

This year has been an exceptionally busy one for the Protein Data Bank. In the last six months, we have received more new sets of atomic coordinates and structure factors than in any prior twelve-month period. These new acquisitions bring the number of atomic coordinate sets available for distribution to 183 and the number of structure factor sets to 43. We are also in the process of preparing 13 coordinate entries for which data have been deposited very recently.

We now offer a printed listing service, covering printed listings of individual atomic coordinate data sets and programs or all bibliographic entries for \$58 (£33) per listing, postage included. It has unfortunately been necessary to raise the cost of magnetic tape and microfiche distributions somewhat, and these new charges are listed on the request form included on the last two pages of the newsletter. These charges are limited to the actual cost of preparing and mailing individual tape and microfiche items. User charges account for less than 15 percent of the Brookhaven Protein Data Bank budget, with the major portion of the cost of operating the data base being borne by our grant from the National Science Foundation.

We would like to wish Professor Kakudo well on his retirement from Osaka University and thank him for his efforts on behalf of the Protein Data Bank. Effective April 1, Professor Yasuoka has assumed responsibility for the Data Bank functions in Japan formerly carried out by Professor Kakudo.

Inquiries and suggestions are welcomed and may be addressed to any of the persons listed below.

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 Lensfield Road Cambridge CB2 1EW, England	O. Kennard	0223-66499
		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	N. Yasuoka	(06) 877-5111 ext. 3837

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

23-APR-82

CODE	ITEM	NO. TAPES		AVAILABILITY			
		800	1600	US	UK	JA	AUS
DATAPRT	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		
DGLOTTTP	DIAGONAL PLOTS (LINE PRINTER)	1	1		X		
DIHDLTP	COMPLETE TORSION ANGLES	2	1		X		
DSTNCTTP	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 JAN-82 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

23-APR-82

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. 9 (JUL/81 - JAN/82)		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		
DGLOTFI	DIAGONAL PLOTS (LINE PRINTER)		X		
DIHDLFI	COMPLETE TORSION ANGLES		X		
DSTNCFI	CONNECTIVITY SPECIFICATIONS WITH DISTANCES		X		
FISIPLFI	PHI/PSI PLOTS (LINE PRINTER)		X		
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES		X		

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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	1/82 YES
CONNECT	GENERATE FULL CONNECTIVITY	F.BERNSTEIN	12/81 YES
CONTC	INTERMOLECULAR CONTACTS	L.ANDREWS	10/79 NO
DOPLOT	DIAGONAL PLOTS ON PRINTER	E.SHANSON,F.BERNSTEIN	3/79 YES
D1HDRL	COMPLETE TORSION ANGLES	F.BERNSTEIN	3/80 YES
DSTNCE	CALC DISTANCES FROM CONECT RECORDS	F.BERNSTEIN	3/79 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
PHIPS1	MAIN-CHAIN TORSION ANGLES	ANDREWS,WILLIAMS,BERNSTEIN	6/79 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
THEOD	*MEASURE COORDINATES WITH THEODOLITE	L.LEBIODA	1/82 NO
TORSRU	COMPLETE TORSION ANGLES	G.GREEKE	10/79 NO
TOTALS	VALIDATION OF MASTER RECORD	L.ANDREWS,F.BERNSTEIN	5/78 YES

