

We are very pleased to report that requests for data from Protein Data Bank users are running at an all-time high. At the present rate, we project that Brookhaven will fill approximately 160 orders for this year; up from the previous annual high of 119. These totals do not include requests received by the centers in England, Australia and Japan.

The Data Bank now has 274 atomic coordinate and 104 structure factor entries available for distribution, while the total size of the data base has grown to 47 Mbytes for coordinates and 99 Mbytes for structure factors. By improving data processing software, we continue to be able to handle most new depositions within several weeks of receipt.

Tom Koetzle will be attending the European Crystallographic Meeting in Turin, Italy, September 2-6. Tom will bring a display to Turin describing the Protein Data Bank, and he looks forward to meeting many European users at the Conference.

Inquiries may be addressed to any of the persons listed below. The order 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	03-418-7333
Japan	Institute for Protein Research	Y. Katsube	(06) 877-5111
	Osaka University Yamadaoka, 3-2, Suita, Osaka 565, Japan	K. Yoshida	ext. 3912

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

CODE	ITEM	12-JUN-85				
		NO. TAPES	AVAILABILITY			
		800 1600 6250	US UK JA AUS			
DATAPRTP	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, 3	2	1	X	X	X
YEAR89H	COORDINATE ENTRIES (TABLES 3, 7, 9)	1	1	X	X	
YEAR89T	NEW OR REVISED COORDINATE ENTRIES FOR 1984	1	1	X	X	
PAR185F	NEW OR REVISED COORD ENTRIES 1985 (TO DATE)	1	1	X	X	
NONST1F	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 4)	2	1	X	X	X
NONST2F	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 5)	2	1	X	X	X
NONST3F	STRUCTURE FACTOR HOLDINGS (PART 3 - TABLE 6)	1	1	X	X	X
BENDERPT	PARAMETERS FOR BENT-WIRE MODELS	1	1	X		
BLDKITP	MODEL BUILDER'S KIT					PLEASE INQUIRE AT US CENTER
CONNECTP	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS	2	1	X		
DOPLOT	DIAGONAL PLOTS (LINE PRINTER)	1	1	X		
D1HORL	COMPLETE TORSION ANGLES	2	1	X		
DSTNCTP	CONNECTIVITY SPECIFICATIONS WITH DISTANCES	1	1	X		
FIS1PLP	PHI/PSI PLOTS (LINE PRINTER)	1	1	X		
PHI5PTP	LISTS OF PHI/PSI/OMEGA VALUES	1	1	X		

* NEW OR REPLACEMENT ENTRY SINCE APR-85 NEWSLETTER

TABLE 2. PROTEIN DATA BANK, INFORMATION AVAILABLE ON MICROFICHE

CODE	ITEM	12-JUN-85			
		AVAILABILITY			
		US UK JA AUS			
DATAPRF	ALL CURRENT PROGRAMS, BIBLIOGRAPHIC ENTRIES, COORDINATE ENTRIES (TABLES 3, 7, 9)		X	X	X
YEAR89H	NEW OR REVISED COORDINATE ENTRIES FOR 1984		X		
PAR185F	NEW OR REVISED COORDINATE ENTRIES 1985 (TO DATE)		X		
NONST1F	STRUCTURE FACTOR HOLDINGS (PART 1 - TABLE 4)		X	X	X
NONST2F	STRUCTURE FACTOR HOLDINGS (PART 2 - TABLE 5)		X	X	X
NONST3F	STRUCTURE FACTOR HOLDINGS (PART 3 - TABLE 6)		X	X	X
CORR18F	LIST OF CORRECTIONS NO. 16 (JAN/85 - JUL/85)		X	X	X
BENDERF	PARAMETERS FOR BENT-WIRE MODELS		X		
BLDKITF	MODEL BUILDER'S KIT				PLEASE INQUIRE AT US CENTER
CONNECTF	CONNECTIVITY SPECIFICATIONS FOR ALL ATOMS		X		
DOPLOTF	DIAGONAL PLOTS (LINE PRINTER)		X		
D1HORLF	COMPLETE TORSION ANGLES		X		
DSTNCTF	CONNECTIVITY SPECIFICATIONS WITH DISTANCES		X		
FIS1PLF	PHI/PSI PLOTS (LINE PRINTER)		X		
PHI5PLF	LISTS OF PHI/PSI/OMEGA VALUES		X		

* NEW OR REPLACEMENT ENTRY SINCE APR-85 NEWSLETTER

TABLE 3. PROTEIN DATA BANK, AVAILABLE PROGRAMS

NAME	PURPOSE	AUTHOR(S)	12-JUN-85	
			REV DATE/	SUPPORTED
BENDER	PARAMETERS FOR BENT-WIRE MODELS	G. WILLIAMS	4/82	YES
BLDKIT	MODEL BUILDER'S KIT	E. ABOLA	2/84	YES
CHIRAL	CHECK CHIRALITY	E. ABOLA	1/82	YES
CONNECT	GENERATE FULL CONNECTIVITY	F. BERNSTEIN	8/82	YES
CONCTC	INTERMOLECULAR CONTACTS	L. ANDREWS	5/83	NO
DOPLOT	DIAGONAL PLOTS ON PRINTER	E. SHANSON, F. BERNSTEIN	1/83	YES
D1HORL	COMPLETE TORSION ANGLES	E. ABOLA	3/80	YES
DRCTRY	DIRECTORY OF PDB DISTRIBUTION TAPE	E. ABOLA	5/84	YES
DSSP	SECONDARY STRUCTURE, SOLVENT EXPOSURE	H. KABSCH, C. SANDER	12/83	NO
DSTNCE	CALC. DISTANCES FROM CONECT RECORDS	F. BERNSTEIN	8/82	YES
FIS1PL	PHI/PSI PLOTS ON PRINTER	F. BERNSTEIN	5/79	YES
LSM	COLOR-CODED ALPHA-CARBON MODELS	R. MATELA, R. FLETTERICK	3/82	NO
NAMOD	BALL-AND-STICK MODEL DISPLAY	Y. BEPPU	11/78	NO
PHI5P1	MAIN-CHAIN TORSION ANGLES	ANDREWS, WILLIAMS, BERNSTEIN	2/79	YES
REFMTI	REFORMAT DATA FOR SUPERTAB, SUPERB	L. RELLICK, J. DUANE	12/83	NO
STERED	EXTENDED C, 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	11/82	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-85 NEWSLETTER

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

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

IDENT CODE	MOLECULE	DEPOSITOR	12-JUN-85	
			DATE/	CODE
RIACTSF	ACTINIDIN	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
RCYC501	CYTOCHROME C550	R. TIMKOVICH	4/76	SF
R1ZNASF	DNA (A, D-1000-CCGG) SPACE GROUP P 43 21 2	H. DREW, R. DICKERSON	1/81	SF
R1BNASF	DNA (A, D-1000-CCGG) SPACE GROUP P 21	H. DREW, R. DICKERSON	1/81	SF
R0PD04	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	6/75	SF
R2GPDF	AP0-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79	SF
R2M4BSF	HEMOGLOBIN (HORSE, AQUO MET AND CO)	LADNER, HEIDNER, PERUTZ	6/80	SF
R1FDHSF	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/80	SF
R4JMDCH02	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	5/75	SF
LAMPY1	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	9/75	SF
RLDH05	LACTATE DEHYDROGENASE	M. ROSSMANN	8/75	SF
RLDH07	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	8/75	SF
RLSDHSF	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)	U. GRAU, M. ROSSMANN	1/81	SF
RLZHSF	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	C. BLAKE, D. RICE	6/81	SF
RLZHSF	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)	C. BLAKE, D. RICE	6/81	SF
RNEMYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76	SF
RDEMYSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76	SF
R4TNASF	TRANSFER RNA (YEAST, PHE)	A. JACK, J. LADNER, A. KLUG	6/80	SF

