

All of our contributors and users will be pleased to know that the National Institutes of Health have awarded funds to the Protein Data Bank to help support our services. These funds will assist us in bearing the increasing costs of processing a higher volume of new data and of maintaining a rapidly growing data base.

Table 3, which lists the currently available atomic coordinate holdings, has been reorganized so that the structures which were not derived directly from experimental data are identified as "model" and listed separately. These data sets have also been grouped separately (at the end) on our distribution tape (DATAPRTP) and microfiche (DATAPRFI).

We are trying a simpler method of preparing the tables for this Newsletter. If anyone has a strong opinion, favorable or not, about their legibility please let us know. Postal costs limit us to three sheets of paper; this then implies small print.

Enrique Abola will be attending the August Snowmass ACA meeting and will be happy to receive comments from users. As always, inquiries and suggests may be addressed to any 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. 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 and U. S. National Institutes of Health.

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

CODE	ITEM	06-JUL-83						
		NO. TAPES AVAILABILITY 800 1600 6250 US UK JA AUS						
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 4, 7)	2	2	1	X	X	X	X
NONST1TP	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 5)	2	1	1	X	X	X	X
NONST2TP	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 6)	2	1	1	X	X	X	X
BENDERTP	PARAMETERS FOR BENT-WIRE MODELS	2	1	1	X	X	X	X
BLDKITTP	MODEL BUILDER'S KIT	PLEASE	INQUIRE	AT	US	CENTER		
CONNECTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	1	X			
DGPLOTTP	DIAGONAL PLOTS (LINE PRINTER)	1	1	1	X			
D1HORLTP	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			
PHIPSIPT	LISTS OF PHI/PSI/OMEGA VALUES	1	1	1	X			

* NEW OR REPLACEMENT ENTRY SINCE APR-83 NEWSLETTER

TABLE 4. PROTEIN DATA BANK, AVAILABLE PROGRAMS

06-JUL-83				
NAME	PURPOSE	AUTHOR(S)	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 FULL CONNECTIVITY	F.BERNSTEIN	8/82	YES
CONTACT	INTERMOLECULAR CONTACTS	L.ANDREWS	9/82	NO
DGPLOT	DIAGONAL PLOTS ON PRINTER	E.SHWANSON,F.BERNSTEIN	1/83	YES
D1HORL	COMPLETE TORSION ANGLES	E.ABOLA	3/80	YES
DSTNCE	CALC DISTANCES FROM CONNECT RECORDS	F.BERNSTEIN	8/82	YES
FIS1PL	PHI/PSI PLOTS ON PRINTER	F.BERNSTEIN	5/79	YES
HASRP	HEAVY ATOM SEARCH-REFINEMENT PACKAGE	TERWILLIGER,EISENBERG,KIM	2/83	NO
LSH	COLOR-CODED ALPHA-CARBON MODELS	R.MATELA,R.FLETTERICK	3/82	NO
NAIWD	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	M.ROSSMANN	6/79	NO
TAPDIR	PRINT DIRECTORY OF TAPE CONTENTS	H.BERNSTEIN,F.BERNSTEIN	11/79	YES
THEOD	MEASURE COORDINATES WITH THEODOLITE	L.LEBIDOA	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 APR-83 NEWSLETTER

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

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

06-JUL-83				
CODE	ITEM	AVAILABILITY US UK JA AUS		
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. 12 (JAN/83 - JUL/83)	X	X	X
BENDRF1	PARAMETERS FOR BENT-WIRE MODELS	X		
BLDKITF1	MODEL BUILDER'S KIT	PLEASE	INQUIRE	AT US CENTER
CONNECTF1	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	X		
DGPLOTF1	DIAGONAL PLOTS (LINE PRINTER)	X		
D1HORLF1	COMPLETE TORSION ANGLES	X		
DSTNCF1	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	X		
FIS1PLF1	PHI/PSI PLOTS (LINE PRINTER)	X		
PHIPSI1F1	LISTS OF PHI/PSI/OMEGA VALUES	X		

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

06-JUL-83				
IDEN	MOLECULE	DEPOSITOR	DATE/	CODE
R1ACTSF	ACTININ	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	2/74	SF
R2BSC5F	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
RCYCS501	CYTOCHROME C550	R.TINKOVICH	4/76	SF
R1ZNASF	DNA (Z', CCGG, HIGH-SALT, SYNTHETIC)	H.DREW,R.DICKERSON	1/81	SF
R1BNASF	DNA (B, CCGGAATTCGGG, SYNTHETIC, 290 DEG K)	H.DREW,R.DICKERSON	1/81	SF
R6PD04F	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M.ROSSMANN	8/75	SF
RG6P04F	APF-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M.ROSSMANN	12/79	SF
R2M4BSF	HEMOGLOBIN (HORSE, ADO MET AND CO)	LADNER,HEIDNER,PERUTZ	6/80	SF
R1FDHSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J.FRIER	6/80	SF
RHM2HO2F	HEMOGLOBIN (HUMAN, DEOXY)	M.PERTZ,G.FERMI	5/75	SF
LAMPY1F	HEMOGLOBIN (LAMPREY)	HENDRICKSON,LOVE,KARLE	5/73	SF
RLDH07F	LACTATE DEHYDROGENASE	M.ROSSMANN	8/75	SF
R2LDH07F	LACTATE DEHYDROGENASE/ANAD/PYRUVATE	M.ROSSMANN	8/75	SF
R2LDHSF	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
RMTMYS1F	MYOGLOBIN (SPERM WHALE, MET)	T.TAKANO	6/76	SF
RDEHS1F	MYOGLOBIN (SPERM WHALE, DEOXY)	T.TAKANO	6/76	SF
RRLBY02F	RUDEOXIN	L.JENSEN	3/74	SF
RHTNASF	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)

