

The Protein Data Bank is pleased to announce the installation of its new microVAX computer system with three processors connected on a local area network, which is expected to be fully operational in the near future.

The atomic coordinate and bibliographic entry distribution tape (DATAPRTP) can now be ordered in the following formats:

Distribution Medium	Tape Format
9-Track (6250/1600/800 cpi) tape	Unlabelled format VAX/VMS COPY format VAX/VMS BACKUP format
DEC - TK50	VAX/VMS COPY format VAX/VMS BACKUP format

The rates for these services are given on the order form on pp. 5-6 of this newsletter.

The Data Bank has also acquired new computer hardware and software which makes it convenient to distribute individual coordinate files on IBM-PC 350K floppy diskettes. This service is being offered on a trial basis and those interested should contact Brookhaven directly.

Future plans include the distribution of tapes directly readable on a VAX/ULTRIX computer as well as 1/4" cartridge tapes for the IRIS workstation. On-line access to the Data Bank through dial-up lines to Brookhaven should be available by the end of this year.

We are pleased to announce that Brookhaven can accept order forms and purchase orders by facsimile. The number to use is (United States) 516-282-3000. The original purchase order should also be sent to Brookhaven by mail.

<u>Area</u>	<u>Address of Center</u>	<u>Name</u>	<u>Phone</u>
Worldwide except Australia and Japan	Protein Data Bank	E. E. Abola	516-282-4383
	Chemistry Department	F. C. Bernstein	516-282-4382
	Brookhaven National Laboratory	S. H. Bryant	516-282-4382
	Upton, New York 11973, USA (BITNET address: ABOLA@BNLDAG)	T. F. Koetzle J. C. Weng	516-282-4384 516-282-4382
Australia	CSIRO Central Information Service P. O. Box 89, East Melbourne Victoria 3002, Australia	T. Graddon	03-418-7266
Japan	Institute for Protein Research Osaka University Yamadaoka, 3-2, Suita, Osaka 565, Japan	Y. Katsube K. Yoshida	(06) 877-5111 ext. 3912

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

CODE	ITEM	16-APR-87		
		AVAILABILITY	USA	JAP AUS
DATAPRTP	ALL CURRENT COORDINATE ENTRIES (TABLE 8), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 10 - NO COORDINATES IN BIB ENTRIES)	X	X	X
YEAR86PT	NEW OR REVISED COORDINATE ENTRIES FOR 1986	X		
PART87PT	NEW OR REVISED COORDINATE ENTRIES 1987 (TO DATE)	X		
PDBPGMTP	COMPUTER PROGRAMS AND MISCELLANEOUS FILES (TABLE 3, PARTS A AND B)	X		
NONST1PT	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 4)	X	X	
NONST2PT	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 5)	X	X	
NONST3PT	STRUCTURE FACTOR HOLDINGS (PART 3 - TABLE 6)	X	X	
NONST4PT	STRUCTURE FACTOR HOLDINGS (PART 4 - TABLE 7)	X	X	
BENDERPT	PARAMETERS FOR BENT-WIRE MODELS	X		
BLDKITPT	MODEL BUILDER'S KIT			PLEASE INQUIRE AT US CENTER
CONECTPT	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X		
DOPLOTP	DIAGONAL PLOTS (LINE PRINTER)	X		
DIHDLPT	COMPLETE TORSION ANGLES	X		
DSTNCTPT	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X		
FIS1PLPT	PHI/PSI PLOTS (LINE PRINTER)	X		
PH1PS1PT	LISTS OF PHI/PSI/OMEGA VALUES	X		

* NEW OR REPLACEMENT ENTRY SINCE JAN-87 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	16-APR-87		
		AVAILABILITY	USA	JAP AUS
DATAPRF1	ALL CURRENT COORDINATE ENTRIES (TABLE 8), COMPUTER PROGRAMS (TABLE 3, PART A), ALL CURRENT BIBLIOGRAPHIC ENTRIES (TABLE 10 - NO COORDINATES IN BIB ENTRIES)	X	X	
YEAR86F1	NEW OR REVISED COORDINATE ENTRIES FOR 1986	X		
PART87F1	NEW OR REVISED COORDINATE ENTRIES 1987 (TO DATE)	X		
CORR19F1	LIST OF CORRECTIONS NO. 19 (JULY/86 - JAN/87)	X	X	X
NONST1F1	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 4)	X	X	
NONST2F1	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 5)	X	X	
NONST3F1	STRUCTURE FACTOR HOLDINGS (PART 3 - TABLE 6)	X	X	
NONST4F1	STRUCTURE FACTOR HOLDINGS (PART 4 - TABLE 7)	X	X	
BENDERF1	PARAMETERS FOR BENT-WIRE MODELS	X		
BLDKITF1	MODEL BUILDER'S KIT			PLEASE INQUIRE AT US CENTER
CONECTF1	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X		
DOPLOTF1	DIAGONAL PLOTS (LINE PRINTER)	X		
DIHDLF1	COMPLETE TORSION ANGLES	X		
DSTNCF1	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X		
FIS1PLF1	PHI/PSI PLOTS (LINE PRINTER)	X		
PH1PS1F1	LISTS OF PHI/PSI/OMEGA VALUES	X		

