The Model Resolution Function – A Technique for Estimating the Quality of Approximation of Particles by Models in Small-Angle X-ray or Neutron Scattering

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Abstract

Although the quality of a structure model obtained from small-angle X-ray or neutron scattering curves for polymers can be determined qualitatively by comparing the isotropic scattering curve calculated for the model with the experimental scattering data for a solution of polymer molecules, other methods are needed for a more precise evaluation. A model resolution function has been defined to permit quantitative comparisons. With this function, the quality of the approximation can be assessed, and the structure resolution can be determined. An overinterpretation of scattering curves by use of complex but uniform-density models can thus be avoided. Furthermore, the value of the Porod volume calculated from the scattering data has been found to depend strongly on the interval in which the scattering data are recorded or selected for evaluation. The calculations with the atomic model curves showed that it is impossible to compute physically meaningful values of the hydration of the molecules from the Porod volume and the dry volume by use of extrapolated scattering curves with an insufficient resolution. The theory of the model resolution function and the interpretation of the Porod volume have been verified and tested with experimental scattering curves from solutions of RNA molecules.

I. Introduction

In small-angle X-ray or neutron scattering studies, the shape of biological macromolecules must usually be determined by trial and error (Damaschun, Müller & Bielka, 1979). In other words, the experimental scattering curve or electron distance distribution function is compared with curves or distance distribution functions computed from models. The model is adjusted until the curves from the model and the experiment agree within experimental uncertainty. The model often will fit the data only within a certain interval of scattering angles θ, beginning with the angle θ = 0. As a measure of the quality of the fit, factors called R factors (Feigin, 1971), in analogy with crystal structure analysis, have been employed. These factors are defined by the equations

\[ R_1(s_1,s_2) = \frac{1}{s_2 - s_1} \int_{s_1}^{s_2} \frac{|I_{\text{exp}}(s) - I_{\text{mod}}(s)|}{I_{\text{exp}}(s)} \, ds \] (1)

\[ R_2(s_1,s_2) = \int_{s_1}^{s_2} |I_{\text{exp}}(s) - I_{\text{mod}}(s)|^2 \, ds / \int_{s_1}^{s_2} I_{\text{exp}}(s)^2 \, ds \] (2)

The data often can be compared with the model only within an interval between \( s_1 \) and \( s_2 \), where \( s = 4\pi \sin \theta / \lambda \), \( 2\theta \) is the scattering angle and \( \lambda \) is the wavelength. In automated curve-fitting techniques (Walter, Kranold, Göcke, Damaschun & Müller, 1975; Sjöberg, 1977; Müller, Damaschun & Hübner, 1979) based on Marquardt’s (1963) method, the minimum of

\[ r(\beta) = \sum_{k=1}^{m} \left\{ w_k [I_{\text{mod}}(s_k,\beta) - I_{\text{exp}}(s_k)] \right\}^2 \] (3)

is evaluated and used as the criterion for the quality of the fit. In (3), \( \beta \) is the parameter vector of the model, and the \( w_k \) are weighting factors. Each of equations (1)–(3) defines a different model as ‘best’. From a function called the model resolution function, which we introduce in the next section, the structure resolution for a given model can be determined. For biological substances, such as nucleic acids, proteins and polysaccharides, one can show that the maximum structure resolution attainable with homogeneous models can also be calculated by use of scattering curves computed from models that employ atomic coordinates. An ‘overinterpretation’ of the data resulting from the use of molecular models with homogeneous electron density distributions (shape models) is thus avoided. We also discuss the relation between the attainable structure resolution and the molecular volume \( V_p \) calculated for RNA molecules.

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II. Theory

For scattering of monochromatic radiation with wavelength \( \lambda \),

\[ s \leq 4\pi/\lambda. \]  

(4)

Usually, however, the equipment does not allow data to be obtained at such large \( s \), but only for

\[ s \leq 4\pi/2. \]  

(4)

where \( S_{\text{diff}} \) in general is much smaller than \( 4\pi/2 \). Moreover, in order to provide sufficient intensity, diffractometers usually use slit collimation, and in this case the largest attainable \( s \) value is even smaller and is given by

\[ s_{\text{max}} = (s_{\text{diff}}/t_{\text{max}})^{1/2}, \]  

(5)

where \( t_{\text{max}} \) is the \( s \) value corresponding to the largest angle in the profile of the primary beam. The experimental scattering curve \( I_{\text{exp}}(s) \), after correction for collimation effects, can be written

\[ I_{\text{exp}}(s) = G(s)I(s), \]  

(6)

where \( I(s) \) is the scattering curve that would have been obtained for point collimation, and

\[ G(s) = \begin{cases} 1 & s \leq s_{\text{max}} \\ 0 & s > s_{\text{max}} \end{cases}. \]  

(7)

The function \( G(s) \) in (7) specifies the interval of \( s \) that is accessible in the experiment.

