18.5–6 REAL-TIME DOCKING SYSTEM FOR ANALYSIS OF ENZYME-SUBSTRATE INTERACTIONS. By A.Metcalfe*+, D.M. Blow*,& W.V.Wright+@, *Biophysics Group, Blackett Laboratory, Imperial College, London SW7 2BZ and +IBM UK Scientific Centre, Athelstan House, St Clement St, Winchester SO23 9UT, England.

The forces acting between an enzyme and another molecule regarded as a substrate are modelled as follows :
1. Electrostatic interactions between charged groups;
2. Hydrogen bond interactions using potential function of Levitt (J.Mol.Biol.168,595:1983);
3. Van der Waals' interactions using potential functions of Levitt (loc.cit);
4. Entropic 'hydrophobic' effects assumed proportional to solvent-accessible area. A correction is included for molecular surface associated with hydrophilic groups.

In calculation, enzyme and substrate are considered rigid bodies, and only forces acting between enzyme and substrate molecules are considered. The force and couple acting on the substrate are evaluated on demand, and the substrate can move under these forces, or an additional steering force and couple can be imposed by the operator. No system for relaxation of conformation of either molecule is included within this system.
Forces are computed on an IBM 4341 and the interacting molecules are displayed through the Winchester Graphics System, which allows control of viewpoint, scale and viewport clipping. Overall force and couple are displayed, and the strongest interactions of each type may be identified.
The system has been used to study enzyme-substrate interactions in cases where accurate coordinates are known from crystallography, as a preliminary to hypothetical docking experiments.
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18.6–1 SHELX-84: A PROGRAM SYSTEM FOR CRYSTAL STRUCTURE SOLUTION AND REFINEMENT. By George Sheldrick, Anorganisch-Chemisches Institut der Universität, Tammannstraße 4, D-3400 Göttingen, F.R.G.

It is hoped to release at least part of SHELX-84, the successor to the widely used SHELX-76 program for mainframe computers, at the Hamburg I.U.Cr. Meeting.

In addition to random-start numerical multisolution direct methods, the structure solution part includes E-normalisation and statistics, Fouriers, Peak-search and unique molecule assembly, and a variety of options for partial structure expansion. A number of computational aids to Patterson interpretation have been added, including derivation of heavy atom co-ordinates consistent with the Harker sections, heavy-atom refinement and a minimum-function correlation table for analysis of pseudo-symmetry problems. Both the Patterson and the direct methods routines have already been employed successfully for the location of heavy atoms from protein isomorphous delta(F) data.

The structure refinement part extends the constraints (e.g. rigid groups) and restraints (e.g. bond lengths) used in SHELX-76, and includes flexible automatic matrix blocking, and refinement of absorption, extinction, twin, and absolute configuration parameters. Preparation of tables and compliance with the requirements of Acta Cryst. have been simplified, and a number of features have been automated, e.g. choice of asymmetric unit for Fourier calculations, $U_{(ij)}$ constraints for special positions, generation of hydrogen atoms, setting up bond length constraints.

SHELX-84 provides more or less the same facilities as the program "X" in the mini-computer SHELXTL package; it is *not* intended to incorporate other facilities of SHELXTL such as molecular graphics.

SHELX-84 is written in a very simple subset of FORTRAN in the same inimitable style as SHELX-76. It may be run on a wide variety of 32(or more)-bit computers without significant alteration. All routines are valid for all space groups, in conventional settings or otherwise. Storage is allocated dynamically using large single dimension array which resides in blank common, so that there are *no restrictions* on the *number* of reflections, phase relations, scattering factor types, atoms, constraints, restraints, twin components, Fourier peaks, etc. which can be processed. This technique is particularly suitable for virtual memory machines, but is *not compatible with 16-bit micro- and mini-computers.* The program has been designed to be easy to use, with extensive use of default settings which may be changed, if necessary, by experienced users. For example a routine direct methods job requires only the title, cell, symmetry and approximate cell contents, followed by the four-letter word 'TREF'; the corresponding Patterson analysis is initiated by the word 'PATT'.

18.6–2 A MICRO-COMPUTER PROGRAM TO DETECT HIGHER LATTICE SYMMETRY. By A. Mugnoli, Istituto di Chimica Fisica, Università di Genova, Corso Europa, I-16132 Genova, Italy.

Measurement of lattice parameters by an automatic diffractometer can lead to an unsuitable unit cell: sometimes a higher symmetry has been overlooked (Herbstein & Marsh, Acta Cryst.(1982) B38, 1051; Davies, Kopf & Weiss, Acta Cryst. (1982) B38, 2251). The present program NEWLAT performs a further metrical test of the results given by our diffractometer and is routinely used in this Institute.

The program adopts the B-matrix algorithm by Santoro, Mighell & Rodgers (Acta Cryst. (1980) A36, 796). Starting from a given unit cell, new cells are generated, distributed in crystal systems and sorted according to a figure of merit. Tolerances on lattice parameters may be input or assumed as default values. For each solution the output gives the new cell parameters, the transformation matrix for the input unit cell and a figure of merit. As recommended by Clegg (Acta Cryst.(1981) A37, 913) a list of couples of nearly orthogonal vectors is also obtained along with angles between all the vectors perpendicular to a given one.

NEWLAT has been tested on several published cases of lately recognized higher symmetry; it always has lead to the correct crystal system. The program is written in Fortran IV language and runs on a Micro PDP-11 computer.