

NEWSLETTER

Frances Bernstein and Thomas Koetzle will be attending the XIIth Congress and General Assembly of the I.U.Cr. in Ottawa, Canada. Tom will be participating in the Microsymposium on Data Bases and Data Centers on Wednesday, August 19 from 1030-1300. In addition, there will be an exhibit by the Protein Data Bank in the conference lounge that will primarily be attended by Frances when she is not attending sessions. Copies of all our literature will be available and we are looking forward to meeting you there.

We are pleased to announce the availability of two new documents. We have prepared an "Introduction to the Protein Data Bank" outlining our purpose and general procedures. In addition, we have completed the list of "Sources of Visual Aids for Macromolecular Structure". This initial listing includes two books and seventeen suppliers of visual aid material. We expect to update both of these documents as appropriate and user comments on them are most welcome. Either or both may be ordered by completing item 3 on the Request Form.

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	516-282-4383
		F. C. Bernstein	516-282-4382
		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 Osaka, Japan	M. Kakudo	(06) 877-5111 ext. 3836

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

CODE	ITEM	01-JUL-81		AVAILABILITY			
		NO. TAPES 800 1600		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		
CONNECTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	X			
DSPLOTTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	X			
DIHDLRTP	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 APR-81 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	01-JUL-81			
		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	
CORR07FI	LIST OF CORRECTIONS NO. 7 (JUL/80-JAN/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			
FISIFLFI	PHI/PSI PLOTS (LINE PRINTER)	X			
PHIPSIFI	LISTS OF PHI/PSI/OMEGA VALUES	X			

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TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

Table with columns: IDENT, MOLECULE, DEPOSITOR(S), DATE/STATUS, and a large list of protein entries such as ACID PROTEINASE, CYTOCHROME B5, and HEMERYTHRIN B.

* NEW OR REPLACEMENT ENTRY SINCE APR-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
CONCT	INTERMOLECULAR CONTACTS	L. ANDREWS	10/79 NO
DOPLOT	DIAGONAL PLOTS ON PRINTER	E. SWANSON, F. BERNSTEIN	3/79 YES
DIHORL	COMPLETE TORSION ANGLES	E. ABOLA	3/80 YES
DSTNCE	CALC DISTANCES FROM CONECT RECORDS	F. BERNSTEIN	3/79 YES
FISLPL	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	H. ROSSMANN	6/79 NO
TAPOIR	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

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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, BIBLIOGRAPHIC ENTRIES

NAME	PURPOSE	AUTHOR(S)	REV DATE/ SUPPORTED
OEAP	ACID PROTEINASE (ENDOTHIA PARASITICA)		
OAF1	APOFERRITIN (HORSE)		
OMAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE		
OCTS	CITRATE SYNTHASE (PIG)		
OCTX	ALPHA COBRATOXIN		
OCN1	CONCAVALIN A (DEMETALLIZED)		
OCN2	CONCAVALIN A (DEMETALLIZED)		
OCYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)		
OCCY	CYTOCHROME C* (RHODOSPIRILLUM MOLISCHIANUM)		
OCY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)		
OSCI	CYTOCHROME C555 (CHLOROBBIUM THIOSULFATOPHILUM)		
OEZ2	ELASTASE COMPLEX (PIG)		
OETU	ELONGATION FACTOR TU COMPLEX (E. COLI)		
OE8X	ERABUTOXIN B		
OFD1	FERREDOXIN (AZOTOBACTER VINLANDII)		
OFX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)		
OFX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)		
OGP1	GLUTATHIONE PEROXIDASE (BOVINE)		
OGG1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)		
OH8G	HEMOGLOBIN (GLYCERA DIBRANCHIATA)		
OPH4	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)		
OUJ1	IMMUNOGLOBULIN, BENGE-JONES FRAGMENT (KAPPA) AU		
OR0Y	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)		
OMBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)		
OMB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)		
OMB4	MYOGLOBIN (SPERM WHALE, OXY)		
OSN3	*SCORPION NEUROTOXIN VARIANT-3		
OPFK	PHOSPHOFUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)		
OPP1	PHOSPHOLIPASE A2 (PORCINE)		
OPPA	PHOSPHORYLASE A (RABBIT)		
OPB1	PHOSPHORYLASE B (RABBIT)		
ORX5	RELAXIN (PORCINE, MODEL)		
ORSA	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)		
OTMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)		
OTBV	VIRUS (TOMATO BUSHY STUNT)		

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TABLE 5. PROTEIN DATA BANK, STRUCTURE FACTOR HOLDINGS

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
R1ACTSF	ACTINININ	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
R1ZNASF	DNA (Z', CGCG, HIGH-SALT, SYNTHETIC)	H. DREW, R. DICKERSON	1/81 SF
R1BNASF	*DNA (B, CGCGAATTCGG, SYNTHETIC)	H. DREW, R. DICKERSON	1/81 SF
RGPD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	8/75 SF
R2GPDF	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79 SF
R1HMH5F	*HENERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81 SF
R2MH5F	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER, HEIDNER, PERUTZ	6/80 SF
R1FDH5F	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/80 SF
RHUMDEH02	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	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
RDEHYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76 SF
R3RSASF	*RIBONUCLEASE A	A. WLODAWER	5/81 SF
RUBY02	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 APR-81 NEWSLETTER

CODES

SF STRUCTURE FACTORS

TABLE 7. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

01-JUL-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 '1MBN1' FOR SPERM-WHALE MYOGLOBIN, '1MBN2' 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.

