

We are pleased to announce that, effective immediately, data tapes distributed from Brookhaven and Cambridge will be available at 6250 cpi as well as 1600 cpi and 800 cpi. We would prefer, however, that data deposition tapes continue to be written at 1600 cpi or 800 cpi so that we can read them on our minicomputer before sending them to our central computer.

At this time we would like to thank the numerous users (about 190) who took the time to fill out our November questionnaire which dealt with the problem that the coordinate files (DATAPRTP) would shortly not be able to fit on one tape at 1600 cpi. More than half these users can read tapes at 6250 cpi. The option to keep on supplying the entire data base (on one tape at 6250 cpi for \$181, or two tapes at 1600 cpi for \$220) was preferred by a wide margin overall. Even among users who cannot read 6250 cpi tapes this option was slightly preferred over the second option - subdivision of the data base. The third option, data compression, was less favored. We expect to run out of space on one tape at 1600 cpi about the time that our next Newsletter will be published (April) and at that time we will revise our order form.

Those of you who have been reading this Newsletter since Number 7 in December 1978 will recall that we awarded a prize for the 100th distributable data entry. We are pleased to say that one of Dr. Emil Harutyunyan's leghemoglobin entries is our 200th distributable data entry. His prize (in these days of tight budgets) is a free copy of DATAPRTP. Please note that we have processed substantially more than 100 entries in the last four years, because many data entries are replacements.

Inquiries and suggestions are welcomed and may be addressed to any of the persons listed below. The request form on pages 5-6 of this Newsletter may be used to order data from Brookhaven or Cambridge; users in Australia or Japan should contact their centers for detailed information.

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 Yamadaoka, 3-2, Suita, 565 Japan	N. Yasuoka	(06) 877-5111 ext. 3912

Supported by the U. S. National Science Foundation

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

CODE	ITEM	18-JAN-83			
		NO. TAPES	AVAILABILITY	US	UK
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	2	1	1	X X X X
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	2	1	1	X X X
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	2	1	1	X X X
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	1	1	1	X
BLDK1TP	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER			
CONECTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	1	X
DGDIOTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	1	X
DIHDLRTP	COMPLETE TORSION ANGLES	2	1	1	X
DSTNCEP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	2	1	1	X
FIS1PLTP	PHI/PSI PLOTS (LINE PRINTER)	1	1	1	X
PHIPS1TP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	1	X

TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

NAME	PURPOSE	AUTHOR(S)	18-JAN-83	
			REV DATE/SUPPORTED	
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G. WILLIAMS	4/82	YES
BLDKIT	MODEL BUILDER'S KIT	E. ABOLA	5/82	YES
CHIRAL	CHECK CHIRALITY	E. ABOLA	1/82	YES
CONNECT	GENERATE CONNECTIVITY	F. BERNSTEIN	8/82	YES
CONCTC	INTERMOLECULAR CONTACTS	L. ANDREWS	9/82	NO
DGDIOT	DIAGONAL PLOTS ON PRINTER	E. SWANSON, F. BERNSTEIN	1/83	YES
DIHDLR	COMPLETE TORSION ANGLES	E. ABOLA	3/80	YES
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
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	11/79	YES
THEOD	MEASURE COORDINATES WITH THEODOLITE	L. LEBIODA	1/82	NO
TORSRU	COMPLETE TORSION ANGLES	G. REEKE	10/79	NO
TOTALS	VALIDATION OF MASTER RECORD	L. ANDREWS, F. BERNSTEIN	3/82	YES

\* NEW OR REPLACEMENT ENTRY SINCE OCT-82 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

DEAP	ITEM	18-JAN-83	
		REV DATE/SUPPORTED	
DEAP	ACID PROTEINASE (ENDOTHELIA PARASITICA)		
OADC	ADH-NADH-DIMETHYLSULFOXIDE COMPLEX		
OAF1	POPOFERRITIN (HORSE)		
OMAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE		
ORNB	BARNASE (BACILLUS AMYLOLIQUEFACIENS)		
OICB	CALCIUM-BINDING PROTEIN (MINOR A FORM, BOVINE)		
OPTC	D-ALANYL-CARBOXYPEPTIDASE-TRANSEPTIDASE		
OZPF	D-ALANYL-D-ALANINE PEPTIDASE (Zn2+ G PEPTIDASE)		
OCTS	CITRATE SYNTHASE (PIG)		
OCN2	CONCAVALIN A (DEMETALLIZED)		
OCRO	CRO REPRESSOR		
OGCR	GAMMA-CRYSTALLIN II (CALF)		
OCYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)		
OCY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)		
OC51	CYTOCHROME C555 (CHLOROBLUM THIOSULFATOPHILUM)		
OC3A	DES-ARG77-C3A ANAPHYLATOXIN		
OCDF	DIHYDROFLATE REDUCTASE (CHICKEN LIVER)		
DANB	DNA (GGTATACC)		
DANB	DNA (GG+UA+UACC)		
DESZ	ELASTASE COMPLEX (PIG)		
OETU	ELONGATION FACTOR TU COMPLEX (E. COLI)		
OEBX	ERABUTOXIN B		
OFX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)		
OFX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)		
OGAP	CATABOLITE GENE ACTIVATOR PROTEIN		
OGGI	GLUTATHIONE PEROXIDASE (BOVINE)		
OGD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)		
OHMG	HEMAGGLUTININ		
ODCH	HEMOGLOBIN (COBALT, DEOXY)		
OHBO	HEMOGLOBIN (GLYCERA DIBRANCHIATA)		
OPHH	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)		
OAUI	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU		
ORQY	IMMUNOGLOBULIN, BENCE-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		
OINI	INSULIN (PORCINE)		
OIN2	INSULIN (PORCINE)		
OLRP	N-TERMINAL DOMAIN OF LAMBDA REPRESSOR		
OLZ1	LYSOZYME (HUMAN)		
OLZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)		
OLZ6	LYSOZYME (STREPTOMYCES ERYTHRAEUS)		
OCTF	L7/L12 (E. COLI, C-TERMINUS)		
OMBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)		
OMB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)		
OPFK	PHOSPHOFRUCTOKINASE (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)		
ORST	RIBONUCLEASE ST (STREPTOMYCES ERYTHRAEUS)		
ORNT	RIBONUCLEASE T1-2(PRIME)-GUANYLIC ACID (ASPERGILLUS ORYZAE)		
OFMT	INITIATOR TRANSFER RNA (E. COLI, F/MET)		
OTA1	TRANSFER RNA (YEAST, ASP, A FORM)		
OTA2	TRANSFER RNA (YEAST, ASP, B FORM)		
OTRI	TRANSFER RNA (YEAST, PHE)		
OMTS	METHIONYL TRANSFER RNA SYNTHETASE		
OGN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)		
OUTG	UTEROGLOBIN (RABBIT)		
OSTV	VIRUS (SATELLITE TOBACCO NECROSIS)		
OTMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)		
OTBV	VIRUS (TOMATO BUSHY STUNT)		