06-JUL-83				
IDEN	MOLECULE	DEPOSITOR	DATE/	CODE
R1CCR5F	*CYTOCHROME C (RICE)	H.OCHI,N.TANAKA	3/83	SF
R5S1CSF	CYTOCHROME C551 (OXIDIZED)	T.TAKANO,R.DICKERSON	9/81	SF
R5S1CSF	CYTOCHROME C551 (REDUCED)	T.TAKANO,R.DICKERSON	9/81	SF
R1ANAS2F	DNA (A,D-1000-CCGG)SPACE GROUP P 43 21 2	B.CONNER,R.DICKERSON	6/82	SF
R1ANAS2F	DNA (A,D-1000-CCGG)SPACE GROUP P 21	B.CONNER,R.DICKERSON	6/82	SF
R2BNAS5F	DNA (B, CCGGAATTCGGG, SYNTHETIC, 16 DEG K)	H.DREW,R.DICKERSON	11/81	SF
R2BNAS5F	DNA (B, 9-BR-CCGGAATTCGGG, 20 DEG C)	KOPKA,FRATINI,DICKERSON2/82	SF	
R2KNAS5F	DNA (B, 9-CCGGAATTCGGG, 7 DEG C)	KOPKA,FRATINI,DICKERSON2/82	SF	
R1GAASF	GLUTAMINASE-ASPARAGINASE (ACTINOBACTER)	H.AMMON	12/82	SF
R1GASSF	GLUTAMINASE-ASPARAGINASE (PSEUDOMONAS 7A)	H.AMMON	12/82	SF
R1HM5F	*HEMERYTHRIN (MET)	STENKAMP,STIEKER,JENSEN	2/83	SF
R1HMZ5F	*HEMERYTHRIN (AZIDO, MET)	STENKAMP,STIEKER,JENSEN	2/83	SF
R2IN5SF	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 (FLURO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH5SF	LEGHEMOGLOBIN (FLURO MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH6SF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH6SF	LEGHEMOGLOBIN (NICOTINATE MET)	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LH7SF	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R2LH7SF	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN,HARUTYUNYAN	4/82	SF
R1LYM5F	*LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	HOGLE,RAO,SUNDARALINGAM7/82	SF	
R1MLTSF	MELITTIN	TERWILLIGER,EISENBERG	8/81	SF
R1O10VF	OVOMUCOID FRAGMENT	E.PAPAMAKOS,R.HUBER	1/82	SF
R2B2PSF	PROPHOSPHOLIPASE A2 (BOVINE)	D.I.KSTRA,HOL.DRENTH	9/81	SF
R1PYPSF	INORGANIC PYROPHOSPHATASE	E.HARUTYUNYAN ET AL.	2/83	SF
R1RN3SF	RIBONUCLEASE A	BORKAKOTI,MOSS,PALMER	6/82	SF
R4RSASFX	RIBONUCLEASE A (XRAY)	A.WLODAWEK	6/82	SF
R4RSASFN	RIBONUCLEASE A (NEUTRON)	A.WLODAWEK	6/82	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
R1TPOSF	TRYPSIN (ORTHORHOMBIC)	BODE,WALTER,HUBER	9/82	SF
R3PTNSF	TRYPSIN (TRIGONAL, 2.4M (NH4)2SO4)	J.WALTER,R.HUBER	10/81	SF
R3PTBSF	TRYPSIN (BENZAMIDINE, INHIBITED)	BODE,SCHLAGER,WALTER	9/82	SF
R1TPPSF	TRYPSIN (P-AMINO-PHENYL-PYRUVATE)	WALTER,BODE,HUBER	9/81	SF
R4PT1SF	TRYPSIN INHIBITOR (BOVINE, PANCREAS)	R.HUBER,J.DEISENHOFER	9/82	SF
R2PT2SF	TRYPSIN/TRYPSIN INHIBITOR COMPLEX	R.HUBER,J.DEISENHOFER	9/82	SF
R1TPASF	TRYPSIN (ANHYDRO)/TRYPSIN INHIBITOR	HUBER,BODE,DEISENHOFER	9/82	SF
R2TGASF	TRYPSINOGEN (2.4M MGSO4)	J.WALTER,R.HUBER	10/81	SF
R1TGCSF	TRYPSINOGEN (5 CH3OH, 5 H2O)	J.WALTER,R.HUBER	10/81	SF
R1GTGSF	TRYPSINOGEN (173 DEG K, .7 CH3OH, .3 HOH)	J.WALTER,R.HUBER	10/81	SF
R2GTGSF	TRYPSINOGEN (103 DEG K, .7 CH3OH, .3 HOH)	J.WALTER,R.HUBER	10/81	SF
R2TPGSF	TRYPSINOGEN/TRYPSIN INHIBITOR	R.HUBER ET AL.	9/82	SF
R3TP1SF	TRYPSINOGEN/TRYPSIN INHIBITOR/ILE-VAL	R.HUBER ET AL.	9/82	SF
R2TP1SF	TRYPSINOGEN/PTI/ILE-VAL (MERCURATED)	J.WALTER,R.HUBER	10/81	SF
R1TGSSF	TRYPSINOGEN/PTI	R.HUBER ET AL.	9/82	SF

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TABLE 7. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

