10.9: Real-space residual

The real-space residual, RSR, 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.

$$\mathrm{RSR} = \frac{\sum |\rho_{obs} - \rho_{calc}|}{\sum |\rho_{obs} + \rho_{calc}|}$$

(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.)

The measure of similarity is often provided in the form of a graph of RSR values against residue number, showing clearly which residues give best and worst agreement with the experimental electron-density map. For nucleic acid structures, RSR may also be calculated separately for base, sugar and phosphate moieties of the nucleic acid monomer. RSR is generally considered an excellent model-validation tool.