Brookhaven National Laboratory

Protein Data Bank

Newsletter

The Protein Data Bank continues to grow. During the past year we distributed 375 data sets to 31 laboratories. These figures do not include data distributed outside North America by the Crystallographic Data Centre in Cambridge, England. The Bank is now supported by a grant from the NSF molecular biology division, so for the moment at least we are financially secure. We are currently in the process of converting all atomic coordinate files to a compact 80-column card image format. This new format will include many improvements, such as ordering of atoms in a totally standard fashion, and inclusion of atom connectivities where these are not completely specified by the primary structure.   Details of the new format will be announced in the next newsletter. In the meantime, atomic coordinate data will continue to be available in the 132-column "Diamond-like" format.

A pre-addressed form has been enclosed for your use to help us keep our mailing list current. This form must be returned if you wish to remain on the mailing list. Please note any address corrections where appropriate. On the back of the form we have included space to be filled in if you wish to request data from the Data Bank.

Data Distribution

To obtain data from the Bank, please fill out the enclosed request form and send a new 2400' reel of magnetic tape to

T. F. Koetzle
Chemistry Department
Brookhaven National Laboratory
Upton, New York 11973
Tel: 516-345-4384

Individuals with a computing account at Brookhaven may extract atomic coordinates from the Bank using program SEARCH, as outlined in the first newsletter (September, 1974). Up-to-date documentation on use of the Brookhaven computing system is available upon request.

Data Deposition

New coordinate sets received will be processed directly into the 80-column format. Persons wishing to deposit data should contact T. Koetzle to obtain deposition forms.

Macromolecules available in old format

Protein	Investigators	Holdings[a]
Carboxypeptidase A (bovine)	W. N. Lipscomb	AC
α-Chymotrypsin (bovine)	D. M. Blow	AC,TA,SF
Chymotrypsinogen (bovine)	J. Kraut	AC
Concanavalin A (jack bean)	G. M. Edelman	AC,TA
	K. D. Hardman	AC
Cu,Zn Superoxide dismutase (bovine)	D.&J. Richardson	AC
Cytochrome b_5 (calf liver)	F. S. Mathews	AC,TA
Cytochrome c_2 (R. rubrum)	J. Kraut	AC
D-Glyceraldehyde-3-Phosphate dehydrogenase (lobster)	M. G. Rossmann	AC,TA
Flavodoxin (clostridium MP)	M. L. Ludwig	AC,TA
Hemoglobin (horse oxy, deoxy; human deoxy)	M. F. Perutz	AC,TA
Hemoglobin (sea lamprey)	W. E. Love	AC,TA,SF
High Potential Iron Protein (chromatium)	J. Kraut	AC
Lactate dehydrogenase (dog fish)	M. G. Rossmann	AC,TA
Lysozyme (hen egg white)	R. Diamond	AC,TA
	D. C. Phillips	
Myogen (carp)	R. H. Kretsinger	AC,SF
Myoglobin (sperm whale)	J. C. Kendrew	AC
	H. C. Watson	
Nuclease (S. aureus)	F. A. Cotton	AC
Pancreatic Trypsin Inhibitor (bovine)	R. Huber	AC,TA
Papain (papaya latex)	J. Drenth	AC,TA
Ribonuclease-S (bovine)	F. M. Richards	AC
	H. W. Wyckoff	
Rubredoxin (C. pasteurianum)	L. H. Jensen	AC,SF
Subtilisin BPN' (B. amylolique faciens)	J. Kraut	AC
Thermolysin (B. thermoproteolyticus)	B. W. Matthews	AC

[a]AC - atomic coordinates; TA - torsion angles; SF - structure factors and phases.

Programs available

None are currently available.

I wish to remain on the Protein Data Bank mailing list. Please note any address correction above.

Fold 1

Dr. T. F. Koetzle
Chemistry Department
Brookhaven National Laboratory
Upton, New York   11973

Fold 2

PROTEIN DATA BANK REQUEST

Name:

Address:
  (and telephone)

Please send,
                (i)   all current parameter sets   ____
                (ii)   the parameter sets listed   ____
                (iii) all available PDB programs   ____
                (iv)   the programs listed below   ____

      Out-of-date parameter sets are not distributed unless specifically
requested. Parameter sets and programs obtained from the Data Bank are not
to be used for purposes involving financial gain to the recipient or his
institution.

      A NEW 2400' reel of magnetic tape which I would like written

          ____ 7 track   , ____ 9 track
          ____ 556 bpi   , ____ 800 bpi ,   ____ 1600 bpi (9 track only)
          ____ EBCDIC   , ____ ASCII   ,   ____ BCD
          ____ Unlabelled , ____ Labelled (User's label _____ retained)
   is   ____ Enclosed   , ____ Sent Separately

      Tapes are normally blocked because the entire Protein Data Bank will not
fit on one unblocked tape.   ____   Check here if blocked tapes cannot be handled.

Parameter Sets Requested

Programs Requested