06-JUL-83				
IDEN	MOLECULE	DEPOSITOR	DATE/	CODE
0EAP	ACID PROTEINASE (ENDOTHRAL PARASITICA)			
0ADC	ADH-NADH-DIMETHYLSULFOXIDE COMPLEX			
0AF1	APOFERRITIN (HORSE)			
0MAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE			
0RNB	BARNASE (BACILLUS AMYLOLIQUEFACIENS)			
0ICA	CALCULONIN PROTEIN (MINKER A FORM,BOVINE)			
0C01	*CALOTROPIN D1 (CALOTROPIS GIGANTEA)			
0PTE	D-ALANYL-CARBOXYPEPTIDASE -TRANSEPTIDASE			
0ZGP	D-ALANYL-D-ALANINE PEPTIDASE (ZNP+ G PEPTIDASE)			
0CTS	CITRATE SYNTHASE (PIG)			
00NE	CONCAVALIN A (DEMETALLIZED)			
0CRO	CRO REPRESSOR			
0GCR	GAMMA-CRYSTALLIN II (CALF)			
0CYP	CYTOCHROME C PEROXIDASE (SACCHAROMYCES CEREVISIAE)			
0CY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)			
05C1	CYTOCHROME C555 (CHLOROBIUM THIOSULFATOPHILUM)			
0CSA	DES-AR77-03A ANAPHYLATOXIN			
0CDF	DIHYDROFLATE REDUCTASE (CHICKEN LIVER)			
0ANB	DNA (GGTATACC)			
0ANB	DNA (GG-UU-UACC)			
0ESZ	ELASTASE COMPLEX (PIG)			
0ETU	ELONGATION FACTOR TU COMPLEX (E. COLI)			
0E8B	ERABUTOXIN B			
0FX1	FLAVODOXIN (DESULFOVIBRIO VULGARIS)			
0FX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)			
0GAP	CATABOLITE GENE ACTIVATOR PROTEIN			
0GP1	GLUTATHIONE PEROXIDASE (BOVINE)			
0G01	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)			
0HG6	HEMAGGLUTININ			
0DCH	HEMOGLOBIN (COBALT, DEOXY)			
0HBG	HEMOGLOBIN (GLYCERA DIBRANCHIATA)			
0PH4	P-HYDROXYBENZONATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)			
0AU1	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU			
0ROV	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER, KAPPA) ROY			
0MCP	IMMUNOGLOBULIN FAB (KAPPA) MCP63			
0IG1	IMMUNOGLOBULIN G1 (KAPPA) DOB			
0INI	INSULIN (PORCINE)			
0INE	INSULIN (PORCINE)			
0LRF	5'-TERMINAL DOMAIN OF LAMBDA REPRESSOR			
0L21	LYSOZYME (HUMAN)			
0L25	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)			
0L26	LYSOZYME (STREPTOMYCES ERYTHRAEUS)			
0CTF	L7/L12 (E. COLI, C-TERMINUS)			
0MBA	*MYOGLOBIN (APLYSIA LIMACINA)			
0MBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)			
0MB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)			
0PFK	PHOSPHOFUCTOKINASE (BACILLUS STEAROTHERMOPHILUS)			
0PP2	PHOSPHOLIPASE A2 (RATTLESNAKE)			
0PPA	PHOSPHORYLASE A (RABBIT)			
0PB1	PHOSPHORYLASE (RABBIT)			
0RX5	RELAXIN (PORCINE, MODEL)			
0RSA	RIBONUCLEASE A (BOVINE)			
0RST	RIBONUCLEASE ST (STREPTOMYCES ERYTHRAEUS)			
0RNT	RIBONUCLEASE T1-2(PHME)-GUANYLIC ACID (ASPERGILLUS ORYZAE)			
0T14	*THIOREDOXIN REDUCTASE (BACTERIOPHAGE T4)			
0FM1	INITIATOR TRANSFER RNA (E. COLI, F/MET)			
0TA1	TRANSFER RNA (YEAST, ASP. A FORM)			
0TA2	TRANSFER RNA (YEAST, ASP. B FORM)			
0TRI	TRANSFER RNA (YEAST, PHE)			
0MT5	METHIONYL TRANSFER RNA SYNTHETASE			
0YPI	*TRIOSE PHOSPHATE ISOMERASE (SACCHAROMYCES CEREVISIAE)			
0GN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)			
0UTG	UTEROGLOBIN (RABBIT)			
0STV	VIRUS (SATELLITE TOBACCO NECROSIS)			
0TMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)			
0TBV	VIRUS (TOMATO BUSHY STUNT)			

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TABLE 3. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