\* NEW OR REPLACEMENT ENTRY SINCE OCT-82 NEWSLETTER

TABLE 2. PROTEIN DATA BANK. INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	18-JAN-83			
		AVAILABILITY	US	UK	JA
DATAPRF1	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	X	X	X	
NONST1F1	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	X	X	X	
NONST2F1	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	X	X	X	
CORR1F1	LIST OF CORRECTIONS NO. 11 (JUL/82 - JAN/83)	X	X	X	
BENDERF1	PARAMETERS FOR BENT-WIRE MODELS	PLEASE INQUIRE AT US CENTER			
BLDK1F1	MODEL BUILDER'S KIT	PLEASE INQUIRE AT US CENTER			
CONECTF1	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X			
DGDIOTF1	DIAGONAL PLOTS (LINE PRINTER)	X			
DIHDLRF1	COMPLETE TORSION ANGLES	X			
DSTNCF1	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X			
FIS1PLF1	PHI/PSI PLOTS (LINE PRINTER)	X			
PHIPS1F1	LISTS OF PHI/PSI/OMEGA VALUES	X			

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

IDENT CODE	MOLECULE	18-JAN-83	
		DEPOSITOR	DATE/ CODE
RIACTSF	ACTINININ	E. BAKER	7/77 SF
CHYMOF	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	4/73 SF
RCARF04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCARF05	CALCIUM-BINDING PARVALBUMIN	F. S. MATHEWS	12/77 SF
R2B5CSF	CYTOCHROME B5	T. TAKANO, R. DICKERSON	7/80 SF
R3CY1SF	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80 SF
R4CY1SF	CYTOCHROME C (ALBACORE, REDUCED)	R. KRETSINGER	8/75 SF
RQCV5501	CYTOCHROME C550	R. STENKAMP	6/81 SF
R1ZNASF	DNA (Z1, CGCG, HIGH-SALT, SYNTHETIC)	H. DREW, R. DICKERSON	1/81 SF
R1ZNASF	DNA (B, CGCGAATTCGGC, SYNTHETIC, 290 DEG K)	H. DREW, R. DICKERSON	1/81 SF
R1BNASF	GLYCERALDEHYDE 3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	12/79 SF
R2GDSF	AP0-GLYCERALDEHYDE 3-P-DEHYDROGENASE	M. ROSSMANN	8/75 SF
R1HMF5F	HEMERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81 SF
R2HMF5F	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER, HEIDNER, PERUTZ	6/80 SF
R1FDH5F	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/80 SF
RHMUDH02	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	5/75 SF
LAMPY1F	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)	J. GRUBB, 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
R1MCT5F1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76 SF
R0EMYSF1	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

