difference between Laue-case and Bragg-case diffraction. Rays affected by the Bragg surface give rise to a high-intensity region on dark-field profiles. The profiles of this peak are *not* well predicted by an approximate Green-function method based on truncated planar Bragg surfaces. As d increases so as to be much greater than about ξ_1, the Bragg peak begins to consist of several narrowly-spaced fringes contained within a broad envelope.

There is some experimental evidence for the presence of such Bragg peaks on X-ray topographs of cylindrical crystals (see *e.g.* Saldin & Buckley-Golder, 1977). In the instance cited above the diameter was of the order of a hundred extinction distances. The narrow Bragg fringes expected were smeared out to form a wide high-intensity region near F_1 on the photographs in this case since they were projection (or traverse) topographs. One method of computing the form of such peaks would be by means of an extension of our calculations and the use of the reciprocity theorem (Kato, 1968).

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On the Evaluation of Root-Mean-Square Errors in Atomic Coordinates in Protein Crystallography

BY Z. S. DEREWENDA, A. M. BRZOZOWSKI, A. STĘPIEŃ AND M. J. GRABOWSKI

Department of Crystallography, Institute of Chemistry, University of Łódź, 91 416 *Łódź, Nowotki* 16, *Poland*

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Abstract

The calculation of standard deviations for atomic coordinates in human deoxyhaemoglobin A on the basis of various reciprocal-space residuals has shown the resulting values to be in good agreement with each other. Evidence is presented that such calculations may be more reliable than is commonly accepted. It is also shown that Wilson's statistics may be applied successfully to low- and high-angle protein diffraction data.

Introduction

It is usually assumed that the calculation of standard deviations of atomic coordinates in a model of a protein molecule is rather difficult. However, the knowledge of its value may prove very helpful, for example in estimating the credibility of the orientation of a known protein molecule in an unknown crystal lattice, found using various molecular replacement techniques.

It is interesting that various reciprocal-space residuals may serve both as correlation functions in rotation and translation function searches (Nixon & North, 1976) and as a basis of $|\overline{\Delta r}|$ evaluation (Luzzati, 1952; Parthasarathy & Parthasarathi, 1972; Nixon & North, 1976). Attention has also been paid to the physical interpretation of refinement based on the minimization of some of these residuals (Wilson, 1976).

On the other hand, the search for the correct orientation of a protein molecule with the molecular replacement method was frequently based on a strictly mathematical assumption that a unique set of correct values of rotational and translational parameters

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should give a minimum value of the residual. This is obvious in the case of asymmetric monomeric proteins, or even polymeric molecules with axes of pseudo-symmetry, which may produce an approximate fit at several orientations, if a fine sampling grid is used. In the case of a coarse grid (especially in rotational searches), the minimum value of the residual may sometimes refer to such an approximate fit. The calculation of $|\overline{\Delta r}|$ from the values of reciprocal-space residuals, if proved credible, should give an *a priori* indication of erroneous orientation.

In this paper we present the results of $|\overline{\Delta r}|$ determination for human deoxyhaemoglobin A in space group $P2_12_12$ crystallized from polyethylene glycol (PEG) solutions (Ward, Wishner, Lattman & Love, 1975).

1. Reciprocal-space residuals

The following reciprocal-space residuals may be used as correlation functions:

$$R_1 = \sum |F_o - F_c| / \sum F_o \tag{1}$$

$$R_2 = \sum |F_o^2 - F_c^2| / \sum F_o^2 \tag{2}$$

$$R_3 = \sum (F_o - F_c)^2 / \sum F_o^2 \tag{3}$$

$$R_4 = \sum (F_o^2 - F_c^2)^2 / \sum F_o^4. \tag{4}$$

1.1 R_1 *residual*

The R_1 residual, commonly used in crystallography, should not be confused with the R factor used by Luzzati (1952) to derive the average error in atomic coordinates. Luzzati points out that the R factor expressed by