CODES

SF STRUCTURE FACTORS

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

IDENT CODE	MOLECULE	DEPOSITOR	12-JUN-85	
			DATE/	CODE
R1ICBSF	CALCIUM-BINDING PROTEIN (INTESTINAL)	D. SZEBENI, K. MOFFAT	7/83	SF
R1ICRSF	CYTOCHROME C (RICE)	H. OCHI, N. TANAKA	3/83	SF
R351CSF	CYTOCHROME C551 (OXIDIZED)	T. TAKANO, R. DICKERSON	9/81	SF
R451CSF	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, CCGGAATTCGG, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81	SF
R3BNASF	DNA (B, 9-BR-CCGGAATTCGG, 20 DEG C)	KOPKA, FRATINI, DICKERSON/2/82	SF	
R4BNASF	DNA (B, 9-BR-CCGGAATTCGG, 7 DEG C)	KOPKA, FRATINI, DICKERSON/2/82	SF	
R5BNASF	DNA (B, CCGGAATTCGG, SYNTHETIC)/CISPLATIN	WING, P. JURA, DREW, DICKSON	8/83	SF
R1GAA5F	GLUTAMINASE-ASPARAGINASE (ACINETOBACTER)	H. AMMON	12/82	SF
R1GAS5F	GLUTAMINASE-ASPARAGINASE (PSEUDOMONAS 7A)	H. AMMON	12/82	SF
R1HM95F	HEMERYTHRIN (MET)	STENKAMP, SIEKER, JENSEN	2/83	SF
R1HM95F	HEMERYTHRIN (AZIDO, MET)	STENKAMP, SIEKER, JENSEN	2/83	SF
R1HNS5F	INSULIN (BOVINE, 2-ZINC) DES-PHE B1	C. REYNOLDS, G. DOOSON	5/82	SF
RLH15F	LEGHEMOGLOBIN (ACETATE, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH15F	LEGHEMOGLOBIN (ACETATE, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH25F	LEGHEMOGLOBIN (AQUO, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH35F	LEGHEMOGLOBIN (CYANO, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH35F	LEGHEMOGLOBIN (CYANO, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH45F	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH45F	LEGHEMOGLOBIN (DEOXY)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH55F	LEGHEMOGLOBIN (FLUORO, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH55F	LEGHEMOGLOBIN (FLUORO, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH65F	LEGHEMOGLOBIN (NICOTINATE, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH65F	LEGHEMOGLOBIN (NICOTINATE, MET)	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH75F	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RLH75F	LEGHEMOGLOBIN (FERRO)/NITROSOBENZENE	VAINSHTEIN, HARUTYUNYAN	4/82	SF
RILM5F	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)	HOGLE, RAO, SUNDARALINGAM/2/82	SF	
R1MLT5F	MELTILLIGER	TERWILLIGER, EISENBERG	8/81	SF
R1OV05F	OMOVUICOID FRAGMENT	E. PAPAMOKOS, R. HUBER	1/82	SF
R2BP25F	PROPHOSPHOLIPASE A2 (BOVINE)	D. JAKSTRA, HOL, DRENTH	5/81	SF
R1R35F	INORGANIC PYROPHOSPHATASE	E. HARUTYUNYAN, ET AL.	2/83	SF
R1RN35F	RIBONUCLEASE A	BORKAKOTI, MOSS, PALMER	6/82	SF
R3TLN5F	THERMOLYSIN (NATIVE)	B. MATTHEWS, M. HOLMES	2/82	SF
R2PTN5F	TRYPsin (ORTHORHOMBIC, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81	SF
R1TP05F	TRYPsin (ORTHORHOMBIC)	BODE, WALTER, HUBER	9/82	SF
R1TP05F	TRYPsin (TRIGONAL, 2.4M (NH4)2SO4)	J. WALTER, R. HUBER	10/81	SF
R3PTB5F	TRYPsin (BENZAMIDINE, INHIBITED)	BODE, SCHWAGER, WALTER	9/82	SF
R1TPP5F	TRYPsin/P-AMIDINO-PHENYL-PYRUVATE	WALTER, BODE, HUBER	9/82	SF
R4PT15F	TRYPsin INHIBITOR (BOVINE, PANCREAS)	R. HUBER, J. DEISENHOFER	9/82	SF
R2PTC5F	TRYPsin/TRYPsin INHIBITOR COMPLEX	R. HUBER, J. DEISENHOFER	9/82	SF
R1TPA5F	TRYPsin (ANHYDRO)/TRYPsin INHIBITOR	HUBER, BODE, DEISENHOFER	5/82	SF
R2TGA5F	TRYPsin (GENE, 2.4M MSS04)	J. WALTER, R. HUBER	10/81	SF
R1TGC5F	TRYPsin (GENE, 5 CH3OH, .5 HOH)	J. WALTER, R. HUBER	10/81	SF
R1TGT5F	TRYPsin (GENE, 173 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81	SF
R2TGT5F	TRYPsin (GENE, 103 DEG K, .7 CH3OH, .3 HOH)	J. WALTER, R. HUBER	10/81	SF
R2TGS5F	TRYPsin (GENE)/TRYPsin INHIBITOR	R. HUBER ET AL.	6/82	SF
R2TGS5F	TRYPsin (GENE)/TRYPsin INHIBITOR/ILE-VAL	R. HUBER ET AL.	9/82	SF
R2TPI5F	TRYPsin (GENE)/PTI/ILE-VAL (MERCURATED)	J. WALTER, R. HUBER	10/81	SF
R1TGS5F	TRYPsin (GENE)/PTI	R. HUBER ET AL.	9/82	SF