The highest structure resolution attainable for a set of measured data can be defined by the correlation function \( C(r) \) in real space. For an intensity function \( I(s) \) known for all reciprocal space \( s \),

\[ rC(r) = \frac{1}{2\pi^2} \int \frac{I(s)s}{\sin sr} ds. \]  

(8)

For the corrected experimental intensity \( I_{\text{exp}}(s) \),

\[ [rC(r)]_{\text{exp}} = \frac{1}{2\pi^2} \int \frac{I_{\text{exp}}(s)s}{\sin sr} ds. \]  

(9)

From the convolution theorem for Fourier sine transforms, the experimental function \( [rC(r)]_{\text{exp}} \) can be expressed as

\[ [rC(r)]_{\text{exp}} = g(r)*[rC(r)], \]  

(10)

where the asterisk denotes convolution, and \( g(r) \), the Fourier cosine transform of \( G(s) \), is given by

\[ g(r) = \mathcal{F}[G(s)] = \sin(s_{\text{max}}r)/r. \]  

(11)

From the function \( g(r) \), several different definitions of the maximum resolution \( A \) can be obtained. For example, in crystal structure analysis, the full width

\[ A = 2\pi/s_{\text{max}} \]  

(12)

of the base of the principal maximum is defined as the resolution, while in small-angle scattering (Damaschun, Müller & Bielka, 1979), by analogy with the sampling theorem in information theory (Brillouin, 1956), the half width

\[ A = \pi/s_{\text{max}} \]  

(13)

has been employed. When \( s_{\text{max}} \) is chosen to provide favorable experimental conditions, rather than being determined by the diffractometer, analogous definitions can be introduced. Damaschun, Müller & Bielka (1979) also used the structure resolution as a test of fits with models. When the experimental scattering curve agreed within experimental error with the curve calculated for the model for \( s \leq s_{\text{res}}^{\text{mod}} \), the resolution of the model was defined to be

\[ A_{\text{res}}^{\text{mod}} = \pi/s_{\text{res}}^{\text{mod}}. \]  

(14)

We will now modify (8) to take account of the contribution of the scattering curve for \( s > s_{\text{max}} \) in tests of a model or in determination of structure resolution. For the function \([rC(r)]_{\text{mod}}\) of a model,

\[ [rC(r)]_{\text{mod}} = \frac{1}{2\pi^2} \int \frac{I_{\text{mod}}(s)s}{\sin sr} ds. \]  

(15)

By multiplying the numerator and the denominator of the integrand in (15) by \( I_{\text{exp}}(s) \), we obtain

\[ [rC(r)]_{\text{mod}} = \frac{1}{2\pi^2} \int \frac{I_{\text{exp}}(s)s[I_{\text{mod}}(s)/I_{\text{exp}}(s)]\sin sr}{\sin sr} ds. \]  

(16)

As in (9) and (10), the convolution theorem gives

\[ [rC(r)]_{\text{mod}} = \mathcal{MRF}(r)*[rC(r)]_{\exp} \]  

(17)

where the asterisk denotes a convolution, and

\[ \mathcal{MRF}(r) = \frac{1}{2\pi^2} \int \frac{[I_{\text{mod}}(s)/I_{\text{exp}}(s)]\cos sr}{\sin sr} ds. \]  

(18)

Normally \( I_{\text{exp}}(s) \) has no zeros for \( s < \infty \) and, as we explain below, for large \( s \) we extrapolate the ratio \( I_{\text{mod}}(s)/I_{\text{exp}}(s) \) with a function of \( s \) that guarantees that the integral in (18) converges. If in other cases the experimental and model curves decay with the same power of \( s \), we subtract a constant before transformation, so that the integrand in (18) goes to zero for large \( s \). We therefore can assume that this integral exists.