$$R = (\overline{||F_o| - |F_c||}) / \overline{|F_o|} \tag{5}$$

is a function of D only, where the latter defines the error of the model, as expressed by

$$D(\mathbf{s}) = \overline{\cos 2\pi(\Delta r \times \mathbf{s})}, \tag{6}$$

while R_1 (1) depends on the values of $\mathbf{s}_{max}$ ($|s| = 2 \sin\theta/\lambda$) and the atomic scattering factors. In order to obtain an accurate value of $|\overline{\Delta r}|$, the R (5) factor should be calculated for shells of constant $|s|$. In the case of protein crystals, the reciprocal lattice is very densely packed, and the R_1 residual, calculated for shells of data, is a fairly good approximation of the R factor of Luzzati. Hence, the calculation of D from protein data sets seems to be more reliable than in the case of simple organic or inorganic crystals. When the value of D is known, $|\overline{\Delta r}|$ may be calculated with equations (49), (50) and (51) of Luzzati (1952).

1.2. R_2 *residual*

The R_2 residual is a rarely used factor. It has never been used, at least to our knowledge, to calculate D and hence $|\overline{\Delta r}|$, but the numerator of (2) – $\sum |F_o^2 - F_c^2|$ – appears in the equation for the r.m.s. error in the difference Fourier synthesis – $\langle \Delta\delta^2 \rangle$ – derived by Henderson & Moffat (1971),

$$\langle \Delta\delta^2 \rangle = \frac{2}{V^2 h} \sum \Delta F^2(h). \tag{7}$$

1.3. R_3 *residual*

The physical interpretation of refinement based on the minimization of the R_3 residual was given by Wilson (1976). He points out that the minimum of R',

$$R' = \sum |F_o - F_c|^2, \tag{8}$$

corresponds to the best fit, in the least-squares sense, between the observed and calculated electron densities. If the model is correctly oriented and there are small errors in coordinates,

$$R'' = \sum \big||F_o| - |F_c|\big|^2 \tag{9}$$

is a good approximation of R'.

Parthasarathy & Parthasarathi (1972) have shown that, provided Wilson's (1949) distribution functions apply, it is possible, with the value of R_3, to calculate $|\overline{\Delta r}|$ even if an incomplete model has been used. They derived expressions for R_3 as a function of D and σ^2; the latter is a measure of the incompleteness of the model, and may be easily calculated (10) if we know the number of atoms the structure contains (N) and the number of atoms in the model (C).

$$\sigma_1^2 = \sum_i^C f_i^2 / \sum_i^N f_i^2. \tag{10}$$

Assuming that there is no error in the intensity data, we may use (11) and (12) to calculate the value of D for centric and acentric cases, respectively:

$$R_3 = 1 + \sigma_1^2 - (4\sigma_1^2/\pi)\,|(1 - \sigma_1^2 D^2)^{1/2} + \sigma_1 D \sin^{-1}(\sigma_1 D)|, \tag{11}$$

$$R_3 = 1 + \sigma_1^2 - 2\sigma_1 \left| \int^{\pi/2} \xi^{1/2}\, d\varphi - \frac{1 - \sigma_1^2 D^2}{2} \int^{\pi/2} \xi^{-1/2}\, d\varphi \right|, \tag{12}$$

where $\xi = 1 - \sigma_1^2 D^2 \sin^2\varphi$.

According to Parthasarathy & Parthasarathi (1972), (11) and (12) hold only for triclinic space groups.

1.4. R_4 residual

Wilson (1976) also gave a physical interpretation of the refinement based on the minimization of the R_4 (4) residual. Such refinement leads to the best fit – in the least-squares sense – between the Patterson syntheses of the observed and calculated intensities. Parthasarathy & Parthasarathi (1972) have derived expressions for R_4 as a function of D and σ_1^2, for centric (13) and acentric (14) cases, when there are no errors in the intensity data.

$$R_4 = 1 + \sigma_1^4 - \tfrac{2}{3}\sigma_1^2 - \tfrac{4}{3}\sigma_1^4 D^2 \qquad (13)$$

$$R_4 = 1 - \sigma_1^2(1 - \sigma_1^2) - \sigma_1^4 D^2. \qquad (14)$$

Moreover, it is possible to apply these expressions to the majority of monoclinic and orthorhombic space groups, provided that Wilson's distribution functions apply.

