

## NEWSLETTER

With the start of the new fiscal year at Brookhaven, we regret to announce that our charges are increasing effective immediately. The charges described here apply only for requests to Brookhaven and Cambridge; users in Japan and Australia should inquire at their respective centers. Each microfiche item will cost \$84.00 (~~47~~) except for the correction fiche which is free. Each tape item will cost \$122.00 (~~68~~) including a new 2400' reel of tape and domestic postage. If Table 1 indicates that the item requires two tapes then the charge will be \$147.00 (~~82~~) including the cost of two tapes and postage. There is an additional charge of \$15.00 (~~8~~) per magnetic tape to cover foreign airmail postage where appropriate.

Over the course of the next few years we anticipate making some changes in the format of our atomic coordinate entries. As far as possible we will do this by adding new types of records; user programs should thus be prepared to handle or ignore record types that are not currently defined. Any revisions to existing record types will be announced well in advance via the Newsletter. Because of user requests we are reserving a class of records for user definition and use. All records beginning with the four letters USER are hereby reserved for user definition and will be ignored by our programs.

We have now received so many structure factor entries that they no longer can fit on one magnetic tape at 1600 cpi. Because these entries do not change we have subdivided them in two items, each of which may be ordered separately. Items NONST1TP and NONST1FI contain "older" structure factor entries and it is expected that this item will not change. Items NONST2TP and NONST2FI will continue to grow as new structure factor entries are received.

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	E. Abola	516-282-4383
	Chemistry Department	F. C. Bernstein	516-282-4382
	Brookhaven National Laboratory Upton, New York 11973 USA	T. F. Koetzle	516-282-4384
Europe and Worldwide	University Chemical Laboratory	O. Kennard	0223-66499
	Lensfield Road Cambridge CB2 1EW, England	S. Bellard	
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002 Australia	C. Garrow	03-419-1333
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

		05-OCT-81				
CODE	ITEM	NO. TAPES		AVAILABILITY		
		800	1600	US	UK	JA AUS
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	2	1	X	X	X X
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	2	1	X	X	X
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	1	1	X	X	X
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	X		
BLDKITTP	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER				
CONNECTTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	X		
DGPLOTPP	DIAGONAL PLOTS (LINE PRINTER)	1	1	X		
DIHDLRTP	COMPLETE TORSION ANGLES	2	1	X		
DSTNCTTP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	X		
FIS1PLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	X		
PHIPSTTP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	X		

\* NEW OR REPLACEMENT ENTRY SINCE JUL-81 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

		05-OCT-81				
CODE	ITEM	AVAILABILITY				
		US	UK	JA AUS		
DATAPRFI	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	X	X	X		
NONST1FI	*STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	X	X	X		
NONST2FI	*STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	X	X	X		
CORROBFI	*LIST OF CORRECTIONS NO. 8 (JAN/81-JUL/81)	X	X	X X		
BENDERFI	PARAMETERS FOR BENT-WIRE MODELS	X				
BLDKITFI	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER				
CONNECTFI	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X				
DGPLOTFI	DIAGONAL PLOTS (LINE PRINTER)	X				
DIHDLRFI	COMPLETE TORSION ANGLES	X				
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X				
FIS1PLFI	PHI/PSI PLOTS (LINE PRINTER)	X				
PHIPSTFI	LISTS OF PHI/PSI/OMEGA VALUES	X				

\* NEW OR REPLACEMENT ENTRY SINCE JUL-81 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