IDENT	MOLECULE	DEPOSITOR(S)	DATE/STATUS		
24PE	ACID PROTEINASE (ENDOTHA PARASITICA)	T. BLUNDELL	9/81	2LH2	LEGHEMOGLOBIN(AQUO MET)
24PP	ACID PROTEINASE (PENICILLIUM ANTHINELLUM)	A. SIELECKI, M. JAMES	1/78 R	1LH3	LEGHEMOGLOBIN(CYANO MET)
1APR	ACID PROTEINASE (RHIZOPUS CHINENSIS)	D. DAVIES	9/79	2LH3	LEGHEMOGLOBIN(CYANO MET)
2ACT	ACTINIDIN	E. BAKER	11/79	1LH4	LEGHEMOGLOBIN(DEOXY)
1ACK	ACTINONANTHIN	V. PLETNEV, A. KUZIN	12/82	2LH5	LEGHEMOGLOBIN(FLUORO MET)
2ABK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77	1LH5	LEGHEMOGLOBIN(FLUORO MET)
1AGA	AGAROSE	S. ARNOTT	5/78	2LH5	LEGHEMOGLOBIN(FLUORO MET)
2MGA	AGGLUTININ (WHEAT GERM)	C. HIGHT	5/80	1LH6	LEGHEMOGLOBIN(NICOTINATE MET)
4ADH	ALCOHOL DEHYDROGENASE (APO)	C.-I. BRANDEL	8/79	2LH6	LEGHEMOGLOBIN(NICOTINATE MET)
1ALP	ALPHA LYTIC PROTEASE	BRAYER, DELBAERE, JAMES	6/79	1LH7	LEGHEMOGLOBIN(FERRO)/NITROSOBENZENE
21AT	TAKA-AMYLASE	KUSUNOKI, MATSUURA, KAKUDO	10/82	2LH7	LEGHEMOGLOBIN(FERRO)/NITROSOBENZENE
1IABP	L-ARABINOSYL-BINDING PROTEIN	F. QUITOCHO, G. GILLILAND	5/80	1LH8	LEGHEMOGLOBIN(NITROSOBENZENE)
1AAT	CYTOSOLIC ASPARTATE AMINOTRANSFERASE	HARUTYUNYAN, MALASHKEVICH	4/82 A	1LH9	LYSOZYME (BACTERIOPHAGE T4)
2ATC	ASPARTATE CARBAHOYLTRANSFERASE	W. LIPSOMB	3/82	1LY2	LYSOZYME (HEN EGG-WHITE, SET W2)
3ATC	ASPARTATE CARBAHOYLTRANSFERASE/CTP	W. LIPSOMB	3/82 R	2LY2	LYSOZYME (HEN EGG-WHITE, SET RS5D)
1AZU	AZURIN	E. ADMAN, L. SIEKER, L. JENSEN	8/80	3LY2	LYSOZYME (HEN EGG-WHITE, SET RS5A)
2BCL	BACTERIOCHLOROPHYLL A-PROTEIN	B. MATTHEWS	1/79 A	5LY2	LYSOZYME (HEN EGG-WHITE, SET RS12A)
1ABX	ALPHA-BUNGAROTOXIN	D. GARG, S. SPENCER, R. STROUD	4/80 A	6LY2	LYSOZYME (HEN EGG-WHITE, SET RS16)
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74	7LY2	LYSOZYME (HEN EGG-WHITE, TRICLINIC)
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74	8LY2	LYSOZYME (HEN EGG-WHITE, INACTIVATED)
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	S. ARNOTT	5/78	1LY3	LYSOZYME (HEN, NAM-NAG-NAM SUBSTRATE ONLY)
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	J. KANNAN	6/78	1LH0	MYOGLOBIN (HEN EGG-WHITE, MONOCLINIC)
1CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	6/78	2LH2	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)
1CAC	CARBONIC ANHYDRASE C (HUMAN)	D. REES, W. LIPSOMB	3/82 R	1LYM	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)
3CPA	CARBOXYPEPTIDASE A/GLYCYLTYROSINE	D. REES, W. LIPSOMB	3/82	1LZ2	LYSOZYME (TURKEY EGG-WHITE)
4CPA	CARBOXYPEPTIDASE A/POTATO INHIBITOR	D. REES, W. LIPSOMB	5/82	2MH0	MALATE DEHYDROGENASE
5CPA	CARBOXYPEPTIDASE A/WATER (BOVINE)	M. SCHMID, J. HERRIOTT	6/76 A	1MLT	MELITTIN
1CPB	CARBOXYPEPTIDASE B (BOVINE)	S. ARNOTT	5/78	1MB5	MYOGLOBIN (SEAL, MET)
1CAR	CARRAGEENAN	M. ROSSMANN	7/82 R	1MBN	MYOGLOBIN (SPERM WHALE, MET)
3CAT	CATALASE (BEEF LIVER)	B. VAINSHTEIN ET AL.	2/83 BN	2MBN	MYOGLOBIN (SPERM WHALE, MET)
4CAT	CATALASE (PENICILLIUM VITALE)	S. ARNOTT	5/78	3MBN	MYOGLOBIN (SPERM WHALE, DEOXY)
1C4S	CHONDROITIN-4-SULFATE	S. ARNOTT	5/78	1MB0	MYOGLOBIN (SPERM WHALE, OXY)
2C4S	CHONDROITIN-4-SULFATE (CA SALT)	D. BLUM	1/78	1MB5	MYOGLOBIN (SPERM WHALE, CO, NEUTRON)
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	A. TULINSKY	8/76	1MRH	MYOHEMERYTHRIN
3CHA	ALPHA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	5/80	1NXB	NEUROTOXIN B (LATICAUDA SEMIFASCIATA)
1GCH	GAMMA-CHYMOTRYPSIN	J. KRAUT, J. BIRKTOFT	3/75	1OVS	NEUROTOXIN I (VARIANT 3)
1OCT	ALPHA COBRATOXIN	W. SAENGER, M. WALKINSHAW	3/82	1OVS	OVOMUCIN (JAPANESE QUAIL)
2CNA	CONCANAVALIN A	G. REEKE, J. BECKER, G. EDELMAN	4/75	1PPT	AVIAN PANCREATIC POLYPEPTIDE
3CNA	CONCANAVALIN A	K. HARDMAN	9/76	8PAP	PAPAIN (NATIVE)
1CN1	CONCANAVALIN A (DEMETALLIZED)	M. SHOHAM	12/81	1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)
1CRN	CRAMBIN	W. HENDRICKSON, M. TEETER	5/81	2PAD	PAPAIN (CYS DERIV OF CYS-25)
2BSC	CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77	3PAD	PAPAIN (OXIDIZED CYS-25)
15B5	CYTOCHROME B5 (E. COLI, OXIDIZED)	BETHGE, CZERWINSKI, MATHEWS	8/79	4PAD	PAPAIN (TOS-LYS, CYS-25)
3CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80	5PAD	PAPAIN (BZOXY-GLY-PHE-GLY, CYS-25)
4CYT	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO, R. DICKERSON	7/80	6PAD	PAPAIN (BZOXY-PHE-ALA, CYS-25)
1CCY	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	8/76	1PEP	PEPSIN (PORCINE)
1CCR	CYTOCHROME C (RICE)	H. OCHI, N. TANAKA	3/83	1PFC	PFC FRAGMENT OF AN IGG
1CCY	CYTOCHROME C (PRIME)	J. KRAUT	8/81	3PGK	PHOSPHOGLYCERATE KINASE (YEAST)
1CC2	CYTOCHROME C2	H. IGUCHI, YASUOKA, KAKUDO	3/73	2PGK	PHOSPHOGLYCERATE KINASE (HORSE)
1CDV	CYTOCHROME C3(D. VULGARIS MIYAZAKI)	R. TIMKOVICH	8/76 A	3PGM	PHOSPHOGLYCERATE MUTASE
15SC	CYTOCHROME C550	MATSUURA, TAKANO, DICKERSON	7/81	1BP2	PHOSPHOLIPASE A2 (BOVINE)
351C	CYTOCHROME C551 (OXIDIZED)	MATSUURA, TAKANO, DICKERSON	7/81	2BP2	PHOSPHOLIPASE A2 (BOVINE)
451C	CYTOCHROME C551 (REDUCED)	MATSUURA, TAKANO, DICKERSON	7/81	1P2P	PHOSPHOLIPASE A2 (PORCINE) TRANSMANINATED
3DFR	DIHYDROFOLATE REDUCTASE (L. CASEI)	J. BOLIN, D. MATHEWS, J. KRAUT	6/82 R	1PCY	PLASTOCYANIN
4DFR	DIHYDROFOLATE REDUCTASE (E. COLI)	B. CONNER, R. DICKERSON	6/82 R	2PAB	PREALBUMIN (HUMAN, PLASMA)
1ANA	DNA(A, 5(PRIME)-D-10DD-CGGG(3(PRIME)))	H. DREW, R. DICKERSON	11/81	2GSA	PROTEINASE A (STREPTOMYCES GRISEUS)