2. The calculation of $|\overline{\Delta r}|$ in protein crystallography

As already stated, it is assumed that the calculations of standard deviations of the atomic positions is rather difficult (Blundell & Johnson, 1976). Luzzati (1952) and Cruickshank (1949) methods of error estimation are usually regarded as upper and lower limits, respectively. Fermi (1975) and Huber *et al.* (1974) have also applied the method of Lipson & Cochran (1966), but Fermi (1975) found the resulting $|\overline{\Delta r}|$ value for the model of deoxyhaemoglobin unreasonably low.

Since the Luzzati method assumes that the sole cause of disagreement between the observed and calculated structure amplitudes is positional errors in the atoms, other inevitable errors (errors in the observed amplitudes, errors in the model structure) lead to overestimation of $|\overline{\Delta r}|$. There is some evidence, however, that this overestimation does not play a significant role, and the Luzzati method gives a much better estimate of the error than other methods. Fermi (1975) found that the error in atomic coordinates of human deoxyhaemoglobin calculated by this method was in good agreement with the overall r.m.s. error calculated from lack of symmetry 0·4–0·5, 0·4, respectively. Chambers & Stroud (1979) have compared the estimates of $|\overline{\Delta r}|$ obtained for two independently refined models of bovine trypsin by the Luzzati method with figures obtained by direct comparison of the coordinate sets, and found the results consistent. Fermi & Perutz (1977) have calculated the R_1 factor between calculated structure amplitudes derived from a model of deoxyhaemoglobin in two positions differing by a rotation of 1·4° about the molecular dyad; this rotation is equivalent to the $|\overline{\Delta r}|$ value of 0·5 Å. Fig. 1 in the paper of Fermi & Perutz (1977) shows the plot of the R_1 value (calculated in shells) against 2 sin θ/λ, and its agreement with the theoretical curve for $|\overline{\Delta r}| = 0{\cdot}5$ Å. We may observe that the overestimation of the error by the Luzzati method is almost insignificant. Moreover, as pointed out by Fermi & Perutz (1977) this calculation proves that the method of Luzzati can be used to estimate $|\overline{\Delta r}|$ even if the latter is not randomly distributed, but results from a rotation of the whole molecule.

Nixon & North (1976) have used the results of Parthasarathy & Parthasarathi (1972) to calculate $|\overline{\Delta r}|$ for human lysozyme in space group $P2_12_12_1$ from the values of R_3 and R_4. This was possible since Wilson's distribution functions were shown to apply surprisingly well to human lysozyme data in both the low- and high-angle parts. The agreement of the results so obtained, even though (11) and (12) are not fully applicable to orthorhombic space groups (see § 1.3), with those calculated by the Luzzati method further increases the credibility of the latter.

3. Human deoxyhaemoglobin A

The structure of human deoxyhaemoglobin A in space group $P2_1$ is known from the work of Fermi (1975). We have used the atomic coordinates kindly provided by Dr O. Kennard from the Protein Data Bank (Bernstein *et al.*, 1977). X-ray diffraction intensities from HbA crystals grown from solutions containing polyethylene glycol (space group $P2_12_12$) were measured to a resolution of 3·5 Å by Ward *et al.* (1975) and a copy of these data was kindly supplied by Dr J. C. Hanson.

All calculations described in this paper were performed with the HbA tetramer positioned in the PEG unit cell as described elsewhere (Derewenda, Dodson, Dodson & Brzozowski, 1981).

Structure factors were calculated from the positions of all non-hydrogen atoms; atomic form factors have been used.

