Rigid-body motion is the main source of diffuse scattering in protein crystallography

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The origin of diffuse X-ray scattering from protein crystals has been the subject of debate over the past three decades regarding whether it arises from correlated atomic motions within the molecule or from rigid-body disorder. Here, a supercell approach to modelling diffuse scattering is presented that uses ensembles of molecular models representing rigid-body motions as well as internal motions as obtained from ensemble refinement. This approach allows oversampling of Miller indices and comparison with equally oversampled diffuse data, thus allowing the maximum information to be extracted from experiments. It is found that most of the diffuse scattering comes from correlated motions within the unit cell, with only a minor contribution from longer-range correlated displacements. Rigid-body motions, and in particular rigid-body translations, make by far the most dominant contribution to the diffuse scattering, and internal motions give only a modest addition. This suggests that modelling biologically relevant protein dynamics from diffuse scattering may present an even larger challenge than was thought.