

MS29-04 Atomic shifts in unrestrained refinement can indicate alternative conformations. Oleg V. Sobolev, Vladimir Y. Lunin, *Institute of Mathematical Problems of Biology, Russian Academy of Sciences, Pushchino, Russia.*
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Unrestrained reciprocal space refinement is stable for the vast majority of atoms when working at atomic resolution. Nevertheless geometrical restraints should be held in refinement for residues that are present in several (alternative) conformations in the crystal used for the X-ray experiment; in the other case such residues deteriorate significantly. We believe that on the contrary, large distortion of a residue in unrestrained refinement may hint the presence of alternative conformations for this residue. To get these hints in a routine way we suggest two procedures that analyze amplitudes of atomic shifts resulted from several cycles of unrestrained refinement. A simple diagram plotting the values of atomic shifts against the residue number may give an idea of the crystallographic order of different parts of the structure at qualitative level. This approach was checked earlier by selective analysis of several structures [1] and has shown promising results. The second approach presents an automatic decision-making procedure that classifies each residue as ‘single conformation’ or ‘multiple conformations’. The procedure is based on the observation that single-conformation and alternative-conformations residues have different mobility in unrestrained refinement. The decision is made either by comparing the observed atomic shifts to a predetermined threshold, or by comparing probabilities of these shifts for residues possessing of single and multiple conformations.

A thorough analysis of 225 atomic resolution structures stored in PDB was conducted to study the mobility of different kinds of residues in unrestrained refinement. The analysis revealed different mobility of different kinds of atoms (*e.g.* ones in main and side chains, or atoms in the core and at the surface of the molecule). These distinctions were taken into account when constructing decision making procedures; the threshold values and probability distributions for atomic shifts were defined differently for different kinds of atoms.

The suggested decision making procedures may be considered as binary classification statistical tests. Standard statistical approaches were applied to evaluate their efficiency. All decision-making procedures have demonstrated approximately equal predictive power. The prediction was more precise for side chains than for main chains. The decision-making procedures based on analysis of atomic shifts were found to be more reliable than similar procedures based on ADP or density values calculated at atomic centers. This study has shown that atomic shifts in unrestrained refinement can be used to predict the residues which should probably have alternative conformations. This prediction may be useful to choose residues for most thoroughly check with electron density maps.

We developed several programs that implement plotting diagrams of atomic shifts and application of decision-making procedures. Their user-friendly versions will be available soon.

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MS29-05 Better data – proper redundancy
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It has repeatedly been demonstrated that high redundancy is a very desirable characteristic of data sets, leading to reduced statistical errors and ultimately more precise intensity information (a recent example is [1]). Consequently, average redundancy is a value usually supplied when diffraction data are reported. However, when space group symmetry is high and unit cells are small, which applies for many solid state compounds, this average number is misleading for reflections with a low number of symmetry equivalents. Examples are *P4/mmm* or *P6/mmm*, where a general reflection *hkl* has 16 or 24 equivalents, respectively, while *00l*-reflections only comprise two equivalent reflections. In a data set with a certain average redundancy, general reflections most likely have been observed many times more often than axial reflections, severely skewing redundancy distribution. Consequently, the intensity information of the axial reflections is based on very few values only and therefore less reliable. In order to achieve high redundancy for *each* reflection, not just the general ones, a data collection strategy program is required. Usually, diffractometer manufacturers include such a program with their packages. Beside these, a lot of software with that purpose has been developed over the last two decades [2-5]. The fact that development is still continuing [6] shows, that scientists are constantly facing new and unique problems which can not be solved using existing software. Unsatisfied with existing options, we developed a data collection strategy software which provides the possibility to take care of the „symmetry affected“ reflections mentioned above. The resulting software turned out to be rather flexible, providing the ability to use a very wide range of indicators beyond redundancy for strategy determination. The program is hardware independent and can easily be configured for use with different goniometers and detectors. Beyond strategy calculation it also contains tools for detailed analysis of measured diffraction data sets.

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