4. Wilson's statistics

As already pointed out (§ 1), the derivation of $|\overline{\Delta r}|$ on the basis of R_3 and R_4 is not possible, unless Wilson's distribution functions apply. Fig. 1 shows histograms of the distributions of observed and calculated structure factors for human HbA data. The solid line is derived from equations (16) and (17) of Nixon & North (1976) taking – as these authors suggest – $\sum$ as the mean F^2 for each shell of data. It is clearly seen that the agreement of the distributions of F_o and F_c with

theoretical curves is good. Hence, as in the case of the lysozyme data, the results of Parthasarathy & Parthasarathi (1972) may be used. It is noteworthy, however, that centric data exhibit deviations from theory greater than acentric data. This effect may be partially explained by the scarcity of weak centric reflections.

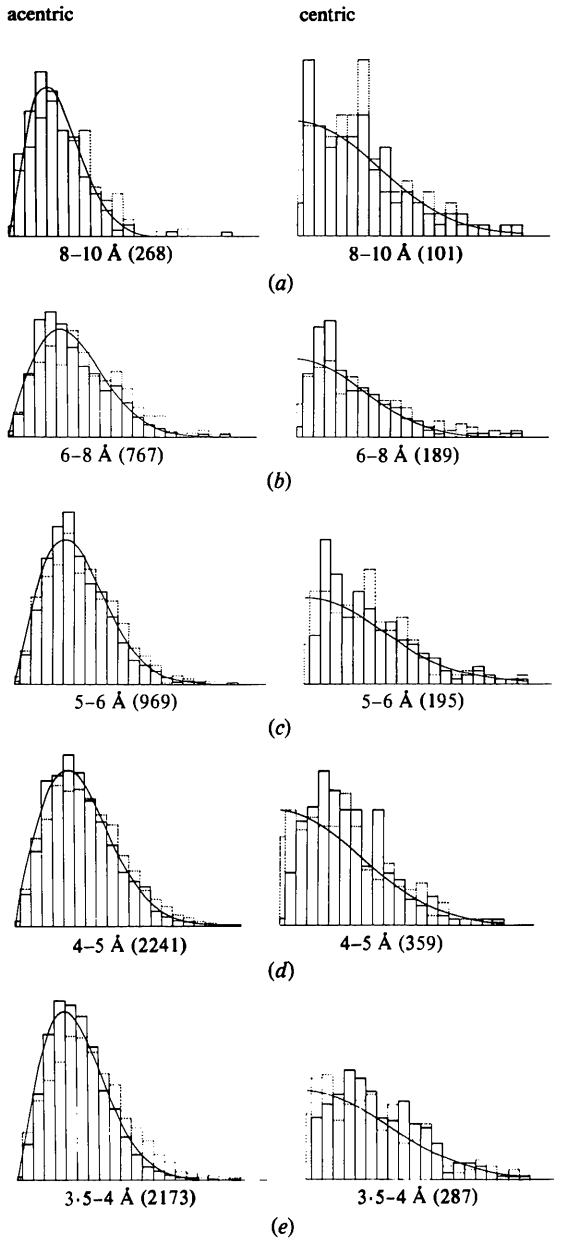


Fig. 1. Distribution functions for structure factors of human deoxyhaemoglobin crystallized from PEG solutions. (*a*) For resolution range 10–8 Å; (*b*) 8–6 Å; (*c*) 6–5 Å; (*d*) 5–4 Å; (*e*) 4–3·5 Å; the solid histograms are F_o, the dotted histograms are F_c. The ordinate is the number of structure factors with value F. The units of F are arbitrary. The number in brackets is the number of reflexions in each set.

