10.8: Real-space correlation coefficient

The real-space correlation coefficient, RSCC, is a measure of the similarity between an electron-density map calculated directly from a structural model and one calculated from experimental data. An advantage of techniques for evaluating goodness of fit in real space is that they can be performed for arbitrary sets of atoms. They are therefore used most often in the refinement of biological macromolecular structures to improve the model fit on a per-residue basis.

$$\mathrm{RSCC} = \frac{\sum |\rho_{obs} - \langle\rho_{obs}\rangle| \sum |\rho_{calc} - \langle\rho_{calc}\rangle|}{\sqrt{\sum |\rho_{obs} - \langle\rho_{obs}\rangle|^2 \sum |\rho_{calc} - \langle\rho_{calc}\rangle|^2}}$$

(ρ's are electron density values at grid points that cover the residue in question, obs and calc refer to experimental and model electron density, respectively.)

This metric is similar to the real-space residual RSR, but does not require that the two densities be scaled against each other.