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

IDENT CODE	MOLECULE	DEPOSITOR	12-JUN-85	
			DATE/	CODE
R1CAT5F	*CATALASE (BEEF LIVER)	M. ROSSMANN	11/81	SF
R4CHAS5F	ALPHA-CHYMOTRYPSIN (BOVINE)	H. TSUKADA, D. BLOW	11/84	SF
R2QCH5F	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	7/84	SF
R1CYP5F	CYTOCHROME C PEROXIDASE (YEAST)	F. INZEL, P. POULOS, KRAUT	11/83	SF
R2C2CSF	CYTOCHROME C2 (OXIDIZED)	BHATIA, F. INZEL, KRAUT	11/83	SF
R3C2CSF	CYTOCHROME C2 (REDUCED)	BHATIA, F. INZEL, KRAUT	11/83	SF
R6BNASF	DNA (B, CCGGAATTCGG, SYNTHETIC)/NETROPSIN	M. KOPKA, R. DICKERSON	8/84	SF
R7BNASF	DNA (B, CCGGAATTCGG, ANISO TEMP FACTORS)	HOLBROOK, DICKERSON, KIM	1/85	SF
R1FX15F	FLAVODOXIN (D, VULGARIS, UNREFINED)	WATENPAUGH, SIEKER, JENSON/10/84	SF	
R2M4BSF	HEMOGLOBIN (HUMAN, DEOXY)	G. FERMI, M. PERUTZ	3/84	SF
R1HM95F	HEMOGLOBIN (HUMAN, OXY)	B. SHANNAN	3/84	SF
R1MCP5F	IGA FAB (KAPPA) MCPG03	G. COHEN ET AL.	7/84	SF
R2MCP5F	IGA FAB (KAPPA) MCPG03/PHOSPHOCHOLINE	PADLAN, COHEN, DAVIES	10/84	SF
R1PFC5F	*1GG PFC FRAGMENT	S. BRYANT ET AL.	4/85	SF
R1LZT5F	*LYSOZYME (HEN EGG-WHITE, TRICLINIC)	HOSON, BROWN, SIEKER, JENSON	4/85	SF
R1MEO5F	MYOGLOBIN (SPERM WHALE, OXY)	S. PHILLIPS	3/84	SF
R1PPO5F	PAPAIN D	J. JANSONIUS	10/84	SF
R3RPF5F	PROTEINASE I (RAT MAST CELL)	S. REMINGTON, B. MATTHEWS	9/84	SF
R5PT15F	PTI (X-RAY)	A. WLODAWER, R. HUBER	10/84	SF
R5PT15F	PTI (NEUTRON)	A. WLODAWER, R. HUBER	10/84	SF
R6R5A5F	*RIBONUCLEASE A (X-RAY)	A. WLODAWER	6/85	SF
R6R5A5F	*RIBONUCLEASE A (NEUTRON)	A. WLODAWER	6/85	SF
R6R5X5F	RUBREDOXIN (C, PASTEURIANUM)	WATENPAUGH, SIEKER, JENSON/10/84	SF	
R2VSB5F	*VIRUS COAT PROTEIN (SBMV, T=1)	M. ROSSMANN	4/85	SF
R4SBV5F	*VIRUS COAT PROTEIN (SOUTHERN BEAN MOSAIC) M. ROSSMANN	M. ROSSMANN	4/85	SF

