Notes

s8b.m2.o5 Constraining and Restraining Parameters for Protein Phasing at Very Low Resolution. K.M. Andersson & C.J. Gilmore *Dept. of Chemistry, Univ. of Glasgow, Glasgow G12 8QQ, Scotland.*
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The speed of which protein structures are solved is limited by two major factors: crystallization and structure solution.

A direct approach to the phase problem is one of the long-time goals in crystallography since only native data need to be used and the time spent on solving structures is thus also an important financial aspect. Direct methods such as Shake-and-Bake, require high-resolution data and only work for rather small proteins (ca. 1200 non-H atoms). For larger proteins, which do not diffract to high, or even medium resolution, other methods need to be developed.

Starting at very low resolution, the electron density is blurred and uniform such that simple shape-approximations can be used to describe the envelope. This low chemical complexity is both an advantage and disadvantage. In order to get initial structure factor phases at this resolution, other phase information than the decoding of the phases through statistical triplet and quartet relations between the structure factor magnitudes must be used. Such intrinsic phase information can be extracted from the space group symmetry, cell parameters, packing coefficients, allowed packing regions and other known parameters which contain information of the position, orientation and shape of the protein molecule [1,2].

When a good envelope with up to 100-150 reliable structure factor phases are obtained, phase extension to the desired resolution, using the prior phase information, hopefully more easily converges to a structure solution of the protein molecule under study.

The use and validity of different restraining and constraining parameters for correctly positioning and modifying the shape of the initial envelopes will be presented.

[1] Andersson K.M. "Positioning a Protein Molecule in the Asymmetric Unit Using Very Low Order Reflections and Packing Restraints." J. Appl. Cryst. (1999), **32**, 530-535.
[2] Andersson K.M. & C.J. Gilmore "On the Macromolecular Phase Problem at Very Low Resolution. The Electron Density Distribution" (2000). Submitted to Acta Cryst. D.