CODES

SF STRUCTURE FACTORS

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

IDENT CODE	MOLECULE	18-JAN-83	
		DEPOSITOR	DATE/ CODE
R351CSF	CYTOCHROME C551 (OXIDIZED)	T. TAKANO, R. DICKERSON	9/81 SF
R51CSF	CYTOCHROME C551 (REDUCED)	T. TAKANO, R. DICKERSON	9/81 SF
R1ANASF	DNA (A, D-1000-CCGG)SPACE GROUP P 43 21 2	B. CONNER, R. DICKERSON	6/82 SF
R1ANAP2	DNA (A, D-1000-CCGG)SPACE GROUP P 21	B. CONNER, R. DICKERSON	6/82 SF
R2BNASF	DNA (B, CGCGAATTCGGC, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81 SF
R3BNASF	DNA (B, 9-BR-CGCGAATTCGGC, 20 DEG C)	KOPKA, FRATINI, DICKERSON2	8/82 SF
R1GASNF	DNA (B, 9-BR-CGCGAATTCGGC, 7 DEG C)	KOPKA, FRATINI, DICKERSON2	8/82 SF
R21NS5F	*GLUTAMINASE-ASPARAGINASE (ACTINOBACTER)	H. AMMON	12/82 SF
R1LH15F	INSULIN (BOVINE, 2-ZINC)DES-PHE B1	C. REYNOLDS, G. DODSON	5/82 SF
R2LH15F	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH25F	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH25F	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH35F	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH35F	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH45F	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH45F	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH55F	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH55F	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH65F	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH65F	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LH75F	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R2LH75F	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	4/82 SF
R1LYMSF	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	HOGLE, RAO, SUNDARALINGAM7	8/82 SF
R1MLT5F	MELITTIN	TERNILLIGER, EISENHOFER	8/81 SF
R1OV05F	OVOMUCOID FRAGMENT	E. PAPANIKOLAS, R. HUBER	1/82 SF
R2BP25F	PROPHOSPHOLIPASE A2 (BOVINE)	D. J. KOSTER, H. DRENTH	9/81 SF
R1RN35F	RIBONUCLEASE A	BORKAKOTI, MOSS, PALMER	6/82 SF
R4RSASF	RIBONUCLEASE A (XRAY)	A. WLODARER	6/82 SF
R4RSASF	RIBONUCLEASE A (NEUTRON)	A. WLODARER	6/82 SF
R3TLNSF	TRYP SIN (ORTHORHOMBIC, 2.4M)	B. MATTHEWS, M. HOLMES	2/82 SF
R2PTNSF	TRYP SIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81 SF
R1TPOSF	TRYP SIN (ORTHORHOMBIC)	BODE, WALTER, HUBER	9/82 SF
R3PTNSF	TRYP SIN (TRIGONAL, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81 SF
R3PTBSF	TRYP SIN (BENZAMIDINE INHIBITED)	BODE, SCHWAGER, WALTER	9/82 SF
R1TPPSF	TRYP SIN/P-AMIDINO-PHENYL-PHYRUVATE	WALTER, BODE, HUBER	9/82 SF
R4PT15F	TRYP SIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	9/82 SF
R2PTCSF	TRYP SIN/TRYP SIN INHIBITOR COMPLEX	R. HUBER, J. DEISENHOFER	9/82 SF
R1TPASF	TRYP SIN (ANHYDRO)/TRYP SIN INHIBITOR	HUBER, BODE, DEISENHOFER	9/82 SF
R2TGASF	TRYP SIN (GENE 5 DNA)	J. WALTER, R. HUBER	10/81 SF
R1TGCSF	TRYP SIN (GENE 5 DNA)	J. WALTER, R. HUBER	10/81 SF
R1TGTSF	TRYP SIN (GENE 5 DNA)	J. WALTER, R. HUBER	10/81 SF
R2TGTSF	TRYP SIN (GENE 5 DNA)	J. WALTER, R. HUBER	10/81 SF
R2TGPSF	TRYP SIN (GENE 5 DNA)	R. HUBER ET AL.	9/82 SF
R3TPI5F	TRYP SIN (GENE 5 DNA)	R. HUBER ET AL.	9/82 SF
R2TPI5F	TRYP SIN (GENE 5 DNA)	R. HUBER ET AL.	10/81 SF
R1TGSSF	TRYP SIN (GENE 5 DNA)	R. HUBER ET AL.	9/82 SF