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*IDENT,26PDD
*INSERT,26PDC.2
REMARK 17
REMARK 17 CORRECTION. CHANGE RESIDUE 6 FROM ASP TO ASN ON DEPOSITORS
REMARK 17 INSTRUCTIONS. 20-APR-81.
*DELETE,26PD.144
SEQRES 1 G 334 ACE SER LYS ILE GLY ILE ASN GLY PHE GLY ARG ILE GLY
*DELETE,26PD.261,268
ATOM 36 N ASN 6 6.007 -18.610 26.457 1.00 0.00
ATOM 37 CA ASN 6 5.396 -17.482 27.175 1.00 0.00
ATOM 38 C ASN 6 4.904 -16.462 26.147 1.00 0.00
ATOM 39 O ASN 6 5.674 -15.614 25.672 1.00 0.00
ATOM 40 CB ASN 6 6.426 -16.862 28.144 1.00 0.00
ATOM 41 ASN 6 5.754 -16.281 29.360 1.00 0.00
ATOM 42 AD1 ASN 6 5.245 -16.934 30.285 1.00 0.00
ATOM 43 AD2 ASN 6 5.791 -15.083 29.450 1.00 0.00
*DELETE,26PDC.9
MASTER 140 0 0 7 26 0 7 15 2507 1 0 26
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*IDENT,1CPAH
*INSERT,1CPAG.5
REMARK 12
REMARK 12 CORRECTION. CHANGE RESIDUE 72 FROM GLN TO GLU ON
REMARK 12 DEPOSITORS INSTRUCTIONS. 20-APR-81.
*DELETE,1CPA.32
SEQRES 6 307 LEU GLY ILE HIS SER ARG GLU TRP ILE THR GLN ALA THR
*DELETE,1CPA.56
HELIX 2 H2 GLU 72 GLU 88 1
*DELETE,1CPA.685,693
ATOM 57 N GLU 72 -4.795 23.159 -3.336 1.00 0.00
ATOM 57B CA GLU 72 -6.178 23.477 -0.029 1.00 0.00
ATOM 57C GLU 72 -7.113 22.267 -0.001 1.00 0.00
ATOM 58O GLU 72 -7.637 21.830 -1.047 1.00 0.00
ATOM 581 CB GLU 72 -6.140 23.944 -1.452 1.00 0.00
ATOM 582 CG GLU 72 -4.796 24.303 -1.913 1.00 0.00
ATOM 583 CD GLU 72 -4.610 25.777 -2.301 1.00 0.00
ATOM 584 OE1 GLU 72 -4.221 26.040 -3.486 1.00 0.00
ATOM 585 OE2 GLU 72 -4.909 26.657 -1.451 1.00 0.00
*DELETE,1CPAG.6
MASTER 78 2 1 8 8 32 0 6 2453 2 6 25
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*IDENT,1GPDE
*INSERT,1GPDE.3
REMARK 20
REMARK 20 CORRECTION. CHANGE RESIDUE 6 OF BOTH CHAINS FROM ASP TO ASN
REMARK 20 ON DEPOSITORS INSTRUCTIONS. 20-APR-81.
*DELETE,1GPD.106
SEQRES 1 G 334 ACE SER LYS ILE GLY ILE ASN GLY PHE GLY ARG ILE GLY
*DELETE,1GPD.132
SEQRES 1 R 334 ACE SER LYS ILE GLY ILE ASN GLY PHE GLY ARG ILE GLY
*DELETE,1GPD.298,305
ATOM 39 N ASN G 6 -7.206 17.820 24.791 1.00 0.00
ATOM 40 CA ASN G 6 -6.944 16.427 25.179 1.00 0.00
ATOM 41 C ASN G 6 -6.513 15.688 23.911 1.00 0.00
ATOM 42 O ASN G 6 -7.263 15.621 22.926 1.00 0.00
ATOM 43 CB ASN G 6 -8.212 15.816 25.815 1.00 0.00
ATOM 44 CG ASN G 6 -7.937 15.306 27.206 1.00 0.00
ATOM 45 AD1 ASN G 6 -8.576 14.433 27.766 1.00 0.00
ATOM 46 AD2 ASN G 6 -6.975 15.778 27.749 1.00 0.00
*DELETE,1GPD.2855,2862
ATOM 2596 N ASN R 6 6.489 -17.410 24.714 1.00 0.00
ATOM 2597 CA ASN R 6 6.183 -16.041 25.154 1.00 0.00
ATOM 2598 C ASN R 6 5.475 -15.010 24.273 1.00 0.00
ATOM 2599 O ASN R 6 6.111 -14.101 23.720 1.00 0.00
ATOM 2600 CB ASN R 6 7.485 -15.324 25.569 1.00 0.00
ATOM 2601 CG ASN R 6 7.697 -15.369 27.059 1.00 0.00
ATOM 2602 AD1 ASN R 6 6.697 -15.823 27.602 1.00 0.00
ATOM 2603 AD2 ASN R 6 6.819 -14.914 27.727 1.00 0.00
*DELETE,1GPDE.4