IDENT	MOLECULE	DEPOSITOR(S)	DATE/ STATUS	MOLECULE	DEPOSITOR(S)	DATE/ STATUS
1A2U	AGAROSE	S. ARNOTT	5/78	4LDH	LACTATE DEHYDROGENASE (PIG)	W. EVENTOFF, M. ROSSMANN
1APP	*ACID PROTEINASE (ENDOTHRIA PARASITICA)	T. BLUNDELL	9/81 RP	3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE (PIG)	M. ROSSMANN
1APR	ACID PROTEINASE (RHIZOPUS CHINENSIS)	M. JAMES, I. HSU	12/79	5LDH	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU, M. ROSSMANN
2ACT	ACTININ	E. BAKER	11/79 R	1HBL	LEGHEMOGLOBIN	VAINSHTEIN, HARUTYUNYAN
2AKG	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77 R	1LZM	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS
2AGA	AGGLUTININ (WHEAT GERM)	C. WRIGHT	5/80 R	1LYZ	LYSOZYME (HEN EGG-WHITE, SET W2)	R. DIAMOND, D. PHILLIPS
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C. -I. BRANDEN	8/76	2LYZ	LYSOZYME (HEN EGG-WHITE, SET R55D)	R. DIAMOND, D. PHILLIPS
2ADH	ALCOHOL DEHYDROGENASE (ORTHO PHEN)	C. -I. BRANDEN	8/76	3LYZ	LYSOZYME (HEN EGG-WHITE, SET R56A)	R. DIAMOND, D. PHILLIPS
4ADH	ALCOHOL DEHYDROGENASE (APO)	C. -I. BRANDEN	8/79	4LYZ	LYSOZYME (HEN EGG-WHITE, SET R59A)	R. DIAMOND, D. PHILLIPS
1ALP	ALPHA LYTIC PROTEASE	BRAYER, DELBAERE, JAMES	6/79	5LYZ	LYSOZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND, D. PHILLIPS
1ABP	L-ARABINOSE-BINDING PROTEIN	F. QUIJOCHO, G. GILLILAND	5/80	6LYZ	LYSOZYME (HEN EGG-WHITE, SET RS16)	R. DIAMOND, D. PHILLIPS
1ATC	ASPARTATE CARBAMOYLTRANSFERASE	CRAMFORD, MONACO, LIPSCOMB	8/79 A	7LYZ	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	A. YONATH
1AZU	AZURIN	E. ADMAN, L. SIEKER, L. JENSEN	8/80	8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY
1ABX	ALPHA-BUNGAROTOXIN	R. AGARD, S. SPENCER, R. STROUD	4/80 A	9LYZ	LYSOZYME (HEN, NAM-NAG-NAM SUBSTRATE ONLY)	J. KELLY, M. JAMES
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74	1LZH	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	ARTYMIUK, BLAKE, RICE, WILSON
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74	2LZH	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	ARTYMIUK, BLAKE, RICE, WILSON
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	8/74	1LZ2	*LYSOZYME (TURKEY EGG-WHITE)	R. BOTT, R. SARMA
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	S. ARNOTT	5/78	1MDH	MALATE DEHYDROGENASE	L. BANASZAK
1CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	6/76	1MLT	*MELITTIN	TERWILLIGER, EISENBERG
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76	1MLP	MUREIN LIPOPROTEIN (HYPOTHETICAL)	A. MCLAUGHLIN
1CPA	CARBOXYPEPTIDASE A (BOVINE)	H. LIPSCOMB	2/73	1MBS	MYOGLOBIN (SEAL, MET)	H. SCLOULDI
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M. SCHMID, J. HERRIOTT	9/76 A	1MBN	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON
1CAR	CARRAGEENAN	S. ARNOTT	5/78	2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO
1CHS	CHONDROITIN-4-SULFATE	S. ARNOTT	5/78	3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO
2CHS	CHONDROITIN-4-SULFATE (CA SALT)	S. ARNOTT	5/78	1MBO	MYOGLOBIN (SPERM WHALE, OXY, NEUTRON)	S. PHILLIPS
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/75 R	1MHR	MYOHEMERYTHRIN	W. HENDRICKSON
3CHA	ALPHA-CHYMOTRYPSIN	A. TULINSKY	8/76	1NXB	NEUROTOXIN B (LATICAUDA SEMIFASCIATA)	D. TERNONGLOU, G. PETSKO