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

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
R2BNASF	DNA(B,CGCGAATTCGGG,SYNTHETIC,16 DEG K)	H.DREW,R.DICKERSON	11/81 SF
R3BNASF	*DNA(B,9-BR-CGCGAATTCGGG,20 DEG C)	J.WALTER,R.HUBER	10/81 SF
R4BNASF	*DNA(B,9-BR-CGCGAATTCGGG, 7 DEG C)	KOPKA,FRATINI,DICKERSON2/82 SF	
R1MLTSF	MELITTIN	TERWILLIGER,EISENBERG	8/81 SF
R2BP2SF	PROPHOSPHOLIPASE A2 (BOVINE)	DIJKSTRA,HOL,DRENTH	9/81 SF
R3TLNSF	*THERMOLYSIN(NATIVE)	B.MATTHEWS,M.HOLMES	2/82 SF
R2PTNSF	TRYPSIN(ORTHORHOMBIC,2.4M (NH4)2SO4)	J.WALTER,R.HUBER	10/81 SF
R3PTNSF	TRYPSIN(TRIGONAL,2.4M (NH4)2SO4)	J.WALTER,R.HUBER	10/81 SF
R2TGSF	TRYPSINOGEN(2.4M MGS04)	J.WALTER,R.HUBER	10/81 SF
R1TGCSF	TRYPSINOGEN(.5 CH3OH, .5 HOH)	J.WALTER,R.HUBER	10/81 SF
R1GTGSF	TRYPSINOGEN(173 DEG K,.7 CH3OH,.3 HOH)	J.WALTER,R.HUBER	10/81 SF
R2TGTSF	TRYPSINOGEN(103 DEG K,.7 CH3OH,.3 HOH)	J.WALTER,R.HUBER	10/81 SF
R2T1SF	TRYPSINOGEN/PT1/ILE-VAL (MERCURATED)	J.WALTER,R.HUBER	10/81 SF

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CODES

SF STRUCTURE FACTORS

also:

R1OVOSF *OVOMUCOID FRAGMENT

E.PAPAMOKOS,R.HUBER 1/82 SF

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
CHYM0F	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(ZI,CGCG,HIGH-SALT,SYNTHETIC)	H.DREW,R.DICKERSON	1/81 SF
R1BNASF	DNA(B,CGCGAATTCGGG,SYNTHETIC,290 DEG K)	H.DREW,R.DICKERSON	1/81 SF
RGPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M.ROSSMANN	8/75 SF
R2GPD5F	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M.ROSSMANN	12/79 SF
R1HMMSF	HEMERYTHRIN (MET, HYDROXO)	R.STENKAMP	6/81 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
R5LDH5F	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
RMEHYSF1	MYOGLOBIN (SPERM WHALE, MET)	T.TAKANO	6/76 SF
R2EHYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T.TAKANO	6/76 SF
R3RSASF	RIBONUCLEASE A	A.WLODAHER	5/81 SF
RURBY02	RUBREDOXIN	L.JENSEN	3/74 SF
R4TNASF	TRANSFER RNA (YEAST, PHE)	A.JACK,J.LADNER,A.KLUG	6/80 SF