MASTER 143 0 6 14 52 0 14 15 5112 2 88 52
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*IDENT,BLYZC
*INSERT,BLYZB.2
REMARK 7
REMARK 7 CORRECTION. CHANGE RESIDUE 103 FROM ASN TO ASP AND CHANGE
REMARK 7 ATOM 788 FROM ND2 TO OD2 AS PER DEPOSITORS INSTRUCTIONS.
REMARK 7 21-MAY-81.
*DELETE,BLYZ.928,935
ATOM 781 N ASP 103 -3.290 29.710 30.060 1.00 0.00
ATOM 782 CA ASP 103 -2.750 30.590 29.010 1.00 0.00
ATOM 783 C ASP 103 -3.230 30.450 27.570 1.00 0.00
ATOM 784 O ASP 103 -2.700 31.100 26.640 1.00 0.00
ATOM 785 CB ASP 103 -1.220 30.450 28.940 1.00 0.00
ATOM 786 CG ASP 103 -0.590 30.560 30.300 1.00 0.00
ATOM 787 OD1 ASP 103 -0.030 29.580 30.700 1.00 0.00
ATOM 788 OD2 ASP 103 -0.680 31.530 31.040 1.00 0.00
*DELETE,BLYZB.6
MASTER 109 0 0 4 5 11 0 6 1000 1 10 10
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*IDENT,3PTIE
*INSERT,3PTID.3
REMARK 9
REMARK 9 CORRECTION. DELETE INITIAL ACE RESIDUE ON DEPOSITORS
REMARK 9 INSTRUCTIONS AND RENUMBER ALL REMAINING ATOMS. REVISE
REMARK 9 SEQRES AND CONECT RECORDS ACCORDINGLY. 27-MAY-81.
*DELETE,3PTI.41,45
SEQRES 1 58 ARG PRO ASP PHE CYS LEU GLU PRO PRO TYR THR GLY PRO
SEQRES 2 58 CYS LYS ALA ARG ILE ILE ARG TYR PHE TYR ASN ALA LYS
SEQRES 3 58 ALA GLY LEU CYS GLN THR PHE VAL TYR GLY CYS ARG
SEQRES 4 58 ALA LYS ARG ASN ASN PHE LYS SER ALA GLU ASP CYS MET
SEQRES 5 58 ARG THR CYS GLY GLY ALA
*DELETE,3PTI.60,564
ATOM 1 N ARG 1 26.522 27.417 -2.687 1.00 0.00
ATOM 2 CA ARG 1 25.603 26.909 -1.661 1.00 0.00
ATOM 3 C ARG 1 25.256 26.217 -4.466 1.00 0.00
ATOM 4 O ARG 1 27.268 25.519 -6.112 1.00 0.00
ATOM 5 CB ARG 1 24.610 25.885 -2.248 1.00 0.00
HETATM 498 O HOH 80 1.512 21.004 16.032 1.00 0.00
HETATM 499 O HOH 82 2.775 12.487 8.809 1.00 0.00
HETATM 500 O HOH 85 22.649 17.990 17.554 1.00 0.00
HETATM 501 O HOH 90 .741 19.373 13.161 1.00 0.00
HETATM 502 O HOH 95 11.965 8.325 14.883 1.00 0.00
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*DELETE,3PTI.565,570
CONECT 43 42 440
CONECT 110 109 302
CONECT 242 241 408
CONECT 302 110 301
CONECT 408 242 407
CONECT 440 43 439
*DELETE,3PTID.4
MASTER 79 4 0 1 2 0 0 6 501 1 6 5
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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. Documentation desired (no charge). If only documentation is requested, enclosure of a self-addressed envelope would be appreciated.

- () 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 (March 1981)
 () Non-Standard Entries (Structure Factors) format description for NONSTDTP and NONSTDFI (May 1981)
 () Data Deposition form

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).

<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 \$81 (£36 from Cambridge). Correction fiche are free.

Item

Cost

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 (£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 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