Table 18.5.7.1. *Comparison of full-matrix $\sigma(r, B_{\rm avg})$ with the diffraction-component precision index (DPI)*

Protein	$(N_i/p)^{1/2}$	R	$d_{\rm min}$ (Å)	DPI $\sigma(r, B_{\rm avg})$ (Å)	Full-matrix $\sigma_{\rm diff}(r, B_{\rm avg})$ (Å)	Reference
Concanavalin A	0.148	0.128	0.94	0.034	0.033	(*a*)
Immunoglobulin	0.476	0.156	1.70	0.221	0.186	(*b*)

References: (*a*) Deacon *et al.* (1997); (*b*) Usón *et al.* (1999).

18.5.7. Examples of the diffraction-component precision index

18.5.7.1. *Full-matrix comparison with the diffraction-component precision index*

The DPI (18.5.6.9) with R was offered as a quick and rough guide for the diffraction-data-only error for an atom with $B = B_{\rm avg}$. The necessary data for the comparison with the two unrestrained full-matrix inversions of Section 18.5.5 are given in Table 18.5.7.1. For concanavalin A with $B_{\rm avg} = 14.8$ Å^2, the full-matrix quadratic (18.5.4.2*b*) gives 0.033 Å for a carbon atom and the DPI gives 0.034 Å for an unspecified atom. For the immunoglobulin with $B_{\rm avg} = 26.8$ Å^2, the full-matrix quadratic (18.5.4.2*a*) gives $\sigma_{\rm diff}(r) = 0.19$ Å for a carbon atom, while the DPI gives 0.22 Å.

For these two structures, the simple DPI formula compares surprisingly well with the unrestrained full-matrix calculations at $B_{\rm avg}$.

For the restrained full-matrix calculations on concanavalin A, the quadratic (18.5.4.2*c*) with $B = B_{\rm avg}$ gives $\sigma_{\rm res}(r) = 0.028$ Å for a carbon atom, which is only 15% smaller than the unrestrained 0.033 Å. This small decrease matches the discussion of $\sigma_{\rm res}(r)$ and $\sigma_{\rm diff}(r)$ in Section 18.5.4.1 following equation (18.5.4.1). But that discussion also indicates that for the immunoglobulin, the restrained $\sigma_{\rm res}(r, B_{\rm avg})$, which was not computed, will be proportionaly much lower than the unrestrained value of $\sigma_{\rm diff}(r, B_{\rm avg}) = 0.19$ Å, since the restraints are relatively more important in the immunoglobulin.

18.5.7.2. *Further examples of the DPI using R*

Table 18.5.7.2 shows a range of examples of the application of the DPI (18.5.6.9) using R to proteins of differing precision, starting with the smallest $d_{\rm min}$. In all the examples, N_i has been set equal to $n_{\rm atoms}$, the total number of atoms. The ninth and tenth columns show $\langle \Delta r \rangle$ values derived from Luzzati (1952) and Read (1986) plots described later in Section 18.5.8.

The first entry is for crambin at 0.83 Å resolution and 130 K (Stec *et al.*, 1995). Their results were obtained from an unrestrained full-matrix anisotropic refinement. Inversion of the full matrix gave s.u.'s $\sigma_{\rm diff}(x) = 0.0096$ Å for backbone atoms, 0.0168 Å for side-chain atoms and 0.0409 Å for solvent atoms, with an average for all atoms of 0.022 Å. The DPI $\sigma(r, B_{\rm avg}) = 0.021$ Å corresponds to $\sigma(x) = 0.012$ Å, which is satisfactorily intermediate between the full-matrix values for the backbone and side-chain atoms.

