Poster Presentation

MS22.P17

aCHESYM: standardized placement of macromolecular models in the unit cell

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Unique choice of the unit cell and the asymmetric unit are well defined and described in the International Tables for Crystallography vol. A. Unfortunately, the placement of molecules within the unit cell is not standardized. Since structure solution programs often use random numbers in their algorithms, the selected set of atomic coordinates may be different even with successive runs of the same program. Although formally correct, an arbitrary choice of molecular placement within the unit cell is confusing and may lead to interpretation errors [1]. With the use of the anti-Cheshire unit cell introduced by Dauter [2], for all space groups without inversion symmetry, it is possible to transform the molecular model such that its center of gravity falls within the anti-Cheshire asymmetric unit cell. It means that for macromolecular crystal structures it should be possible to standardize the placement of the molecules within the unit cell. In consequence, it should be easier for crystallographers and non-crystallographers to compare similar or related crystal structures. An implementation of the anti-Cheshire concept has been programmed in Python as a web service, aCHESYM. The aCHESYM program takes a PDB file as input and transforms the macromolecular model into the desired anti-Cheshire region. The program can also handle structure factor CIF files if the transformation used requires reindexing of the reflection data. The unit cell, coordinates and displacement parameters of all atoms after transformation are saved in a new PDB file. All the calculated transformations are reversible, so there is no danger of data loss. Moreover, the program helps the user to find the most compact assembly of the molecules (chains) in the structure when there are several chains in the asymmetric unit.

[1] *Dauter, Z. Acta Cryst. D69, 2–4.,* ***[2]*** *Dauter, Z. Acta Cryst. D69, 872–878.*

Keywords: computer program, macromolecular crystallography, python