations.

In the near future the Protein Data Bank hopes to publish a brief list of sources for visual aids (other than computer graphics) in the field of protein structure. Included would be models, 35 mm slides, movies and so forth. We presently are contacting about 15 sources; please inform us if you feel you should be included or know of someone else who should be.

A partial list of substantive corrections which have been applied to the atomic coordinate entries since August 1980 is given in Table 7. 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. As indicated in our last Newsletter, we have added bibliographic entries for macromolecular structures for which coordinates are not yet available. (A current list of these entries is presented in Table 6). These bibliographic entries are being actively maintained but the revisions will not be listed in Table 7 and will not appear on the correction fiche.

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	
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 3168 Australia	C. Garrow	544-0633
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

08-JAN-81

CODE	ITEM	NO.TAPES 800	1600	AVAILABILITY US	UK	JA	AUS
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 6)	2	1	X	X	X	X
NONSTDTP	ALL STRUCTURE FACTOR HOLDINGS (TABLE 5)	2	1	X	X	X	
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	X			
BLDKITTP	MODEL BUILDER*S KIT	PLEASE INQUIRE AT US CENTER					
CONECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	X			
DGPLOTTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	X			
DIHDRLTP	COMPLETE TORSION ANGLES	2	1	X			
DSTNCETP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	X			
FISIPLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	X			
PHIPSITP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	X			

* NEW OR REPLACEMENT ENTRY SINCE OCT-80 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

08-JAN-81

CODE	ITEM	AVAILABILITY US	UK	JA	AUS
DATAPRFI	ALL CURRENT COORDINATE ENTRIES AND PROGRAMS (TABLES 3,4)	X	X	X	
NONSTDFI	ALL STRUCTURE FACTOR HOLDINGS (TABLE 5)	X	X	X	
CORR06FI	LIST OF CORRECTIONS NO. 6 (JAN/80-JUL/80)	X	X	X	X
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X			
BLDKITFI	MODEL BUILDER*S KIT	PLEASE INQUIRE AT US CENTER			
CONECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X			
DGPLOTFI	DIAGONAL PLOTS (LINE PRINTER)	X			
DIHDRLFI	COMPLETE TORSION ANGLES	X			
DSTNCEFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X			
FISIPLFI	PHI/PSI PLOTS (LINE PRINTER)	X			
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	X			

* NEW OR REPLACEMENT ENTRY SINCE OCT-80 NEWSLETTER

TABLE 4. PROTEIN DATA BANK. AVAILABLE PROGRAMS

08-JAN-81

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 OCT-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

08-JAN-81

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
RGPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M.ROSSMANN	8/75 SF
R2GPDSF	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M.ROSSMANN	12/79 SF
R2MHBSF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER,HEIDNER,PERUTZ	6/80 SF
R1FDHSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J.FRIER	6/80 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
R4TNASF	TRANSFER RNA (YEAST, PHE)	A.JACK,J.LADNER,A.KLUG	6/80 SF

* NEW OR REPLACEMENT ENTRY SINCE OCT-80 NEWSLETTER

CODES

SF STRUCTURE FACTORS

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

08-JAN-81

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/ STATUS	
1APE	ACID PROTEINASE(ENDOTHIA PARASITICA)	T.BLUNDELL	10/79	
1APP	ACID PROTEINASE(PENICILLIUMJANTHINELLUM)	M.JAMES,T.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	
1ATC	ASPARTATE CARBAMOYLTRANSFERASE	CRAWFORD,MONACO,LIPSCOMB	8/79	A
1AZU	AZURIN	E.ADMAN,L.SIEKER,L.JENSEN	8/80	
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 6I	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	4/75	
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	R
4CYT	CYTOCHROME C (ALBACORE, REDUCED)	T.TAKANO,R.DICKERSON	7/80	R
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	
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	
1GRS	*GLUTATHIONE REDUCTASE (HUMAN)	G.SCHULZ	12/80	AN
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	
1HKG	*HEXOKINASE A - GLUCOSE COMPLEX (YEAST)	W.BENNETT JR.,T.STEITZ	12/80	P
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	
1KGA	KDPG ALDOLASE	A.TULINSKY	8/78	A
1KES	KERATAN SULFATE	S.ARNOTT	5/78	
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)	W.MUSICK,M.ROSSMANN	9/78	
4LDH	LACTATE DEHYDROGENASE (PIG)	W.EVENTOFF,M.ROSSMANN	4/77	R
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE(PIG)	M.ROSSMANN	11/74	
5LDH	*LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U.GRAU,M.ROSSMANN	10/80	N
1HBL	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
1NXB	NEUROTOXIN B (LATICAUDA SEMIFASCIATA)	D.TSERNOGLOU,G.PETSKO	8/80	N
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
1PCY	PLASTOCYANIN	J.GUSS,H.FREEMAN	8/80	
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(CLOSTRIDIUM PASTEURIANUM)	L.JENSEN	1/75	
3RXN	RUBREDOXIN(DESULFOVIBRIO VULGARIS)	E.ADMAN,L.SIEKER,L.JENSEN	9/80	
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	
1TNC	TROPONIN (CA-BINDING COMPONENT,MODEL)	R.KRETSINGER,C.BARRY	6/80	A
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	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	B