Equation (18) is the definition of the model resolution function, which characterizes the structure resolution with which a given model approximates the structure of the molecule from which the model was derived or with which it is tested. The half-width \( A_{\text{MRF}} \) of the model resolution function can serve as a measure of the resolution for the model, or the form of the model resolution function can be compared with the function \( g(r) \) defined by (11).

As we have mentioned, the quotient \( I_{\text{mod}}(s)/I_{\text{exp}}(s) \) should be extrapolated analytically for large \( s \), to avoid termination effects. When this ratio has the form
k/s^n for s ≥ x, with n = 1, 2, 3, ..., the integral

$$MRF_{\text{rest}}(r) = k \int \frac{(\cos sr)}{s^n} ds$$  \hspace{1cm} (19)

can be evaluated analytically (Gerber & Schmidt, 1983), and

$$MRF_{\text{rest}}(r) = kCi(rx) \hspace{1cm} n = 1,$$

$$MRF_{\text{rest}}(r) = k[-\pi r/2 + (\cos rx)/x + rSi(rx)] \hspace{1cm} n = 2,$$

$$MRF_{\text{rest}}(r) = (kr^2/2)[(\cos rx)/r^2 x^2 - (\sin rx)/rx - Ci(rx)] \hspace{1cm} n = 3$$  \hspace{1cm} (20)

where

$$Ci(rx) = \int_{rx}^{\infty} (\cos t)/t dt,$$

and

$$Si(rx) = \int_{0}^{rx} (\sin t)/t dt.$$  \hspace{1cm} (21)

### III. Results and discussion

Scattering curves for molecules in solution can be calculated from the atomic coordinates and atomic structure factors (Müller, 1983). In the algorithm for these calculations, in which the molecular dimensions are evaluated from the van der Waals radii of the atoms, the form and volume of the region from which the solvent is excluded must be exactly specified. This region, often called the solvent-excluded volume of the molecule, is approximated by close-packed cubes with edge 0.05 nm. From the approximate solvent-excluded volume, the molecular surface can be obtained with nearly atomic resolution, but in the interior of the molecule the electron density is uniform. This algorithm thus provides scattering curves for models with and without electron density fluctuations. These scattering curves can be used in studies of the properties of model resolution functions.

For our discussion of the information obtainable from the model resolution function, we calculated the scattering curve for an aqueous solution of RNA double helices with 12 adenine–uracil and guanine–cytosine base pairs in an alternating series in an A-form double helix (Fig. 1).

In these calculations we used the atomic coordinates of Arnott, Hukins & Dover (1972). A computer plot of the molecule is shown in the inset in Fig. 1. The scattering curve of the solvent-excluded volume was normalized to the same zero-angle intensity I(0) as the curve for the RNA double helix, so that the curves could be more easily compared. From fits of the scattering curves for homogeneous models to the scattering curve for the RNA double helix, we found that a hollow cylinder (see the inset in Fig. 1) with outer radius R_o = 1.14 nm, inner radius R_i = 0.26 nm, and length H = 3.375 nm can be used as a rough approximation to the shape of the RNA molecule in solution. We will now discuss the structure resolution of both these models – the excluded-volume body and the hollow cylinder – in relation to the real RNA double helix.

The resolution of a structure model has been determined (Damaschun, Müller & Bießka, 1979) in an experimental investigation by considering the point at which significant differences between the model curve and the experimental curve begin to appear. However, if the experimental error band for the model in Fig. 1 is arbitrarily chosen to be 15%, both the scattering curve for the excluded-volume model and the curve for the hollow cylinder agree with the curve for the RNA molecule for s < 2.2 nm^-1 (see Figs. 1 and 2). The same structure resolution \(A_{\text{res}} \approx 1.43\) nm, as given by (14), thus could be formally assigned to both uniform-density models for the RNA molecule in solution. The
actual structure resolution for these two models, however, must be different, as can be seen both from the different quality of the fits of the two models to the real molecule and also from the behavior of the two scattering curves for \( s > 2.2 \text{ nm}^{-1} \).