1BNA	DNA(B, CGCGAATTCGGG, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81	1RNS	RIBONUCLEASE A
2BNA	DNA(B, CGCGAATTCGGG, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81	2RNX	RIBONUCLEASE S
3BNA	DNA(B, G-B-CGGCAATTCGGG, 20 DEG C)	KOPKA, FRATINI, DICKERSON	2/82	3RNX	RUBREDOXIN(CLOSTRIDIUM PASTEURIANUM)
4BNA	DNA(B, G-B-CGGCAATTCGGG, 20 DEG C)	H. DREW, R. DICKERSON	2/82	2S51	RUBREDOXIN(DESULFOVIBRIO VULGARIS)
1ZNA	DNA(Z', CGCG, HIGH-SALT, SYNTHETIC)	H. DREW, R. DICKERSON	1/81	2S5N	STAPHYLOCOCCAL NUCLEASE
1EED	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76	2S5I	SUBTILISIN INHIBITOR (STREPTOMYCES)
1ECT	ERYTHROCUORIN (REDUCED, DEOXY)	W. STEIGEMANN, E. WEBER	3/79	1SBT	SUBTILISIN BPN, PRIME
1ECO	ERYTHROCUORIN (CARBONMONOXY)	W. STEIGEMANN, E. WEBER	3/79	2SBT	SUBTILISIN NOVO
1ECA	ERYTHROCUORIN (AQUO, MET)	W. STEIGEMANN, E. WEBER	3/79	2S00	SUPEROXIDE DISMUTASE
1ECN	ERYTHROCUORIN (CYANO, MET)	H. STEIGEMANN, E. WEBER	3/79	3TLN	THERMOLYSIN(NATIVE)
2FD1	FERREDOXIN (AZOTOBACTER VINELANDII)	STOUT, GHOSH, FUREY, OODNELL	11/81	4TLN	THERMOLYSIN(L-LEU-NH0H)
1FDX	FERREDOXIN (PEPTOCOCCUS AERGENS)	E. ADMAN, L. SIEKER, L. JENSEN	8/76	5TLN	THERMOLYSIN(H-NH2-PHALONYL--A-G-NTR0AND)
3FXK	FERREDOXIN (SPIRULINA PLATENSIS)	TSUKIHARA, KATSUBE, KAKUDO	12/81	1SRX	THIOREDOXIN (E. COLI, OXIDIZED)
3FXN	FLAVODOXIN (CLOSTRIDIUM MP, OXIDIZED)	M. LODGII	12/77	4TNA	TRANSFER RNA (YEAST, PHE)
4FXN	FLAVODOXIN (CLOSTRIDIUM MP, SEMIQUINONE)	M. LODGII	12/77	6TNA	TRANSFER RNA (YEAST, PHE)
1GN	GLUCAGON	T. BLUNDELL	12/77	8TNA	TRANSFER RNA (YEAST, PHE)
1PG1	GLUCOSE-6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77	1T1T	TRIOSE PHOSPHATE ISOMERASE
2GRS	GLUTATHIONE REDUCTASE (HUMAN)	G. SCHULZ	11/81	2PTN	TRYPSIN(ORTHORHOMBIC, 2.4M (NH4)2SO4)
19PD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	7/75	1TPO	TRYPSIN(ORTHORHOMBIC, 2.4M (NH4)2SO4)
29PD	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79	3PTN	TRYPSIN(BENZAMIDINE INHIBITED)
39PD	*GLYCERALDEHYDE-3-P-DEHYDROGENASE (HUMAN)	H. WATSON, J. CAMPBELL	6/83 P	1TIP	TRYPSIN(BENZAMIDINE INHIBITED)
1HRB	HEMERYTHRIN B	W. HENDRICKSON	6/76 A	3PTP	TRYPSIN(DIP INHIBITED)
1HQ0	HEMERYTHRIN(MET)	STENKAMP, SIEKER, JENSEN	2/83 R	4PTI	TRYPSIN INHIBITOR (BOVINE, PANCREAS)
1HZ	HEMERYTHRIN(AZIDO, MET)	STENKAMP, SIEKER, JENSEN	2/83 R	2PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX
1HD5	HEMOGLOBIN (DEER, SICKLE CELL)	E. APMA, R. SIFLING	10/79	1TPA	TRYPSIN(ANHYDRO)/TRYPSIN INHIBITOR
2MBH	HEMOGLOBIN (HORSE, AQUO MET)	R. LADNER, H. DEDNER, PERUTZ	2/77	1TGN	TRYPSINOGEN
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	11/73	2TGA	TRYPSINOGEN(2.4M MG504)
1HBB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	4/75	1TGC	TRYPSINOGEN(.5 CH3OH, .5 HOH)
1HCO	HEMOGLOBIN (HUMAN, CARBONMONOXY)	J. BALDWIN	8/79	1TGT	TRYPSINOGEN(173 DEG K, .7 CH3OH, .3 HOH)
2HCO	HEMOGLOBIN (HUMAN, CARBONMONOXY, NRG REFND)	J. BALDWIN	8/79	2TGT	TRYPSINOGEN(103 DEG K, .7 CH3OH, .3 HOH)
1FH0	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/83 N	1T0B	TRYPSINOGEN (WITH CA, FROM PEG)
1HBS	HEMOGLOBIN S (HUMAN, SICKLE CELL)	E. PADLAN, L. LOVE	6/82	3TPI	TRYPSINOGEN/TRYPSIN INHIBITOR
1LHB	HEMOGLOBIN (LAMPREY)	H. ENDRICKSON, LOVE, KARLE	3/73	2PTI	TRYPSINOGEN/PTI(ILE-VAL (MERCURATED))
2YAK	HEXOKINASE (YEAST) FORM B11	STEITZ, ANDERSON, STENKAMP	12/80	1T05	TRYPSINOGEN/PSTI
1HKG	HEXOKINASE A - GLUCOSE COMPLEX (YEAST)	W. BENNETT JR., T. STEITZ	4/75	1T51	TYROSYL TRANSFER RNA SYNTHETASE
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	12/77	25BV	VIROUS COAT PROTEIN(SOUTHERN BEAN MOSAIC)
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	11/77		
2HYA	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S. ARNOTT	5/78		
3HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78		
4HYA	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78		
1FB4	*IMMUNOGLOBULIN FAB (LAMBDA) KOL	M. MARQUART, R. HUBER	5/83 N		
3FAB	IMMUNOGLOBULIN FAB, PRIME	R. POLJAK	9/81		
1MC0	IMMUNOGLOBULIN B-J INTACT	SCHIFFER, EDMUNDSON ET AL.	5/78 A		
1RE1	IMMUNOGLOBULIN B-J FRAGMENT(V-DIMER)RE1	O. EPP, R. HUBER	3/76		
2RHE	*IMMUNOGLOBULIN B-J FRAGMENT(V-MIMER)RHE1	FUREY, WANG, YOO, SAX	6/83 RN		
1FC1	IMMUNOGLOBULIN FC (HUMAN)	J. DEISENHOFER	5/81		
1FC2	IMMUNOGLOBULIN FC-FRAGMENT B COMPLEX	J. DEISENHOFER	5/81		
1IG2	*IMMUNOGLOBULIN G1 (LAMBDA) KOL	M. MARQUART, R. HUBER	5/83 N		
1INS	INSULIN (PORCINE, 2-ZINC)	G. DOODSON, D. HODGKIN	7/80		
2INS	INSULIN (BOVINE, 2-ZINC) DES-PHE B1	C. REYNOLDS, G. DOODSON	5/82		
1GF1	INSULIN-LIKE GROWTH FACTOR I (MODEL)	BLUNDELL, BEDARKAR, HUMBEL	12/82		
1GF2	INSULIN-LIKE GROWTH FACTOR II (MODEL)	BLUNDELL, BEDARKAR, HUMBEL	12/82		
1KGA	KOPG ALDOLASE	A. TULINSKY	8/78 A		
1KES	KERATAN SULFATE	S. ARNOTT	5/77		
4LDH	LACTATE DEHYDROGENASE (DOGFLSH)	W. EVENTOFF, M. ROSSMANN	4/78		
3LDH	LACTATE DEHYDROGENASE (MAD/PYRVUATE) (DOGFL)	M. ROSSMANN	11/74		
5LDH	LACTATE DEHYDROGENASE (S-LAC/MAD) (PIG)	U. GRAU, H. ROSSMANN	10/80		
1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)	W. MUSICK, M. ROSSMANN	9/78		
1LH1	LEGHEMOGLOBIN(ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 R		
2LH1	LEGHEMOGLOBIN(ACETATE MET)	VAINSHTEIN, HARUTYUNYAN	4/82 R		
1LH2	LEGHEMOGLOBIN(AQUO MET)	VAINSHTEIN, HARUTYUNYAN	4/82		

