

BROOKHAVEN NATIONAL LABORATORY

PROTEIN DATA BANK

NEWSLETTER

Number 5

November, 1977

We are pleased to announce that the National Science Foundation has extended funding of primary Protein Data Bank activities for three years, starting November 1, 1977. By virtue of this ongoing financial support, the Data Bank will be able to continue to expand services to our community of users. We also have a new distribution center, C.S.I.R.O. (Melbourne), which will take over distribution of data in Australia (see addresses below).

The Bank now includes a total of 84 atomic coordinate entries, seven of which have been added since distribution of the last issue of this Newsletter (Number 4, May 1977). A list of the coordinate holdings, with identification codes to be used in requesting data, is shown in Table 1. In addition, the Bank holds 15 sets of structure factors and phases. These are listed in Table 2, along with two additional non-standard entries containing torsion angle data.

A large number of minor revisions to the atomic coordinate data have been made since distribution of the last Newsletter. The most important revisions, which involve corrections of atomic coordinates or changes in secondary structure specifications, are given in Table 3. The full listing of revisions is too bulky to reproduce here, but is available on microfiche at no charge from Brookhaven. To order this listing, please check the appropriate box on the request form attached to this Newsletter. Most changes involve corrections of typographical errors, clarifications of remarks, etc.

At this time, we wish to emphasize the advantages of including structure factor-phase information in the Protein Data Bank. Preservation and dissemination of these primary crystallographic data are an important part of the Bank's archival function. Contributors are urged to deposit structure factor-phase data, for native structures and heavy-atom derivatives. Also, receipt of atomic coordinate data for hypothetical structures, based on energy calculations or model building, will be welcomed. The methods used to derive these data will be clearly identified, and the data will be distributed in the normal fashion.

A large part of the work necessary to make the Protein Data Bank bibliographic and sequence information available for interactive search has now been accomplished, thanks to funds provided by the National Institutes of Health. We hope that within three to six months, this portion of the file will be included as part of the NIH/EPA Chemical Information System on CYPHERNET (see *Science* 195, 253 (1977)). In order to adapt the protein file to this interactive system, certain stylistic changes have been made to the bibliographic data, and a few additional record types included. These minor changes already are reflected in the format of some of the newest atomic coordinate entries. A revised description of file record formats will be available shortly, and can be ordered by checking the appropriate box on the request form.

A communication describing the Protein Data Bank has recently been published in J. Mol. Biol. 112, 535 (1977).

Unfortunately, due to changes in Department of Energy accounting procedures and in order to cover a higher percentage of costs, it is necessary for Brookhaven to increase charges for distribution of data. These new charges, which are effective immediately, are detailed on the request form. At this writing, Melbourne and Tokyo have set no distribution charges, but Cambridge plans to implement a small charge in 1978. If you wish to receive data, please fill out the request form and mail it, together with a new 2400 foot reel of magnetic tape, to the appropriate center listed below. (Note: Brookhaven finds it convenient to supply a new tape for this purpose, and will do so for a small additional charge.) Users' comments and suggestions are always welcome.

AREA	ADDRESS OF CENTER	NAMES
The Americas	Chemistry Department Brookhaven National Laboratory Upton, New York 11973 USA	F. C. Bernstein (tel. 516-345-4382) T. F. Koetzle (tel. 516-345-4384) G.J.B. Williams (tel. 516-345-4383)
Europe and Worldwide	University Chemical Laboratory Lensfield Road Cambridge CB2 1EW, England	O. Kennard (tel. (0223)66499)
Australia	C.S.I.R.O. Division of Applied Organic Chemistry Box 4331 G.P.O. Melbourne, Victoria 3001 Australia	B. J. Poppleton
Japan	Department of Chemistry Faculty of Science The University of Tokyo Bunkyo-ku, Tokyo, Japan	M. Tasumi

