

Figures of Merit

What is $R(F)$? (also known as $R1$)

$$R_F = \frac{\sum_{hkl} \left| |F_o(hkl)| - |F_c(hkl)| \right|}{\sum_{hkl} |F_o(hkl)|}$$

What is $wR(F^2)$ (also known as $wR2$)

$$wR_{F^2} = \left[\frac{\sum_{hkl} \left[w \left(F_o^2(hkl) - F_c^2(hkl) \right)^2 \right]}{\sum_{hkl} \left(F_o^2(hkl) \right)^2} \right]^{1/2}$$

What is $S(F^2)$ (also known as Goof or $S2$)

$$S_{F^2} = \left[\frac{\sum_{hkl} \left[w \left(F_o^2(hkl) - F_c^2(hkl) \right)^2 \right]}{N_{data} - N_{parameters}} \right]^{1/2}$$

What is R_{int}

$$R_{int} = \frac{\sum_{hkl} \left| F_o^2(hkl) - \overline{F_o^2(hkl)} \right|}{\sum_{hkl} F_o^2(hkl)}$$

What is R_{sigma} ?

$$R_{\text{sigma}} = \frac{\sum_{hkl} \sigma(F_o^2(hkl))}{\sum_{hkl} F_o^2(hkl)}$$

What is R_{sym} ?

$$R_{\text{sym}} = \frac{\sum_{hkl} \sum_{i=1}^n |I_i(hkl) - I_i(\bar{h}\bar{k}\bar{l})|}{\sum_{hkl} \sum_{i=1}^n I_i(hkl)}$$

What is R_{merge}

$$R_{\text{merge}} = \frac{\sum_{hkl} \sum_{i=1}^n |I(hkl) - I_i(hkl)|}{\sum_{hkl} N \times I(hkl)}$$

What is V_m , V_{protien} and V_{solvent} ?

$$V_m = 2.15 \text{ \AA}^3 / \text{Daltons} \quad [\text{Mathews, J. Mol. Biol. (1968) } \mathbf{33}, 491-497]$$

$$V_{\text{protien}} = 1.23 / V_m$$

$$V_{\text{solvent}} = 1 - V_{\text{protein}}$$

What is F_n

$$F_n = \frac{1}{\langle \Delta 2\theta \rangle} \times \frac{N}{N(\theta)_{\text{calculated}}}$$

What is M_{20} ?

$$M_{20} = \frac{Q_{20}}{2 \langle Q \rangle N_{20}}$$

where Q_{20} is the Q (quadratic form) value for the 20th observation, $\langle Q \rangle$ is the average discrepancy for the first 20 observations, N_{20} are the number of Q values that are indexed.

What are the Quadratic Forms?

Cubic	$Q = (h^2 + k^2 + l^2)a_{11}$
Tetragonal	$Q = (h^2 + k^2)a_{11} + l^2 a_{33}$
Hexagonal	$Q = (h^2 + hk + l^2)a_{11} + l^2 a_{33}$
Orthorhombic	$Q = h^2 a_{11} + k^2 a_{22} + l^2 a_{33}$
Monoclinic	$Q = h^2 a_{11} + k^2 a_{22} + l^2 a_{33} + hla_{13}$
Triclinic	$Q = h^2 a_{11} + k^2 a_{22} + l^2 a_{33} + hka_{12} + hla_{13} + kla_{23}$

$$a_{11} = a^{*2} \quad a_{22} = b^{*2} \quad a_{33} = c^{*2} \quad a_{12} = 2a^* b^* \cos \gamma^* \quad a_{13} = 2a^* c^* \cos \beta^* \quad a_{23} = 2b^* c^* \cos \alpha^*$$