CODES

SF STRUCTURE FACTORS

\* NEW OR REPLACEMENT ENTRY SINCE OCT-82 NEWSLETTER

TABLE 3. PROTEIN DATA BANK. ATOMIC COORDINATE HOLDINGS

IDENT	MOLECULE	DEPOSITOR(S)	DATE/STATUS			
2APE	ACID PROTEINASE (ENDOTHELIAL PARASITICA)	T. BLUNDELL	9/81 R	1LH1	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN 4/82 R
1APP	ACID PROTEINASE (PENICILLIUM JANTHINELLUM)	M. JAMES, I. HSU	12/79	2LH1	LEGHEMOGLOBIN (ACETATE MET)	VAINSHTEIN, HARUTYUNYAN 4/82
1APR	ACID PROTEINASE (RHIZOPUS CHINENSIS)	D. DAVIES	8/79	1LH2	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN, HARUTYUNYAN 4/82
2ACT	ACTININ	E. BAKER	11/79 R	2LH2	LEGHEMOGLOBIN (AQUO MET)	VAINSHTEIN, HARUTYUNYAN 4/82
1ACX	*ACTINOXANTHIN	V. PLETNEV, A. KUZIN	12/82 N	1LH3	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN 4/82
2ADK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77 R	2LH3	LEGHEMOGLOBIN (CYANO MET)	VAINSHTEIN, HARUTYUNYAN 4/82
1AGA	AGAROSE	S. ARNOTT	5/78	1LH4	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN 4/82
2AGA	AGGLUTININ (WHEAT GERM)	C. WRIGHT	5/80 R	2LH4	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN 4/82
4ADH	ALCOHOL DEHYDROGENASE (APO)	C. T. BRANDEN	8/79	1LH5	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN 4/82
1ALP	ALPHA LYTIC PROTEASE	BRAYER, DELBAERE, JAMES	6/79	2LH5	LEGHEMOGLOBIN (FLUORO MET)	VAINSHTEIN, HARUTYUNYAN 4/82
1ATA	TAKA-AMYLASE	KUSUNOKI, MATSUURA, KAKUDO	3/82 B	1LH6	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN 4/82
1ABP	L-ARABINOSE-BINDING PROTEIN	F. QUIOCHO, G. GILLILAND	5/80	2LH6	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN, HARUTYUNYAN 4/82
1AAT	CYTOSOLIC ASPARTATE AMINOTRANSFERASE	HARUTYUNYAN, MALASHKEVICH	4/82 A	1LH7	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN 4/82
2ATC	ASPARTATE CARBAMOYLTRANSFERASE	W. LIPSOMB	3/82	2LH7	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN 4/82
3ATC	ASPARTATE CARBAMOYLTRANSFERASE/CTP	W. LIPSOMB	3/82 R	1LZM	LYSOZYME (BACTERIOPHAGE T4)	B. MATTHEWS 3/77
1AZU	AZURIN	E. ADMAN, L. SIEKER, L. JENSEN	8/80	1LZV	LYSOZYME (HEN EGG-WHITE, SET W2)	R. DIAMOND, D. PHILLIPS 2/75
2BCL	BACTERIOCHLOROPHYLL A-PROTEIN	B. MATTHEWS	1/79 RA	2LYZ	LYSOZYME (HEN EGG-WHITE, SET RSSD)	R. DIAMOND, D. PHILLIPS 2/75
1ABX	ALPHA-BUNGAROTOXIN	D. AGARD, S. SPENCER, R. STROUD	4/80 A	3LYZ	LYSOZYME (HEN EGG-WHITE, SET R56A)	R. DIAMOND, D. PHILLIPS 2/75
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74	4LYZ	LYSOZYME (HEN EGG-WHITE, SET R56A)	R. DIAMOND, D. PHILLIPS 2/75
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74	5LYZ	LYSOZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND, D. PHILLIPS 2/75
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	8/74	6LYZ	LYSOZYME (HEN EGG-WHITE, SET RS16)	R. DIAMOND, D. PHILLIPS 2/75
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	S. ARNOTT	5/78	7LYZ	LYSOZYME (HEN EGG-WHITE, TRICLINIC)	A. YONATH 5/77
1CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	6/76	8LYZ	LYSOZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY 9/77
1CAC	CARBONIC ANHYDRASE C (HUMAN)	K. KANNAN	5/76	9LYZ	LYSOZYME (HEN, NAM-NAG-NAM, SUBSTRATE ONLY)	J. KELLY, M. JAMES 12/79
3CPA	CARBOXYPEPTIDASE A (GLYCYLTYROSINE)	D. REES, W. LIPSOMB	3/82 R	1LH2H	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	ARTYMIUK, BLAKE, RICE, WILSON 6/81 A
4CPA	CARBOXYPEPTIDASE A/POTATO INHIBITOR	D. REES, W. LIPSOMB	3/82	2LH2H	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	ARTYMIUK, BLAKE, RICE, WILSON 6/81 A
5CPA	CARBOXYPEPTIDASE A/WATER (BOVINE)	D. REES, W. LIPSOMB	5/82	1LYM	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	HOGLE, RAO, SUNDARLINGAM 7/82
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M. SCHMID, J. HERRIOTT	9/76 A	1LZ2	LYSOZYME (TURKEY EGG-WHITE)	R. BOTT, R. SARMA 9/81 A
1CAR	CARRAGEENAN	S. ARNOTT	5/78	1MDH	MALATE DEHYDROGENASE	L. BANASZAK 6/76 A
3CAT	CATALASE (BEEF LIVER)	M. ROSSMANN	7/82 R	1MLT	MELITTIN	TERWILLIGER, EISENBERG 8/81
1CNS	CHONDROITIN-4-SULFATE	S. ARNOTT	5/78	1MLP	MUREIN LIPOPROTEIN (HYPOTHETICAL)	A. MCLACHLAN 8/78
2CNS	CHONDROITIN-4-SULFATE (CA SALT)	S. ARNOTT	5/78	1MB5	MYOGLOBIN (SEAL, MET)	H. SCOULOUDI 3/79
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/78 R	1MBN	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON 4/73
3CHA	ALPHA-CHYMOTRYPSIN	A. TULINSKY	8/76	2MBN	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO 9/76
2GCH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	5/80 R	3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO 9/76
1CHG	CHYMOTRYPSINOGEN	J. KRAUT, J. BIRKTOFT	3/75	1MBD	MYOGLOBIN (SPERM WHALE, DEOXY)	S. PHILLIPS 8/81