CODES

SF STRUCTURE FACTORS

TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
DEAP	ACID PROTEINASE (ENDOTHA PARASITICA)		
DADC	ADH-NADH-DIMETHYLSULFOXIDE COMPLEX		
DAF1	APOFERRITIN (HORSE)		
OMAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE		
O1CB	CALCIUM-BINDING PROTEIN (MINOR A FORM,BOVINE)		
OCPE	CARBOXYPEPTIDASE A-INHIBITOR COMPLEX		
OCTS	CITRATE SYNTHASE (PIG)		
OCTX	ALPHA COBRATOXIN		
OCN2	CONCAVALIN A (DEMETALLIZED)		
OCRO	CRO REPRESSOR		
OGCR	GAMMA-CRYSTALLIN II (CALF)		
OCYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)		
OCY3	CYTOCHROME C3 (DESULFOVIBRIO THIOSULFURICANS NORWAY)		
OSCI	CYTOCHROME C555 (CHLOROBIVM THIOSULFATOPHILUM)		
OC3A	DES-ARG77-C3A ANAPHYLATOXIN		
OE2S	ELASTASE COMPLEX (PIG)		
OETU	ELONGATION FACTOR TU COMPLEX (E. COLI)		
OE8X	ERABUTOXIN B		
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	HEMAGGLUTININ		
OH6G	HEMOGLOBIN (GLYCERA DIBRANCHIATA)		
OPHH	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)		
DAU1	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU		
OR0Y	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY		
OKCP	IMMUNOGLOBULIN FAB (KAPPA) MCP603		
OFB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL		
O1G1	IMMUNOGLOBULIN G1 (KAPPA) DOB		
O1G2	IMMUNOGLOBULIN G1 (LAMBDA) KOL		
O1N1	INSULIN (PORCINE)		
O1N2	INSULIN (PORCINE)		
OGF1	INSULIN-LIKE GROWTH FACTOR I (HUMAN)		
OGF2	INSULIN-LIKE GROWTH FACTOR II (HUMAN)		
OLZ1	LYSOZYME (HUMAN)		
OLZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)		
OLZ6	LYSOZYME (STREPTOMYCES ERYTHRAEUS)		
OCF	L7/L12 (E. COLI, C-TERMINUS)		
OMB5	MYOGLOBIN (SPERM WHALE, CARBON MONOXIDE, NEUTRON STUDY)		
OMBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)		
OMB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)		
OSN3	SCORPION NEUROTOXIN VARIANT-3		
OOVO	OVOMUCOID FRAGMENT		
OPFK	PHOSPHOFUCTOKININASE (BACILLUS STEAROTHERMOPHILUS)		
OBP1	PHOSPHOLIPASE A2 (PORCINE)		
OPP2	PHOSPHOLIPASE A2 (RATTLESNAKE)		
OPPA	PHOSPHORYLASE A (RABBIT)		
OPB1	PHOSPHORYLASE B (RABBIT)		
ORX5	RELAXIN (PORCINE, MODEL)		
ORSA	RIBONUCLEASE A (BOVINE)		
OR33	RIBONUCLEASE A (BOVINE, NEUTRON STUDY)		
OFHT	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)		
OMTS	METHIONYL TRANSFER RNA SYNTHETASE		
OTS1	TYROSYL TRANSFER RNA SYNTHETASE (BACILLUS STEAROTHERMOPHILUS)		
OGN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)		
OUTG	UTEROGLOBIN (RABBIT)		
OTMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)		
OTBV	VIRUS (TOMATO BUSHY STUNT)		

* NEW OR REPLACEMENT ENTRY SINCE JAN-82 NEWSLETTER

REQUEST FORM

(Please include a self-addressed label)

1. Name _____ Date _____
 Address _____ Telephone _____

2. Documentation desired (no charge).

- () Latest Newsletter
 () Introduction to The Protein Data Bank (June 1981)
 () Sources of Visual Aids for Macromolecular Structure (May 1982)
 () Atomic Coordinate Entry Format Description for DATAPRTP and
 DATAPRFI (December 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 (April 1982)
 () Data Deposition form

3. Please send the following magnetic tape items (from Table 1). Each
 1-tape item costs \$154 (~~£~~ 87); each 2-tape item costs \$188 (~~£~~ 106).
 Domestic postage is included.

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

Total _____

4. Tape format desired (all tapes are unlabelled)

	Availability	
	US	UK
() 9 track, 1600 cpi, EBCDIC	yes	yes
() 9 track, 800 cpi, EBCDIC	yes	yes
() 9 track, 1600 cpi, ASCII	yes	yes
() 9 track, 800 cpi, ASCII	yes	yes
() 7 track, 800 cpi, BCD	yes	please inquire

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.

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$92 (£ 52 from Cambridge), postage included. Correction fiche are free.

<u>Item</u>	<u>Cost</u>
-------------	-------------

Total _____

6. Please send the following printed listings. Each listing costs \$58, (£ 33), postage included.

<u>Ident Code</u> (From Table 3)	<u>Cost</u>
----------------------------------	-------------

Total _____

7. 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) = _____

8. Total charges

Magnetic tape charges (3 above) _____

Microfiche charges (5 above) _____

Printed listing charges (6 above) _____

Air mail postage charges (7 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