* NEW OR REPLACEMENT ENTRY SINCE APR-85 NEWSLETTER

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TABLE 7. PROTEIN DATA BANK, ATOMIC COORDINATE HOLDINGS

IDENT	MOLECULE	DEPOSITOR(S)	DATE/STATUS		
2APE	ACID PROTEINASE (ENDOTHA PARASITICA)	T. BLUNDELL	9/81	1PFC	IGG PFC FRAGMENT
2APP	ACID PROTEINASE (PENICILLIUM JANTHINELLUM)	A. SIELECKI, M. JAMES	1/83	11G2	IMMUNOGLOBULIN G1 (LAMBDA) KOL
1APR	ACID PROTEINASE (RHIZOPUS CHINENSIS)	D. DAVIES	8/79	11N5	INSULIN (PORCINE, 2-ZINC)
2ACT	ACTINIDIN	E. BAKER	11/79	21N5	INSULIN (BOVINE, 2-ZINC) DES-PHE BI
1ACK1	ACTINOLACTIN	V. CLETNYV, A. KUZIN	12/82	2PKA	KALLIKREIN A (PORCINE)
2ADK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77	2KA1	KALLIKREIN A (PORCINE)/PTI (BOVINE)
1AGA	AGAROSE	S. ARNOTT	5/78	1KGA	KDGP ALDOLASE
2HGA	AGGLUTININ (WHEAT GERM)	C. WRIGHT	5/80	1KES	KERATAN SULFATE
4ADH	ALCOHOL DEHYDROGENASE (APO)	C. -I. BRANDEN	8/79	4LDH	LACTATE DEHYDROGENASE (DOGFISH)
5ADH	ALCOHOL DEHYDROGENASE (APO) /ADP-RIBOSE	H. EKLUND, T. A. JONES	1/84	3LDH	LACTATE DEHYDROGENASE/ANAD/PYRUVATE (DOGFISH)
6ADH	ALCOHOL DEHYDROGENASE (Holo) /NADH/DMSO	H. EKLUND	12/82	5LDH	LACTATE DEHYDROGENASE/S-LAC/NAD (PIG)
7ADH	ALCOHOL DEHYDROGENASE (ISONICOTINIMIDYLATED)	B. PLAPP, H. EKLUND	1/84	1LDX	LACTATE DEHYDROGENASE (MOUSE TESTES)
2ALP	*ALPHA-LYTIC PROTEASE	M. FUJINAGA, M. JAMES	3/85 R	1LH1	LEGEHEMOGLOBIN (ACETATE MET)
2TAA	ALPHA-AMYLASE	KUSUNOKI, MATSUURA, KAKUDO	10/82	2LH1	LEGEHEMOGLOBIN (ACETATE MET)
5AP1	ALPHA 1-ANTI TRYPSIN (MODIFIED, TETRAGONAL)	J.R. HUBER ET AL.	10/84	2LH2	LEGEHEMOGLOBIN (AQUO MET)
6AP1	ALPHA 1-ANTI TRYPSIN (MODIFIED, HEXAGONAL)	R. KABER ET AL.	10/84	2LH3	LEGEHEMOGLOBIN (AQUO MET)
1ABP	L-ARABINOSE-BINDING PROTEIN	F. QUICHO, G. GILLILAND	5/80	1LH3	LEGEHEMOGLOBIN (CYANO MET)
1AAT	CYTOSOLIC ASPARTATE AMINOTRANSFERASE	HARUTYUNYAN, MALASHKEVICH	4/82 A	2LH3	LEGEHEMOGLOBIN (CYANO MET)
2ATC	ASPARTATE CARBAMOYLTRANSFERASE	W. LIPSCOMB	3/82	1LH4	LEGEHEMOGLOBIN (DEOXY)
4ATC	ASPARTATE CARBAMOYLTRANSFERASE	W. LIPSCOMB	4/84	2LH4	LEGEHEMOGLOBIN (DEOXY)
5ATC	ASPARTATE CARBAMOYLTRANSFERASE/CTP	W. LIPSCOMB	4/84 R	4LY2	LYSOZYME (HEN EGG-WHITE, SET R59A)
1AZA	AZURIN (ALCALIGENES DENITRIFICANS)	E. BAKER, G. NORRIS	5/84	2LH5	LEGEHEMOGLOBIN (FLUORO MET)
1AZU	AZURIN (PSEUDOMONAS AERUGINOSA)	E. ADMAN, L. SIEKER, L. JENSEN	8/80	1LH6	LEGEHEMOGLOBIN (NICOTINATE MET)
2BCL	BACTERIOCHLOROPHYLL A-PROTEIN	B. MATTHEWS	1/79 A	2LH6	LEGEHEMOGLOBIN (NICOTINATE MET)
1ABX	ALPHA-BUNGAROTOXIN	D. AGARD, S. SPENCER, R. STROUD	4/80 A	1LH7	LEGEHEMOGLOBIN (FERRO) /NITROSOBENZENE
1CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74	1LH8	LEGEHEMOGLOBIN (FERRO) /NITROSOBENZENE
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6H	R. KRETSINGER	8/74	1LZM	LYSOZYME (BACTERIOPHAGE T4)
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6I	R. KRETSINGER	8/74	1LY2	LYSOZYME (HEN EGG-WHITE, SET W2)
11CB	CALCIUM-BINDING PROTEIN (INTESTINAL)	D. SZEBENYI, K. MOFFAT	7/83	2LY2	LYSOZYME (HEN EGG-WHITE, SET R55D)
1CAP	CAPSULAR POLYSACCHARIDE (E. COLI M41)	S. ARNOTT	5/78	3LY2	LYSOZYME (HEN EGG-WHITE, SET R56A)
2CAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANNAN	10/83	4LY2	LYSOZYME (HEN EGG-WHITE, SET R59A)
1CAC	CARBONIC ANHYDRASE C (HUMAN)	H. LIPSCOMB	5/76	5LY2	LYSOZYME (HEN EGG-WHITE, SET R512A)
3CPA	CARBOXYPEPTIDASE A/GLYCYLTYROSINE	D. REES, W. LIPSCOMB	3/82	6LY2	LYSOZYME (HEN EGG-WHITE, SET R516)
4CPA	CARBOXYPEPTIDASE A/POTATO INHIBITOR	D. REES, W. LIPSCOMB	3/82	7LY2	LYSOZYME (HEN EGG-WHITE, TRICLINIC)
5CPA	CARBOXYPEPTIDASE A/WATER (BOVINE)	D. REES, W. LIPSCOMB	5/82	1LZ7	*LYSOZYME (HEN EGG-WHITE, TRICLINIC)
1CPB	CARBOXYPEPTIDASE B (BOVINE)	M. SCHMID, J. HERRIOTT	6/76 A	8LY2	LYSOZYME (HEN EGG-WHITE, INACTIVATED)
1CAR	CARRAGEENAN	S. ARNOTT	5/78	9LY2	LYSOZYME (HEN NAN-NAG-NAM SUBSTRATE ONLY)
7CAT	CATALASE (BEEF LIVER)	F. I.TA, M. ROSSMANN	11/84 R	1LZH	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)
8CAT	CATALASE (BEEF LIVER)	F. I.TA, M. ROSSMANN	11/84 R	2LZH	LYSOZYME (HEN EGG-WHITE, ORTHORHOMBIC)
4CAT	CATALASE (PENICILLIUM VITALE)	B. VAINSHTEIN ET AL.	2/83 B	1LYM	LYSOZYME (HEN EGG-WHITE, MONOCLINIC)
1CH5	CHONDROITIN-4-SULFATE	S. ARNOTT	5/78	2LH1	LYSOZYME (HUMAN)
1CH5	CHONDROITIN-4-SULFATE (CA SALT)	S. ARNOTT	5/78	2LH2	LYSOZYME (TURKEY EGG-WHITE)
2CHA	ALPHA-CHYMOTRYPSIN (TOSYL)	D. BLOW	1/75	1MD1	MALATE DEHYDROGENASE
4CHA	ALPHA-CHYMOTRYPSIN (BOVINE)	H. TSUKADA, D. BLOW	11/84	1MLT	MELITTIN
5CHA	ALPHA-CHYMOTRYPSIN (BOVINE)	R. BLEVINS, A. TULINSKY	1/85 R	1MT2	*CD2ZN METALLOTHIONEIN (ISOFORM 11)
2GCH	GAMMA-CHYMOTRYPSIN	COHEN, DAVIES, SILVERTON	5/80	1MB5	MYOGLOBIN (SEAL, MET)
1CHG	CHYMOTRYPSINOGEN	J. KRAUT, J. BIRKTOFF	3/75	1MN	MYOGLOBIN (SPERM WHALE, MET)
1CTA	CITRATE SYNTHASE (PIG)	REMINGTON, WIEGAND, HUBER	1/84	2MB	MYOGLOBIN (SPERM WHALE, MET)
2CTA	CITRATE SYNTHASE (PIG, COA, CITRATE CMLX)	REMINGTON, WIEGAND, HUBER	1/84	3MB	MYOGLOBIN (SPERM WHALE, DEOXY)
3CTA	CITRATE SYNTHASE (CHICKEN, COA, CITRATE)	REMINGTON, WIEGAND, HUBER	1/84	1MBD	MYOGLOBIN (SPERM WHALE, DEOXY)
4CTA	CITRATE SYNTHASE (PIG, OXALOACETATE CMLX)	REMINGTON, WIEGAND, HUBER	1/84	1MB0	MYOGLOBIN (SPERM WHALE, OXY)
1CTX	ALPHA COBRATOXIN	W. SAENGER, M. WALKINSHAW	3/82	1MB5	MYOGLOBIN (SPERM WHALE, CO, NEUTRON)
2CNA	CONCANAVALIN A	G. RECKE, J. BECKER, G. EDELMAN	4/75	1MK4	MYOHEMERIN
3CNA	CONCANAVALIN A	K. HARDMAN	9/76	1NXB	NEUROTOXIN B (LATICAUDA SEMIFASCIATA)
1CN1	CONCANAVALIN A (DEMETALLIZED)	M. SHOHAM	12/81	1SN3	SCORPION NEUROTOXIN (VARIANT 3)
1CRN	CRAMBIN	H. HENDRICKSON, M. TEETER	5/81	1OPV	OVONUCLO THIRD DOMAIN (JAPANESE QUAIL)
2BSC	CYTOCHROME B5 (OXIDIZED)	F. S. MATHEWS	12/77	10V1	AVIAN PANCREATIC POLYPEPTIDE
156B	CYTOCHROME B556 (E. COLI, OXIDIZED)	BETHES, CZEZINSKI, MATHEWS	8/79	9PAP	PAPAIN (ACTIVE)
3CYT	CYTOCHROME C (ALBACORE, OXIDIZED)	T. TAKANO, R. DICKERSON	7/80	1PAD	PAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)
4CYT	CYTOCHROME C (ALBACORE, REDUCED)	T. TAKANO, R. DICKERSON	7/80	2PAD	PAPAIN (CYS DERIV OF CYS-25)
1CYC	CYTOCHROME C (BONITO, HEART)	M. KAKUDO	8/76	3PAD	PAPAIN (OXIDIZED CYS-25)
1OCR	CYTOCHROME C (RICE)	H. OCHI, N. TANAKA	3/83	4PAD	PAPAIN (TOS-LYS, CYS-25)
1OCY	CYTOCHROME C (PRIME)	P. WEBER, R. SALEMME	8/81	5PAD	PAPAIN (BZOO-GLY-PHE-GLY, CYS-25)
1CCY	CYTOCHROME C (PEROXIDASE (YEAST))	B. FINZEL, T. POLJUS, J. KRAUT	11/83	6PAD	PAPAIN (BZOO-PHE-ALA, CYS-25)
2CCY	CYTOCHROME C2 (OXIDIZED)	G. BHATIA, B. FINZEL, J. KRAUT	11/83	1PAP	PAPAIN D
3CCY	CYTOCHROME C2 (REDUCED)	G. BHATIA, B. FINZEL, J. KRAUT	11/83	1PEP	PEPSIN (PORCINE)
2CDV	CYTOCHROME C3 (DESULFOVIBRIO VULGARIS)	N. YASUOKA, M. KAKUDO	11/83	3PKG	PHOSPHOGLYCERATE KINASE (YEAST)