* NEW OR REPLACEMENT ENTRY SINCE JAN-87 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, COMPUTER PROGRAMS AND MISCELLANEOUS FILES

NAME	PURPOSE	AUTHOR(S)	16-APR-87	
			REV DATE/	SUPPORTED
PART A - AVAILABLE ON DATAPRTP, DATAPRF1, PDBPGMTP				
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G.WILLIAMS	4/82	YES
BLDKIT	MODEL BUILDER'S KIT	E.ABOLA	2/84	YES
BRUKPT	MAKE VAX/VMS FILES FROM PDB TAPE	H.BOSSHARD	8/85	NO
CONECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	8/82	YES
CONCTC	INTERMOLECULAR CONTACTS	L.ANDREWS	5/83	NO
DGLOTP	DIAGONAL PLOTS ON PRINTER	E.SHANSON,F.BERNSTEIN	3/82	NO
DIHDL	COMPLETE TORSION ANGLES	E.ABOLA	3/80	YES
DRCTRY	DIRECTORY OF PDB DISTRIBUTION TAPE	E.ABOLA	7/86	YES
DSP	SECONDARY STRUCTURE, SOLVENT EXPOSURE	KABSCH,C.SANDER	12/83	NO
DSTNCE	CALC DISTANCES FROM CONECT RECORDS	F.BERNSTEIN	8/82	YES
FIS1PL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79	YES
LSM	COLOR-CODED ALPHA-CARBON MODELS	R.MATELA,R.FLETTERICK	3/82	NO
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y.BEPPU	11/78	NO
PH1PS1	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	2/79	YES
REFMTE	REFORMAT DATA FOR SUPERTAB,SUPERB	L.RELLICK,J.DUANE	12/83	NO
STEREO	EXTRACT X,Y,Z FROM STEREO DIAGRAMS	H.ROSSMANN	2/74	YES
TAPDIR	PRINT DIRECTORY OF TAPE CONTENTS	H.BERNSTEIN,F.BERNSTEIN	6/79	NO
THEOD	MEASURE COORDINATES WITH THEODOLITE	L.LEBLOD	1/82	NO
TORSUR	COMPLETE TORSION ANGLES	G.GREEK	10/79	NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	3/82	YES
PART B - AVAILABLE ON PDBPGMTP				
ALB	SECONDARY STRUCT. CALC., PREDICTION A.FINKELSTEIN,O.PTITSYN		10/85	NO
CRYSTAL	DATA BASE - PROTEIN CRYSTALLIZATION G.GILLILAND		12/84	NO

* NEW OR REPLACEMENT ENTRY SINCE JAN-87 NEWSLETTER

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

TABLE 4. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 1, SEE ALSO TABLES 5,6,7)

IDENT CODE	MOLECULE	DEPOSITOR	16-APR-87	
			DATE/	CODE
RIACTSF	ACTINININ	E.BAKER	7/77	SF
CHYMF	ALPHA-CHYMOTRYPSIN (TOSYL)	D.BLOW	4/73	SF
RCARP04	CALCIUM-BINDING PARVALBUMIN	R.KRETSINGER	2/74	SF
RCARP05	CALCIUM-BINDING PARVALBUMIN	R.KRETSINGER	1/81	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
RCV5501	CYTOCHROME C550	R.TIMKOVICH	4/76	SF
R1ZNASF	DNA (Z-PRIME), CGCG, HIGH-SALT, SYNTHETIC	H.DREW,R.DICKERSON	1/81	SF
R1BNASF	DNA (B, CGCGAATTCGCG, SYNTHETIC, 290 K)	H.DREW,R.DICKERSON	1/81	SF
RGPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTRIM)	M.ROSSMANN	8/75	SF
R2GPDF	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M.ROSSMANN	12/79	SF
R2HBSF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER,HEIDNER,PERUTZ	6/80	SF
R1FDH5F	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J.FRIER	6/80	SF
R1HJDEH02	HEMOGLOBIN (HUMAN, DEOXY)	H.PERUTZ,G.FERMI	5/75	SF
LAMPFY1	HEMOGLOBIN (LAMPREY)	HENDRIKSON,LOVE,KARLE	5/73	SF
RLD06	LACTATE DEHYDROGENASE	M.ROSSMANN	8/75	SF
RLD07	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M.ROSSMANN	8/75	SF
RLD08F	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U.GRAU,M.ROSSMANN	1/81	SF
R1LZHSF	LYSOZYME (HEN EGG-WHITE, MONOCLONIC)	C.BLAKE,D.RICE	6/81	SF
R2LZHSF	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	C.BLAKE,D.RICE	6/81	SF
RMEYMSF1	MYOGLOBIN (SPERM WHALE, MET)	T.TAKANO	6/76	SF
RDEYMSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T.TAKANO	6/76	SF
R4TNASF	TRANSFER RNA (YEAST, PHE)	A.JACK,J.LADNER,A.KLUG	6/80	SF