The model resolution function, unlike the structure resolution \( R_{\text{mod}} \), correctly predicts the difference in the quality of the fits. In Fig. 2, we have plotted the unnormalized ratios \( I_{\text{mod}}(s)/I_x(s) \), where \( I_x(s) \) is the scattering curve of the RNA molecule in solution. [Since the curve was calculated from atomic coordinates, rather than being measured, we use the notation \( I_x(s) \) rather than \( I_{\text{exp}}(s) \).] If we choose the excluded-volume body as the uniform-density model of the molecule in solution, we obtain a structure resolution \( A_{\text{MRF}} = 0.57 \text{ nm} \) from the model resolution function (Fig. 3) but for the hollow cylinder we get 1.0–1.3 nm. In Fig. 3 we have also plotted the normalized resolution function \( \sin (2\pi x)/2\pi x \) for \( s_{\text{mod}} = 2.2 \text{ nm}^{-1} \), which is the basis for (14). A comparison of the two model resolution curves with this function shows that both the excluded-volume body and the hollow cylinder have a higher structure resolution than would be expected from (14).

Furthermore, since the excluded-volume body is by definition the best uniform-density approximation for the real molecule, we can conclude that there is no physically correct uniform-density structure model for RNA molecules with a resolution better than 0.57 nm.

The uniform-density body (the excluded-volume body) can be considered to be the scattering molecule that would be obtained from a series of measurements of the scattering from a solution of molecules in which the effects of electron density fluctuations in the interior of the molecule are cancelled experimentally by contrast variation (Stuhrmann & Kirste, 1965). As can be seen from Fig. 3, the hollow cylinder with the measurements given above thus gives a somewhat higher resolution for this 'molecule' than when the cylinder is used as a model of the real RNA oligomer. This conclusion, however, cannot be made from the value of the full base width \( A_{\text{MRF}} = 0.75 \text{ nm} \) alone but is possible only after consideration of the \( x \) dependence of the model resolution function curves (Fig. 3).

As the atomic structure of natural RNA molecules in solution, such as tRNA or ribosomal RNA, is not known, fits of simple geometric or complex bodies are necessary to determine the structure of these molecules. If suggestions about the base pairing are available from other physicochemical techniques, double-helical and single-strand regions can be adequately modeled by hollow cylinders or cylinders

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**Fig. 2.** Quotient function \( I_{\text{mod}}(s)/I_x(s) \) for the \( A \)-form double helix. 
- The function \( G(s) \) defined in (6) and (7) for \( s_{\text{max}} = 2.2 \text{ nm}^{-1} \).
- The scattered intensity of the excluded-volume uniform-density body divided by the scattered intensity for the RNA double helix in solution.
- The scattered intensity of the hollow cylinder divided by the scattered intensity of the uniform-density excluded-volume body.
- The scattered intensity of the hollow cylinder divided by the intensity of the RNA double helix in solution.

**Fig. 3.** Normalized model resolution functions for the \( A \)-form RNA double helix.
- The curve \( \sin (2\pi x)/2\pi x \).
- The RNA double helix modeled by the excluded-volume uniform-density body.
- The uniform-density excluded-volume body modeled by a hollow cylinder.
- The RNA double helix modeled by a hollow cylinder.
respectively, and by trial and error the spatial arrangement of these building blocks that corresponds to the large molecule can be determined. In this modeling process, however, the resolution of the model cannot be higher than that of the subunits in the model, so that, for models of RNA molecules, it cannot be greater than about 1.0 or 1.3 nm (Fig. 3). In Fig. 4, the ratios of the experimental and calculated curves from two suggested structure models based on different pathways for the nucleotide strand are plotted for ribosomal 5S RNA from rat liver (Müller, Welfle, Damaschun & Bielka, 1981; Müller, Damaschun, Böhme, Fabian & Welfle, 1982). The molecule was approximated by uniform and hollow cylinders.

Projections of the models are shown in the inset in Fig. 4. The model resolution function for both models is plotted in Fig. 5. The resolution of about 0.9 to 1.5 nm is the best value possible for this macromolecule model with homogeneous cylindrical and hollow cylindrical subunits. Because of the similarity of the models (see the projections in the inset in Fig. 5), a resolution of about 1.2 nm does not permit a clear choice between the two models. An unambiguous determination of the position of the sugar–phosphate backbone within the electron density distribution of the model is therefore impossible with models composed of subunits with uniform electron density. Only by introduction of physically based electron density inhomogeneities, for example, by specifying phosphate groups, sugar and bases as scattering centers for nucleic acids (Müller, 1983), can the model structure resolution be improved significantly.