3CC5	CYTOCHROME C5 (OXIDIZED, AZOTOBACTER VULGARIS)	D. C. STOUT, D. CARTER	8/84	2PKP	PHOSPHOGLYCERATE KINASE (HORSE)
1551	CYTOCHROME C551 (OXIDIZED)	H. W. LUCH	8/78	3PKP	PHOSPHOGLYCERATE KINASE (HORSE)
351C	CYTOCHROME C551 (OXIDIZED)	MATSUURA, TAKANO, DICKERSON	7/81	1BP2	PROPHOSPHOLIPASE A2 (BOVINE)
451C	CYTOCHROME C551 (REDUCED)	MATSUURA, TAKANO, DICKERSON	7/81	2BP2	PROPHOSPHOLIPASE A2 (BOVINE)
30FR	DIHYDROFLAVONE REDUCTASE (L. CASEI)	J. BOLIN, D. MATTHEWS, J. KRAUT	6/82	3BP2	PROPHOSPHOLIPASE A2 (BOVINE) TRANSAMINATED
40FR	DIHYDROFLAVONE REDUCTASE (E. COLI)	J. BOLIN, D. MATTHEWS, J. KRAUT	6/82	1P2P	PHOSPHOLIPASE A2 (PORCINE)
1ANA	DNA (5'-P-PPIME-3')-D-1000-CGGG-3' (PRIME1)	B. CONNER, R. DICKERSON	6/82	1PCY	PLASTOCYANIN (POPLAR, CU2+)
1BN4	DNA (B. COCCOAAITCCGG, SYNTHETIC, 230 DEG K)	H. DREW, R. DICKERSON	11/81	2PCY	PLASTOCYANIN (POPLAR, APO)
2BN4	DNA (B. COCCOAAITCCGG, SYNTHETIC, 16 DEG K)	H. DREW, R. DICKERSON	11/81	2PAB	PREALBUMIN (HUMAN, PLASMA)
3BN4	DNA (B. 9-BR-CGGCAATTCGG, SYNTH, 20 DEG C)	KOPKA, FRATINI, DICKERSON	2/82	35GB	PROTEINASE B (STREP, GRISEUS) /OMTK3
4BN4	DNA (B. 9-BR-CGGCAATTCGG, SYNTH, 7 DEG C)	KOPKA, FRATINI, DICKERSON	2/82	35GB	PROTEINASE B (STREP, GRISEUS) /OMTK3
5BN4	DNA (B. COCCOAAITCCGG, SYNTHETIC) /CISPLATIN	H. NG, P. JURA, DREW, DICKERSON	8/83	1IPY	INORGANIC PYROPHOSPHATASE
6BN4	DNA (B. 9-BR-CGGCAATTCGG, SYNTH) /NETROSPIN	KOPKA, R. DICKERSON	8/84	1PYK	PYRUVATE KINASE (CAT)
7BN4	DNA (B. COCCOAAITCCGG, ANISO TEMP FACTORS)	HOLBROOK, DICKERSON, KIM	1/85	1RH0	RHOANASE
1ZNA	DNA (Z', CCGG, HIGH-SALT, SYNTHETIC)	H. DREW, R. DICKERSON	1/81	5RKA	*RIBONUCLEASE A (X-RAY+NEUTRON)
1EST	ELASTASE (PORCINE, TOSYL)	H. WATSON	5/76	1RN3	RIBONUCLEASE A
1ECD	ERYTHROCYRURIN (REDUCED, DEOXY)	W. STEIGEMANN, E. WEBER	3/79	1RNB	RIBONUCLEASE B
1ECD	ERYTHROCYRURIN (CARBONMONOXID)	W. STEIGEMANN, E. WEBER	3/79	4RXN	RUBREDUOXIN (C. PASTEURIANUM, UNCONST REF)
1ECA	ERYTHROCYRURIN (AQUO, MET)	W. STEIGEMANN, E. WEBER	3/79	5RXN	RUBREDUOXIN (C. PASTEURIANUM, NRG+XTAL REF)
1ECN	ERYTHROCYRURIN (CYANO, MET)	W. STEIGEMANN, E. WEBER	3/79	3RXN	RUBREDUOXIN (DESULFOVIBRIO VULGARIS)
2FD1	FERRIDOXIN (AZOTOBACTER VINELANDII)	STOUT, GOSH, FUREY, O'DONNELL	11/81	2SN5	STAPHYLOCOCCAL NUCLEASE
1FDX	FERRIDOXIN (PEPTOCOCCUS AEROGESUS)	E. ADMAN, L. SIEKER, L. JENSEN	8/76	39B2	PROTEINASE B (BACT. MAST CELL)
3FXC	FERRIDOXIN (SPRULIN PLATENSIS)	TSUKIHARA, KATSUBE, KAKUDO	12/81	1SBT	SUBTILISIN INHIBITOR (STREPTOMYCES)
3FXN	FLAVODIOLIN (CLOSTRIDIUM MF OXIDIZED)	M. LUDWIG	12/77	1SPT	SUBTILISIN BPN-PRIME
4FXN	FLAVODIOLIN (CLOSTRIDIUM MF SEMIQUINONE)	M. LUDWIG	12/77	2SBT	SUBTILISIN NOVO
1FX1	FLAVODIOLIN (D. VULGARIS, UNREFINED)	WATENPAUGH, SIEKER, JENSEN	10/84	151C	SUBTILISIN BPN(PRIME)/SSI COMPLEX
1GPB	GALACTOSE-BINDING PROTEIN	S. MOUBRAY, G. PETSKO	8/83 A	250D	SUPEROXIDISE DISMUTASE
1GCN	GLUCAGON	T. BLUNDELL	10/77	31LN	THERMOLYSIN (NATIVE)
1P01	GLUCOSE 6-PHOSPHATE ISOMERASE	H. MUIRHEAD	7/77 A	4TLN	THERMOLYSIN (LEU-NH2)
2GR5	GLUTATHIONE REDUCTASE (HUMAN)	G. SCHULZ	11/81	5TLN	THERMOLYSIN (HONH-BZMALONYL-A-G-NITROALD)
1GPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTR)	M. ROSSMANN	7/75	7TLN	THERMOLYSIN (CHCCO (NH-OH)LEUCO3)
2OPD	APD-GLYCERALDEHYDE-3-P-DEHYDROGENASE	M. ROSSMANN	12/79	1SRX	THIOPYRIMIDINE (E. COLI, OXIDIZED)
3OPD	GLYCERALDEHYDE-3-P-DEHYDROGENASE (HUMAN)	H. WATSON, J. CAMPBELL	6/83	4TNA	TRANSFER RNA (YEAST, PHE)
1HR8	HEMERYTHRIN B	W. HENDRICKSON	6/76 A	6TNA	TRANSFER RNA (YEAST, PHE)
1HRQ	HEMERYTHRIN (MET)	STENKAMP, SIEKER, JENSEN	2/83	8TNA	TRANSFER RNA (YEAST, PHE)
1HRZ	HEMERYTHRIN (AZIDIO, MET)	STENKAMP, SIEKER, JENSEN	2/83	1T1M	TRIOSE PHOSPHATE ISOMERASE
1HR3	HEMERYTHRIN (AZIDIO, MET, SIPHONOSOMA)	SMITH, HENDRICKSON, ADDISON	5/83	2TNC	TROPONIN-C (TURKEY)
1H05	HEMOGLOBIN (DEER, SINGLE CELL)	E. AMMA, R. GIRLING	10/79	2PTN	TRYPSIN (ORTHORHOMBIC, 2.4M (NH4)2SO4)
2HHB	HEMOGLOBIN (HORSE, AQUO MET)	R. LADNER, HEIDNER, PERUTZ	2/77	1TPD	TRYPSIN (ORTHORHOMBIC, 5 HOH)
2HH1	HEMOGLOBIN (HORSE, DEOXY)	R. LADNER, HEIDNER, PERUTZ	11/73	3PTN	TRYPSIN (TRIGONAL, 2.4M (NH4)2SO4)
2HHB	HEMOGLOBIN (HUMAN, DEOXY)	G. FERMI, M. PERUTZ	3/84 R	3PTB	TRYPSIN (BENZAMIDINE INHIBITED)
3HHB	HEMOGLOBIN (HUMAN, DEOXY, SYMMETRY AVRGD)	G. FERMI, M. PERUTZ	3/84 R	1TPP	TRYPSIN/P-AMIDINO-PHENYL-PYRUVATE
4HHB	HEMOGLOBIN (HUMAN, DEOXY, UNRESTRAINED)	G. FERMI, M. PERUTZ	3/84 R	3PTP	TRYPSIN (DIP INHIBITED)
1HCO	HEMOGLOBIN (HUMAN, CARBONMONOXID)	J. BALDWIN	8/79	4PT1	TRYPSIN INHIBITOR (BOVINE, PANCREAS)
2HCO	HEMOGLOBIN (HUMAN, CARBONMONOXID, NRG REFND)	R. LADNER, HEIDNER, PERUTZ	2/77	1T81	TRYPSIN INHIBITOR (BOVINE, XRAY+NEUTRON)
1HHH	HEMOGLOBIN (HUMAN, OXY)	B. SHAANAN	8/83	2PTC	TRYPSIN/TRYPSIN INHIBITOR COMPLEX
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. FRIER	6/76	1TPA	TRYPSIN (ANHYDRO)/TRYPSIN INHIBITOR
1H85	HEMOGLOBIN S (HUMAN, SINGLE CELL)	E. PADLAN, W. LOVE	6/82	1TRN	TRYPSINOGEN
1LH8	HEMOGLOBIN (LAMPREY)	HENDRICKSON, LOVE, KARLE	3/73	2TGA	TRYPSINOGEN (2.4M MGSO4)
2YHX	HEXOKINASE (YEAST) FORM B111	STEITZ, ANDERSON, STENKAMP	12/80	11G6	TRYPSINOGEN (5 CH3OH, 5 HOH)
1HK6	HEXOKINASE A - GLUCOSE COMPLEX (YEAST)	R. BODNE ET AL., J. STEINKAMP	3/79	1GTG	TRYPSINOGEN (173 DEG K, .7 CH3OH, .3 HOH)
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75	2TGT	TRYPSINOGEN (103 DEG K, .7 CH3OH, .3 HOH)
1HYA	HYALURONIC ACID (NA SALT, 3-FOLD HELIX)	S. ARNOTT	11/77	1TGB	TRYPSINOGEN (WITH CA, FROM PEG)
2HYA	HYALURONIC ACID (NA SALT, 4-FOLD HELIX)	S. ARNOTT	5/78	2TGP	TRYPSINOGEN/TRYPSIN INHIBITOR
3HYA	HYALURONIC ACID (NA SALT, 2-FOLD HELIX)	S. ARNOTT	5/78	3TPT	TRYPSIN INHIBITOR (BOVINE, ILE-VAL)
1HYH	HYALURONIC ACID (CA SALT, 3-FOLD HELIX)	S. ARNOTT	5/78	2TPI	TRYPSINOGEN/PTI (ILE-VAL (MERCURATED))
1MCP	IGA FAB (KAPPA)MCP603	SATOH, COHEN, PADLAN, DAVIES	7/84	1TGS	TRYPSINOGEN/PTI
2MCP	IGA FAB (KAPPA)MCP603/PHOSPHOCOLINE	E. PADLAN, G. COHEN, D. DAVIES	10/84	1T51	TRYOSYL TRANSFER RNA SYNTHETASE
1FB4	IMMUNOGLOBULIN FAB (LAMBDA) KOL	M. MARQUART, R. HUBER	5/83	1GN5	GENE 5 DNA-UNWINDING PROTEIN (E. COLI)
3FAB	IMMUNOGLOBULIN FAB, PRIME, NEW	R. POLJAK	9/81	25TV	VIRUS (SATELLITE TOBACCO NECROSIS)
1MCG	IMMUNOGLOBULIN B - J CONTACT	R. COLLEGER, EDMUNDSON ET AL.	5/78 A	4VIR5	VIRUS (SOUTHERN BEAN MOSAIC)
1RE1	IMMUNOGLOBULIN B - J FRAGMENT (V-DIMER) RE1	R. EPP, R. HUBER	3/78 A	2TBV	VIRUS (TOMATO BUSHY STUNT)
2RHE	IMMUNOGLOBULIN B - J FRAGMENT (V-NMIMER) RHE	FUREY, HANG, YOO, SAX	6/83		
1FC1	IMMUNOGLOBULIN FC (HUMAN)	J. DEISENHOFER	5/81		
1FC2	IMMUNOGLOBULIN FC-FRAGMENT B COMPLEX	J. DEISENHOFER	5/81		

