comprehensive implementation of the fundamentals of crystallography (symmetries, Fourier, scattering, etc). As the foundation of the macromolecular suite PHENIX, it has a certain connotation which is undeserved since the algorithms and data structures it features are correct for any crystal structure.

As part of the EPSRC grant "Age Concern" we developed a companion library, the Small Molecule Toolbox (smtbx). It shares the same philosophy as the cctbx: it is designed to make the writing of short scripts easy as well as to make it possible to build or to integrate it into large programs. It provides tools covering the whole workflow of small molecule work but we will focus on refinement in this talk.

The smtbx provides full matrix least-squares, restraints on bond lengths, angles, or dihedral angles, and special position constraints as well as the wealth of geometrical constraints available in ShelX; the both of merohedral and non-merohedral twin refinement; a solvent disorder modelling similar to the SQUEEZE procedure in PLATON.

More importantly, its modular and open design ease the addition of new features. We will present one such new tool to model water molecules.

[1] R. Grosse-Kunstleve et al, http://cctbx.sourceforge.net/

Keywords: refinement, full matrix, constraints

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On the refinement of routine single crystal X-ray data only to mimic single crystal neutron structural results

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In the case of organic compounds single crystal neutron diffraction is a source of reliable structural data particularly hydrogen atom positions and their ADPs. In consequence, neutron geometry of organic molecules is usually more reliable then single crystal X-ray diffraction structural data, although no doubt this is the X-ray diffraction technique which is by far the most popular among crystallographers to acquire structural information.

One can ask then a question whether it is possible to refine single crystal X-ray diffraction data only in such a way as to mimic the geometry of molecules obtained from single crystal neutron diffraction experiments.

In this contribution will present results of our analysis focused on comparison of structural neutron and X-ray results obtained for a series of five crystals of model compounds of increasing complexity and quality of data.

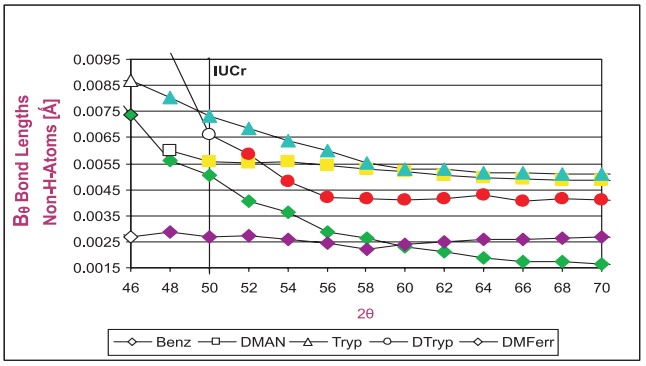

Fig. 1. Average differences between the neutron and X-ray bond lengths for the non-H-atoms obtained for a series of model compounds as a function of diffraction 2θ angle.

For each crystal, we have performed series of refinements as a function of resolution (sin θ/λ, in fact as a function of diffraction 2θ angle) using the neutron structural results as the reference ones. Will present a number of dependences of different parameters characterising the quality of X-ray data sets and average differences between particular neutron and X-ray structural parameters on 2θ diffraction angle. The results obtained influence understanding of benchmarks commonly accepted by IUCr and used in different checkcif programs, in particular 2θ limit equal to 50° for the MoKα X-ray radiation. One example of such a dependence is shown in figure below.

Keywords: neutron, X-ray, refinement

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On a method for the absolute scaling of refined atomic B factors

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The comparison of crystallographic models representing different functional and/or physical states of the same protein might seem easy if big conformational differences are detected by simple visual inspection. The precision of the models must be immediately considered if subtle structural changes are at play or if the aim is to evaluate small internal changes that occur in combination with for example large scale rigid-body changes. While the estimation of the positional uncertainty of crystallographic models has been extensively studied and a few methods have been developed to perform error-inclusive coordinate comparisons, the comparison of isotropic atomic B factors (Bi) has received less attention. One problem is to estimate standard uncertainties for refined Bi, but in addition, it is known that direct quantitative comparisons of Bi are flawed by several sources of model-specific variations (such as refinement strategies, data resolution, etc) ultimately contributing to a general scaling problem (inaccuracy). Precise and accurate comparison of Bi among several (frequently many) models would represent a rich source of information about dynamics and plasticity, often neglected in crystallographic approaches, despite the general acceptance of using Bi as a critical parameter in model refinement. The development of new methods to bring refined B factors to a common absolute scale would thus represent a genuine contribution, especially relevant to tackle the problem of "protein allostery without conformational change" (i.e. without a change in the shape: conformational entropy modulation). In this work we propose a method to compare atomic B factors, based on Cruickshank's approach to predict atomic positional standard uncertainties (psu's) in crystallographic models [1]. The method we are now proposing uses Cruickshank's psu's to build a correction index that, once applied to invididual refined atomic B factors, generates a set of scaled B factors to be used for comparison purposes. This approach assumes that the psu's integrate all sources of position uncertainty: dynamic (temperature-dependent), static and model error. Among other interesting applications, direct comparison of room and cryogenic temperature models are possible. Different sets of protein models consisting of apo and complexed forms revealed a previously overlooked inverse relationship between Bavg and Rfree, warning about the need for adequate and complete model refinement strategies to ensure accurate structural comparisons. We show evidence supporting that the Wilson B factor value can act as a universal attractor leading to inaccurate models. As a practical example we have used