Sevcik *et al.* (1996) carried out restrained anisotropic full-matrix refinements on data from two slightly different crystals of ribonuclease Sa, with $d_{\rm min}$ of 1.15 and 1.20 Å. They inverted full-matrix blocks containing parameters of 20 residues to estimate coordinate errors. The overall r.m.s. coordinate error for protein atoms is given as 0.03 Å, and for all atoms (including waters and ligands) as 0.07 Å for MGMP and 0.05 Å for MSA. The DPI gives $\sigma(r, B_{\rm avg}) = 0.05$ Å for both structures.

The next entries concern the two lower-resolution (1.8 and 1.95 Å) studies of TGF-β2 (Daopin *et al.*, 1994). The DPI gives $\sigma(r) = 0.16$ Å for 1TGI and 0.24 Å for 1TGF. This indicates an r.m.s. position difference between the structures for atoms with $B_i = B_{\rm avg}$ of $(0.16^2 + 0.24^2)^{1/2} = 0.29$ Å. Daopin *et al.* reported the differences between the two determinations, omitting poor parts, as $\langle \Delta r \rangle_{\rm rms} = 0.15$ Å (main chain) and 0.29 Å (all atoms).

Human diferric lactoferrin (Haridas *et al.*, 1995) is an example of a large protein at the lower resolution of 2.2 Å, with a high value of $(N_i/p)^{1/2}$, leading to $\sigma(r, B_{\rm avg}) = 0.43$ Å.

Three crystal forms of thaumatin were studied by Ko *et al.* (1994). The orthorhombic and tetragonal forms diffracted to 1.75 Å, but the monoclinic $C2$ form diffracted only to 2.6 Å. The structures with 1552 protein atoms were successfully refined with restraints by *XPLOR* and *TNT*. For the monoclinic form, the number of parameters exceeds the number of diffraction observations, so (N_i/p) is negative and no estimate by (18.5.6.9) of the diffraction-data-only error is possible. The DPI (18.5.6.9) gives 0.17 and 0.16 Å for the orthorhombic and tetragonal forms, respectively.

18.5.7.3. *Examples of the DPI using $R_{\rm free}$*

As in the case of monoclinic thaumatin, for low-resolution structures the number of parameters may exceed the number of diffraction data. To circumvent this difficulty, it was proposed in Section 18.5.6.3 to replace $p = n_{\rm obs} - n_{\rm params}$ by $n_{\rm obs}$ and R by $R_{\rm free}$ in a revised formula (18.5.6.10) for the DPI. Table 18.5.7.3 shows examples for some structures for which both R and $R_{\rm free}$ were

Table 18.5.7.2. *Examples of diffraction-component precision indices (DPIs)*

Protein	N_i	$n_{\rm obs}$	$(N_i/p)^{1/2}$	$C^{-1/3}$	R	$d_{\rm min}$ (Å)	DPI $\sigma(r, B_{\rm avg})$ (Å)	Luzzati $\langle \Delta r \rangle$ (Å)	Read $\langle \Delta r \rangle$ (Å)	Reference
Crambin	447	23759	0.150	1.074	0.090	0.83	0.021	0.055		(*a*)
Ribonuclease MGMP	1958	62845	0.208	1.046	0.109	1.15	0.047		0.08	(*b*)
Ribonuclease MSA	1832	60670	0.204	1.016	0.106	1.20	0.045		0.05	(*b*)
TGF-β2 1TGI	948	~14000	0.305	~1.0	0.173	1.80	0.16	0.21	0.18	(*c*)
TGF-β2 1TFG	974	~11000	0.370	~1.0	0.188	1.95	0.24	0.23		(*c*)
Lactoferrin	5907	39113	0.618	1.036	0.179	2.20	0.43	0.25–0.30	0.35	(*d*)
Thaumatin C2	1552	4622	*	1.10	0.184	2.60	—	0.25		(*e*)

References: (*a*) Stec *et al.* (1995); (*b*) Sevcik *et al.* (1996); (*c*) Daopin *et al.* (1994); (*d*) Haridas *et al.* (1995); (*e*) Ko *et al.* (1994).
* (N_i/p) negative.

references