2CHC	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	5/80 R	1PPT	AVIAN PANCREATIC POLYPEPTIDE	T. BLUNDELL
1CAT	CATALASE (BEEF LIVER)	M. ROSSMANN	6/81 A	8PAP	PAPAIN (NATIVE)	J. DRENTH
1CHG	CHYMOTRYPSINOGEN	J. KRAUT, J. BIRKTOFT	3/75	1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)	J. DRENTH
2CNA	CONCAVALIN A	G. REEKE, J. BECKER, G. EDELMAN	4/75	2PAD	PAPAIN (CYS DERIV OF CYS-25)	J. DRENTH
3CNA	CONCAVALIN A	K. HARDMAN	9/76 R	3PAD	PAPAIN (OXIDIZED CYS-25)	J. DRENTH
1CRN	CRAMBIN	W. HENDRICKSON, M. TEETER	5/81	4PAD	PAPAIN (TOS-LYS, CYS-25)	J. DRENTH
2BSC	CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77 R	5PAD	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH
156B	CYTOCHROME B562 (E. COLI, OXIDIZED)	BETHGE, CZERWINSKI, MATHEWS	8/79	6PAD	PAPAIN (BZOXY-PHE-ALA, CYS-25)	J. DRENTH
3CVT	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80 R	1PEP	PEPSIN (PORCINE)	N. ANDREEVA ET AL.
4CVT	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO, R. DICKERSON	7/80 R	1PGK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON
1CYC	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	8/76	2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE
1CCY	*CYTOCHROME C PRIME	P. WEBER, R. SALEMME	8/81 P	2PGH	PHOSPHOLIPASE A2 (BOVINE)	H. C. WATSON
1C2C	CYTOCHROME C2	J. KRAUT	3/73	1BP2	PHOSPHOLIPASE A2 (BOVINE)	B. DIJKSTRA, J. DRENTH
155C	CYTOCHROME C550	R. TIMKOVICH	8/76	2BP2	PHOSPHOLIPASE A2	B. DIJKSTRA, W. HOL, J. DRENTH
351C	CYTOCHROME C551 (OXIDIZED)	MATSUURA, TAKANO, DICKERSON	7/81	1PCY	PLASTOCYANIN	J. GUSS, H. FREEMAN
451C	CYTOCHROME C551 (REDUCED)	MATSUURA, TAKANO, DICKERSON	7/81	2PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, C. BLAKE
1DFR	DIHYDROFOLATE REDUCTASE (L. CASE1)	J. BOLIN, D. MATTHEWS, J. KRAUT	3/80	1PKY	PYRUVATE KINASE (CAT)	H. MUIRHEAD
2DFR	DIHYDROFOLATE REDUCTASE (E. COLI)	J. BOLIN, D. MATTHEWS, J. KRAUT	3/80	1RLX	RELAXIN (MODEL, CONFORMATION A, UNREFINED)	A. EVANS, A. NORTH
1BNA	DNA (B. COCCACATCOCCO, SYNTHETIC)	H. DREW, R. DICKERSON	1/81	3RLX	RELAXIN (MODEL, CONFORMATION B, UNREFINED)	A. EVANS, A. NORTH
1ZNA	DNA (Z1, CGCG, HIGH-SALT, SYNTHETIC)	H. DREW, R. DICKERSON	1/81	4RLX	RELAXIN (MODEL, CONFORMATION A, REFINED)	A. EVANS, A. NORTH
2ZNA	DNA (Z-1, CGCGCG, SYNTHETIC, MODEL)	A. RICH	2/81	1RHO	RHODANES	W. HOL
3ZNA	DNA (Z-11, CGCGCG, SYNTHETIC, MODEL)	A. RICH	2/81	3RSA	RIBONUCLEASE A	A. WLODANER
1EST	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76	1RNS	RIBONUCLEASE S	H. WYCKOFF, F. RICHARDS
1ECD	ERYTHROCRUORIN (REDUCED, DEOXY)	W. STEIGEMANN, E. WEBER	3/79	2RXN	RUBREDOXIN (CLOSTRIDIUM PASTEURIANUM)	L. JENSEN
1ECO	ERYTHROCRUORIN (CARBONMONOXY)	W. STEIGEMANN, E. WEBER	3/79	3RXN	RUBREDOXIN (DESULFOVIBRIO VULGARIS)	E. ADMAN, L. SIEKER, L. JENSEN
1ECA	ERYTHROCRUORIN (AQUO, MET)	W. STEIGEMANN, E. WEBER	3/79	1SNS	STAPHYLOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN
1ECN	ERYTHROCRUORIN (CYANO, MET)	W. STEIGEMANN, E. WEBER	3/79	1SGA	STREPTOMYCES GRISEUS PROTEINASE A	BRAYER, DELBAERE, JAMES
1FDX	FERRIDOXIN (PEPTOCOCCUS AEROGENES)	E. ADMAN, L. SIEKER, L. JENSEN	8/76	2SGB	STREPTOMYCES GRISEUS PROTEINASE B	DELBAERE, BRAYER, JAMES