CODES
SF STRUCTURE FACTORS

TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 2, SEE ALSO TABLES 4,6,7)

IDENT CODE	MOLECULE	DEPOSITOR	16-APR-87	
			DATE/	CODE
R1CCRSF	CYTOCHROME C (RICE)	H.OCHI,N.TANAKA	3/83	SF
R3L1CSF	CYTOCHROME C551 (OXIDIZED)	T.TAKANO,R.DICKERSON	9/81	SF
R4S1CSF	CYTOCHROME C551 (REDUCED)	T.TAKANO,R.DICKERSON	9/81	SF
R1ANASF	DNA (A,D-10DD-CGCG)SPACE GROUP P 43 21 2	B.CONNER,R.DICKERSON	6/82	SF
R1ANAP2	DNA (A,D-10DD-CGCG)SPACE GROUP P 21	B.CONNER,R.DICKERSON	6/82	SF
R2BNASF	DNA (B,CGCGAATTCGCG,SYNTHETIC,16 K)	H.DREW,R.DICKERSON	11/81	SF
R3BNASF	DNA (B,9-BR-CGCGAATTCGCG,20 DEG C)	KOPKA,FRATINI,DICKERSON	2/82	SF
R4BNASF	DNA (B,9-BR-CGCGAATTCGCG,7 DEG C)	KOPKA,FRATINI,DICKERSON	2/82	SF
R1GAASF	DNA (B,CGCGAATTCGCG,SYNTHETIC)/CISPLATIN	WING,JARA,DREW,DOCKRSN	8/83	SF
R1GASFS	GLUTAMINASE-ASPARAGINASE (ACINETOBACTER)	H.AMMON	12/82	SF
R1GASFS	GLUTAMINASE-ASPARAGINASE (PSEUDOMONAS 7A)	H.AMMON	12/82	SF
R1HM0SF	HEMERYTHRIN (MET)	STENKAMP,SIEKER,JENSEN	2/83	SF
R1HM2SF	HEMERYTHRIN (AZIDO, MET)	STENKAMP,SIEKER,JENSEN	2/83	SF
R2INSFS	INSULIN (BOVINE, 2-ZINC)DES-PHE B1	C.REYNOLDS,G.DODSON	5/82	SF
R1LH1SF	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH1SF	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH2SF	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH2SF	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH3SF	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH3SF	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH4SF	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH4SF	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH5SF	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH5SF	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH6SF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH6SF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH75FR	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	2/83	SF
R2LH75FR	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LYM5F	LYSOZYME (HEN EGG-WHITE, MONOCLONIC)	HOGLE,RAO,SUNDARALINGAM	7/82	SF
R1LIT5F	MELITIN	TERWILLIGER,EISENBERG	8/81	SF
R10V0SF	OVUMUCOID FRAGMENT (JAPANESE QUAIL)	E.PAPAMKOS,R.HUBER	1/82	SF
R2BP2SF	PROPHOSPHOLIPASE A2 (BOVINE)	D.IKSTRA,HOL,DRENTH	9/81	SF
R10V0SF	INORGANIC PYROPHOSPHATASE	E.HARUTYUNYAN ET AL.	2/83	SF
R1RN3SF	RIBONUCLEASE A	BORKAKOTI,M.OSS,PALMER	6/82	SF
R3TLNSF	TRYPHOSIN (NATIVE)	B.MATTHEWS,M.HOLMES	2/82	SF
R1RN2SF	TRYPHOSIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J.HALTER,R.HUBER	10/81	SF
R1RPOSF	TRYPHOSIN (ORTHORHOMBIC)	BODE,WALTER,HUBER	9/82	SF
R3PTNSF	TRYPHOSIN (TRIGONAL, 2.4M (NH4)2SO4)	J.HALTER,R.HUBER	10/81	SF
R3PTNSF	TRYPHOSIN (BENZAMIDINE INHIBITED)	BODE,SCHWAGER,WALTER	9/82	SF
R1TPPSF	TRYPHOSIN (P-AMIDINO-PHENYL-PYRUVATE)	WALTER,BODE,HUBER	9/82	SF
R1PT1SF	TRYPHOSIN INHIBITOR (BOVINE, PANCREAS)	R.HUBER,J.DEISENHOFER	9/82	SF
R1PT2SF	TRYPHOSIN INHIBITOR (COMPLEX)	R.HUBER,J.DEISENHOFER	9/82	SF
R1PT3SF	TRYPHOSIN (ANHYDRO)/TRYPHOSIN INHIBITOR	HUBER,BODE,DEISENHOFER	9/82	SF
R2TGSF	TRYPHOSIN (2.4M MGS04)	J.HALTER,R.HUBER	10/81	SF
R1TGSF	TRYPHOSIN (5 CH3OH, .5 HOH)	J.HALTER,R.HUBER	10/81	SF
R1TGT5F	TRYPHOSIN (173 K, .7 CH3OH, .3 HOH)	J.HALTER,R.HUBER	10/81	SF
R2TGT5F	TRYPHOSIN (103 K, .7 CH3OH, .3 HOH)	J.HALTER,R.HUBER	10/81	SF
R2TGT5F	TRYPHOSIN (TRYPSIN INHIBITOR)	J.HALTER ET AL.	9/82	SF
R3TPI5F	TRYPHOSIN (TRYPSIN INHIBITOR)/ILE-VAL	R.HUBER ET AL.	9/82	SF
R2TPI5F	TRYPHOSIN (PTI)/ILE-VAL (MERCURATED)	J.HALTER,R.HUBER	10/81	SF
R1TGS5F	TRYPHOSIN/PSTI	R.HUBER ET AL.	9/82	SF

