**m32.p05**

## Automatic building of nucleic acids structures

Frantisek Pavelcik[a], B. Schneider[b]

*[a]Department of Inorganic Chemistry, PRIF UK, 84215 Bratislava, Slovak Republic; and Department of Chemical Drugs, FaF VFU, 61242 Brno, Czech Republic. [b]Institute of Organic Chemistry and Biochemistry, Academy of Sciences of Czech Republic, 16610 Prague, Czech Republic. Email: pavelcik@fns.uniba.sk*

**Keywords: nucleic acids, model building, automatic structure solution**

Molecular fragments are located in an electron density map by a phased rotation conformation and translation function, as implemented in the program NUT [1]. Two types of backbone fragments can be used. A rigid double helical fragment NAhelix of 90 atoms is used to locate stretches of regular A-RNA (DNA) structures. The position and orientation of the fragment can be refined. NAhelix is suitable for low-resolution structures. Typical RNA structure contains about 70% of the double-helical conformation. The second fragment is RNAbone (17 atoms), which represents mononucleotide of phosphate-sugar-phosphate type. The fragment is flexible and all backbone torsion angles can be varied during the search. For computation reasons the search is restricted by a table of allowed conformations. The most frequent conformations were determined by a conformation family generator [2] utilizing knowledge of sugar-phosphate-sugar conformation families [3]. The RNAbone is suitable for intermediate resolution (2.0-3.0Å). Individual fragments are connected into polynucleotide chains by a program HEL [4]. In the case of RNAbone also side-chains can be build. The PDB file is a result of connecting. The procedures were tested on RNA/DNA structures ranging form small nucleotide (1QYL) to ribosome (1FFK, 1J5E). About 65% to 100% of the structure can be built, depending on resolution, fragment used and phase quality.

[1] Pavelcik, F. (2006). J. Appl. Cryst. submitted.
[2] Pavelcik, F. & Vanco, J. (2006). J. Appl. Cryst. 39, accepted.
[3] Schneider, B., Moravek, Z. & Berman, H. M. (2004). Nucl. Acids Res. 32, 1666-1677.
[4] Pavelcik, F. (2006). J. Appl. Cryst. 39, 287.

**m32.p06**

## "Recent developments in version 6.0 of the CCP4 crystallographic program suite"

F. Remacle, P.J Briggs

*CCP4 group, Computer sciences and engineering department, CCLRC Daresbury Laboratory, Warrington, WA4 4AD*

**Keywords: software for crystallography, macromolecular crystallography, structure determination**

The Collaborative Computational Project Number 4 in Protein Crystallography was set up to assemble a comprehensive collection of software to satisfy the computational requirements in macromolecular X-ray crystallography. The project is currently coordinated at CCLRC Daresbury Laboratory. The resulting collection of software, commonly known as the CCP4 program suite, is now distributed to academic and commercial users world-wide via periodic releases - the most recent of which is version 6.0.

This poster will outline the new features in the CCP4 program suite:
- New programs included in the suite: CCP4 Molecular Graphics, Phaser, Coot, Chooch, BP3, pirate, superpose, chainsaw Pdb_merge.
- New versions of existing programs such as Refmac5, Mosflm, sfcheck, molrep, ...
- New functionalities in various programs part of the suite
- CCP4 interface now include new tools, has more programs available and has new functionalities.
- New user-friendly automated downloading and installation.

An overview of on-going development work within the CCP4 group will also be included.