MODEL STRUCTURES

Z2NA	DNA(2-I, CGCGCG, SYNTHETIC, MODEL)	A.RICH	2/81
Z3NA	DNA(2-II, CGCGCG, SYNTHETIC, MODEL)	A.RICH	2/81
IDNN	DNA(ATCGGCTAAG, . . . , MODEL)	J.SUSSMAN,E.TRIFONOV	11/85
I1GE	IMMUNOGLOBULIN E(F C FRAGMENT)MODEL	E.PADLAN,D.DAVIES	11/82
1GF1	INSULIN-LIKE GROWTH FACTOR I (MODEL)	BLUNDELL,BEDARKAR,HUMBEL	12/82
1GF2	INSULIN-LIKE GROWTH FACTOR II (MODEL)	BLUNDELL,BEDARKAR,HUMBEL	12/82
1MLP	MURINE LI.FOPROTEIN (MODEL)	A.MCLACHLAN	8/78
1RLX	RELAXIN(MODEL, CONFORMATION A, UNREFINED)	A.EVANS,A.NORTH	3/78
2RLX	RELAXIN(MODEL, CONFORMATION B, UNREFINED)	A.EVANS,A.NORTH	3/78
3RLX	RELAXIN(MODEL, CONFORMATION A, REFINED)	A.EVANS,A.NORTH	3/78
4RLX	RELAXIN(MODEL, CONFORMATION B, REFINED)	A.EVANS,A.NORTH	3/78
1TNC	TROPONIN (CA-BINDING COMPONENT,MODEL)	R.KRETSINGER,C.D.BARRY	6/80 A

* NEW OR REPLACEMENT ENTRY SINCE APR-85 NEWSLETTER

STATUS CODES

BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
R	RECENT (1984-1985) REPLACEMENT FOR AN OUT-OF-DATE PARAMETER SET

TABLE 8. COORDINATE AND STRUCTURE FACTOR ENTRIES IN PREPARATION

12-JUN-85			
1CY3	*CYTOCHROME C3	R.HASER,M.FREY,F.PAYAN	6/85 P
1GP1	*GLUTATHIONE PEROXIDASE (BOVINE)	O.EPP,R.LADENSTEIN	6/85 P
20V0	*OVOMUCOID THIRD DOMAIN(SILVER PHEASANT)	W.BODE,O.EPP	6/85 N
9TNA	*TRANSFER RNA(YEAST, ASP)	WESTHOF,DUMAS,MORAS	6/85 N
4TP1	*TRYPSINOGEN/ARG-15-PTI/VAL-VAL	W.BODE,J.WALTER	6/85 N
1R16P	*GLUTATHIONE PEROXIDASE (BOVINE)	O.EPP,R.LADENSTEIN	6/85 SF
R20V0SF	*OVOMUCOID THIRD DOMAIN(SILVER PHEASANT)	W.BODE,O.EPP	6/85 SF