1CTX	ALPHA COBRATOXIN	W. SAENGER, M. WALKINSHAW	3/82	1MB0	MYOGLOBIN (SPERM WHALE, OXY)	S. PHILLIPS 8/81
2CNA	CONCAVALIN A	G. REEKE, J. BECKER, G. EDELMAN	4/75	1MB5	MYOGLOBIN (SPERM WHALE, CO, NEUTRON)	HANSON, NORVELL, SCHOENBORN 11/82 N
3CNA	CONCAVALIN A	K. HARDMAN	9/76 R	1MHR	MYOHEMERYTHRIN	W. HENDRICKSON 6/76 A
1CN1	CONCAVALIN A (DEMETALLIZED)	M. SHOHAM	12/81	1NXB	NEUROTOXIN B (LATICAUDA SEMIFASCIATA)	D. TERNER, G. PETSKO 8/80
1CRN	CRAMBIN	W. HENDRICKSON, M. TEETER	5/81	1SN3	*SCORPION NEUROTOXIN (VARIANT 3)	C. BUGG ET AL. 12/82
2B5C	CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77 R	1OV0	OVUMUCOID THIRD DOMAIN (JAPANESE QUAIL)	E. PAPAMOKOS, R. HUBER 1/82
156B	CYTOCHROME B5(2) (E. COLI, OXIDIZED)	BETHGE, CZERWINSKI, MATHEWS	8/79	1PPT	AVIAN PANCREATIC POLYPEPTIDE	T. BLUNDELL 1/81
3CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80 R	9PAP	PAPAIN (NATIVE)	J. DRENTH 11/76 R
4CYT	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO, R. DICKERSON	7/80 R	1PAD	PAPAIN (ACE-AL-ALA-PHE-ALA, CYS-25)	J. DRENTH 11/76 R
1CYT	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	8/76	2PAD	PAPAIN (CYS DERIV OF CYS-25)	J. DRENTH 11/76 R
1CCY	CYTOCHROME C. PRIME.	P. WEBER, R. SALEMME	8/81	3PAD	PAPAIN (OXIDIZED CYS-25)	J. DRENTH 11/76 R
1CC2	CYTOCHROME C2	J. KRAUT	3/73	4PAD	PAPAIN (TOS-LYS, CYS-25)	J. DRENTH 11/76 R
1CDV	CYTOCHROME C3(D. VULGARIS MIYAZAKI)	HIGUCHI, YASUOKA, KAKUDO	1/82 A	5PAD	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)	J. DRENTH 11/76 R
155C	CYTOCHROME C5(D) (OXIDIZED)	R. TIMKOVICH	8/76	6PAD	PAPAIN (BZOXY-PHE-ALA, CYS-25)	J. DRENTH 11/76 R
351C	CYTOCHROME C5(1) (OXIDIZED)	MATSUURA, TAKANO, DICKERSON	7/81 R	1PEP	PEPSIN (PORCINE)	N. ANDREEVA ET AL. 7/78 A
451C	CYTOCHROME C5(1) (REDUCED)	MATSUURA, TAKANO, DICKERSON	7/81	1PFC	PFC FRAGMENT OF AN IGG	L. M. AMZEL 10/81
3DFR	DIHYDROFLAVONE REDUCTASE (L. CASEI)	J. BOLIN, D. MATTHEWS, J. KRAUT	6/82 R	3PKK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON 7/82
4DFR	DIHYDROFLAVONE REDUCTASE (E. COLI)	J. BOLIN, D. MATTHEWS, J. KRAUT	6/82 R	4PKK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE 9/76 B
1ANA	DNA (A, 5-PRIME)-D-1000-CCGG-3(PRIME)	B. CONNER, R. DICKERSON	6/82	3PGM	PHOSPHOGLYCERATE MUTASE	H. WATSON 4/82 R
1BNA	DNA (B, CGCGAATTCGCG, SYNTHETIC, 290 DEG K)	H. DREW, R. DICKERSON	1/81	1BP2	PHOSPHOLIPASE A2 (BOVINE)	B. DIJKSTRA, J. DRENTH 4/81
2BNA	DNA (B, CGCGAATTCGCG, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81	2BP2	PROPHOSPHOLIPASE A2	B. DIJKSTRA, W. HOL, J. DRENTH 6/81
3BNA	DNA (B, 9-BR-CGCGAATTCGCG, 20 DEG C)	KOPKA, FRATINI, DICKERSON	2/82	1PCY	PLASTOCYANIN	J. GUSS, H. FREEMAN 8/80
4BNA	DNA (B, 9-BR-CGCGAATTCGCG, 7 DEG C)	KOPKA, FRATINI, DICKERSON	2/82	2PAB	PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, C. BLAKE 9/77 R
1ZNA	DNA (Z, CGCC, HIGH-SALT, SYNTHETIC)	H. REW, R. DICKERSON	1/81	1PYK	PYRUVATE KINASE (CAT)	H. MURHEAD 1/80 A
2ZNA	DNA (Z-1, CGCCGG, SYNTHETIC, MODEL)	A. RICH	2/81	1RLX	RELAXIN (MODEL, CONFORMATION A, UNREFINED)	A. EVANS, A. NORTH 3/78
3ZNA	DNA (Z-1, CGCCGG, SYNTHETIC, MODEL)	A. RICH	2/81	2RLX	RELAXIN (MODEL, CONFORMATION B, UNREFINED)	A. EVANS, A. NORTH 3/78
1DNN	*DNA (ATCGGTAAG... MODEL)	J. SUSSMAN, E. TRIFONOV	11/82 N	3RLX	RELAXIN (MODEL, CONFORMATION A, REFINED)	A. EVANS, A. NORTH 3/78
1EST	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76	4RLX	RELAXIN (MODEL, CONFORMATION B, REFINED)	A. EVANS, A. NORTH 3/78
1ECD	ERYTHROCYRUCORIN (REDUCED, DEOXY)	W. STEIGEMANN, E. WEBER	3/79	1RHD	RHODANASE	W. HOL 12/77
1ECO	ERYTHROCYRUCORIN (CARBONMONOXO)	W. STEIGEMANN, E. WEBER	3/79	4RSA	RIBONUCLEASE A (XRAY+NEUTRON)	A. WLODAWER 6/82 R
1ECA	ERYTHROCYRUCORIN (AQUO, MET)	W. STEIGEMANN, E. WEBER	3/79	1RN3	RIBONUCLEASE A	BORKAKOTI, MOSS, PALMER 10/81
1ECN	ERYTHROCYRUCORIN (CYANO, MET)	W. STEIGEMANN, E. WEBER	3/79	1RNS	RIBONUCLEASE S	H. WYCKOFF, F. RICHARDS 4/73
2FD1	FERREDOXIN (AZOTOBACTER VINELANDII)	STOUT, GHOSH, FUREY, O'DONNELL	11/81 R	2RXN	RUBREDOXIN (CLOSTRIDIUM PASTEURIANUM)	L. JENSEN 1/75
1FDX	FERREDOXIN (PEPTOCOCCUS AERGENES)	E. ADMAN, L. SIEKER, L. JENSEN	8/76	3RXN	RUBREDOXIN (DESULFOVIBRIO VULGARIS)	E. ADMAN, L. SIEKER, L. JENSEN 5/82 R
1FXD	FERREDOXIN (SPIRULINA PLATENSIS)	TSUKIHARA, KATSUBE, KAKUDO	12/81 R	2SNS	STAPHYLOCOCCAL NUCLEASE	M. LEGG, F. A. COTTON, E. HAZEN 5/80 R
3FXN	FLAVODOXIN (CLOSTRIDIUM MP, OXIDIZED)	M. LUDWIG	12/77 R	1SGA	STREPTOMYCES GRISEUS PROTEINASE A	BRAYER, DELBAERE, JAMES 6/78
4FXN	FLAVODOXIN (CLOSTRIDIUM MP, SEMIQUINONE)	M. LUDWIG	12/77	25GB	STREPTOMYCES GRISEUS PROTEINASE B	DELBAERE, BRAYER, JAMES 6/79 R
1GCA	GLUCAGON	T. BLUNDELL	10/77	25S1	SUBTILISIN INHIBITOR (STREPTOMYCES)	Y. MITSUI ET AL. 4/80 R
