A specialised software for statistical applications in macromolecular crystallography

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Keywords: Macromolecular crystallography

A new package for applications in macromolecular structural crystallography, **cRy**, has been developed in the renowned *R* statistical platform. This is the first software of its kind and it is supposed to provide a bridge between the large communities of crystallographers and professional statisticians. At present macromolecular crystallographers make heavy use of large systems of programs, like CCP4 [1] or PHENIX [2], mainly written in Fortran, C/C++ or Python. These programs handle the several statistical operations, normally carried out in crystallography, with *ad hoc* routines, usually developed by different authors, often not sharing a common statistical platform. Data and results are exchanged through files with well-defined formats. The **cRy** package reads and writes files in the most commonly used crystallographic formats, carries out all major crystallographic calculations and provides an interface between the crystallographic data structure and the statistical objects and tools offered by *R*. **cRy** provides, thus, that common statistical platform that, at present, is still lacking in structural crystallography. The code has been developed using S4 classes.

References

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