CODES
SF STRUCTURE FACTORS

TABLE 6. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 3, SEE ALSO TABLES 4,5,7)

IDENT CODE	MOLECULE	DEPOSITOR	16-APR-87	
			DATE/	CODE
R1CATSF	CATALASE (BEEF LIVER)	M.ROSSMANN	11/81	SF
R1CHASF	ALPHA-CHYMOTRYPSIN (BOVINE)	H.TSUKADA,D.BLOW	11/84	SF
R2GCHSF	GAMMA-CHYMOTRYPSIN	C.MEN,DAVIES,SILVERTON	7/85	SF
R2C2CSF	CYTOCHROME C2 (OXIDIZED)	BHATIA,FINZEL,KRAU	11/83	SF
R3C2CSF	CYTOCHROME C2 (REDUCED)	BHATIA,FINZEL,KRAU	11/83	SF
R2ANASF	DNA (A, CGGCGCCCG, SYNTHETIC)	MCCALL,BROWN,KENNARD	8/85	SF
R2BNASF	DNA (B, CGCGAATTCGCG, SYNTHETIC)/NETROPSIN	M.KOPKA,R.DICKERSON	8/84	SF
R1BNASF	MELITIN (BOVINE INHIBITOR COMPLEX)	HOLBROOK,DICKERSON,KIM	1/85	SF
R1FX1SF	FLAVOXYDIN (D. VULGARIS, UNREFINED)	H.WALTER ET AL.	10/85	SF
R1G1P5F	GLUTATHIONE PEROXIDASE (BOVINE)	O.EPP,R.LET	6/85	SF
R2HHSF	HEMOGLOBIN (HUMAN, DEOXY)	G.FERMI,L.PERUTZ	3/84	SF
R1HHSF	HEMOGLOBIN (HUMAN, OXY)	B.SHAANAN	3/84	SF
R1H0SF	IGA FAB (KAPPA)MCP603	G.COHEN ET AL.	7/84	SF
R2MCP5F	IGA FAB (KAPPA)MCP603/PHOSPHOCHOLINE	PADLAN,COHEN,DAVIES	10/84	SF
R1PFC5F	GG PFC FRAGMENT	O.EPP,R.LET	4/85	SF
R1LZTSF	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	HOSON,BRNN,SIEKER,JENSEN	4/85	SF
R1M0SF	MYOGLOBIN (SPERM WHALE, OXY)	S.PHILLIPS	3/84	SF
R2V0SF	OVUMUCOID THIRD DOMAIN (SILVER PHEASANT)	H.BODE,O.EPP	6/85	SF
R1P0SF	PAPAIN D	J.JANSONIUS	10/84	SF
R3RPF2F	PROTEINASE II (RAT MAST CELL)	S.RENINGTON,B.MATTHEWS	9/84	SF
R5PT1SF	PTI (X-RAY)	A.WLODAWER,R.HUBER	10/84	SF
R5PT1SF	PTI (NEUTRON)	A.WLODAWER,R.HUBER	10/84	SF
R5R5ASF	RIBONUCLEASE A (X-RAY)	A.WLODAWER	6/85	SF
R5R5ASF	RIBONUCLEASE A (NEUTRON)	A.WLODAWER	6/85	SF
R5R5ASF	RUBREDOXIN (C. PASTEURIANUM)	WATENPAUGH,SIEKER,JENSEN	10/84	SF
R2V5SF	VIRUS COAT PROTEIN (SBIW T=1)	M.ROSSMANN	4/85	SF
R5B5SF	VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC)	M.ROSSMANN	4/85	SF

CODES
SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS (PART 4, SEE ALSO TABLES 4,5,6)