5. Derivation of $|\overline{\Delta r}|$ value with various reciprocal-space residuals

5.1. *Derivation of D and* $|\overline{\Delta r}|$ *by the Luzzati* (1952) *method*

Fig. 2 shows a plot of R_1, $\overline{F}_o$ and $\overline{F}_c$ against s ($2 \sin \theta/\lambda$). The calculations were performed for shells of data, and an overall scale factor and isotropic temperature factor (20 Å^2) were applied. The solid line is derived from equation (51) and Table 1 of Luzzati (1952). As observed by Fermi (1975) there is complete disagreement of the R_1 factor with the theoretical curve at low resolution. Note that the maxima of R_1 correspond to regions where there is considerable disagreement between the values of $\overline{F}_o$ and $\overline{F}_c$.

The use of individual scale factors, calculated independently for each shell of data, improved the agreement in the low-resolution range, having, however, no effect on the resulting $|\overline{\Delta r}|$ value. Furthermore, characteristic minima and maxima of R_1 remained (see Fig. 4).

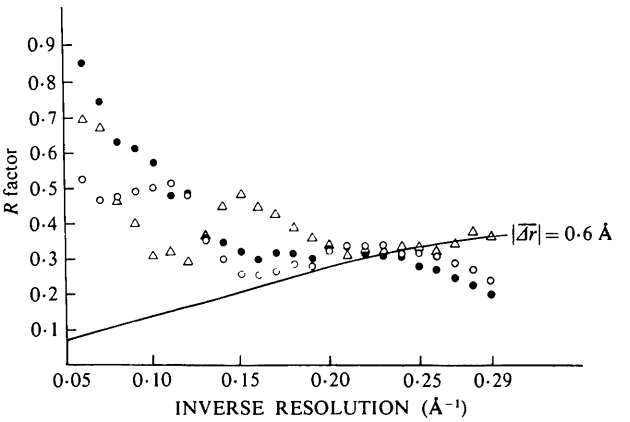


Fig. 2. R_1 factor as a function of inverse resolution. △ R_1 factor; ● $\overline{F}_c$; ○ $\overline{F}_c$. Theoretical curve drawn according to Luzzati (1952). Other details in the text.

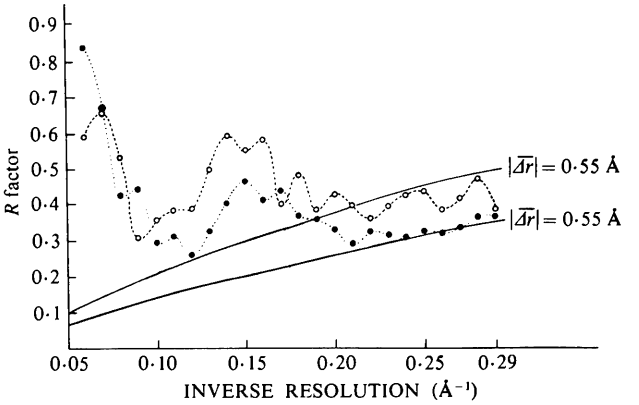


Fig. 3. R_1 as a function of inverse resolution, for centric and acentric data sets. ○ Centric data; ● acentric data. Solid curves drawn according to Luzzati (1952) for centric (upper curve) and acentric cases.

Table 1. *Root-mean-square error in deoxyhaemoglobin atomic coordinates calculated from different reciprocal-space residuals for shells of data, separated into centric and acentric regions*

