

Publication

Bias reduction in phase refinement by modified interference functions: Introducing the gamma correction

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The chemical, physical and symmetry constraints of an electron-density map impose relationships between structure factors, and these relationships are exploited during refinement. However, constraints often allow an artificially high correlation between the model and the original structure factors, a flaw known as model or refinement bias. Elimination of the bias component of a constrained model, the component insensitive to constraints, enhances the power of phase-refinement techniques. The scale of the bias component, here denoted as gamma, is shown to be equal in magnitude to the origin vector of the interference function G that defines the relationships between the structure factors. The gamma correction leads to solvent flipping in the case of phase improvement by solvent flattening, and other types of constraint allow a similar treatment.

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