Hydrogen Bond Computing Server (HBCS): An online web server to compute hydrogen bond interactions with their precision

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CALCULATION OF ATOMIC COORDINATE ERROR:

Diffraction precision index (DPI) was first introduced by Cruickshank (Cruickshank, 1999) as a quantitative descriptor to estimate the coordinate error $\sigma(x, B_{avg})$ of an 'average atom' *i.e.* whose B factor is the average B factor of the refined model. DPI, derived from experimental crystallographic parameters, is computationally very efficient unlike the full-matrix error estimate. Though it is an approximation, it has been shown that the DPI agrees very well with the full-matrix error estimate (Cruickshank, 1999). The coordinate error of each atom can be calculated using equation (1), which takes account of the B factor of an individual atom versus that of an average atom,

$$Atomic\ coordinate\ error = DPI\ \left(B_{atom}/B_{average}\right)^{1/2} \qquad (1)$$

The overall DPI itself can be calculated using equation 2

$$\sigma(x, B_{avg}) = (N_i/p)^{1/2} C^{-1/3} R_{work} d_{min} \qquad (2a)$$

$$\sigma(x, B_{avg}) = (N_i/n_{obs})^{1/2} C^{-1/3} R_{free} d_{min} \qquad (2b)$$

where N_i is the number of fully occupied atoms, $p = n_{obs} - n_{params}$, n_{obs} is the number of reflections used in the refinement, n_{params} is the number of parameters, C is the diffraction data completeness, d_{min} is the resolution of the diffraction data and the R (reliability) factor (either R_{work} or R_{free}).

Finally, the precision of any interatomic distance (d) and angle (θ) can be quantified by harnessing the atomic displacement parameters of any individual interacting atoms (labeled 'A', 'B' and 'C' in equation 3 and 4). A more detailed discussion on this subject has been presented by the authors elsewhere (Kumar *et al.*, 2015, Gurusaran *et al.*, 2014).

$$\sigma_d = (\sigma_A^2 + \sigma_B^2)^{1/2} \quad (3)$$

$$\sigma_\theta = \left(\frac{\sigma_A^2}{d_{AB}^2} + \frac{\sigma_B^2 d_{AC}^2}{d_{AB}^2 d_{BC}^2} + \frac{\sigma_C^2}{d_{BC}^2}\right)^{1/2} \quad (4)$$

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