Resolution Min	Max	R_1	D	$\overline{\lvert\Delta r\rvert}$	R_3	D	$\overline{\lvert\Delta r\rvert}$	R_4	D	$\overline{\lvert\Delta r\rvert}$	Number of reflexions
Centric data											
10·0	8·0	0·3486	0·926	0·896	0·1185	0·929	0·877	0·1591	0·938	0·818	101
8·0	6·0	0·5222	0·810	1·154	0·2874	0·803	1·178	0·5024	0·789	1·224	189
6·0	5·0	0·3936	0·902	0·641	0·1712	0·893	0·665	0·2878	0·884	0·693	195
5·0	4·0	0·3994	0·900	0·525	0·1954	0·876	0·588	0·3703	0·850	0·652	359
4·0	3·5	0·4166	0·893	0·453	0·2109	0·864	0·515	0·3266	0·870	0·530	287
Acentric data											
10·0	8·0	0·2664	0·908	1·004	0·0234	0·912	0·981	0·1536	0·920	0·933	268
8·0	6·0	0·3500	0·819	1·150	0·1381	0·840	1·050	0·2839	0·846	1·028	767
6·0	5·0	0·3459	0·830	0·853	0·1403	0·837	0·833	0·3118	0·830	0·853	969
5·0	4·0	0·3175	0·860	0·628	0·1199	0·865	0·616	0·2479	0·867	0·611	2241
4·0	3·5	0·3393	0·837	0·568	0·1364	0·842	0·559	0·2941	0·840	0·562	2173

Table 2. *Root-mean-square error in deoxyhaemoglobin atomic coordinates determined with complete and partial model structures.*

Column 3 contains the average $\overline{\lvert\Delta r\rvert}$ for the complete model; R_3 and R_4 refer to the values of F_c calculated for a partial model. Only acentric data have been used in these calculations.

Resolution		Complete model	Incomplete model					
					$\sigma_1^2 = 1{\cdot}0$		$\sigma_1^2 = 0{\cdot}95$	
Min	Max	$\overline{\lvert\Delta r\rvert}$ (Å)	R_3	R_4	$\overline{\lvert\Delta r\rvert}(R_3)$	$\overline{\lvert\Delta r\rvert}(R_4)$	$\overline{\lvert\Delta r\rvert}(R_3)$	$\overline{\lvert\Delta r\rvert}(R_4)$
4·44	4·26	0·60	0·121	0·263	0·61	0·61	0·56	0·58
4·26	4·08	0·52	0·116	0·218	0·56	0·54	0·49	0·49
4·08	3·92	0·57	0·135	0·283	0·60	0·60	0·56	0·56
3·92	3·77	0·55	0·130	0·291	0·56	0·58	0·52	0·54
3·77	3·64	0·56	0·142	0·308	0·56	0·56	0·54	0·54
3·64	3·51	0·59	0·162	0·343	0·60	0·59	0·57	0·57

It needs to be emphasized that Luzzati (1952) derived expressions for $\overline{\lvert\Delta r\rvert}$ independently for centric and acentric cases; hence, it seems justified to separate the centric and acentric data for calculations. Such a procedure was followed by Nixon & North (1976) in their studies of human lysozyme. Fig. 3 shows a plot of R_1-centric and R_1-acentric against $\lvert s\rvert$. It can be seen that for $\lvert s\rvert > 0{\cdot}21$ Å^{-1} the values of R_1-acentric are in much better agreement with the theoretical curve ($\overline{\lvert\Delta r\rvert} = 0{\cdot}55$ Å) than the values obtained for centric data. This effect may be at least partially explained by the worse agreement of the centric data (Fig. 1) with the theoretical Wilson distribution functions.

5.2. *Derivation of* $\overline{\lvert\Delta r\rvert}$ *from* R_3 *and* R_4 *– complete model structure*

Table 1 shows statistics of the values of R_1, R_3 and R_4, with the resulting values of D and $\overline{\lvert\Delta r\rvert}$, calculated independently for each shell of data. Individual scale factors were applied and centric and acentric data were treated separately. A significant discrepancy between centric and acentric data in the cases of R_3 and R_4 residuals was probably due to analogous reasons to those in the case of R_1 (see § 5.1). We assume that the results based on the analysis of acentric data are more reliable; they are plotted in Fig. 4 against $\lvert s\rvert$ and compared with the theoretical curves. The latter were calculated with Table 1 and equation (51) of Luzzati (1952), and from (11) to (14) by numerical methods, where necessary. It may be seen that, although for $\lvert s\rvert$

