It is known that X-ray intensities from a crystal containing similar atoms follow either the centric or the acentric Wilson distribution depending on whether the crystal is centrosymmetric or not. Crystallographers exploit this property to resolve space group ambiguities of a crystal from a statistical study of the observed intensities. A number of statistical parameters of the two Wilson distributions (e.g., Wilson's ratio, variance, higher moments of intensities) as well as other quantitative statistical criteria for goodness of fit (e.g., chi-square test, Kolmogorov test, Neyman-Barton smooth test etc.) have been suggested in the literature for this purpose. From the point of view of the Theory of Statistics none of these can be classified as a 'best test'. A 'best test' (also called the most powerful test) is the one for which the critical region is such that the type II error is minimized. Such a test can be constructed using Neyman-Pearson Lemma. In this paper a best test to distinguish between the two Wilson distributions is discussed. The effect of data truncation due to unobserved reflections is also taken into account in the theoretical treatment.

One of the most fundamental concepts in science is the concept of information. The proof by Shannon (The Math­ematical Theory of Communication, 1948, Bell Syst. Tech. J., 21, 379-423; 623-656) that there exists a unique and consistent measure of the information content, followed by the development by Jaynes (see Collected Works: Papers on Probability, Statistics, and Statistical Physics, 1981, Dordrecht-Holland: Reidel) of a general information-theoretic approach to problems of statistical inference, provides a very powerful framework for treating such problems of which statistical mechanics, image processing, and crystallographic inversion (i.e., structure estimation) may be regarded as particular examples.

We shall describe some of the fundamental concepts involved in information-theoretic based approaches to the crystallographic inversion problem and show how practical methods of structure refinement may be developed which are aimed at macromolecular structure determination (Wilkins, Varghese and Lehmann, Acta Cryst. 1983, A39, 47). Particular attention will be given to the roles of prior information, event-space and choice of constraint functions (Steenstrup and Wilkins, 1984, Acta Cryst. A40) with a view to relating recent articles on the inversion problem (e.g., Britten and Collins, Acta Cryst., 1982, A38, 129, and Piro, Acta Cryst., 1983, A39, 61).