On the information content of X-ray diffraction data

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The prominent role that likelihood-based methods play in macromolecular crystallography suggests that it is worth examining the closely-related concept of information. The process of carrying out a diffraction experiment yields information about the true values of the diffraction intensities; can a measure of the information added by the diffraction experiment provide a useful criterion to test whether we have collected actual data and not just *hkl* values? Are such measures useful for defining the resolution limit? From an alternative point of view, an experimental observation adds information to our knowledge of the parameters of a model by restricting their allowed values; can a comparison of the total amount of information available to determine parameter values be used to justify rational choices of model parameterization (*e.g.* the number of parameters used to describe thermal displacements)? Finally, do these considerations shed light on the problem of how many parameters are required to describe electron density in the crystal accurately and whether that number of parameters can be determined with sufficient precision using the available data?