The model structure resolution that can be and that is attained plays an important role not only in the assessment of shape models or tertiary structure models but also in the calculation and the estimation of the reliability of structure parameters. While the radius of gyration $R_g$ (Guinier, Fournet, Walker & Yudowitch, 1955) or the maximum diameter $L$ (Damaschun, Müller & Pürschel, 1968) of a protein or nucleic acid can usually be determined quite accurately from experimental scattering curves, the volume

$$V_p = \frac{2\pi^2}{\int_0^\infty s^2 I(s) \, ds}$$

obtained from the zero-angle intensity and the Porod invariant (Porod, 1951) depends on the structure resolution. Especially for small molecules (molecular weight less than 50 000) with a highly developed surface structure, the reduction in the shape resolution by the contributions of the electron density fluctuations inside the molecule can lead to an incorrect interpretation of the results. In Fig. 1 a significant effect from the atomic electron density fluctuations on the form of the scattering curve is noticeable for scattering vectors greater than 2 nm$^{-1}$. For example, values of the Porod invariant (Damaschun et al., 1978) calculated from the original scattering curve do not correspond to the geometric volume of the molecule. Two approximation procedures have been proposed for replacing the long series of measurements (Stuhrmann & Kirste, 1965) required for eliminating the effects of the electron density fluctuations in the

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![Fig. 4. Quotient functions for rat liver ribosomal 5S RNA. The scattered intensity of model I divided by the measured intensity. The scattered intensity for model II divided by the experimental intensity.](image)

![Fig. 5. Normalized model resolution functions for rat liver ribosomal 5S RNA. The resolution function for model I. The resolution function for model II. The insert shows a superposition of the two models.](image)
interior of the molecule. However, by subtraction of a constant (Luzzati, Witz & Nicolaieff, 1961; Kratky, 1963) or by analytical extrapolation of the scattering curve by the equation

$$I(s) = \frac{k}{s^4}$$  \hspace{1cm} (24)$$

in a region of the scattering curve in which the contribution of the electron density variations of the internal structure is not appreciable (for proteins and nucleic acids, for \( s \leq 2 \text{ nm}^{-1} \)), the information content and therefore the resolution is reduced. In Fig. 1 the scattering curves of the RNA dodecamer and the uniform excluded-volume body are shown for an analytic extrapolation \( k/s^4 \). The ratios \( I_{\text{mod}}(s)/I_x(s) \) are plotted in Fig. 6. In this plot, \( I_{\text{mod}}(s) \) is identical to \( LI_x(s) \) for \( s \leq s^* = 3-2 \text{ nm}^{-1} \), while, for \( s > s^* \), \( I_{\text{mod}}(s) \) is extrapolated by (24). In Fig. 6, the quotient function for the experimental rat liver 5S rRNA also is plotted, and \( I_{\text{mod}}(s) \) is the experimental curve that was extrapolated using (24) for \( s > s^* = 1.8 \text{ nm}^{-1} \). Model resolutions of 0.9 and 0.77 nm for the oligonucleotides and 1.0 nm for the 5S rRNA were obtained with the modified extrapolated scattering curves in Fig. 7. From these analytically extrapolated scattering curves the volume \( V_p \) was also calculated from (23). For the excluded-volume body and a resolution of 0.77 nm the volume determined from the extrapolated scattering curve was about 60% greater than the actual volume 6.52 nm\(^3\) (Table 1), calculated from \( N = 52 \ 120 \) cubes. The volume \( V_p = 6.42 \text{ nm}^3 \) computed from (23) for the entire scattering curve (\( A \leq 0.05 \text{ nm} \)) differs by only 2% from the correct value. For the A-RNA oligomer in solution, a volume about 70% too large is likewise obtained from the analytically extrapolated scattering curve (\( A_{\text{MRF}} = 0.9 \text{ nm} \)) (Table 1). The \( V_p \) values computed from poorly resolved scattering curves are not the volumes of the hydrated molecules but at best are quantities for which the deviation from the dry volume of the molecule is a measure that characterizes the resolution. In particular, there is no physical basis for calculating the solvation of a globular protein (Fedorov, 1981) or of nucleic acids from the equation