1PGI	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77	1SBT	SUBTILISIN BPN, PRIME.	J. KRAUT 8/72
2GRS	GLUTATHIONE REDUCTASE (HUMAN)	G. SCHULZ	11/81 R	2SBT	SUBTILISIN NOVO	J. DRENTH 9/76
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	7/75	25OD	SUPEROXIDE DISMUTASE	J. RICHARDSON, D. RICHARDSON 3/80 R
2GPD	APO-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79	31LN	THERMOLYSIN (NATIVE)	B. MATTHEWS, M. HOLMES 2/82 R
1HRB	HEMERYTHRIN B	W. HENDRICKSON	6/76 A	4TLN	THERMOLYSIN (NON-BZMALONYL-A-G-NITROANL)	B. MATTHEWS, M. HOLMES 2/82
1HMB	HEMERYTHRIN (MET, HYDROXO)	R. STENKAMP	6/81 R	6TLN	THERMOLYSIN (CH2CO(N-OH)LEUCOCH3)	B. MATTHEWS, M. HOLMES 2/82
1HDS	HEMOGLOBIN (DEER, SICKLE CELL)	E. AMMA, R. GIRLING	10/79	19RX	THIOREDOXIN (E. COLI, OXIDIZED)	B. O. SODERBERG 5/76 A
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	R. LADNER, HEIDNER, PERUTZ	2/77 R	4TNA	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG 4/78 R
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73	5TNA	TRANSFER RNA (YEAST, PHE)	S. H. KIM ET AL. 11/78 R
1LHB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	4/75	8TNA	TRANSFER RNA (YEAST, PHE)	M. SUNDARLINGAM 2/79 R
1HCO	HEMOGLOBIN (HUMAN, CARBONMONOXO)	J. BALDWIN	8/79	11TM	TRIOSE PHOSPHATE ISOMERASE	I. WILSON, D. PHILLIPS 9/76
2HCO	HEMOGLOBIN (HUMAN, CARBONMONOXO, NRG REFND)	J. BALDWIN	8/79	11TC	TRONPIN (CA-BINDING COMPONENT, MODEL)	R. KRETSINGER, C. BARRY 6/80 A
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	8/76	2PTN	TRYPSIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER, W. BODE 10/81 R
1LHB	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	3/73	1TPO	TRYPSIN (ORTHORHOMBIC)	W. BODE, J. WALTER, R. HUBER 9/82
2YHK	HEXOKINASE (YEAST) FORM B111	STEITZ, ANDERSON, STENKAMP	3/78 R	3PTN	TRYPSIN (TRIGONAL, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER, W. BODE 10/81
1HK6	HEXOKINASE A - GLUCOSE COMPLEX (YEAST)	W. BENNETT JR., T. STEITZ	12/80	3PTB	TRYPSIN (BENZAMIDINE INHIBITED)	W. BODE, P. SCHWAGER, J. WALTER 9/82 R
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75	3PTP	TRYPSIN (P-AMIDINO-PHENYL-PYRUVATE INHIBITED)	J. WALTER, W. BODE, R. HUBER 9/82
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	11/77	4FTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER 9/82 R
2HYA	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S. ARNOTT	5/78	2PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R. HUBER, J. DEISENHOFER 9/82 R
3HYA	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S. ARNOTT	5/78	1TPA	TRYPSIN (ANHYDRO)/TRYPSIN INHIBITOR	HUBER, BODE, DEISENHOFER 9/82
4HYA	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78	1TGN	TRYPSINOGEN	A. KOSSIAKOFF, R. STROUD 9/79
3FAB	IMMUNOGLOBULIN F-AB, PRIME, NEW	R. POLJAK	9/81 R	2TGA	TRYPSINOGEN (2.4M MGSO4)	J. WALTER, R. HUBER, W. BODE 10/81 R
1MCG	IMMUNOGLOBULIN B-J FRAGMENT	SCHIFFER, EDMUNDSON ET AL.	5/78 A	1TGC	TRYPSINOGEN (.5 CH3OH, .5 HOH)	J. WALTER, R. HUBER, W. BODE 10/81
1RE1	IMMUNOGLOBULIN B-J FRAGMENT (V-DIMER) RE1	O. EPP, R. YUO	5/78 A	1TGT	TRYPSINOGEN (173 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER, W. BODE 10/81
1RHE	IMMUNOGLOBULIN B-J FRAGMENT (V-MMER) RHE	B. WANG, C. HOO, M. SAX	12/77 A	2TGT	TRYPSINOGEN (103 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER, W. BODE 10/81
1FC1	IMMUNOGLOBULIN FC (HUMAN)	J. DEISENHOFER	5/81	1TGB	TRYPSINOGEN (WITH CA FROM PEG)	W. BODE, FEHLHAMMER, HUBER 3/79
1FC2	IMMUNOGLOBULIN FC-FRAGMENT B COMPLEX	J. DEISENHOFER	5/81	2TGP	TRYPSINOGEN/TRYPSIN INHIBITOR	R. HUBER ET AL. 9/82 R
1INS	INSULIN (PORCINE, 2-ZINC)	C. REYNOLDS, G. DODSON	7/80	3TPI	TRYPSINOGEN/TRYPSIN INHIBITOR/ILE-VAL	R. HUBER ET AL. 9/82 R
2INS	INSULIN (BOVINE, 2-ZINC) DES-PHE B1	G. DODSON, G. DODSON	5/82	2TPI	TRYPSINOGEN/PTI/ILE-VAL (MERCURATED)	J. WALTER, R. HUBER, W. BODE 10/81
1GF1	*INSULIN-LIKE GROWTH FACTOR I	BLUNDELL, BEDARKAR, HUMBEL	12/82 N	1TGS	TRYPSINOGEN/PSTI	R. HUBER ET AL. 9/82
1GF2	*INSULIN-LIKE GROWTH FACTOR II	BLUNDELL, BEDARKAR, HUMBEL	12/82 N	1TS1	TYROSYL TRANSFER RNA SYNTHETASE	BHAT, BLON, BRICK, NYBORG 7/82 A
1KGA	KDGP ALDOLASE	A. TULINSKY	8/78	25BV	VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC)	M. ROSSMANN 5/82 R
1KES	KERATAN SULFATE	S. ARNOTT	5/78			
4LDH	LACTATE DEHYDROGENASE (DOG FISH)	W. EVENTOFF, M. ROSSMANN	4/77 R			
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE (DOG F)	M. ROSSMANN	11/74			
5LDH	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU, M. ROSSMANN	10/80			
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)	W. MUSICK, M. ROSSMANN	9/78			