* NEW OR REPLACEMENT ENTRY SINCE APR-85 NEWSLETTER

STATUS CODES

A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
N	NEW ENTRY AWAITING APPROVAL BY DEPOSITOR
P	IN PREPARATION
R	REPLACEMENT FOR ENTRY IN TABLE 7
SF	STRUCTURE FACTORS

TABLE 9. PROTEIN DATA BANK, BIBLIOGRAPHIC ENTRIES

12-JUN-85			
DEAP	ACID PROTEINASE (ENDOTHIA PARASITICA)		
OADC	ADH-NADH-DIMETHYLSULFOXIDE COMPLEX		
DAF1	APOFERRITIN (HORSE)		
OMAA	MITOCHONDRIAL ASPARTATE AMINOTRANSFERASE		
ORNB	BARNASE (BACILLUS AMYLOLIQUEFACIENS)		
OC01	CALOTROPIN D1 (CALOTROPIS GIGANTEA)		
OPT2	D-ALANYL-CARBOXYPEPTIDASE-TRANSEPTIDASE		
OZGP	D-ALANYL-D-ALANINE PEPTIDASE (Zn2+ 6 PEPTIDASE)		
OGC1	*GAMMA-CHYMOTRYPSIN - INACTIVATOR COMPLEX		
OCN2	CONCAVANE A (DEMETALLIZED)		
OCRO	CRO REPRESSOR		
OGCR	GAMMA-CRYSTALLIN II (CALF)		
OCY3	CYTOCHROME C3 (DESULFOVIBRIO DESULFURICANS NORWAY)		
OSC1	CYTOCHROME C555 (CHLOROBILIUM SULFATOPHILUM)		
OC3A	DES-AR077-C3A ANAPHYLATOXIN		
OCDF	DIIHYDROGLUTE REDUCTASE (CHICKEN LIVER)		
OANB	DNA(GGTATACC)		
OANB	DNA(GGUAUACC)		
ODP1	*DNA POLYMERASE I		
UESZ	ELASTASE COMPLEX (PIG)		
DETU	ELONGATION FACTOR TU COMPLEX (E. COLI)		
DEBX	ERABUTOXIN B		
OFX1	FERRIDOXIN I (APHANOTHECE SACRUM)		
OFX3	FLAVODOXIN(OXIDIZED,ANACYSTIS NIDULANS)		
OFX2	FLAVODOXIN (REDUCED, CLOSTRIDIUM MP)		
OG8P	D-GALACTOSE-BINDING PROTEIN(ESCHERICHIA COLI)		
OGAP	CATABOLITE GENE ACTIVATOR PROTEIN		
OGP1	GLUTATHIONE PEROXIDASE (BOVINE)		
OGD1	D-GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE (BACILLUS STEAROTHERMOPHILUS)		
OHMG	HEMAGGLUTININ		
OHF1	HEMOCYANIN(PANULIRUS INTERRUPTUS)		
ODCH	HEMOGLOBIN (COBALT, DEOXY)		
OH8G	HEMOGLOBIN (GLYCERA DIBRANCHIATA)		
OPH4	P-HYDROXYBENZOATE HYDROXYLASE (PSEUDOMONAS FLUORESCENS)		
DAU1	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (KAPPA) AU		
OR0Y	IMMUNOGLOBULIN, BENCE-JONES FRAGMENT (V-MONOMER,KAPPA) ROY		
OIG1	IMMUNOGLOBULIN G1 (KAPPA) DOB		
O1N4	INSULIN (HUMAN)		
O1N1	INSULIN (PORCINE)		
O1N2	INSULIN (PORCINE)		
O1N3	DESPENTAPEPTIDE INSULIN(BEEF)		
OLRP	N-TERMINAL DOMAIN OF LAMBDA REPRESSOR		
OLGM	LYSOZYME (EMBDOEN GOOSE)		
OLZ5	LYSOZYME (HEN EGG-WHITE, NEUTRON STUDY)		
OLZT	LYSOZYME (HEN EGG-WHITE, HIGH-TEMPERATURE)		
OLZ6	LYSOZYME (STREPTOMYCES ERYTHRAEUS)		
OTEL	LYSOZYME (TORTOISE EGG-WHITE)		
OC1F	L7/L12 (E. COLI, C-TERMINUS)		
OB2M	*BETA2-MICROGLOBULIN		
OMBA	MYOGLOBIN (APLYSIA LIMACINA)		
OMBM	MYOGLOBIN (SPERM WHALE, MET, TEMPERATURE STUDIES)		
OMB3	MYOGLOBIN (SPERM WHALE, MET, NEUTRON STUDY)		
OPFK	PHOSPHOTRICKINASE (BACILLUS STEAROTHERMOPHILUS)		
OPP2	PHOSPHOLIPASE A2 (RATTLESNAKE)		
OPPA	PHOSPHORYLASE A (RABBIT)		
OPB1	PHOSPHORYLASE B (RABBIT)		
ORX5	RELAXIN (PORCINE, MODEL)		
OR5A	RIBONUCLEASE A (BOVINE)		
OR5B	RIBONUCLEASE (BOVINE SEMINAL)		
ORB1	RIBONUCLEASE B1(BINASE)		
OR5T	RIBONUCLEASE ST (STREPTOMYCES ERYTHREUS)		
ORNT	RIBONUCLEASE T1-2(PRIME)-GUANYLIC ACID (ASPERGILLUS ORYZAE)		
OSBP	*SULFATE-BINDING PROTEIN		
OSDE	FE-SUPEROXIDE DISMUTASE (ESCHERICHIA COLI)		
OSDP	FE-SUPEROXIDE DISMUTASE (PSEUDOMONAS OVALIS)		
OTH1	*THAUMATIN		
OT4T	THIOREDOXIN REDUCTASE (BACTERIOPHAGE T4)		
OFMT	INITIATOR TRANSFER RNA (E. COLI, F/MET)		
OTAI	TRANSFER RNA (YEAST, ASP, A FORM)		
OTAZ	TRANSFER RNA (YEAST, ASP, B FORM)		
OTRI	TRANSFER RNA (YEAST, PHE)		
OMTS	METHIONYL TRANSFER RNA SYNTHETASE		
OYP1	TRIOSE PHOSPHATE ISOMERASE (SACCHAROMYCES CEREVISIAE)		
OUTG	UTEROGLOBIN (RABBIT)		
OTMV	VIRUS PROTEIN DISK (TOBACCO MOSAIC)		

* NEW OR REPLACEMENT ENTRY SINCE APR-85 NEWSLETTER

TABLE 10. SUBSTANTIVE CORRECTIONS TO COORDINATE ENTRIES AND PROGRAMS

12-JUN-85

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 '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 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,3ATCC
*INSERT,3ATCB,6
REMARK 8
REMARK 8 CORRECTION. THIS ENTRY IS OBSOLETE. 02-JAN-85.
*INSERT,3ATC,9
REVDAT 4 02-JAN-85 3ATCC 3 OBSLTE
*INSERT,3ATC,3
OBSLTE 02-JAN-85 3ATC 5ATC
*DELETE,3ATCB,7
MASTER 65 9 2 24 40 0 10 9 7056 4 10 72