* NEW OR REPLACEMENT ENTRY SINCE OCT-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 6. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

08-JAN-81

0EAP	ACID PROTEINASE (ENDOTHIA PARASITICA)
0AF1	APOFERRITIN (HORSE)
0MAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
0CTS	CITRATE SYNTHASE (PIG)
0CTX	ALPHA COBRATOXIN
0CN1	CONCANAVALIN A (DEMETALLIZED)
0CN2	CONCANAVALIN A (DEMETALLIZED)
0CYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)
0CCY	CYTOCHROME C* (RHODOSPIRILLUM MOLISCHIANUM)
0CY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)
05C1	CYTOCHROME C555 (CHLOROBIUM THIOSULFATOPHILUM)
0ESZ	ELASTASE COMPLEX (PIG)
0ETU	ELONGATION FACTOR TU COMPLEX (E. COLI)
0EBX	*ERABUTOXIN B
0FD1	FERREDOXIN (AZOTOBACTER VINLANDII)
0FX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)
0FX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)
0GP1	GLUTATHIONE PEROXIDASE (BOVINE)
0GD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)
0HBG	HEMOGLOBIN (GLYCERA DIBRANCHIATA)
0PHH	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)
0AUI	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU
0ROY	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY
0MCP	IMMUNOGLOBULIN FAB (KAPPA) MCP603
0FB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL
0FC2	IMMUNOGLOBULIN FC (HUMAN) - FRAGMENT B OF PROTEIN A (STAPH AUREUS) COMPLEX
0FC1	IMMUNOGLOBULIN FC (HUMAN)
0IG1	IMMUNOGLOBULIN G1 (KAPPA) DOB
0IG2	IMMUNOGLOBULIN G1 (LAMBDA) KOL
0IN2	INSULIN (PORCINE)
0GF1	INSULIN-LIKE GROWTH FACTOR I (HUMAN)
0GF2	INSULIN-LIKE GROWTH FACTOR II (HUMAN)
0LZ1	LYSOZYME (HUMAN)
0LZ2	LYSOZYME (TURKEY)
0LZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)
0CTF	L7/L12 (E. COLI, C-TERMINUS)
0MB5	MYOGLOBIN (SPERM WHALE, CARBON MONOXIDE, NEUTRON STUDY)
0MBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)
0MB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)
0MB4	MYOGLOBIN (SPERM WHALE, OXY)
0PFK	PHOSPHOFRUCTOKINASE (BACILLUS STEAROTHERMOPHILIUS)
0BP2	PHOSPHOLIPASE A2 (BOVINE)
0BP1	PHOSPHOLIPASE A2 (PORCINE)
0PPA	PHOSPHORYLASE A (RABBIT)
0PB1	PHOSPHORYLASE B (RABBIT)
0RX5	RELAXIN (PORCINE, MODEL)
0RSA	RIBONUCLEASE A (BOVINE)
0RN3	RIBONUCLEASE A (BOVINE)
0FMT	INITIATOR TRANSFER RNA (E. COLI, F/MET)
0TR1	TRANSFER RNA (YEAST, PHE)
0TS1	TYROSYL TRANSFER RNA SYNTHETASE (BACILLUS STEAROTHERMOPHILUS)
0GN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)
0UTG	UTEROGLOBIN (RABBIT)
0TMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)
0TBV	VIRUS (TOMATO BUSHY STUNT)