$$w = \bar{v}d(V_p/V_{\text{dry}} - 1).$$  \hspace{1cm} (25)$$

In (25), \( \bar{v} \) is the partial specific volume; \( d \) is the mass density of the solvent; and \( V_{\text{dry}} \) is the dry volume of the molecule. At high resolution, \( V_p \) approaches the dry volume of the molecules (Table 1). For natural RNA molecules like ribosomal 5S RNA and tRNA\(^{\text{Phe}} \) (for which the model resolution function is not shown) (Müller, Damaschun, Wilhelm, Welfle, & Pilz, 1982), an approximation analogous to (24) with \( A_{\text{MRF}} = 1 \text{ nm} \) also gave a volume \( V_p \) about 60 to 70% larger than the dry volume.

### IV. Conclusions

The resolution for a given model can be computed from the model resolution function for a macromolecule. For the models we have discussed, the

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**Fig. 6.** Quotient functions for the RNA dodecamer and for 5S RNA.

- The scattered intensity for the RNA double helix in solution extrapolated by \( k/s^4 \) for \( s^* \geq 3-2 \text{ nm}^{-1} \) divided by the exact intensity.
- The scattered intensity of the uniform-density RNA dodecamer extrapolated by \( k/s^4 \) for \( s > 3-2 \text{ nm}^{-1} \) divided by the exact intensity.
- The experimental scattering curve for 5S RNA extrapolated by \( k/s^4 \) for \( s > 1.8 \text{ nm}^{-1} \) divided by the exact intensity.

**Fig. 7.** The normalized resolution functions for the models listed in Fig. 6. The same symbols are used to identify the curves as in Fig. 6.
Table 1. *Volume, model structure resolution and apparent solvation of RNA models [poly (A-G)<sub>6</sub> poly(C-U)<sub>6</sub>] and natural RNA molecules*

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<th>$V_{dry}$ (nm&lt;sup&gt;3&lt;/sup&gt;)&lt;sup&gt;a&lt;/sup&gt;</th>
<th>$V_{model}$ (nm&lt;sup&gt;3&lt;/sup&gt;)</th>
<th>$V_p$ (nm&lt;sup&gt;3&lt;/sup&gt;)</th>
<th>$A_{MRF}$ (nm)</th>
<th>$w$ (g H&lt;sub&gt;2&lt;/sub&gt;O/g RNA)&lt;sup&gt;b&lt;/sup&gt;</th>
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<td>Excluded volume</td>
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<td>(tail extrapolated)</td>
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<tr>
<td>Exact curve (not</td>
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<td>extrapolated)</td>
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<td>36.6</td>
<td>1.0</td>
<td>0.34</td>
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*a $V_{dry}$ is the dry volume determined by the equation $V_{dry} = N_A\bar{v}/M$, where $N_A$ is Avogadro’s number, $\bar{v} = 0.54$ cm<sup>3</sup> g<sup>-1</sup>, and $M$ is the molecular weight.

*b The values of $w$ were calculated from (25).

The numerical value $A_{MRF}$ is smaller than the value determined from the scattering vector $s_{mod}$ by the procedure suggested by Damaschun, Müller & Bielka (1979). The value of the resolution calculated from the model resolution function is independent of the scale and weighting employed in the comparison of the scattering curves. With this evaluation of the resolution of subunits used for modelling complex structures, there is no overinterpretation of the experimental scattering curve of such complex particles, so that the analysis provides only information that can be legitimately deduced from the data.

In analyses of scattering curves of nucleic acid molecules and globular proteins (Fedorov, 1981) by models, when the resolution of the model increases, the volume $V_p$ of the model should in general approach the dry volume. The value of the ‘solvation’ that is calculated from the volume $V_p$ and the dry volume $V_{dry}$ has no physical basis, since it is a quantity that depends only on the resolution. If physically based information about the hydration is to be obtained, the results from small-angle scattering, as well as from other methods such as quasielastic light scattering, must be considered in an analysis like the one we have described (Müller, Zirwer, Damaschun, Welfle, Gast & Plietz, 1983).

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References