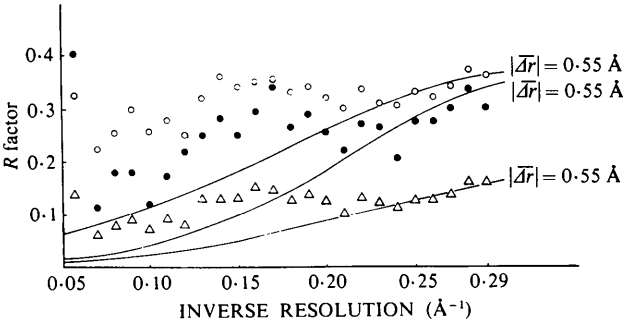


Fig. 4. R_1, R_3 and R_4 as functions of inverse resolution. Individual scale factors were applied for every shell of data. ○ R_1; △ R_3; ● R_4. Only acentric data were used in the calculation. Solid lines derived as described in the text.

$> 0{\cdot}21$ Å^{-1} all methods lead to the same value of $|\overline{\Delta r}|$, R_3 is the least-noisy function.

5.3. *Derivation of* $|\overline{\Delta r}|$ *from* R_3 *and* R_4 – *incomplete model structure*

Nixon & North (1976) have observed that for the values of R_3 and R_4 the corresponding values of D were not sensitive to the value chosen for σ_1^2.

During our structure-factor calculations the haem groups of haemoglobin were handled separately, so a set of F_c based on a partial model consisting of globin atoms only was available. We have calculated the values of D and $|\overline{\Delta r}|$ from this set of data and all three previously described methods.

Table 2 shows the results of the calculations with two values of σ_1^2, 1·0 and 0·95, the latter corresponding to the actual value for the globin model. Only acentric data for $|s| > 0{\cdot}22$ are included in the table.

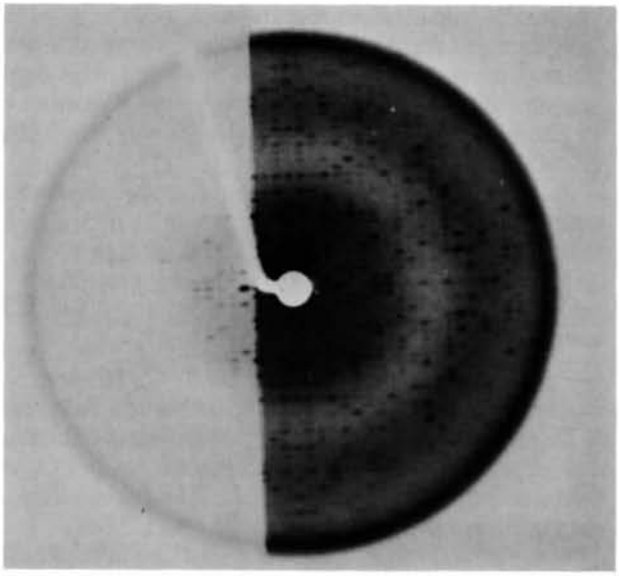
It is evident that, although the use of $\sigma_1^2 = 0{\cdot}95$ leads to lower values of $|\overline{\Delta \mathbf{r}}|$, the difference is small and both results are close to the value of $|\overline{\Delta \mathbf{r}}|$ calculated for a complete model. It is possible that the value of 0·95 was too high to produce any significant differences, but we did not carry out calculations for models of lower σ_1^2.