* NEW OR REPLACEMENT ENTRY SINCE APR-83 NEWSLETTER

STATUS CODES

- BLANK BLANK ENTRY AVAILABLE FOR DISTRIBUTION
- A ALPHA CARBON ATOMS ONLY
- B BACKBONE ONLY
- N NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
- P IN PREPARATION
- R RECENT (1982-1983) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 8. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

06-JUL-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 '*IDENT' DIRECTIVE. THIS IDENTIFIES THE CORRECTION SET, E.G. AS 'IMBNB' 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 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,IAZUC
*INSERT,IAZUB.13
REMARK 8
REMARK 8 CORRECTION. FIX ATOM NUMBERING FOR RESIDUE 3. FIX CONECT
REMARK 8 RECORDS ACCORDINGLY. 07-MAR-83.
*DELETE,IAZU.75,79
ATOM 16 CA CYS 3 38.580 29.790 -2.990 1.00 0.00
ATOM 17 C CYS 3 37.520 28.910 -2.340 1.00 0.00
ATOM 18 O CYS 3 36.440 28.390 -2.810 1.00 0.00
ATOM 19 CB CYS 3 39.100 28.730 -4.060 1.00 0.00
ATOM 20 C CYS 3 40.750 28.870 -4.810 1.00 0.00
*DELETE,IAZU.1007,100B
CONECT 20 19 194
CONECT 194 20 193
*DELETE,IAZUB.14
MASTER 59 0 1 0 0 0 0 6 931 1 7 10

*IDENT,IINSE
*INSERT,IINSD.2
REMARK 13
REMARK 13 CORRECTION. CORRECT MTRIX TRANSFORMATION. REVISE REMARKS
REMARK 13 5 AND 7. CORRECT FORMUL RECORD. 07-MAR-83.
*DELETE,IINS.108,113
REMARK 5 QUASI-TWO-FOLD AXIS THAT TRANSFORMS MOLECULE I INTO
REMARK 5 MOLECULE II IS GIVEN IN THE MTRIX RECORDS BELOW. APPLYING
REMARK 5 THE THREE-FOLD CRYSTALLOGRAPHIC AXIS YIELDS A HEXAMER
REMARK 5 AROUND THE AXIS. THERE ARE TWO ZINC IONS SITUATED ON THIS
REMARK 5 THREE-FOLD AXIS. COORDINATES FOR THE ZINC IONS AND SOME
REMARK 5 WATER MOLECULES ARE INCLUDED BELOW WITH A BLANK CHAIN
REMARK 5 INDICATOR.
*DELETE,IINS.126,131
REMARK 7 *ZNI* COMPRISES RESIDUE HIS B 10 AND WATER HOH 4201 AND
REMARK 7 THEIR TWO CRYSTALLOGRAPHICALLY-RELATED EQUIVALENTS. SITE
REMARK 7 *ZNE* COMPRISES RESIDUE HIS D 10 AND WATER HOH 4513 AND
REMARK 7 THEIR TWO CRYSTALLOGRAPHICALLY-RELATED EQUIVALENTS. SITE
REMARK 7 *ZNI* IS OCTAEDRALLY COORDINATED AROUND ZNI AND SITE *ZNE*
REMARK 7 IS OCTAEDRALLY COORDINATED AROUND ZNE. THE TWO SITES ARE
*DELETE,IINS.175
FORMUL 7 HOH *88(H2 O)
*DELETE,IINS.213,215
MTRIX1 1 -.878620 -.476960 -.023050 0.00000 1
MTRIX2 1 -.477430 .878370 -.022860 0.00000 1
MTRIX3 1 .009350 -.031090 -.999470 0.00000 1
*DELETE,IINS0.
MASTER 158 11 2 6 2 4 12 9 917 4 12 10

*IDENT,IAATA
*INSERT,IAAT.64
REMARK 7
REMARK 7 CORRECTION. INSERT ARGININE AS RESIDUE 120 AND ADJUST
REMARK 7 CA COORDINATES FOR RESIDUES 115-127. REVISE SEGRES
REMARK 7 RECORDS ACCORDINGLY. CORRECT COMMENTS ON HELIX RECORDS.
REMARK 7 INSERT TITLE AND REVISE AUTHOR LIST FOR REFERENCE 2.
REMARK 7 CORRECT SPELLING ERROR IN REMARK 4. 07-MAR-83.
*DELETE,IAAT.17,18
REMARK 1 AUTH YU.M.TORCHINSKY,E.G.HARUTYUNYAN,V.N.MALASHKEVICH,
REMARK 1 AUTH 2 M.KODHAKINA,V.L.MAKAROV,A.E.BRAUNSTEIN
REMARK 1 TITL ASPARTATE TRANSAMINASE FROM CHICKEN HEART CYTOSOL.
REMARK 1 TITL 2 THREE DIMENSIONAL STRUCTURE AND REORIENTATION OF
REMARK 1 TITL 3 THE COENZYME IN THE ACTIVE SITE
*DELETE,IAAT.51
REMARK 4 BY AVERAGING ELECTRON DENSITIES FOR THE TWO SUBUNITS.
*DELETE,IAAT.105
HELIX 9 H9 ASN 232 SER 245 1 HAS A BEND NEAR N-TERMINUS
*DELETE,IAAT.08
HELIX 12 H12 GLN 314 SER 343 1 HAS A BEND IN THE MIDDLE
*DELETE,IAAT.65,96
SEGRES 1 411 ALA ALA SER ILE PHE ALA ALA VAL PRO ARG ALA PRO
SEGRES 2 411 VAL ALA VAL PHE LYS LEU THR ALA ASP PHE ARG GLU ASP

