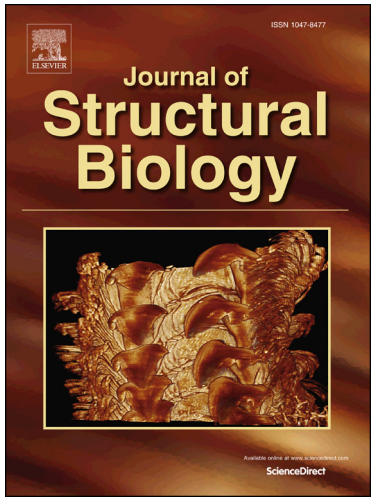

Analytical symmetry detection in protein assemblies. I. Cyclic symmetries

Guillaume Pagès, Elvira Kinzina, Sergei Grudinin

PII: S1047-8477(18)30112-6
DOI: https://doi.org/10.1016/j.jsb.2018.04.004
Reference: YJSBI 7184

To appear in: *Journal of Structural Biology*

Please cite this article as: Pagès, G., Kinzina, E., Grudinin, S., Analytical symmetry detection in protein assemblies. I. Cyclic symmetries, *Journal of Structural Biology* (2018), doi: https://doi.org/10.1016/j.jsb.2018.04.004

Analytical symmetry detection in protein assemblies. I. Cyclic symmetries

Guillaume Pagès[a], Elvira Kinzina,[b], Sergei Grudinin[a]

[a] *Inria, Univ. Grenoble Alpes, CNRS, Grenoble INP, LJK, Grenoble, 38000, France*
[b] *Moscow Institute of Physics and Technology, Dolgoprudny, 141701, Russia*

Abstract

Symmetry in protein, and, more generally, in macromolecular assemblies is a key point to understand their structure, stability and function. Many symmetrical assemblies are currently present in the Protein Data Bank (PDB) and some of them are among the largest solved structures, thus an efficient computational method is needed for the exhaustive analysis of these. The cyclic symmetry groups represent the most common assemblies in the PDB. These are also the building blocks for higher-order symmetries. This paper presents a mathematical formulation to find the position and the orientation of the symmetry axis in a cyclic symmetrical protein assembly, and also to assess the quality of this symmetry. Our method can also detect symmetries in partial assemblies.

We provide an efficient C++ implementation of the method and demonstrate its efficiency on several examples including partial assemblies and pseudo symmetries. We also compare the method with two other published techniques and show that it is significantly faster on all the tested examples. Our method produces results with a machine precision, its cost function is solely based on 3D Euclidean geometry, and most of the operations are performed analytically. The method is available at http://team.inria.fr/nano-d/software/ananas. The graphical user interface of the method built for the SAMSON platform is available at http://samson-connect.net.

Keywords: Point-Group Symmetry, Protein Structure, Protein Assemblies, Continuous Optimization

Email address: sergei.grudinin@inria.fr (Sergei Grudinin)