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A PROTEIN STRUCTURE IS ONLY AS GOOD AS THE DATA *

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Benno P. Schoenborn

DE84 012904

Biology Department
Brookhaven National Laboratory
Upton, NY 11973

INTRODUCTION

In the interpretation of any protein structure derived from diffraction data, one has to try to assess the reliability of the derived atomic positions and atomic species. In the neutron case, it is possible to localize hydrogen atoms (1). This, however, just about doubles the total number of atoms to be derived with about the same number of reflections. In addition, neutron data are often of poorer statistical quality than their x-ray counterparts because of low source flux and the very high background caused by the incoherent scattering of hydrogen atoms. Thus in neutron protein crystallography there is a higher uncertainty in the measured structure factor, in addition to uncertainties in phasing and refinement.

In order to gain some insight into the reliability of the derived atomic structure, the observed atomic densities of all hydrogen atoms bound to the α -carbon have been tabulated (2). This histogram (Figure 1) shows an approximate symmetric distribution centered on -3.8 F units, the theoretical scattering length of hydrogen atoms. The width of this distribution is a good indication of the errors to be expected in the determination of hydrogen-deuterium exchange. The fractional occupancy (X) is evaluated from the observed scattering density (P) at the amide proton position:

$$X = \frac{P + 3.7}{+10.3}.$$

From the histogram (Figure 1), the expected error in P is $\sim 1/3$ the density of an H atom or ~ 1.2 F units. These data, however, imply that up to $\sim 10\%$ of the observed exchange data may have a very large error.

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