IDENT CODE	MOLECULE	DEPOSITOR	16-APR-87	
			DATE/	CODE
R3MGASF	AGGLUTININ (WHEAT GERM, ISOLECTIN 2)	C.WRIGHT	8/86	SF
R2AZASF	AZURIN (ALCALIGENES DENITRIFICANS)	E.BAKER,G.NORRIS	10/86	SF
R1C1BSF	CALCIUM-BINDING PROTEIN (INTESTINAL)	D.SZEBENYI,K.HOFFAT	9/86	SF
R2C1BSF	CYTOCHROME C (PRIME)	B.FINZEL ET AL.	8/85	SF
R2C1P5F	CYTOCHROME C PEROXIDASE (YEAST)	FINZEL,POULOS,KRAU	8/85	SF
R2BNASF	DNA (CGCGAATTCGCG, SYNTHETIC)/HOECHST 33258P	P.JURA,R.DICKERSON	8/86	SF
R1DN4SF	*DNA-1-BR-CG-BR-CG-BR-CG, SYNTHETIC, 18 DEG C,D.MORAS ET AL.		12/86	SF
R1DN5SF	*DNA-1-BR-CG-BR-CG-BR-CG, SYNTHETIC, 37 DEG C,D.MORAS ET AL.		12/86	SF
R1RHSF	LYS 7-DNP-LYS 41 RIBONUCLEASE A	B.FINZEL ET AL.	9/85	SF

continued from Page 3

1TPO	TRYP SIN (ORTHORHOMBIC)	W. BODE, J. WALTER, R. HUBER	9/82
3FTN	TRYP SIN (TRIGONAL, 2 NH (NH ₄) ₂ SO ₄)	J. WALTER, R. HUBER, W. BODE	10/81
3PTB	TRYP SIN (BENZAMIDINE INHIBITED)	W. BODE, P. SCHLAGER, J. WALTER	9/82
1TPP	TRYP SIN (P-AMIDINO-PHENYL-PYRUVATE	J. WALTER, W. BODE, R. HUBER	9/82
3PTP	TRYP SIN (DIP INHIBITED)	J. CHAMBERS, R. STROUD	12/77
4PTI	TRYP SIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	9/82
5PTI	TRYP SIN INHIBITOR (BOVINE, XRAY+NEUTRON)	A. WLODAWER, R. HUBER	10/84
2PTC	TRYP SIN/TRYP SIN INHIBITOR COMPLEX	R. HUBER, J. DEISENHOFER	9/82
1TPA	TRYP SIN (ANHYDRO)/TRYP SIN INHIBITOR	HUBER, BODE, DEISENHOFER	9/82
1TGN	TRYP SIN OGEN	A. KOSSIAKOFF, R. STROUD	9/79
2TGA	TRYP SIN OGEN (2.4M MGSO ₄)	J. WALTER, R. HUBER, W. BODE	10/81
1TGC	TRYP SIN OGEN (.5 CH ₃ OH, .5 HOH)	J. WALTER, R. HUBER, W. BODE	10/81
1TGT	TRYP SIN OGEN (173 K, .7 CH ₃ OH, .3 HOH)	J. WALTER, R. HUBER, W. BODE	10/81
2TGT	TRYP SIN OGEN (103 K, .7 CH ₃ OH, .3 HOH)	J. WALTER, R. HUBER, W. BODE	10/81
1TGB	TRYP SIN OGEN (WITH CA, FROM PEG)	BODE, FEHLHAMMER, HUBER	3/79
2TGD	TRYP SIN OGEN (DIP-INHIBITED, BOVINE)	M. JONES, R. STROUD	3/86
2TGP	TRYP SIN OGEN/TRYP SIN INHIBITOR	R. HUBER ET AL.	9/82
3TPI	TRYP SIN OGEN/TRYP SIN INHIBITOR/ILE-VAL	R. HUBER ET AL.	9/82
2TPI	TRYP SIN OGEN/PTI/ILE-VAL (MERCURATED)	J. WALTER, R. HUBER, W. BODE	10/81
4TPI	TRYP SIN OGEN/ARG-15-PTI/VAL-VAL	W. BODE, J. WALTER	6/85
1TOS	TRYP SIN OGEN/PTI	R. HUBER ET AL.	9/82
1TS1	TYROSYL TRANSFER RNA SYNTHETASE	BHAT, BLOW, BRICK, NYBORG	7/82 A
1UBO	*UBIQUITIN (HUMAN)	VIJAY-KUMAR, BUGG, COOK	1/87
2RHV	RHINOVIRUS 14 (HUMAN)	ROSSMANN, ARNOLD, VRIEND	4/86 R
25TV	VIRUS (SATELLITE TOBACCO NECROSIS)	T. A. JONES, L. LILJAS	6/84
45BV	VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC)	M. ROSSMANN	4/85 R
2TBV	VIRUS (TOMATO BUSHY STUNT)	S. HARRISON	6/84