TABLE 1. PROTEIN DATA BANK. ATOMIC COORDINATE HOLDINGS
87-NOV-77

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ STATUS	IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
IACT	*ACTINIDIN	E. BAKER	7/77	RIACTS	ACTINIDIN	E. BAKER	7/77 SF
2ADK	ADENYLATE KINASE (PORCINE MUSCLE)	G. SCHULZ	3/77 R	CHYHOP	ALPHA-CHYDROTRYPSIN (TOSYL)	D. BLOW	4/73 SF
1ADH	ALCOHOL DEHYDROGENASE (ADP-RIB)	C.-I. BRANDEN	8/76	RCARP04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
2ADH	ALCOHOL DEHYDROGENASE (TOOTHENCH)	C.-I. BRANDEN	8/76	RCARP05	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
1CPV	BALFOUR CYTOCHROME C (BALBACORE) ONLY IN CORE	M. MATTHEWS	2/77	RCYTB582	CYTOCOCHROME B5	F. S. HATHEWS	5/73 TA
2CPV	CALCIUM-BINDING PARVALBUMIN SET 6A	R. KRETSINGER	8/74	RTNUOK281	CYTOCOCHROME C (BALBACORE, OXIDIZED)	R. DICKERSON	5/76 SF
3CPV	CALCIUM-BINDING PARVALBUMIN SET 6B	R. KRETSINGER	8/74	RTNUOK282	CYTOCOCHROME C (BALBACORE, REDUCED)	R. DICKERSON	5/76 SF
ICAB	CARBONIC ANHYDRASE B (HUMAN)	K. KANMAN	6/76	RCYC558	CYTOCOCHROME C558	R. TIMKOVICH	4/76 SF
1CAR	CARBONIC ANHYDRASE C (HUMAN)	K. KANMAN	5/76	RGPDB4	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTRM)	M. ROSSMANN	8/75 SF
1CPA	CARBOXYPEPTIDASE A (BovINE)	V. LIPSCOMB	2/73	RHUMDEH02	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	5/75 SF
1CPB	*CARBOXYPEPTIDASE B (BovINE)	H. SCHMID, J. HERRIOTT	9/76 A	LAMPRT1	HEMOGLOBIN (LAHPREY)	H. HENRICKSON, LOVE, KARLE	5/75 SF
2CRA	ALPHA-CHYDROTRYPSIN (TOSVL)	D. BLOW	1/75 R	RLDH02	LACTATE DEHYDROGENASE	M. ROSSMANN	8/75 SF
3CRA	ALPHA-CHYDROTRYPSIN	F. ULINSKY	8/75	RLDH03	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	8/75 SF
1GCH	GAAMA-CHYDROTRYPSIN	A. COHEN, JAMES, SILVERTON	2/77	RHETHYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76 SF
1GCH	GAAMA-CHYDROTRYPSIN	J. KAUT, J. BIRKTOFT	3/75	ROEYNSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76 SF
2CMA	CONCANAVALIN A	REEKS, BECKER, EDELMAN	4/75	RRUBYB2	RUBREDOXIN	L. JENSEN	3/74 SF
3CMA	CONCANAVALIN A	K. HARDMAN	9/76 R	TORSNAW1	TORSION ANGLES (11 PROTEINS)	T. WU, E. KABAT	5/73 TA
1BEC	CYTOCOCHROME B5	F. S. MATHEWS	8/72 D				
1CYT	CYTOCOCHROME C (BALBACORE, OXIDIZED)	R. DICKERSON	9/76				
2CYT	CYTOCOCHROME C (BALBACORE, REDUCED)	R. DICKERSON	9/76				
1CYC	CYTOCOCHROME C (BONITO, HEART)	M. KAKUDO	8/76				
1C2C	CYTOCOCHROME C2	J. KRAUT	3/73				
1M5C	CYTOCOCHROME C558	R. TIMKOVICH	8/76				
TEST	ELASTASE (PORCINE, TOSVL)	H. WATSON	5/76				
IF04	FERRODOXIN	ADAMSON, SIEKER, JENSEN	8/76				
1LHN	FLAVOPORPHIN (CLOSTRIDIUM MP, OXIDIZED)	M. LUDWIG	10/77 N				
2FXN	*FLAVOPORPHIN (CLOSTRIDIUM MP, REDUCED)	M. LUDWIG	10/77 N				
ICGN	*GLUCAGON	T. BLUNDELL	10/77 N				
1PGI	*GLUCOSE-6-PHOSPHATE ISOMERASE	H. MURHEAD	7/77				
1GP0	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTRM)	M. ROSSMANN	7/75				
2MHB	HEMOGLOBIN (HORSE, AQUO MET)	LAADER, HEITNER, PERUTZ	2/77 R				
2DHB	HEMOGLOBIN (HORSE, DEOXY)	M. PERUTZ, G. FERMI	1/73				
1HHB	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	4/75				
