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Algebraic Direct Methods for Very Low Resolution Protein Structure Determination. D.Y. Guo, Robert H. Blessing, Hauptman-Woodward Medical Research Inst., Buffalo, NY, and Dept. of Structural Biology, SUNY, Buffalo, NY.

Using a zeroth approximation of the crystallographic asymmetric unit as a sphere of uniform electron density, a sphere radius R_m and position r_m are found by a grid search for the position in the unique subvolume of the unit cell that yields the largest nearest-neighbor distance to a symmetry equivalent point. The approximate radius R_m determines values of $u_{hkl} = 2\pi R_m/d_{hkl}$ for unitary structure factor values, $f(u) = \exp(-0.1\ u^2) \approx \Phi(u) = 3(\sin u - u \cos u)/u^3$. The diffraction resolution limit $d_{min} = 2\pi\ R_m/u$ at $u \approx 4.5$, where $\Phi(u)$ has its first node, defines the low-resolution core of reflections used to generate structure invariant triplets for application of an exact algebraic minimum function derived from earlier results [Hauptman *et al*. (2002). *Acta Cryst*. A58, 361-369].

Optimization of the position of the molecule center r by means of the minimum function is restricted by the molecular packing requirement that $|\Delta r| = |r - r_m|$ should be small. This restriction is enforced by a packing figure of merit,

$$\text{FOM} = a\,|\Delta r| + b\ , \quad a = 1/(c\,R_m)\ , \quad b = (c-1)/c\ , \quad c \geq 1, \quad \text{and} \ |\Delta r| < R_m,$$
$$\text{FOM} = 1, \qquad \text{if} \ |\Delta r| \geq R_m,$$

where c is an adjustable parameter that controls the strength of the packing restriction. The figure of merit is linear in $|\Delta r|$, and has its minimum value FOM = $(c - 1)/c$ at $|\Delta r| = 0$, and its maximum value FOM =1 for $|\Delta r| \geq R_m$.

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