MODEL STRUCTURES

2ZNA	DNA (Z-I, CGCGCG, SYNTHETIC, MODEL)	A. RICH	2/81
3ZNA	DNA (Z-II, CGCGCG, SYNTHETIC, MODEL)	A. RICH	2/81
1DNN	DNA (ATCGCTAAG... MODEL)	J. SUSSMAN, E. TRIFONOV	11/82
1IGE	IMMUNOGLOBULIN E (FC FRAGMENT) MODEL	E. PADLAN, D. DAVIES	1/85
1GF1	INSULIN-LIKE GROWTH FACTOR I (MODEL)	BLUNDELL, BEDARKAR, HUMBEL	12/82
1GF2	INSULIN-LIKE GROWTH FACTOR II (MODEL)	BLUNDELL, BEDARKAR, HUMBEL	12/82
1MLP	MUREIN LIPOPROTEIN (MODEL)	A. MCLAUGHLIN	6/78
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
WRLX	RELAXIN (MODEL, CONFORMATION B, REFINED)	A. EVANS, A. NORTH	3/78
1TNC	TROPONIN (CA-BINDING COMPONENT, MODEL)	R. KRETSINGER, C. D. BARRY	6/80 A

* NEW OR REPLACEMENT ENTRY SINCE JAN-87 NEWSLETTER

STATUS CODES

BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
R	RECENT (1985-1987) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 10. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES (NO COORDINATES)