1FXC	FERRIDOXIN (SPIRULINA PLATENSIS)	M. KAKUDO	8/79	2S51	SUBTILISIN INHIBITOR (STREPTOMYCES)	Y. MIYAJI ET AL.
1FDI	FERRIDOXIN (AZOTOBACTER VINELANDII)	STOUT, GHOSH, FUREY, O'DONNELL	1/81	1SBT	SUBTILISIN BPN	J. KRAUT
3FXN	FLAVODOXIN (CLOSTRIDIUM MP, OXIDIZED)	M. LUDWIG	12/77 R	2SBT	SUBTILISIN NOVO	J. DRENTH
4FXN	FLAVODOXIN (CLOSTRIDIUM MP, SEMIQUINONE)	M. LUDWIG	12/77	2S0D	SUPEROXIDE DISMUTASE	J. RICHARDSON, D. RICHARDSON
1GCN	GLUCAGON	T. BLUNDELL	10/77	1TLN	THERMOLYSIN (UNREFINED)	B. MATTHEWS
1PGI	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77	2TLN	THERMOLYSIN (REFINED)	B. MATTHEWS
1GRS	GLUTATHIONE REDUCTASE (HUMAN)	G. SCHULZ	12/80 A	1SRX	THIOREDOXIN (E. COLI, OXIDIZED)	B. -O. SODERBERG
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	7/75	4TNA	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG
2GPD	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79	6TNA	TRANSFER RNA (YEAST, PHE)	S. -H. KIM ET AL.
1HRB	HEMERYTHRIN B	W. HENDRICKSON	6/76 A	8TNA	TRANSFER RNA (YEAST, PHE)	W. SUNDARALINGAM
1HMB	HEMERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81 R	1TIM	TIROSE PHOSPHATE ISOMERASE	I. WILSON, D. PHILLIPS
1HDS	HEMOGLOBIN (DEER, SICKLE CELL)	E. AMMA, R. GIRLING	10/79	1TNC	TROPONIN (CA-BINDING COMPONENT, MODEL)	R. KRETSINGER, C. BARRY
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	R. LADNER, HEIDNER, PERUTZ	2/77 R	1PTN	TRYP SIN (NATIVE, PHB)	FEHLHAMMER, BODE, SCHWAGER
1HMB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73	2PTB	TRYP SIN (BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHWAGER
1HHC	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	4/75	1PTC	TRYP SIN/TRYP SIN INHIBITOR COMPLEX	R. HUBER, W. BODE
1HCO	HEMOGLOBIN (HUMAN, CARBONMONOXY)	J. BALDWIN	8/79	3PTI	TRYP SIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER
2HCO	HEMOGLOBIN (HUMAN, CARBONMONOXY, NRG REFND)	J. BALDWIN	8/79	3PTP	TRYP SIN (DIP INHIBITED)	J. CHAMBERS, R. STROUD
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	8/76	1TGP	TRYP SIN/TRYPSIN INHIBITOR	W. BODE, P. SCHWAGER, R. HUBER
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	3/73	1TPI	TRYP SIN/TRYPSIN INHIBITOR/ILE-VAL	W. BODE, P. SCHWAGER, R. HUBER
1HKG	HEXOKINASE A - GLUCOSE COMPLEX (YEAST)	W. BENNETT JR., T. STEITZ	12/80	1TGA	TRYP SIN/TRYPSIN (MGSO4, WITHOUT CA)	BODE, FEHLHAMMER, HUBER
2YHX	HEXOKINASE (YEAST) FORM BIII	STEITZ, ANDERSON, STENKAMP	3/78 R	1TGB	TRYP SIN/TRYPSIN (WITH CA, FROM PEG)	BODE, FEHLHAMMER, HUBER
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75	1TGN	TRYP SIN/TRYPSIN	A. KOSSIAKOFF, R. STROUD
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	11/77	1SBV	VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC)	M. ROSSMANN
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			
3FAB	*IMMUNOGLOBULIN FAB* NEW	R. POLJAK	9/81 RP			
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-MINMER)RHE	B. WANG, C. YOO, M. SAX	12/77 A			
1FC1	IMMUNOGLOBULIN FC (HUMAN)	J. DEISENHOFER	5/81			
1FC2	IMMUNOGLOBULIN FC-FRAGMENT B COMPLEX	J. DEISENHOFER	5/81			
1INS	INSULIN (PORCINE, 2-ZINC)	G. DODSON, D. HODGKIN	7/80			
1KGA	KDGP ALDOLASE	A. TULINSKY	8/78 A			
1KES	KERATAN SULFATE	S. ARNOTT	5/78			
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)	W. MUSICK, M. ROSSMANN	9/78			