1FDH	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	J. PRIER	8/75				
1LHM	HEMOGLOBIN (HUMAN, FETAL, DEOXY)	H. HENRICKSON, LOVE, KARLE	3/73				
1HDX	HEMOGLOBIN (YEAST) FORM BIII	T. STEITZ	9/76 B				
1HIP	HIGH POTENTIAL IRON PROTEIN	J. KRAUT	4/75				
1FAB	IMMUNOGLOBULIN FAB' (NEW)	R. POLJAK	8/75				
1REI	IMMUNOGLOBULIN B-3 J FRAGMENT REI	O. EPP, R. HUBER	3/76				
4LDH	LACTATE DEHYDROGENASE	V. EVENTOFF, H. ROSSMANN	4/77 R				
3LDH	LACTATE DEHYDROGENASE/NAD/PYRUVATE	M. ROSSMANN	11/74 D				
1LZM	LYSODZYME (BACTERIOPHAGE TA)	B. MATTHEWS	3/77				
1LYZ	LYSODZYME (HEN EGG-WHITE, SET W2)	R. DIAMOND, D. PHILLIPS	2/75				
2LYZ	LYSODZYME (HEN EGG-WHITE, SET R5D)	R. DIAMOND, D. PHILLIPS	2/75				
3LYZ	LYSODZYME (HEN EGG-WHITE, SET R5A)	R. DIAMOND, D. PHILLIPS	2/75				
4LYZ	LYSODZYME (HEN EGG-WHITE, SET R5B)	R. DIAMOND, D. PHILLIPS	2/75				
5LYZ	LYSODZYME (HEN EGG-WHITE, SET RS12A)	R. DIAMOND, D. PHILLIPS	2/75				
6LYZ	LYSODZYME (HEN EGG-WHITE, SET RS16A)	R. DIAMOND, D. PHILLIPS	2/75				
7LYZ	LYSODZYME (HEN EGG-WHITE, TRICLINIC)	A. YOHATH	5/77				
8LYZ	*LYSODZYME (HEN EGG-WHITE, INACTIVATED)	S. OATLEY	9/77				
1MDH	MALATE DEHYDROGENASE	L. BANASZAK	6/76 A				
1HMB	MYOGLOBIN (SPERM WHALE, MET)	H. WATSON	4/73				
2HMB	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	9/76				
3HMB	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	9/76				
8PAP	PAAPAIN, NATIVE	J. DRENTH	11/76 R				
1PAP	PAAPAIN (ACE-ALA-ALA-PHE-ALA, CYS-25)	J. DRENTH	11/76 R				
2PAP	PAAPAIN (INTERFERON OF CYS-25)	J. DRENTH	11/76 R				
3PAP	PAAPAIN (OXIDIZED CYS-25)	J. DRENTH	11/76 R				
4PAP	PAAPAIN (TOS-LYS, CYS-25)	J. DRENTH	11/76 R				
5PAP	PAAPAIN (B2OXY-GLY-PHE-GLY, CYS-25)	J. DRENTH	11/76 R				
6PAP	PAAPAIN (B2OXY-PHE-ALA, CYS-25)	J. DRENTH	11/76 R				
1PGK	PHOSPHOGLYCERATE KINASE (YEAST)	H. WATSON	5/76 A				
2PGK	PHOSPHOGLYCERATE KINASE (HORSE)	P. EVANS, C. BLAKE	9/76 B				
2PAB	*PREALBUMIN (HUMAN, PLASMA)	S. OATLEY, C. BLAKE	9/77 R				
1RNS	RIBONUCLEASE S	H. WYCKOFF, F. RICHARDS	4/75				
1RNS	STREPTOCOCCAL NUCLEASE	F. A. COTTON, E. HAZEN	4/73				
1SGC	STREPTOTHYME GRISSEUS PROTEINASE B	M. JAMES	5/76 A				
1SBT	SUBTILISIN BPM'	J. KRAUT	8/72				
2SBT	SUBTILISIN NOVO	J. DRENTH	9/76				
1SDO	SUPEROXIDE DISMUTASE	J. AND D. RICHARDSON	8/75 A				
1TLN	Thermolysin (UNREFINED)	B. MATTHEWS	4/75				
2TLN	Thermolysin (REFINED)	B. MATTHEWS	4/75				
1SRX	THIOREDOKIN (OXIDIZED)	B.-O. SODERBERG	5/76 A				
1TNA	TRANSFER RNA (YEAST, PHE)	J. SOISSANT, S.-H. KIM	12/75				
2TNA	TRANSFER RNA (YEAST, PHE)	M. SUNDARAMURTHY	5/76 D				
3TNA	TRANSFER RNA (YEAST, PHE)	JACK, LADNER, KLUK	2/77				
1TPH	TAURINE PHOSPHATE ISOMERASE	J. WILSON, D. PHILLIPS	9/76				
1PTN	TRYPsin (NATIVE, PH9)	FEHLHAMMER, BODE, SCHWAGER	1/77				
2PTB	TRYPsin(BENZAMIDINE INHIBITED, PH7)	FEHLHAMMER, BODE, SCHWAGER	1/77				
1PTC	TRYPsin/TRYPsin INHIBITOR COMPLEX	R. HUBER, V. BODE	11/76				
3PTI	TRYPsin INHIBITOR (BovINE, PANCREAS)	R. HUBER, J. DEISENHOFER	11/76				
2PTP	TRYPsin (DIP INHIBITED)	J. CHAMBERS, R. STROUD	4/77				