* NEW OR REPLACEMENT ENTRY SINCE OCT-80 NEWSLETTER

TABLE 7. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

08-JAN-81

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 ↑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 PARTICULAR RECORD AFTER WHICH INFORMATION IS TO BE INSERTED. THE RECORDS TO BE INSERTED FOLLOW IMMEDIATELY AFTER ↑*INSERT↑ IN THE CORRECTION SET. WITHIN EACH CORRECTION NEW RECORDS PLACED IN THE FILE ARE GIVEN THE ↑IDENT↑ NAME AND NUMBERED SEQUENTIALLY.

```
*IDENT,2DFRA
*INSERT,2DFR.67
REMARK   7
REMARK   7 CORRECTION. CHANGE RESOLUTION FROM 2.5 TO 2.0 ANGSTROMS.
REMARK   7 09-OCT-80.
*DELETE,2DFR.36
REMARK   2 RESOLUTION. 2.0 ANGSTROMS.
*DELETE,2DFR.2551
MASTER       63    0    2    8   16    0   10    9 2339    1   70   26

*IDENT,1PCYA
*INSERT,1PCY.46
REMARK   6
REMARK   6 CORRECTION. FIX (1,1) ELEMENT OF SCALE MATRIX.  05-NOV-80.
*DELETE,1PCY.83
SCALE1       .033772  0.000000  0.000000        0.00000
*DELETE,1PCY.907
MASTER       42    2    1    1    9    9    0    6  783    1   37    8

*IDENT,1ATCB
*INSERT,1ATCA.4
REMARK   9
REMARK   9 CORRECTION.  CORRECT X-COORDINATE OF ALL ATOMS AND ZN
REMARK   9  HETATM.  CORRECT ORIGX, SCALE, AND MTRIX TRANSFORMATIONS.
REMARK   9  04-DEC-80.
*DELETE,1ATC.49,57
ORIGX1       .866025   .500000  0.000000        0.00000
ORIGX2      -.500000   .866025  0.000000        0.00000
ORIGX3      0.000000  0.000000  1.000000      -35.05600
SCALE1       .008190   .004729  0.000000        0.00000
SCALE2      -.000000   .009457  0.000000        0.00000
SCALE3      0.000000  0.000000   .007037        -.00000
MTRIX1   1  -.258446  -.966042  0.000000       110.87925
MTRIX2   1  -.966042   .258446  0.000000        85.11150
MTRIX3   1 0.000000  0.000000 -1.000000        70.11200
*DELETE,1ATC.58,471
ATOM       1  CA  UNK R   1      18.637  82.120  51.256  1.00  0.00
ATOM       2  CA  UNK R   2      21.802  81.638  50.156  1.00  0.00
ATOM       3  CA  UNK R   3      23.401  81.869  47.356  1.00  0.00
ATOM       4  CA  UNK R   4      26.526  82.056  45.056  1.00  0.00
ATOM       5  CA  UNK R   5      27.115  83.436  41.656  1.00  0.00
  .
  .
  .
ATOM     412  CA  UNK C 303      58.912  56.761  80.956  1.00  0.00
ATOM     413  CA  UNK C 304      61.971  55.063  80.156  1.00  0.00
ATOM     414  CA  UNK C 305      64.483  56.513  81.856  1.00  0.00
*DELETE,1ATC.473
HETATM  416 ZN   ZN     1      53.843  64.342  46.256  1.00  0.00
*DELETE,1ATCA.5
MASTER       43    0    1    0    0    0    0    9  415    1    0    2
```

REQUEST FORM

1. Name _____ Date _____
   Address _____ Telephone _____
   _____
   _____

2. Tape format desired (all tapes are unlabelled)

   ( ) 9 track, 1600 cpi, EBCDIC
   ( ) 9 track, 800 cpi, EBCDIC
   ( ) 9 track, 1600 cpi, ASCII
   ( ) 9 track, 800 cpi, ASCII
   ( ) 7 track, 800 cpi, BCD

   Only the first two formats are normally prepared at Cambridge; please inquire for availability of other formats.

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

3. ( ) Please send a description of the atomic coordinate entries at no charge (latest revision March 1979).

4. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs $96 (45); each 2-tape item costs $116 (53).

Item	Number of Tapes	Cost

Total _____

5. Please send the following microfiche items (from Table 2). Each microfiche item costs $81 (36 from Cambridge). Correction fiche are free.

Item	Cost

Total _____

6. Air mail postage from Brookhaven to destinations outside U. S. and Canada or from Cambridge to destinations outside the United Kingdom. A postage surcharge of $15 (5) is required per magnetic tape (not per item).

Number of tapes x $15.00 (5) = _____

7. Total charges

Magnetic tape charges (4 above) _____

Microfiche charges (5 above) _____

Air mail postage charges (6 above). _____

Total _____

For Brookhaven only:

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

Payment to the order of Brookhaven National Laboratory

by ( ) check
( ) purchase order number _____

is ( ) enclosed
( ) sent separately to the Protein Data Bank

Please return to

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

or

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