SEGRES 31 411 LEU THR THR LYS ASN LEU ASP TYR VAL ALA LYS SER ILE
SEGRES 32 411 HIS GLU ALA VAL THR LYS ILE GLN
*DELETE,IAAT.239,536
ATOM 843 CA GLY 115 -300 11.100 -23.000 1.00 0.00
ATOM 847 CA ALA 116 -2.300 9.300 -20.700 1.00 0.00
ATOM 852 CA GLU 117 1.100 7.800 -19.100 1.00 0.00
ATOM 861 CA PHE 118 3.000 10.100 -18.200 1.00 0.00
ATOM 872 CA LEU 119 -4.600 12.400 -17.400 1.00 0.00
ATOM 880 CA ARG 120 -3.300 10.400 -14.100 1.00 0.00
ATOM 891 CA ARG 121 3.900 9.500 -14.800 1.00 0.00
ATOM 902 CA TRP 122 4.700 12.900 -14.400 1.00 0.00
ATOM 916 CA TYR 123 2.000 15.600 -12.700 1.00 0.00
ATOM 928 CA ASN 124 -1.700 16.200 -9.100 1.00 0.00
ATOM 936 CA GLY 125 4.100 14.400 -7.500 1.00 0.00
ATOM 940 CA ASN 126 6.800 11.200 -9.700 1.00 0.00
ATOM 948 CA ASN 127 3.400 8.600 -8.900 1.00 0.00
ATOM 956 CA ASN 128 -2.200 11.200 -8.300 1.00 0.00
ATOM 964 CA THR 129 -3.100 8.300 -8.300 1.00 0.00
ATOM 971 CA ALA 130 -5.800 10.800 -7.500 1.00 0.00

ATOM 3206 CA LYS 410 -46.100 -1.100 -28.200 1.00 0.00
ATOM 3215 CA ILE 411 -42.600 -1.700 -26.500 1.00 0.00
ATOM 3223 CA GLN 412 -43.000 1.600 -24.000 1.00 0.00
TER 3232 GLN 412

*DELETE,IAAT.537
MASTER 66 0 0 15 7 0 0 6 411 1 0 32

*IDENT,3CATB
*INSERT,3CATA.3
REMARK 8
REMARK 8 CORRECTION. FIX ATOM NUMBERING FOR RESIDUE 5. 07-MAR-83.
*DELETE,3CAT.143,147
ATOM 34 CA ASP 5 -3.879 21.699 33.558 1.00 20.00
ATOM 35 C ASP 5 -4.494 22.048 32.138 1.00 20.00
ATOM 36 O ASP 5 -5.646 21.701 31.841 1.00 20.00
ATOM 37 CB ASP 5 -4.013 20.200 34.018 1.00 20.00
ATOM 39 CG ASP 5 -3.495 19.100 33.065 1.00 20.00
*DELETE,3CAT.4
MASTER 67 0 1 13 9 0 0 9 4029 0 43 39

*IDENT,4CPAB
*INSERT,4CPAA.8
REMARK 8
REMARK 8 CORRECTION. CORRECT RESIDUE NUMBERING FOR PC1 (CHAIN 1).
REMARK 8 FORMERLY RESIDUE GLU 1 2 (FORMERLY GLU 1 1) TO GLX 1 2.
REMARK 8 REVISE SEGRES RECORDS. 07-MAR-83.
*DELETE,4CPA.66,68
SEGRES 1 38 GLX GLX HIS ALA ASP PRO ILE LYS ASN LYS PRO CYS LYS
SEGRES 2 1 38 THR HIS ASP ASP CYS SER GLY ALA TRP PHE CYS GLN ALA
SEGRES 3 1 38 CYS TRP ASN SER ALA ARG THR CYS GLY PRO TYR VAL
*DELETE,4CPA.2579,2668
ATOM 2449 N GLX I 2 -14.463 -16.664 -1.443 1.00 23.73
ATOM 2450 CA GLX I 2 -13.386 -16.604 -2.426 1.00 29.49
ATOM 2451 C GLX I 2 -12.828 -15.227 -2.806 1.00 31.92
ATOM 2452 O GLX I 2 -11.632 -15.318 -3.276 1.00 37.34
ATOM 2453 CB GLX I 2 -13.815 -17.229 -3.786 1.00 23.88
ATOM 2454 CG GLX I 2 -13.280 -16.825 -5.123 1.00 25.96
ATOM 2455 CD GLX I 2 -12.527 -17.669 -6.090 1.00 35.96
ATOM 2456 AE1 GLX I 2 -11.768 -18.704 -5.944 1.00 40.06
ATOM 2457 AE2 GLX I 2 -12.724 -17.305 -7.323 1.00 35.50
ATOM 2458 N HIS I 3 -13.533 -14.127 -2.931 1.00 29.25
ATOM 2459 CA HIS I 3 -12.977 -12.661 -3.454 1.00 25.22

ATOM 2731 CG1 VAL I 38 -14.265 .381 11.058 1.00 3.00
ATOM 2732 CG2 VAL I 38 -15.015 .865 13.397 1.00 3.88
ATOM 2733 OXT VAL I 38 -12.092 .329 15.226 1.00 20.39
TER 2734 VAL I 38
ATOM 2735 N GLY G 1 -11.303 .403 17.922 1.00 3.00
ATOM 2736 CA GLY G 1 -12.735 .680 17.882 1.00 4.29
ATOM 2737 C GLY G 1 -13.053 2.177 18.164 1.00 9.80
ATOM 2738 O GLY G 1 -13.624 2.944 17.307 1.00 9.36
ATOM 2739 OXT GLY G 1 -13.281 2.474 19.404 1.00 15.06
TER 2740 GLY G 1