16-APR-87

0EAP	ACID PROTEINASE (ENDOTHELA PARASITICA)
0HG1	AGGLUTININ (WHEAT GERM, ISOLECTIN I)
0HOE	ALPHA-AMYLASE INHIBITOR HOE-467A (STREPTOMYCES TENDAE 4158)
0AF1	APOFERITIN (HUMAN)
0HAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE
0RNB	BARNASE (BACILLUS AMYLOLIQUEFACIENS)
0CPT	CALCIUM-BINDING PARVALBUMIN - TERBIUM COMPLEX
0CD1	CALOTROPIN D1 (CALOTROPIS GIGANTEA)
0CPS	CARBOXYPEPTIDASE A (ALPHA)/GLYCYL-L-TYROSINE (-9 DEGREES C)
0ZGB	D-ALANYL-D-ALANINE PEPTIDASE (ZNF+ G PEPTIDASE)
02GP	*GAMMA-CHYMOTRYPSIN/3-BENZYL-6-CHLORO-2-PYRONE
0GCI	GAMMA-CHYMOTRYPSIN - INACTIVATOR COMPLEX
0CN2	CONCANAVALIN A (DEMETALLIZED)
0CRO	CRO REPRESSOR
05C1	CYTOCHROME C555 (CHLOROBBIUM THIOSULFATOPHILUM)
0CFF	*CYTOCHROME P450CAM (SUBSTRATE-FREE)
0DN1	DEOXYRIBONUCLEASE I (DNASE I)
0C3A	DES-ARG77-C3A ANAPHYLATOXIN
0CDF	DIHYDROFOLATE REDUCTASE (CHICKEN LIVER)
0DF5	R67 DIHYDROFOLATE REDUCTASE (ESCHERICHIA COLI)
0EFH	DNA (CGCAATTCGG, SYNTHETIC)
0DN3	DNA (CGCGAATTACGG, SYNTHETIC)
0DAC	DNA (CGCTACCG, SYNTHETIC) COMPLEX WITH TRIOSTIN
0DN6	DNA (GGATGGGAG, SYNTHETIC)
0DN1	DNA (GGGGTCCC, SYNTHETIC)
0ANB	DNA (GGGTATACC)
0ANB	DNA (GG-HUACC)
0GTC	DNA (A, GGGGCTC, SYNTHETIC)
0DPI	DNA POLYMERASE I
0ESC	ELASTASE COMPLEX WITH TWO MOLECULES OF ACE-ALA-PRO-ALA
0ESZ	ELASTASE COMPLEX (PIG)
0EFG	ELONGATION FACTOR TU (TRYP SIN-MODIFIED)
0ETU	ELONGATION FACTOR TU COMPLEX (ESCHERICHIA COLI)
0EXA	EXOTOXIN A (PSEUDOMONAS AERUGINOSA)
0FDL	FAB (IGG D1.3) COMPLEX WITH LYSOZYME
0FXI	FERRDOXIN I (APHANOTHECE SACRUM)
0FX3	FLAVODOXIN (OXIDIZED, ANACYSTIS NIDULANS)
0FX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)
0GBP	D-GALACTOSE-BINDING PROTEIN (ESCHERICHIA COLI)
0GLS	GLUTAMINE SYNTHETASE (SALMONELLA TYPHIMURUM)
0GD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)
0GD2	*D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)
0GOX	GLYCOLATE OXIDASE (SPINACH)
0HP1	HEMOGLOBIN (HUMAN, INTERRUPTUS)
0DCH	HEMOGLOBIN (COBALT, DEOXY)
0HBG	HEMOGLOBIN (GLYCERA DIBRANCHIATA)
0HBT	HEMOGLOBIN (T STATE, HUMAN)
0PHH	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)
0AUJ	IMMUNOGLOBULIN, (RENCE-JONES FRAGMENT (KAPPA) AU)
0ROY	IMMUNOGLOBULIN, (RENCE-JONES FRAGMENT (V-MONOMER, KAPPA) ROY)
0IG1	IMMUNOGLOBULIN G1 (KAPPA) DOB
01N4	INSULIN (HUMAN)
01N1	INSULIN (PORCINE)
01N2	INSULIN (PORCINE)
01N3	DESPRATPEPTIDE INSULIN (BEEF)
0LRP	N-TERMINAL DOMAIN OF LAMBDA REPRESSOR
0GLM	LYSOZYME (EMBDEN GOOSE)
0LZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)
0LZE	LYSOZYME (HEN EGG-WHITE, DEUTERATED ETHANOL)
0LZT	LYSOZYME (HEN EGG-WHITE, HIGH-TEMPERATURE)
0LZ5	LYSOZYME (STREPTHAUREUS)
0TEL	LYSOZYME (TORTOISE EGG-WHITE)
0B2M	BETA2-MICROGLOBULIN
0HMD	MITOCHONDRIAL MALATE DEHYDROGENASE (PORCINE)
0HBA	MYOGLOBIN (APLYSIA LIMACINA)
0HBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)
0HBS	MYOGLOBIN (SPERM WHALE, NEUTRON STUDY)
0HBC	*MYOGLOBIN (SPERM WHALE, CARBONMONOXY, 260 K)
0PSG	PEPSINOGEN (PORCINE)
0PFK	PHOSPHOFRUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)
0PGL	PHOSPHOGLUCOMUTASE (RABBIT)
0PPA	PHOSPHORYLASE A (RABBIT)
0PBI	PHOSPHORYLASE B (RABBIT)
0PRC	PHOTOSYNTHETIC REACTION CENTER (RHODOSPIROBRIONUM RUBRUM)
0CPC	C-PHYCOCYANIN (AGHNELLUM QUADRUPPLICATUM)
0PF1	PROTHROMBIN FRAGMENT 1 (BOVINE)
0RX5	RELAXIN (PORCINE, MODEL)
0RSA	RIBONUCLEASE A (BOVINE)
0RIA	RIBONUCLEASE A (BOVINE) COMPLEX WITH DNA (AAAA)
0RBS	RIBONUCLEASE (BOVINE SEMINAL)
0RBI	RIBONUCLEASE BI (BINASE)
0RST	RIBONUCLEASE ST (STREPTOMYCES ERYTHREUS)
0RNT	RIBONUCLEASE T1-2 (LYRINE)-GUANYLIC ACID (ASPERGILLUS ORYZAE)
05EC	SUBTILISIN CARLSBERG - EGLIN-C COMPLEX (BACILLUS SUBTILIS AND LEECH)
0CSE	*SUBTILISIN CARLSBERG - EGLIN-C COMPLEX (BACILLUS SUBTILIS AND LEECH)
0SNI	SUBTILISIN NOVO - CHYMOTRYPSINOGEN INHIBITOR 2 COMPLEX
0SBP	SULFATE-BINDING PROTEIN
0SDE	FE-SUPEROXIDE DISMUTASE (ESCHERICHIA COLI)
0SDP	FE-SUPEROXIDE DISMUTASE (PSEUDOMONAS OVALIS)
0SDM	MN-SUPEROXIDE DISMUTASE (THERMUS THERMOPHILUS)
0TH1	THAUMATIN
0TLP	THERMOLYSIN (BACILLUS THERMOPROTEOLYTICUS) COMPLEX WITH PHOSPHORAMIDON
0TLL	THERMOLYSIN (BACILLUS THERMOPROTEOLYTICUS) COMPLEX WITH P-LEU-NH2
0TTH	THIOREDOXIN REDUCTASE (BACTERIOPHAGE T4)
0FTI	INITIATOR TRANSFER RNA (E. COLI, F/MET)
0TA1	TRANSFER RNA (YEAST, ASP, A FORM)
0TR1	TRANSFER RNA (YEAST, PHE)
0MTS	METHIONYL TRANSFER RNA SYNTHETASE
0TMD	*TRIMETHYLAMINE DEHYDROGENASE
0YPI	TRIOSE PHOSPHATE ISOMERASE (SACCHAROMYCES CEREVISIAE)
0WRP	TRP REPRESSOR (ESCHERICHIA COLI)
0NTP	*BETA TRYP SIN (NEUTRON) / MONOISOPROPYLPHOSPHORYL INHIBITED
0UTG	UTEROGLOBIN (RABBIT)
0AD2	ADENOVIRUS TYPE 2 HEXON (AD2)
0PLV	VIRUS (POLIO, HUMAN)
0THV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)