* NEW OR REPLACEMENT ENTRY SINCE LAST NEWSLETTER (MAY/77)

STATUS CODES

BLANK	STANDARD ENTRY AVAILABLE FOR DISTRIBUTION
A	ALPHA CARBON ATOMS ONLY
B	BACKBONE ONLY
D	NEW DATA HAS BEEN PROMISED
H	NEW ENTRY WITH DEPOSITOR FOR APPROVAL
P	IN PREPARATION
R	REPLACES AN OUT-OF-DATE PARAMETER SET

TABLE 2. PROTEIN DATA BANK NON-STANDARD ENTRIES

86-NOV-77

IDENT CODE	MOLECULE	DEPOSITOR	DATE/ CODE
RIACTS	ACTINIDIN	E. BAKER	7/77 SF
CHYHOP	ALPHA-CHYDROTRYPSIN (TOSYL)	D. BLOW	4/73 SF
RCARP04	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCARP05	CALCIUM-BINDING PARVALBUMIN	R. KRETSINGER	2/74 SF
RCYTB582	CYTOCOCHROME B5	F. S. HATHEWS	5/75 SF
RTNUOK281	CYTOCOCHROME C (BALBACORE, OXIDIZED)	R. DICKERSON	5/76 SF
RTNUOK282	CYTOCOCHROME C (BALBACORE, REDUCED)	R. DICKERSON	5/76 SF
RCYC558	CYTOCOCHROME C558	R. TIMKOVICH	4/76 SF
RGPDB4	GLYCERALDEHYDE-3-P-DEHYDROGENASE (LOBSTRM)	M. ROSSMANN	8/75 SF
RHUMDEH02	HEMOGLOBIN (HUMAN, DEOXY)	M. PERUTZ, G. FERMI	5/75 SF
LAMPRT1	HEMOGLOBIN (LAHPREY)	H. HENRICKSON, LOVE, KARLE	5/75 SF
RLDH02	LACTATE DEHYDROGENASE	M. ROSSMANN	8/75 SF
RHETHYSF1	MYOGLOBIN (SPERM WHALE, MET)	T. TAKANO	6/76 SF
ROEYNSF1	MYOGLOBIN (SPERM WHALE, DEOXY)	T. TAKANO	6/76 SF
RRUBYB2	RUBREDOXIN	L. JENSEN	3/74 SF
TORSNAW1	TORSION ANGLES (11 PROTEINS)	T. WU, E. KABAT	5/73 TA

*NOTE: IN SOME CASES, MORE RECENT TORSION ANGLES THAN THOSE CONTAINED IN THE ABOVE ENTRIES MAY BE CALCULATED FROM THE APPROPRIATE ATOMIC COORDINATE ENTRIES LISTED IN TABLE 1.