*DELETE,4CPAA.9
MASTER 38 2 1 8 8 36 0 9 2728 3 0 28

*IDENT,2INSA
*INSERT,2INS.155
REMARK 9
REMARK 9 CORRECTION. CORRECT JOURNAL NAME FOR REFERENCES 2 AND 4.
REMARK 9 UPDATE JRNL REFERENCE TO REFLECT PUBLICATION. CORRECT
REMARK 9 MTRIX TRANSFORMATION. REVISE REMARKS 5 AND 7. 07-MAR-83.
*DELETE,2INS.11,12
JRNL REF ACTA CRYSTALLOGR.,SECT.B V. 38 3028 1982
JRNL REFN ASTM ACBCAR DK ISSN 0567-7408
*DELETE,2INS.25,26
REMARK 1 REF ACTA CRYSTALLOGR.,SECT.A V. 34 782 1978
REMARK 1 REFN ASTM ACACBN DK ISSN 0567-7394
*DELETE,2INS.36,37
REMARK 1 REF ACTA CRYSTALLOGR.,SECT.A V. 32 311 1976
REMARK 1 REFN ASTM ACACBN DK ISSN 0567-7394
*DELETE,2INS.115,120
REMARK 5 QUASI-TWO-FOLD AXIS THAT TRANSFORMS MOLECULE I INTO
REMARK 5 MOLECULE II IS GIVEN IN THE MTRIX RECORDS BELOW. APPLYING
REMARK 5 THE THREE-FOLD CRYSTALLOGRAPHIC AXIS YIELDS A HEXAMER
REMARK 5 AROUND THE AXIS. THERE ARE TWO ZINC IONS SITUATED ON THIS
REMARK 5 THREE-FOLD AXIS. COORDINATES FOR THE ZINC IONS AND SOME
REMARK 5 WATER MOLECULES ARE INCLUDED BELOW WITH A BLANK CHAIN
REMARK 5 INDICATOR.
*DELETE,2INS.133,138
REMARK 7 *ZNI* COMPRISES RESIDUE HIS B 10 AND WATER HOH 201 AND
REMARK 7 THEIR TWO CRYSTALLOGRAPHICALLY-RELATED EQUIVALENTS. SITE
REMARK 7 *ZNE* COMPRISES RESIDUE HIS D 10 AND WATER HOH 513 AND
REMARK 7 THEIR TWO CRYSTALLOGRAPHICALLY-RELATED EQUIVALENTS. SITE
REMARK 7 *ZNI* IS OCTAEDRALLY COORDINATED AROUND ZNI AND SITE *ZNE*
REMARK 7 IS OCTAEDRALLY COORDINATED AROUND ZNE. THE TWO SITES ARE
*DELETE,2INS.219,221
MTRIX1 1 -.880000 -.020000 0.00000 1
MTRIX2 1 -.880000 -.020000 0.00000 1
MTRIX3 1 -.010000 -.030000 -1.00000 1
*DELETE,2INS.1202
MASTER 148 11 2 6 2 4 12 9 964 4 12 10

*IDENT,1AATB
*INSERT,1AATA.12
REMARK 8
REMARK 8 CORRECTION. INSERT SCALE RECORDS. 19-APR-83.
*INSERT,1AAT.122
SCALE1 1 -.012320 -.002000 -.009930 .80000
SCALE2 1 .005240 -.000600 .006630 .69800
SCALE3 1 -.001150 .007950 .000180 .44900
*DELETE,1AATA.346
MASTER 68 0 0 15 7 0 0 9 411 1 0 32

*IDENT,CONTC3
*DELETE,CONTC2.1
C LAST REVISION. 5/83
*INSERT,CONTC2.3
C
C CORRECTION. REPLACE BAD RECORDS. 12-MAY-83.
*DELETE,CONTC1.492,493
DIMENSION A(9), B(9)
J = 0

*IDENT,1MBNG
*INSERT,1MBNP.3
REMARK 22
REMARK 22 CORRECTION. CHANGE RESIDUE 122 FROM ASN TO ASP. ADD
REMARK 22 REFERENCE. 12-MAY-83.
*INSERT,1MBNG.6
REMARK 1 REFERENCE 1
REMARK 1 AUTH J.C.KENDREW
REMARK 1 TITL MYOGLOBIN AND THE STRUCTURE OF PROTEINS (NOBEL
REMARK 1 TITL 2 LECTURE, DECEMBER 11, 1962) 103 1963
REMARK 1 REF PRIX NOBEL
REMARK 1 REFN ASTM PRIXL SW 195N 0546-8175 935
*DELETE,1MBNG.7
REMARK 1 REFERENCE 2
*DELETE,1MBNG.13
REMARK 1 REFERENCE 3
*DELETE,1MBN.43
SEGRES 10 458 ARG HIS PRO GLY ASP PHE GLY ALA ASP ALA GLN GLY ALA
*DELETE,1MBN.1041,1048
ATOM 970 N ASP 122 18.100 4.900 19.700 1.00 0.00
ATOM 971 CA ASP 122 17.100 5.900 20.100 1.00 0.00
ATOM 972 C ASP 122 15.900 6.000 19.200 1.00 0.00
ATOM 973 O ASP 122 14.800 6.400 19.700 1.00 0.00
ATOM 974 CB ASP 122 18.000 7.100 20.300 1.00 0.00
ATOM 975 CG ASP 122 19.400 6.800 20.700 1.00 0.00
ATOM 976 OD1 ASP 122 19.600 6.600 22.100 1.00 0.00
ATOM 977 OD2 ASP 122 20.300 6.700 20.000 1.00 0.00
*DELETE,1MBNP.5
MASTER 92 6 1 8 0 3 3 6 1260 1 46 12

*IDENT,3MBNG
*INSERT,3MBNF.3
REMARK 12
REMARK 12 CORRECTION. CHANGE RESIDUE 122 FROM ASN TO ASP UPON
REMARK 12 DEPOSITOR'S INSTRUCTIONS. 12-MAY-83.
*DELETE,3MBN.52
SEGRES 10 153 ARG HIS PRO GLY ASP PHE GLY ALA ASP ALA GLN GLY ALA
*DELETE,3MBN.1042,1049
ATOM 970 N ASP 122 17.454 4.599 19.755 3.61 1.71
ATOM 971 CA ASP 122 15.565 5.681 20.207 3.18 1.51
ATOM 972 C ASP 122 15.619 6.313 19.194 2.75 1.25
ATOM 973 O ASP 122 14.855 7.238 19.507 4.32 1.32
ATOM 974 CB ASP 122 17.410 6.835 20.792 1.04 2.50
ATOM 975 CG ASP 122 18.506 6.317 21.688 1.25 1.10
ATOM 976 OD1 ASP 122 19.768 6.767 21.399 4.21 1.65
ATOM 977 OD2 ASP 122 18.346 5.510 22.586 4.21 1.65
*DELETE,3MBNF.4
MASTER 83 0 3 8 0 0 0 6 1327 1 45 12

```

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 (July 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 (April 1983)
 Non-Standard Entries (Structure Factors) format description for NONST2TP and NONST2FI (April 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
<input type="checkbox"/> 9 track, 6250 cpi, EBCDIC	yes	yes
<input type="checkbox"/> 9 track, 1600 cpi, EBCDIC	yes	yes
<input type="checkbox"/> 9 track, 800 cpi, EBCDIC	yes	yes
<input type="checkbox"/> 9 track, 6250 cpi, ASCII	yes	yes
<input type="checkbox"/> 9 track, 1600 cpi, ASCII	yes	yes
<input type="checkbox"/> 9 track, 800 cpi, ASCII	yes	yes
<input type="checkbox"/> 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</u> (From Table 3)	<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) _____

Foreign 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