Local protein structure validation revisited

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Motivation
Structure validation by computational methods is an important tool in protein crystallography. Stereochemical criteria are mainly used to distinguish locally between distorted and adequately refined models. However, the readily available criteria are not sufficient to clearly establish the global quality, producing only rough indications instead.
Methods
A new criterion, called TAP, measuring local sequence to structure fitness based on torsion angle propensities normalized against the global optimum is introduced.
Results
It is shown to correlate well with experimental parameters for global X-ray accuracy. The TAP score can be used directly to validate the correctness of refined X-ray models. It is shown to have a two to five times higher correlation with experimental quality measures than previous methods. Highly selective TAP thresholds are derived to recognize over 99% of the top experimental structures in the absence of experimental information. Estimating the local interactions can help in the accurate determination of protein conformation by experimental and computational means.

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