\* NEW OR REPLACEMENT ENTRY SINCE OCT-82 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 REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 8. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

18-JAN-83

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 'IMBNA' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK 'IMBN' FOR SPERM-WHALE MYOGLOBIN, 'IMBNB' 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,155CF
\*INSERT,155CE.7
REMARK 10 CORRECTION. IDENTIFY RESIDUES 122 TO 134 AS UNK RATHER THAN
REMARK 10 GLY. 25-OCT-82.
\*DELETE,155C.35,36
SEQRES 10 135 ASP ASP PRO ASP ALA UNK UNK UNK UNK UNK UNK UNK UNK
SEQRES 11 135 UNK UNK UNK UNK UNK
\*DELETE,155C.38,41
FTNOTE 1 SIDE CHAIN ATOMS FOR RESIDUES 122 TO 134 ARE NOT INCLUDED
FTNOTE 1 BECAUSE THE SEQUENCE IN THIS REGION IS NOT DEFINITELY
FTNOTE 1 KNOWN. THE RESIDUES HAVE BEEN LABELLED AS UNK.

Table with columns for ATOM ID, Residue Name, Chain, Residue Number, and B-factor. Includes entries for residues 922-953, 954-966, 967-974, and 975-987.

\*IDENT,3PGKA
\*INSERT,3PGK.61
REMARK 6 CORRECTION. INTERCHANGE ATOMS OE1 AND OE2 OF GLU 341 AND
REMARK 6 ATOMS OD1 AND OD2 OF ASP 372. CORRECT FORMUL RECORDS.
REMARK 6 ADD REMARK 7 ABOUT ATP AND MP3 INTERACTIONS WITH THE
REMARK 6 PROTEIN. 25-OCT-82.
REMARK 7
REMARK 7 THE FOLLOWING ARE POSSIBLE INTERACTIONS BETWEEN ATP, MP3
REMARK 7 AND THE PROTEIN
REMARK 7
REMARK 7 NH2 ARG 38 OC3 MP3 3
REMARK 7 OG1 THR 391 OC2 MP3 3
REMARK 7 N GLY 393 OH MP3 3
REMARK 7 N ASP 372 O2A ATP 1
REMARK 7 MG MG 2 OD1 ASP 372
REMARK 7 N2 LYS 217 O1B ATP 1
REMARK 7 ND2 ASN 334 O2B ATP 1
REMARK 7 N2 LYS 213 O2A ATP 1
REMARK 7 O3\* ATP 1 OD2 ASP 372
REMARK 7 O2\* ATP 1 OE1 GLU 341
REMARK 7 N6 ATP 1 O LEU 311

\*DELETE,3PGK.99,101
FORMUL 2 ATP C10 H12 N5 O13 P3 ----
FORMUL 3 MG MG1 ++
FORMUL 4 MP3 C3 H4 O7 P1 ---
\*DELETE,3PGK.2769,2770
ATOM 2621 OE1 GLU 341 30.499 -2.090 20.649 1.00 0.00
ATOM 2622 OE2 GLU 341 30.132 -.253 19.430 1.00 0.00
\*DELETE,3PGK.2984,2985
ATOM 2836 OD1 ASP 372 27.703 -6.320 15.823 1.00 0.00
ATOM 2837 OD2 ASP 372 28.198 -5.488 17.838 1.00 0.00
\*DELETE,3PGK.3384
MASTER 68 2 3 14 14 12 0 6 3191 1 43 32

\*IDENT,3FABB
\*INSERT,3FABA.3
REMARK 6
REMARK 6 CORRECTION. INSERT CAUTIONARY NOTE AND ADD FTNOTE 1 TO
REMARK 6 RESIDUE ILE H 100. 25-OCT-82.
REMARK 7
REMARK 7 CAUTION(WARNING). THIS COORDINATE SET SHOULD BE REGARDED
REMARK 7 AS A PRELIMINARY DEPOSITION FROM THE AUTHORS. EXTENSIVE
REMARK 7 CHECKING FOR ERRORS AND FOR POSSIBLE ADJUSTMENTS ARE STILL
REMARK 7 IN PROGRESS AND A NEW AND FINAL SET WILL BE DEPOSITED WHEN
REMARK 7 THIS PROCESS IS COMPLETED.
\*INSERT,3FAB.98
FTNOTE 1
FTNOTE 1 THE CONFORMATION OF THE PEPTIDE GROUP OF RESIDUE ILE H 100
FTNOTE 1 HAS BEEN FOUND TO BE IN NEED OF SOME MINOR ADJUSTMENTS AND
FTNOTE 1 WILL BE CORRECTED IN A SUBSEQUENT DEPOSITION.
\*DELETE,3FAB.2471,2478
ATOM 2330 N ILE H 100 -43.130 32.080 4.920 1.00 0.00 1
ATOM 2331 CA ILE H 100 -43.660 31.620 3.640 1.00 0.00 1
ATOM 2332 C ILE H 100 -43.070 32.360 2.490 1.00 0.00 1
ATOM 2333 O ILE H 100 -42.040 32.980 2.690 1.00 0.00 1
ATOM 2334 CB ILE H 100 -45.220 31.830 5.770 1.00 0.00 1
ATOM 2335 CG1 ILE H 100 -45.510 32.230 5.270 1.00 0.00 1
ATOM 2336 CG2 ILE H 100 -46.050 30.630 3.200 1.00 0.00 1
ATOM 2337 CD1 ILE H 100 -44.720 33.550 5.730 1.00 0.00 1
\*DELETE,3FABA.4
MASTER 70 4 0 4 33 0 0 6 3189 2 10 33