*IDENT,2PTNC
*INSERT,2PTNB,16
REMARK 7
REMARK 7 CORRECTION. CHANGE RESIDUE 165 FROM ASN TO ASP AND CHANGE RESIDUE 7 RESIDUE 186 FROM GLN TO GLU, UPON DEPOSITORS INSTRUCTIONS.
REMARK 7 REVISE ATOM AND SEQRES RECORDS ACCORDINGLY. 14-MAR-85.
*INSERT,2PTN,7
REVDAT 4 14-MAR-85 2PTNC 3 SEQRES ATOM

*DELETE,2PTN,7B
SEQRES 12 223 SER ASP SER SER CYS LYS SER ALA TYR PRO GLY GLN ILE
*DELETE,2PTN,7B
SEQRES 13 223 THR SER ASN MET PHE CYS ALA GLY TYR LEU GLU GLY GLY
*DELETE,2PTN,1164,1171
ATOM 1059 N ASP 165 8.778 6.408 4.722 1.00 24.78
ATOM 1060 CA ASP 165 9.557 7.637 4.878 1.00 24.78
ATOM 1061 C ASP 165 9.210 6.667 3.803 1.00 24.78
ATOM 1062 O ASP 165 9.016 9.871 4.104 0.00 24.78
ATOM 1063 CB ASP 165 11.028 7.228 4.718 1.00 24.78
ATOM 1064 CG ASP 165 11.909 8.467 4.639 0.00 0.00 1
ATOM 1065 OD1 ASP 165 12.700 8.702 5.586 0.00 0.00 1
ATOM 1066 OD2 ASP 165 12.111 8.896 3.410 0.00 0.00 1
*DELETE,2PTN,1326,1333

ATOM 1220 N GLU 186 -5.754 8.910 3.770 1.00 26.16
ATOM 1221 CA GLU 186 -7.166 9.210 3.492 1.00 26.16
ATOM 1222 C GLU 186 -7.801 9.986 4.643 1.00 26.16
ATOM 1223 O GLU 186 -6.841 10.672 4.477 1.00 26.16
ATOM 1224 CB GLU 186 -7.907 7.873 3.289 1.00 26.16
ATOM 1225 CG GLU 186 -9.375 8.068 2.884 1.00 50.77
ATOM 1226 CD GLU 186 -9.937 6.736 2.396 1.00 50.77
ATOM 1227 OE1 GLU 186 -9.363 6.126 1.457 0.00 0.00 1
ATOM 1228 OE2 GLU 186 -11.160 6.467 2.803 0.00 0.00 1
*DELETE,2PTNB,17
MASTER 68 2 1 3 0 0 0 6 1712 1 20 18

*IDENT,2TGPE *IDENT,3PTND *IDENT,1TGTG *IDENT,1TGSO *IDENT,2PTCD
*IDENT,1TPAE *IDENT,3TPIE *IDENT,1TPOC *IDENT,1TGCC *IDENT,2TPIE
*IDENT,3PTBD *IDENT,1TGBG *IDENT,1TTPC *IDENT,2TGAC *IDENT,2TGTG
SEE 2PTN ABOVE

*IDENT,3CHAK
*INSERT,3CHAJ,6
REMARK 16
REMARK 16 CORRECTION. THIS ENTRY IS OBSOLETE. 01-APR-85.
*INSERT,3CHA,3
OBSLTE 01-APR-85 3CHA 5CHA
*INSERT,3CHAD,3
REVDAT 12 01-APR-85 3CHAK 3 OBSLTE
*DELETE,3CHAJ,7
MASTER 88 0 0 1 14 0 0 9 1733 2 10 19

*IDENT,2RXNJ
*INSERT,2RXN1,4
REMARK 19
REMARK 19 CORRECTION. THIS ENTRY IS OBSOLETE. 01-APR-85.
*INSERT,2RXN,3
OBSLTE 01-APR-85 2RXN 4RXN 5RXN
*INSERT,2RXND,1
REVDAT 11 01-APR-85 2RXNJ 3 OBSLTE
*DELETE,2RXN1,5
MASTER 119 0 1 0 0 0 0 6 557 1 5 5

*IDENT,4DFRE
*INSERT,4DFRD,4
REMARK 16
REMARK 16 CORRECTION. CORRECT CONECT RECORDS FOR MTX. 12-JUL-85.
*INSERT,4DFR,8
REVDAT 6 12-JUL-85 4DFRE 2 CONECT
*DELETE,4DFR,3332
CONECT 1295 1294 1296 1300
*DELETE,4DFR,3334
CONECT 1297 1298 1302 1303
*DELETE,4DFR,3337
CONECT 1300 1295 1299 1301
*DELETE,4DFR,3340
CONECT 1303 1297 1304 1305
*DELETE,4DFR,3343
CONECT 1306 1305 1307 1310
*DELETE,4DFR,3374
CONECT 2853 2852 2854 2858
*DELETE,4DFR,3376
CONECT 2855 2856 2860 2861
*DELETE,4DFR,3379
CONECT 2858 2853 2857 2859
*DELETE,4DFR,3382
CONECT 2861 2855 2862 2863
*DELETE,4DFRD,5
MASTER 147 8 5 8 16 24 16 9 3041 2 84 26

*IDENT,3CATD
*INSERT,3CATC,7
REMARK 10
REMARK 10 CORRECTION. THIS ENTRY IS OBSOLETE. 01-APR-85.
*INSERT,3CAT,3
OBSLTE 01-APR-85 3CAT 7CAT 8CAT
*INSERT,3CAT,6
REVDAT 5 01-APR-85 3CATD 3 OBSLTE
*DELETE,3CATC,8
MASTER 71 0 1 13 9 0 0 9 4029 0 43 39

ORDER 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 (January 1984)
 - Sources of Visual Aids for Macromolecular Structure (October 1984)
 - Atomic Coordinate and Bibliographic Entry Format Description for DATAPRTP and DATAPRFI (January 1985)
 - Current DATAPRTP Directory
 - Non-Standard Entries (Structure Factors) Format Description
 - NONST1TP and NONST1FI (April 1985)
 - NONST2TP and NONST2FI (July 1985)
 - NONST3TP and NONST3FI (July 1985)
 - Data Deposition form

3. Please send the following magnetic tape items (from Table 1). Each 1-tape item costs \$184 (£153 from Cambridge). Each 2-tape item costs \$225 (£188). Each 3-tape item costs \$266 (£222). 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 |

All tapes are distributed in blocked form with fixed record length and block size. Brookhaven normally uses a block size of 4800 characters. Please indicate here any difficulties this might cause.

5. Please send the following microfiche items (from Table 2). Each microfiche item costs \$150 (£125), postage included. Correction fiche are free.

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

6. Please send the following printed listings. Each listing costs \$71 (£59), postage included.

<u>Ident Code (From Table 7)</u>	<u>Cost</u>
	Total _____

7. Foreign air mail postage for tapes from Brookhaven to destinations outside the U. S. and Canada or from Cambridge to destinations outside the United Kingdom. A postage surcharge of \$20 (£17) is required per item.

Number of items x \$20.00 (£17) = _____

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	_____

Method of Payment:

Cambridge: Cambridge prefers that no check is sent with order. Inclusion of purchase order is desirable but not mandatory.

Brookhaven: Brookhaven requires that either a check or written purchase order payable to Brookhaven National Laboratory be received before service is provided.

() check
() purchase order number _____
is () enclosed
() sent separately

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

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