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PURY: A General Parameter Set Generator for Geometry of Macromolecular Structures

Miha Andrejašič[a], Dušan Turk[a]

[a]*Department of Biochemistry and Molecular Biology, Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia. E-mail: miha.andrejasic@ijs.si*

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The paper of Engh and Huber [1] with description of accurate geometrical parameters of amino acid residues has set a new standard in the protein crystallography. A similar step forward in the area of nucleic acids was made by Parkinson et al. [2]. As the number of macromolecular structures of complexes with ″hetero″ ligands and their variety is growing, the time has come to prepare a parameter set, which will provide parameters for the existing and coming compounds with the accuracy and precision of the Engh-Huber and Parkinson parameter sets. Since such parameter set extends over thousands of atom types and parameters connecting them, it is clear that it can only be reliably constructed, maintained and updated in an automated manner. With these goals in mind the computer program PURY was written.

The program PURY operates in two modes: the crystal structure database digestion mode and the molecular parameter construction mode. In the digestion mode it generates the entire library of parameters based on high-resolution crystal structures. The program reads an unlimited number of high resolution structures (for example the whole Cambridge Crystallographic Data Base), assigns atom types taking into account the local geometry and updates the digested list. The digested list contains all bonding parameters (bond length and angles, torsional angles and improper geometries such as chirality and planarity) together with the frequency of their appearance, sum and sum of squared values. Using this description the digested list can be anytime expanded with a private structure collections, which will update, and when found necessary expand, the digested list. In the construction mode, the program reads a description of molecule and generates molecular topology entry and corresponding parameter list for refinement and energy calculations. Currently, input in the PDB form and output for MAIN, X-PLOR-CNS programs are supported. Input as well as output formats will be expanded to support interaction with a variety of computer programs used in refinement and energy calculations of macromolecules including a web server support.

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Patterson Deconvolution and SAD Phasing in IL MILIONE

Maria Cristina Burla[a], Rocco Caliandro[b], Benedetta Carrozzini[b], Giovanni Luca Cascarano[b], Liberato De Caro[b], Carmelo Giacovazzo[b], Giampiero Polidori[a], Dritan Siliqi[b]

[a] *Dipartimento di Scienze della Terra, Perugia University, Perugia, Italy.* [b]*IC-CNR, Bari, Italy. E-mail: mariacristina.burla@unipg.it*

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The Single-wavelength Anomalous Dispersion (SAD) method is getting more and more importance in high-throughput determination of protein structures. The method of joint probability distribution functions has been applied by the authors for estimating the structure factor moduli of the anomalous scatterer substructure, both in SAD and MAD (Multi-wavelength Anomalous Dispersion) cases. A classical Direct Methods procedure, combining tangent formula and direct space refinement, has been developed: it proved to be a robust, fast and efficient tool to locate the anomalous substructure both in MAD and SAD cases [1], [2], [3]. More recently the authors have applied an entirely direct space approach to single crystal diffraction data of medium and large structural complexity: it includes an automated Patterson deconvolution method, based on the minimum superposition function, followed by an effective direct-space refinement, consisting of cycles of electron density modification.[4]. This method has been successfully applied to SAD data to find the anomalous scatterer substructure: the application to a large set of test structures proves the efficiency and the robustness of the method. The procedure proved to be able to recover the model of substructures up to 160 anomalous scatterers in the asymmetric unit and is a tool of the package IL MILIONE for the global phasing of proteins.

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