The three independent refinements show that non-equivalence has developed in the moderate and the free refinements (Fig. 2). Like the free refinement, the moderate has non-equivalence in the side chains of the exterior of the molecule and the dimer interface residues but shows excellent equivalence for the main-chain folding and shows the same general trends observed for the free refinement (Fig. 2). Comparison of the r.m.s. deviations of Fig. 2 shows that most of the large deviations of the free refinement also occur in that of the moderate whereas the unrealistically severe equivalence restraint of the tight refinement (4 × less than expected error) was sufficient to suppress all indications of non-equivalence. Moreover, the decrease in non-equivalence was accomplished at the apparent expense of only increasing the R factor slightly (about 2%) and with the loss of some solvent structure.

In cases of non-crystallographic symmetry involving high quality diffraction data, restraining the equivalence drastically could be counter-productive and curtail indications of non-equivalence. Since it is clear that equivalence can be retained with accurate data without an external restraint (Blevins & Tulinsky, 1985*a*, *b*), a more relaxed approach would seem prudent. However, there may be certain advantages to restraining non-crystallographic symmetry with lower-order data or in the low-order refinement of more extensive data because non-equivalence develops sluggishly under such circumstances (Cohen, Matthews & Davies, 1970). In the present case it developed decisively at 2·8 Å resolution.

Finally, the routine application of restrained least squares without examining electron density maps is obviously artificial and will necessarily produce limited results in non-equivalence and an appropriate mix of the two is the correct way to proceed. Non-equivalent changes introduced from maps can be easily accommodated in *PROLSQ* along with a decrease in equivalence restraints since the program calculates using all the atoms in the asymmetric unit. Thus, refinement utilizing non-crystallographic symmetry is no faster (computer-time per cycle) than refining the complete asymmetric unit without a symmetry restraint and the resulting phase angles are not those of a symmetrical molecule; however, such a refinement does give the transformation between related molecules and deviations thereof from average coordinates. Even with an averaged structure, if the phases are assigned to observed amplitudes of a non-equivalent structure, the resulting electron density will show non-equivalence. Such was the case for the tight refinement.

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Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Acta Cryst. (1986). B**42**, 200

Crystal structure analysis: A primer. 2nd ed. By J. P. GLUSKER and K. N. TRUEBLOOD. Pp. xviii + 269. Oxford University Press, 1985. Price hardback £29.00, US $37.50; softback £17.00, US $18.95.

The first edition of this text came out 13 years ago in 1972, and was reviewed then by J. L. Lawrence [*Acta Cryst.* (1972), A**28**, 680], who concluded '... this book can be highly recommended as an undergraduate text ... and ... to any scientist who desires an introduction to structure determination'. Now, in producing their second edition, the authors have made the book still better by updating and judiciously enlarging it. Almost every part has been affected, with modified or expanded text, new (extra) diagrams and photographs, such as the protein-crystal synchrotron-radiation diffraction photograph shown in the section on experimental methods. Direct methods and anomalous dispersion now have a chapter each; four-circle diffractometry is explained in detail, the glossary (a most valuable feature) has been doubled in size, and the index nearly doubled too. Of course, the price has more than doubled: the factor is about seven; but it is to be hoped that at least the paper cover version will nevertheless be within the reach of the students - to whom it is addressed.

One regret - which the authors will surely share. In the year of the award of a Nobel prize in the central core of this subject area, it is sad that this book, despite its 20-page 30-section annotated bibliography, just happens not to contain any reference to the papers, or the names, of Jerry Karle and Herbert Hauptman.

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