\* NEW OR REPLACEMENT ENTRY SINCE JUL-81 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
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
CONNECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	4/79 YES
CONTCCT	INTERMOLECULAR CONTACTS	L.ANDREWS	10/79 NO
DGPILOT	DIAGONAL PLOTS ON PRINTER	E.SWANSON,F.BERNSTEIN	3/79 YES
DIHORL	COMPLETE TORSION ANGLES	E.ABOLA	3/80 YES
DSTNCE	CALC DISTANCES FROM CONNECT RECORDS	F.BERNSTEIN	3/79 YES
FIS1PL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79 YES
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78 NO
PHIPS1	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.REKE	10/79 NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	5/78 YES

\* NEW OR REPLACEMENT ENTRY SINCE JUL-81 NEWSLETTER

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

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

NAME	DESCRIPTION	REV DATE/ SUPPORTED
OEAP	ACID PROTEINASE (ENDOTHIA PARASITICA)	
OADC	*ADH-NADH-DIMETHYLSULFOXIDE COMPLEX	
OAF1	APOFERRITIN (HORSE)	
OMAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE	
OCP2	*CARBOXYPEPTIDASE A-INHIBITOR COMPLEX	
OCT5	CITRATE SYNTHASE (PIG)	
OCTX	ALPHA COBRATOXIN	
OCN1	CONCANAVALIN A (DEMETALLIZED)	
OCN2	CONCANAVALIN A (DEMETALLIZED)	
OCRO	*CRO REPRESSOR	
OCYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)	
OCY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)	
O5C1	CYTOCHROME C555 (CHLOROBBIUM THIOSULFATOPHILUM)	
OC3A	*DES-ARG77-C3A ANAPHYLATOXIN	
OESZ	ELASTASE COMPLEX (PIG)	
OETU	ELONGATION FACTOR TU COMPLEX (E. COLI)	
OEBX	ERABUTOXIN B	
OFD1	FERRIDOXIN (AZOTOBACTER VINLANDII)	
OFX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)	
OFX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)	
OGAP	*CATABOLITE GENE ACTIVATOR PROTEIN	
OGP1	GLUTATHIONE PEROXIDASE (BOVINE)	
OGD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)	
OHMG	*HAEMAGGLUTININ	
OH9G	HEMOGLOBIN (GLYCERA DIBRANCHIATA)	
OPH4	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)	
OAU1	IMMUNOGLOBULIN, BENGE-JONES FRAGMENT (KAPPA) AU	
OROY	IMMUNOGLOBULIN, BENGE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY	
OMCP	IMMUNOGLOBULIN FAB (KAPPA) MCP603	
OFB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL	
OIG1	IMMUNOGLOBULIN G1 (KAPPA) DOB	
OIG2	IMMUNOGLOBULIN G1 (LAMBDA) KOL	
OIN2	INSULIN (PORCINE)	
OGF1	INSULIN-LIKE GROWTH FACTOR I (HUMAN)	
OGF2	INSULIN-LIKE GROWTH FACTOR II (HUMAN)	
OLZ1	LYSOZYME (HUMAN)	
OLZ2	LYSOZYME (TURKEY)	
OLZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)	
OCTF	L7/L12 (E. COLI, C-TERMINUS)	
OMB5	MYOGLOBIN (SPERM WHALE, CARBON MONOXIDE, NEUTRON STUDY)	
OMB1	MYOGLOBIN (SPERM WHALE, MET. TEMPERATURE STUDIES)	
OMB3	MYOGLOBIN (SPERM WHALE, MET. NEUTRON STUDY)	
OMB4	MYOGLOBIN (SPERM WHALE, OXY)	
OSN3	SCORPION NEUROTOXIN VARIANT-3	
OOVO	*OVOMUCOID FRAGMENT	
OPFC	*PFC.PRIME. FRAGMENT OF AN IGG1	
OPFK	PHOSPHOFUCTOKINASE (BACILLUS STEAROTHERMOPHILIUS)	
OBP1	PHOSPHOLIPASE A2 (PORCINE)	
OPPA	PHOSPHORYLASE A (RABBIT)	
OPB1	PHOSPHORYLASE B (RABBIT)	
ORX5	RELAXIN (PORCINE, MODEL)	
ORN5	RIBONUCLEASE A (BOVINE)	
ORN3	RIBONUCLEASE A (BOVINE)	
OFMT	INITIATOR TRANSFER RNA (E. COLI, F/MET)	
OTA1	TRANSFER RNA (YEAST, ASP. A FORM)	
OTA2	TRANSFER RNA (YEAST, ASP. B FORM)	
OTR1	TRANSFER RNA (YEAST, PHE)	
OTS1	TYROSYL TRANSFER RNA SYNTHETASE (BACILLUS STEAROTHERMOPHILUS)	
OGN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)	
OUTG	UTEROGLOBIN (RABBIT)	
OTHV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)	
OTBV	VIRUS (TOMATO BUSHY STUNT)	