TABLE 3. SUBSTANTIVE CORRECTIONS TO PROTEIN DATA BANK ENTRIES

*DELETE, ICAB, 91, B8	HELIX 1 T1 TRP 16 TVR 28	1 CONIGUOUS WITH HELIX B
INSERT, ICABA, 3	1 INSERT, ICABA, 3	5 CONIGUOUS WITH HELIX A
REVERSE, 7	7 REVERSE THEIR ORDER FOR ALL THR RESIDUES. INTERLEAVE	
REMARK, 7	7 CORRECTION. CHANGE ATOM NAME CD TO CD1 FOR ALL ILE	
REMARK, 7	7 RESIDUES. CHANGE ATOM NAMES CG TO OC1 AND CG TO CG2 AND	
REMARK, 7	7 REVERSE THEIR ORDER FOR ALL THR RESIDUES. INTERLEAVE	
REMARK, 7	7 ALTERNATE POSITION ATOMS IN RESIDUES 94, 182,	
REMARK, 7	7 CORRECT RESIDUE NAMING ON HELIX, SHEET, TURN CARDS.	
REMARK, 7	7 CORRECT VECTOR PORTION OF SCALE MATRIX. 23-AUG-77.	
*DELETE, ICAB, 91, B8	HELIX 1 T1 ASP 16 TVR 28	1 CONIGUOUS WITH HELIX E1
SCALE1	S.000000 .B12278 .B000000	.B000000 .B000000
SCALE2	S.000000 .B13598 .B000000	.B000000 .B000000
SCALE3	S.000000 .B026958 .B000000	.B000000 .B000000
*DELETE, ICAB, 251	ATOM 185 CD1 ILE 22	29.857 .26.365 -28.410 1.00 8.00
ATOM	255 OG1 THR 33	29.943 22.347 -.430 1.00 8.00
*DELETE, ICAB, 329	ATOM 265 OG1 THR 33	29.943 22.347 -.430 1.00 8.00
ATOM	275 OG1 THR 35	32.212 22.938 4.940 1.00 8.00
*DELETE, ICAB, 345	ATOM 279 CG2 THR 35	30.807 22.902 6.890 1.00 8.00
ATOM	279 OG1 THR 38	26.452 22.928 1.210 1.00 8.00
*DELETE, ICAB, 366, 367	ATOM 281 CG2 THR 38	25.561 23.162 3.340 1.00 8.00
ATOM	281 OG1 THR 38	26.452 22.928 1.210 1.00 8.00
*DELETE, ICAB, 408, 409	ATOM 334 OG1 THR 42	13.101 15.320 3.160 1.00 8.00
ATOM	334 CG2 THR 42	13.419 17.461 2.110 1.00 8.00
*DELETE, ICAB, 439	ATOM 371 CD1 ILE 47	26.450 19.124 -.5.630 1.00 8.00
ATOM	371 OG1 THR 55	31.181 -2.495 -17.340 1.00 8.00
*DELETE, ICAB, 456, 457	ATOM 404 OG1 THR 55	32.481 -.5.560 -17.930 1.00 8.00
ATOM	431 CG2 THR 55	32.481 -.5.560 -17.930 1.00 8.00
*DELETE, ICAB, 528		

(Table 3 continued)

