

18. REFINEMENT

$$\sigma_{LS, Luzz}(r) = 1.33(N_i/p)^{1/2} [R(s_m)/s_m], \quad (18.5.8.3)$$

where $R(s_m)$ is the value of R at some value of $s = s_m$ on the selected Luzzati curve. Equation (18.5.8.3) provides a means of making a very rough statistical estimate of error for an atom with $B = B_{avg}$ (the average B for fully occupied sites) from a plot of R versus $2 \sin \theta / \lambda$.

The corresponding equation involving R_{free} is

$$\sigma_{LS, Luzz}(r) = 1.33(N_i/n_{obs})^{1/2} [R_{free}(s_m)/s_m]. \quad (18.5.8.4)$$

18.5.8.3. Comments on Luzzati plots

Protein structures always show a great range of B values. The Luzzati theory effectively assumes that all atoms have the same B .

Nonetheless, the Luzzati method applied to high-angle data shells does provide an upper limit for $\langle \Delta r \rangle$ for the atoms with low B . It is an upper limit since experimental errors and model imperfections are not allowed for in the theory.

Low-resolution structures can be determined validly by using restraints, even though the number of diffraction observations is less than the number of atomic coordinates. The Luzzati method, based preferably on R_{free} , can be applied to the atoms of low B in such structures. As the number of observations increases, and the resolution improves, the Luzzati $\langle \Delta r \rangle$ increasingly overestimates the true $\sigma(r)$ of the low- B atoms.

In the use of Luzzati plots, the method of refinement, and its degree of convergence, is irrelevant. A Luzzati plot is a statement for the low- B atoms about the maximum errors associated with a given structure, whether converged or not.

References

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