\*IDENT,2GRSA
\*INSERT,2GRS.68
REMARK 7
REMARK 7 CORRECTION. INSERT NEW PUBLICATION AS REFERENCE 1 AND
REMARK 7 RENUMBER THE OTHERS. INSERT MISSING HET AND FORMUL
REMARK 7 RECORDS. CORRECT ATOM NAME IN FAD. 25-OCT-82.
\*INSERT,2GRS.12
REMARK 1 REFERENCE 1
REMARK 1 AUTH G.E.SCHULZ,R.H.SCHIRMER,E.F.PAI
REMARK 1 TITL /FAD\*-BINDING SITE OF GLUTATHIONE REDUCTASE
REMARK 1 REF J.MOL.BIOL. V. 160 287 1982
REMARK 1 REFN ASTM JMOBOK UK ISSN 0022-2836 070
\*DELETE,2GRS.13
REMARK 1 REFERENCE 2
\*DELETE,2GRS.21
REMARK 1 REFERENCE 3
\*DELETE,2GRS.26
REMARK 1 REFERENCE 4
\*DELETE,2GRS.33
REMARK 1 REFERENCE 5
\*DELETE,2GRS.39
REMARK 1 REFERENCE 6
\*DELETE,2GRS.45
REMARK 1 REFERENCE 7
\*INSERT,2GRS.107
HET FAD 1 53 FLAVIN-ADENINE DINUCLEOTIDE
FORMUL 2 FAD 1 C27 H33 N9 O15 P2
\*DELETE,2GRS.3654
HETATM 3618 A02 FAD 1 178.685 49.537 82.758 1.00 0.00
\*DELETE,2GRS.3758
MASTER 66 2 1 11 26 0 0 6 3551 1 53 37

\*IDENT,3PGKB
\*INSERT,3PGKA.20
REMARK 8
REMARK 8 CORRECTION. DELETE INCORRECT CONECT RECORD. 03-DEC-82.
\*DELETE,3PGK.3372
\*DELETE,3PGKA.28
MASTER 70 2 3 14 14 12 0 6 3191 1 42 32

\*IDENT,DGLOT3
\*DELETE,DGLOT2.4
C LAST REVISION. 1/83
\*INSERT,DGLOT2.13
C
C CORRECTION. INCREASE DIMENSIONS TO ALLOW FOR LARGER STRUCTURES.
C CORRECT HANDLING OF OVERLY LARGE STRUCTURE. DO NOT USE
C VARIABLE ITEM# FOR TWO DIFFERENT PURPOSES. WRITE END-OF-FILE
C BETWEEN PLOTS. 06-JAN-83.

\*DELETE,DGLOT.142,144
DIMENSION IRSNAM(2000),IRSNAM(2000),IRSNAM(2000),IRSNAM(2000)
DIMENSION X(2000),Y(2000),Z(2000)
DATA LIMAT/2000/
\*DELETE,DGLOT.214,215
40 CALL NXTLIN(JUNK,JUNK,JUNK,JUNK,JUNK,JUNK,JUNK,JUNK,JUNK,
1,FTNT,JCDE)
\*INSERT,DGLOT.244
ENDFILE IOUT
\*DELETE,DGLOT.274,276
ITEM=IRSNAM(I)/1000+1
IF ((ITEM.EQ.1) GO TO 120
IROW(I)=ICHAR(ITEM)
\*DELETE,DGLOT.285,287
ITEM=MOD(KX,10)+1
IF ((ITEM.EQ.1).AND.(ICOMP(IROW(IJ),IBLANK).EQ.0)) GO TO 130
IROW(I)=ICHAR(ITEM)
\*DELETE,DGLOT.296,298
ITEM=MOD(KX,10)+1
IF ((ITEM.EQ.1).AND.(ICOMP(IROW(IJ),IBLANK).EQ.0)) GO TO 140
IROW(I)=ICHAR(ITEM)
\*DELETE,DGLOT.306,308
ITEM=MOD(IRSNUM(I),10)+1
IF ((ITEM.EQ.1).AND.(ICOMP(IROW(IJ),IBLANK).EQ.0)) GO TO 150
IROW(I)=ICHAR(ITEM)
\*INSERT,DGLOT.341
ENDFILE IOUT

## 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 (October 1982)  
 ( ) 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 (October 1982)  
 ( ) Non-Standard Entries (Structure Factors) format description for  
 NONST2TP and NONST2FI (January 1983)  
 ( ) Data Deposition form

## 3. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs \$181 (£106 from Cambridge); each 2-tape item costs \$220 (£129). Domestic postage is included.

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

Total \_\_\_\_\_

Special Instructions (to be completed for Brookhaven requests only).  
 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. Tape format desired (all tapes are unlabelled)

	Availability	
	US	UK
( ) 9 track, 6250 cpi, EBCDIC	yes	yes
( ) 9 track, 1600 cpi, EBCDIC	yes	yes
( ) 9 track, 800 cpi, EBCDIC	yes	yes
( ) 9 track, 6250 cpi, ASCII	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 \$111 (£65), postage included. Correction fiche are free.

<u>Item</u>	<u>Cost</u>
	Total _____

6. Please send the following printed listings. Each listing costs \$70, (£41), postage included.

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

7. Foreign 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 (£9) is required per magnetic tape (not per item).

Number of tapes x \$15.00 (£9) = \_\_\_\_\_

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