* NEW OR REPLACEMENT ENTRY SINCE JAN-87 NEWSLETTER

TABLE 9. COORDINATE AND STRUCTURE FACTOR ENTRIES IN PREPARATION

16-APR-87

IDENT CODE	MOLECULE	DEPOSITOR(S)	DATE/STATUS
2APR	*RHIZOPUSPEPSIN (ACID PROTEINASE)	K. SUGUNA, D. DAVIES	3/87 RP
2CPP	*CYTOCHROME P450CAM (PSEUDOMONAS PUTIDA)	T. POULOS, B. FINZEL, A. HOWARD	4/87 P
3GAP	*CATABOLITE GENE ACTIVATOR PROTEIN/CAMP	I. WEBER, T. STEITZ	4/87 RP
2MRH	*MYOHEMERITRIN	S. SHERIFF, HENDRICKSON	4/87 RP
3TNC	*TROPONIN C (CHICKEN)	M. SUNDARALINGAM	4/87 AN
1MEV	*MENGO VIRUS	M. ROSSMANN	2/87 P
2APRSF	*RHIZOPUSPEPSIN (ACID PROTEINASE)	K. SUGUNA, D. DAVIES	3/87 SF
2MRHSF	*MYOHEMERITRIN	SHERIFF, HENDRICKSON	4/87 SF
1MEVSF	*MENGO VIRUS	M. ROSSMANN	2/87 SF

* NEW OR REPLACEMENT ENTRY SINCE JAN-87 NEWSLETTER

STATUS CODES

A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
N	NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
P	IN PREPARATION
R	REPLACEMENT FOR ENTRY IN TABLE 8
SF	STRUCTURE FACTORS

BROOKHAVEN ORDER FORM (Please include a self-addressed label)

1. Name _____ Date _____
Address _____ Telephone _____

2. Documentation desired (no charge).

- Introduction to The Protein Data Bank (June 1986)
- Latest Newsletter
- Atomic Coordinate and Bibliographic Entry Format Description for DATAPRTP and DATAPRFI (January 1985)
- Current DATAPRTP Directory
- Sources of Visual Aids for Macromolecular Structure (September 1986)
- Non-Standard Entries (Structure Factors) Format Description
- Data Deposition form

3. Please send the following magnetic tape items (from Table 1).

	6250 cpi	1600 cpi	800 cpi
DATAPRTP (coordinate tape)			
VAX/VMS BACKUP	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	
VAX/VMS COPY	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	
TK50 VAX/VMS BACKUP	<input type="checkbox"/> \$265		
TK50 VAX/VMS COPY	<input type="checkbox"/> \$265		
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	<input type="checkbox"/> \$326
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285	<input type="checkbox"/> \$326
PDBPGMTP			
VAX/VMS COPY	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244
NONST1TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
NONST2TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
NONST3TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
NONST4TP			
Unlabelled ASCII	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285
Unlabelled EBCDIC	<input type="checkbox"/> \$244	<input type="checkbox"/> \$244	<input type="checkbox"/> \$285

Special order items:

Please inquire at Brookhaven for availability and price.
(Items are described in Table 1.)

YEAR86TP	CONECTTP	DSTNCETP
PART87TP	DGPLOTTP	FISIPLTP
BENDERTP	DIHDRLTP	PHIPSITP

Special Instructions. Please check the appropriate box.

() We are especially interested in the pending entries with the following Ident Codes: _____ . Please delay shipment until the date _____ if any of these entries are expected to be available by that date.

() Normal order-will be processed as soon as possible.

4. Please send the following microfiche items (from Table 2). Each microfiche item costs \$231, postage included. Correction fiche are free.

Items: _____ Total Cost: _____

5. Please send the following printed listings. Each listing costs \$84, postage included.

Ident Code(s) (From Table 7): _____ Total Cost: _____

6. Foreign air mail postage for tapes from Brookhaven to destinations outside the U. S. and Canada. A postage surcharge of \$19 is required per item.

Number of items x \$19.00 = _____

7. Total charges

Magnetic tape charges (3 above) _____

Microfiche charges (4 above) _____

Printed listing charges (5 above) _____

Foreign air mail postage charges (6 above) _____

Bank charge _____

for checks not drawn in US dollars on US bank. \$10 _____

Total _____

Method of Payment:

Brookhaven requires that either a check or written purchase order payable to Brookhaven National Laboratory be received before service is provided. Order forms and purchase orders may be sent by facsimile to (United States) 516-282-3000.

() check is () enclosed

() purchase order number _____ () sent separately

Please return to

Ms. F. C. Bernstein
Chemistry Department
Brookhaven National Laboratory
Upton, New York 11973 USA
(516-282-4382)

It is advisable to send a photocopy of this order form directly to Brookhaven; experience shows that purchasing departments often do not forward this form with the order.