ATOM	462	CD1	ILE	59	44.282	3.677	-19.118	1.88	8.88			
*DELETE,ICAB.596												
ATOM	478	CD1	ILE	68	43.116	6.189	-26.598	1.88	8.88			
*DELETE,ICAB.818,827												
ATOM	744	H	BHIS	94	38.647	18.671	-14.498	.58	8.88			
ATOM	745	CA	AHIS	94	39.928	11.412	-14.678	.58	8.88			
ATOM	746	CB	AHIS	94	39.938	11.364	-14.618	.58	8.88			
ATOM	747	C	AHIS	94	40.869	12.418	-13.538	.58	8.88			
ATOM	748	O	BHIS	94	40.126	12.395	-13.498	.58	8.88			
ATOM	749	O	AHIS	94	39.698	12.731	-12.828	.58	8.88			
ATOM	750	O	BHIS	94	39.154	12.828	-12.658	.58	8.88			
ATOM	751	CB	AHIS	94	39.936	12.895	-16.848	.58	8.88			
ATOM	752	CB	BHIS	94	40.867	12.848	-16.978	.58	8.88			
ATOM	753	CG	BHIS	94	39.698	13.322	-16.158	.58	8.88			
ATOM	754	CG	BHIS	94	39.137	13.272	-16.118	.58	8.88			
ATOM	755	N	ND1BHIS	94	38.619	14.888	-15.638	.58	8.88			
ATOM	756	N	ND1BHIS	94	38.654	13.965	-15.818	.58	8.88			
ATOM	757	CO2AHIS	94	38.581	13.981	-17.238	.58	8.88				
ATOM	758	CD2BHIS	94	38.641	13.985	-17.218	.58	8.88				
ATOM	759	CE1AHIS	94	37.978	15.815	-15.448	.58	8.88				
ATOM	760	CE2AHIS	94	37.984	14.962	-15.448	.58	8.88				
ATOM	761	N	CAZAHIS	94	37.865	15.832	-16.758	.58	8.88			
*DELETE,ICAB.879,888												
ATOM	812	OGL	THR	188	58.863	23.365	-6.888	1.88	8.88			
ATOM	814	CG2	THR	188	53.944	24.379	-6.888	1.88	8.88			
*DELETE,ICAB.942,943												
ATOM	875	OGL	THR	188	26.946	26.119	-4.198	1.88	8.88			
ATOM	877	CG2	THR	188	38.717	25.345	-5.628	1.88	8.88			
*DELETE,ICAB.1280												
ATOM	1142	CD1	ILE	144	32.934	11.821	-5.588	1.88	8.88			
*DELETE,ICAB.1377												
ATOM	1311	CD1	ILE	167	47.948	7.288	-21.278	1.88	8.88			
*DELETE,ICAB.1382,1393												
ATOM	1326	OGL	THR	169	53.886	8.759	-27.548	1.88	8.88			
ATOM	1327	CG2	THR	169	55.152	9.628	-26.668	1.88	8.88			
*DELETE,ICAB.1455,1456												
ATOM	1389	OGL	THR	177	44.855	-5.611	-18.788	1.88	8.88			
ATOM	1398	CG2	THR	177	42.814	-7.877	-28.158	1.88	8.88			
*DELETE,ICAB.1492,1501												
ATOM	1426	N	BSER	182	35.568	1.628	-8.568	.58	8.88			
ATOM	1427	CA	ASER	182	35.893	1.695	-7.398	.58	8.88			
ATOM	1428	CA	BSER	182	35.859	1.692	-7.188	.58	8.88			
ATOM	1429	C	ASER	182	36.281	1.568	-6.418	.58	8.88			
ATOM	1430	C	BSER	182	36.333	1.575	-6.348	.58	8.88			
ATOM	1431	O	ASER	182	36.161	1.974	-5.248	.58	8.88			
ATOM	1432	O	BSER	182	36.361	1.978	-5.179	.58	8.88			
ATOM	1433	CB	ASER	182	34.129	.555	-7.148	.58	8.88			
ATOM	1434	CB	BSER	182	34.866	.579	-6.928	.58	8.88			
ATOM	1435	OC	ASER	182	33.521	.564	-5.819	.58	8.88			
*DELETE,ICAB.1588,1599												
ATOM	1442	OGL	THR	183	38.774	-7.767	-7.948	1.88	8.88			
ATOM	1443	CG2	THR	183	49.721	-5.577	-6.548	1.88	8.88			
*DELETE,ICAB.1591,1592												
ATOM	1525	OGL	THR	193	24.343	17.524	-7.228	1.88	8.88			
ATOM	1526	CG2	THR	193	23.646	17.322	-4.938	1.88	8.88			
*DELETE,ICAB.1635,1636												
ATOM	1569	OGL	THR	199	36.684	28.176	-15.418	1.88	8.88			
ATOM	1578	CG2	THR	199	38.595	21.515	-15.788	1.88	8.88			
*DELETE,ICAB.1788,1789												
ATOM	1642	OGL	THR	288	23.367	16.893	-13.288	1.88	8.88			
ATOM	1643	CG2	THR	288	23.525	16.167	-10.998	1.88	8.88			
*DELETE,ICAB.1731												
ATOM	1665	CD1	ILE	218	25.873	14.265	-6.358	1.88	8.88			
*DELETE,ICAB.1739												
ATOM	1673	CD1	ILE	211	32.666	19.487	-3.828	1.88	8.88			
*DELETE,ICAB.1777												
ATOM	1711	CD1	ILE	216	41.615	9.661	-4.778	1.88	8.88			
*DELETE,ICAB.2022,2023												
ATOM	1956	OGL	THR	248	38.811	28.732	-8.368	1.88	8.88			
ATOM	1957	CG2	THR	248	36.571	28.855	-7.798	1.88	8.88			
*DELETE,ICAB.2877,2878												
ATOM	2011	OGL	THR	255	21.965	25.861	-2.878	1.88	8.88			
ATOM	2012	CG2	THR	255	20.859	24.987	-4.788	1.88	8.88			
*DELETE,ICABA.4												
MASTER	32	18	1	7	18	11	8	6	2824	1	5	21