6. Treatment of low-resolution data

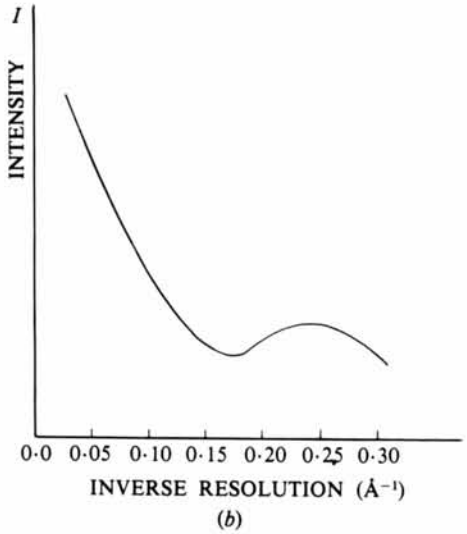
As already pointed out (§§ 5.1, 5.2) there is considerable disagreement of the R-factor values with theoretical curves at low resolution ($|s| < 0{\cdot}21$ Å^{-1}). It is interesting, however, that the minima and maxima of all R factors occur in identical positions in Fig. 1 of Fermi (1975) and in our calculations; moreover, other authors describe similar variations for other proteins [see, for example, Fig. 10.11 of Blundell & Johnson (1976)]. Fermi (1975) suggests that such discrepancies may – at least in part – result from the omission of the solvent molecules from the model structure and from the assumed random spacings of atoms in the theoretical calculations. Fig. 1 of Fermi & Perutz (1977) shows that if the R factor is calculated for structure amplitudes derived from a model in two positions (see § 2) the agreement with the theoretical curve extends below $|s| = 0{\cdot}1$ Å^{-1}. We believe, therefore, that the assumptions of random spacing in theoretical calculations does not play a significant role. Hence, solvent scattering seems to be of major importance. Fig. 5 shows a precession photograph of a haemoglobin crystal grown from polyethylene glycol solution and the radial distribution of the background intensity. The same effect can also be observed with other proteins. The minima and maxima on this plot coincide with the maxima and minima of the R factors on previous figures. Such a background intensity distribution in the region $0{\cdot}1 < |s| < 0{\cdot}21$ Å^{-1} seems to be caused primarily by solvent scattering, as air and glass scatter at different angles (Krieger & Stroud, 1976).

7. Discussion

The results presented in this paper show that the estimation of standard deviations of atomic coordinates of a model protein molecule on the basis of reciprocal-



(*a*)



(*b*)

Fig. 5. (*a*) An overexposed precession photograph of oxyhaemoglobin crystallized from PEG; half of the film was shielded with aluminium foil for data-collection purposes. (*b*) Radial distribution of background intensity on the photograph in (*a*); units of I are arbitrary.

space residuals, R_1, R_3 and R_4, leads to values which are in good agreement with each other. The following points seem noteworthy.

1. There is considerable evidence that the Luzzati method leads to overall values of $|\overline{\Delta r}|$ which are consistent with the actual differences in the model coordinates. Some overestimation of $|\overline{\Delta r}|$ may be caused by the application of 'acentric equations' to the overall data. Our results have shown that different reciprocal-space residuals give results consistent with each other. We have therefore confirmed that these methods may be useful in the determination of $|\overline{\Delta r}|$ in those cases where direct comparison of coordinates is impossible (*e.g.* medium-resolution studies).

2. Our results confirm that Wilson's statistics may be applied successfully to both low- and high-angle protein diffraction data. Hence, the results of Parthasarathy & Parthasarathi (1972) may be used to calculate $|\overline{\Delta r}|$.

3. We have found that the methods used gave consistent results for the region $|s| > 0{\cdot}21$ Å^{-1}. R_3 was found to be the least-noisy function in this region.

4. We have confirmed that the low-angle data is significantly affected by solvent scattering, which is also the cause of high background intensity.

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Interference Effects Among Variants*

BY BERNARD BORIE

The Metals and Ceramics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37830, *USA*

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Abstract

There have been several recent efforts to account for the broadening of the superstructure Bragg maxima and their displacements in reciprocal space observed for partially transformed b.c.c. solid solutions containing the ω phase. They have been concerned with intensity calculations from models for which the ω regions are defective in a variety of senses. All of the models include only one ω variant, while in fact the system must contain four equally likely variants. A method to correct the calculated intensity for interference effects among the variants, omitted from these models, is described. It is applied to a specimen model. Possible applications of the method are discussed.

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