FA5-MS44-P10

Algorithms for Automated Building of Nucleic Acid Structures. Tim Gruene, George M. Sheldrick. *Dept. of Structural Chemistry, University of Göttingen, Germany.*
E-mail: tg@shelx.uni-ac.gwdg.de

Medium to high resolution X-ray structures of DNA and RNA molecules were investigated to find geometric properties useful for automated model building in crystallographic electron density maps. We describe a simple method, starting from a list of electron density "blobs", to identify backbone phosphates and bases based on properties of the local electron density distribution. We have used this knowledge to propose an algorithm for the automated building of nucleic acid models into electron density maps. The algorithm is based on distances and angles involving C1' and the phosphorus atoms and involves the pseudo-torsion angles η' and θ' that describe the ..P-C1'-P-C1'.. chain. These quantities show reasonably narrow distributions and an asymmetry that allows the direction of the phosphate backbone to be established.

Keywords: auto-building, nucleic acids, backbone trace

FA5-MS44-P11

Standard Reference Materials for Validation Crystal-Software. Boris Kodess, Igor Kommel, Sergey Kononogov, Dmitry Shabalin. *Crystals Metrology Dept., National Metrology Institute, VNIIMS-ICS&E, Moscow, Russia.*
E-mail: bnkodess-vm@vniims.ru

The metrological assurance of measurements of crystal characteristics includes development of standard reference materials with certified values of diffraction pattern characteristics (CSRM). Such CSRM allow to estimate the level of divergence of the results, which may occur due to different software. This approach is discussed in the report on the example of obtaining of some microstructure characteristics – values of nano-crystals sizes, micro-strain level, concentration of package defects, on the example of a procedure of obtaining an atomic structure and quantitative phase analysis, including the Rietveld procedures, and on the example of obtaining of characteristics of charge density distributions. Different types of CSRM have been used allowing to determine reliably atomic positions, applying different measurement procedures and computing methods on the basis of different structural complexes; CSRM of austenite steel (the diffraction pattern of which can radically change when microstructure characteristics change) have been used to determine reliably microstructural parameters.
A few of batches of CSRM for phase analysis, which have been certified in different countries on the basis of diffraction properties are known. The report discusses the results of the use of characteristics of various CSRM made in the Russian Federation. The comparison of the characteristics, obtained for CSRM in Russia and USA, NIST (using the same diffractometer installation), gives a very good agreement of these characteristics of CSRMs and the some results for using different Rietveld software. At the same time the difference between the determination results of microstructure parameters can be very substantial and reach up to 10-15 percent. It is because, while obtaining characteristics for this level of crystal substances structure not only different systematic approaches are used but, depending on man-made assumptions an mathematical form of the calculation may differ. As opposed to first and second type CSRM the difference among the results of determination of characteristics of charge density is much more finer and requires more exquisite approaches already at the level of processing of a greater amount of initial data.
The work has been done within the framework of Project on nanomaterials, Federal Agency "Rostekhregulirovanie"-Kontract and Project-ISTC.

Keywords: software validation, charge distribution, nanostructures

FA5-MS44-P12

Protein structure alignment using efficient small fragment clustering. Eugene Krissinel, *CCP4, Research Complex at Harwell, STFC Rutherford Appleton Laboratory, Didcot, United Kingdom*
E-mail: eugene.krissinel@stfc.ac.uk.

Comparison of biomolecules in 3d is a common task, routinely met in various fields of structural biology and protein crystallography. Well-known examples include the inference on protein function from similarity to structures with known function, prediction of binding sites, choice of sequence-remote models for molecular replacement and others. Due to the large size of protein structures, their comparison often starts with the detection of similarity between their simplified representations, such as secondary structure topology or 3d graphs of secondary structure elements. CCP4 Suite of Programs for Protein Crystallography includes SSM (Secondary Structure Matching), a protein structure aligner, which is built on these principles [1]. SSM is widely used and recognized for speed and efficiency (see, e.g., [2]). However, SSM does not work if secondary structure cannot be calculated, which is often the case in crystallographic applications, when refinement is not complete, or if protein chain appears to be fragmented. An alternative approach to protein structure alignment and comparison is proposed, which does not require the initial structural simplifications and, therefore, is free from SSM shortcomings. Instead, the structures are represented as a manifold of overlapping short fragments, which are clustered by their rotation-translation function of best superposition. The final solution is then chosen as one with the maximal Q-score [1], from the set of top-populated clusters after an additional refinement on Ca-level. The procedure is known to be computationally hard, yet it was developed to match the celebrated SSM performance. Analysis of the new algorithm's performance, sensitivity and selectivity is presented.

[1] Krissinel, E. and Henrick, K., Acta Cryst. D, 2004, 60, 2256. [2] Kolodny, R. A.; Koehl, P. and Levitt, M., J. Mol. Biol. 2005, 346, 1173.

Keywords: Protein Structure, Structural Alignment, Structure Comparison