*IDENT,ICVCC												
*INSERT,ICVCB.2												
REMARK	7											
REMARK	7	CORRECTION. CORRECT COORDINATES OF ATOMS 178-182,271,287.										
REMARK	7	699,718. 89-SEP-77.										
*DELETE,ICVC.222,226												
ATOM	178	CB	LVS	25	-26.241	-4.433	11.819	1.88	8.88			
ATOM	179	CG	LVS	25	-25.296	-4.496	18.433	1.88	8.88			
ATOM	180	CD	LVS	25	-24.918	-5.819	9.893	1.88	8.88			
ATOM	181	CE	LVS	25	-23.784	-5.819	8.543	1.88	8.88			
ATOM	182	NZ	LVS	25	-23.668	-6.827	7.661	1.88	8.88			
*DELETE,ICVC.315												
ATOM	271	CE2	PHE	36	-23.658	15.897	9.551	1.88	8.88			
*DELETE,ICVC.331												
ATOM	287	NH2	ARG	38	-25.485	8.797	15.851	1.88	8.88			
*DELETE,ICVC.741												
ATOM	699	DE2	GLU	98	-6.278	11.569	2.243	1.88	8.88			
*DELETE,ICVC.752												
ATOM	718	NH2	ARG	91	-7.538	21.145	5.519	1.88	8.88			
*DELETE,ICVCB.4												
MASTER	23	8	1	5	8	3	8	9	839	1	48	8

*IDENT,ICVTC												
*INSERT,ICVTC.5												
REMARK	18											
REMARK	18	CORRECTION. FIX R(2,2) TERM OF MTRIX TRANSFORMATION.										
REMARK	18	89-SEP-77.										
*DELETE,ICVTA.8												
MTRIX2	1	0.988178	-0.418688	0.082888	-17.993888							
*DELETE,ICVTC.8												
MASTER	52	8	2	18	8	18	8	9	1682	2	95	16

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 ATOMIC COORDINATE 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 583425824, 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 73-88 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 'IMBN1' FOR THE (CHRONOLOGICALLY) FIRST CORRECTION TO DECK 'IMBN' FOR SPERM-WHALE MYOGLOBIN. 'IMBN8' 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.

REQUEST FORM

1. Name: _____ Date: _____
Address: _____ Telephone: _____

2. Send the following information (please check):

- () all current coordinate entries
() parameter sets listed (complete 3. below)
() description of file record formats
() list of revisions on microfiche

3. Parameter sets requested (by ident code please):

4. Tape: I am sending a new 2400 foot reel of magnetic tape () yes () no.

5. Tape format desired:

- () 7 track () 556 bpi () ASCII () Unlabelled (preferred)
() 9 track () 800 bpi () BCD () Labelled-user's label
() 1600 bpi () EBCDIC _____ retained

Tape copies are normally blocked since otherwise the entire contents will not fit on a 2400 foot reel of tape. Indicate the maximum block size allowed if blocks of 5120 characters (bytes) cannot be handled,

Please complete reverse side.

REQUEST FORM

6. Charge (Brookhaven requests only)	Enter Amount
A. Data preparation (unit charge per magnetic tape)	\$ _____
U. S. Department of Energy	\$40.25 ()
Other U. S. Federal Agencies	\$47.45 ()
All others	\$51.00 ()
B. Magnetic tape	\$ 8.59 () \$ _____
(please check if answer to 4. above was <u>NO</u>)	
C. Postage	\$ _____
U. S. and Canada	\$ 2.00 ()
Air Mail to other countries	\$17.00 ()
D. Total charge (A + B + C)	\$ _____
E. Payment to the order of Brookhaven National Laboratory	
by () check	is () enclosed
() purchase order number _____	() sent separately

Mail this completed form to the appropriate center (Brookhaven, Cambridge, Melbourne or Tokyo) at the address listed in the body of the Newsletter.

It is expected that the Protein Data Bank be acknowledged in publications which result from work making use of the Bank's services. We would appreciate receiving reprints of any such publications.