pre-defined number of core objects, so that each structural motif (domain) contained in the structure is represented by one such core. Rather than follow a simplistic approach of assigning the known domain structures to each segment of a low-resolution map, in this work we target a more general unbiased shape identification in terms of domains. No detailed knowledge about the composition of the low-resolution complex is required. A pattern-recognition comparative analysis which makes use of 3rd order moment invariants [1] and the radius of gyration of these shapes and those derived from structures of the unique domains from the PDB [2] results in candidate structural models that can be used for a fit into the density map. We show that the placed candidate models can be employed for subsequent phase extension up to 10-15 Å resolution.

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A Multivariate Likelihood Siras Function for Phasing and Model Refinement. Pavol Skubak[a], Garib N. Murshudov[b], Navraj S. Pannu[a]. [a]*Department of Biophysical Structural Chemistry, Leiden University, the Netherlands,* [b]*York Structural Biology Lab, York, England.*
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Previously, it has has been shown that the use of a multivariate likelihood function to optimally extract information from a single anomalous diffraction (SAD) experiment can improve the results of SAD phasing [1] and model building with iterative refinement [2].
Now a likelihood function based on the multivariate probability distribution of all observed structure factor amplitudes from a single isomorphous replacement with anomalous scattering (SIRAS) experiment has been derived and implemented for use in substructure refinement and phasing as well as macromolecular model refinement. Efficient calculation of a multi-dimensional integration required for function evaluation has been achieved by approximations based on the function's properties.
The use of the function in both SIRAS phasing and protein model building with iterative refinement was essential for successful automated model building in test cases presented.

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