\* NEW OR REPLACEMENT ENTRY SINCE JUL-81 NEWSLETTER

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 1, SEE ALSO TABLE 6)

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
RIACTSF	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
R1ZNASF	DNA(Z1,CGCG,HIGH-SALT,SYNTHETIC)	H. DREW,R. DICKERSON	1/81 SF
R1BNASF	DNA(B,CGCGAATTCGCG,SYNTHETIC)	H. DREW,R. DICKERSON	1/81 SF
R6PD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE(LOBSTR)	M. ROSSMANN	9/75 SF
R2OPDSF	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79 SF
R1HMSF	HEMERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81 SF
R2HBSF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER,HEIDNER,PERUTZ	6/80 SF
R1FDHSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/80 SF
R1HMDH02	HEMOGLOBIN (HUMAN,DEOXY)	M. PERUTZ,G. FERMI	5/75 SF
LAMPYR1	HEMOGLOBIN (LAMPREY)	HENDRICKSON,LOVE,KARLE	5/73 SF
RLDH06	LACTATE DEHYDROGENASE	M. ROSSMANN	8/75 SF
RLDH07	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	9/75 SF
R5LDHSF	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU,M. ROSSMANN	1/81 SF
R1LZHSF	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	C. BLAKE,D.RICE	6/81 SF
R2LZHSF	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	C. BLAKE,D.RICE	6/81 SF
RMETYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76 SF
RDEMYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76 SF
R3RSASF	RIBONUCLEASE A	A. WLODAMER	5/81 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 JUL-81 NEWSLETTER

CODES

SF STRUCTURE FACTORS

TABLE 6. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 2, SEE ALSO TABLE 5)

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R351CSF	*CYTOCHROME C551 (OXIDIZED)	T. TAKANO, R. DICKERSON	9/81 SF
R451CSF	*CYTOCHROME C551 (REDUCED)	T. TAKANO, R. DICKERSON	9/81 SF
R1MLTSF	*MELITTIN	TERNILLIGER,EISENBERG	8/81 SF
R2BP2SF	*PROPHOSPHOLIPASE A2 (BOVINE)	DIJKSTRA,HOL,DRENTH	9/81 SF

\* NEW OR REPLACEMENT ENTRY SINCE JUL-81 NEWSLETTER

CODES

SF STRUCTURE FACTORS

## REQUEST FORM

(Please include a self-addressed label)

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. Documentation desired (no charge).

- ( ) Latest Newsletter  
 ( ) Introduction to The Protein Data Bank (June 1981)  
 ( ) Sources of Visual Aids for Macromolecular Structure (June 1981)  
 ( ) Atomic Coordinate Entry Format Description for DATAPRTP and DATAPRFI (July 1981)  
 ( ) Non-Standard Entries (Structure Factors) format description for NONST1TP and NONST1FI (September 1981)  
 ( ) Non-Standard Entries (Structure Factors) format description for NONST2TP and NONST2FI (September 1981)  
 ( ) Data Deposition form

4. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs \$122 (~~£~~68); each 2-tape item costs \$147 (~~£~~82). Domestic postage is included.

<u>Item</u>	<u>Number of Tapes</u>	<u>Cost</u>
-------------	------------------------	-------------

Total \_\_\_\_\_

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$84 (£47 from Cambridge). Correction fiche are free.

ItemCost

Total \_\_\_\_\_

6. Air mail postage from Brookhaven to destinations outside the U. S. and Canada or from Cambridge to destinations outside the United Kingdom. A postage surcharge of \$15 (£8) is required per magnetic tape (not per item).

Number of tapes x \$15.00 (£8) = \_\_\_\_\_

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 is ( ) enclosed  
 ( ) purchase order number \_\_\_\_\_ ( ) 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