

MOTIVATION:

We introduce the iRMSD, a new type of RMSD, independent from any structure superposition and suitable for evaluating sequence alignments of proteins with known structures.

RESULTS: We demonstrate that the iRMSD is equivalent to the standard RMSD although much simpler to compute and we also show that it is suitable for comparing sequence alignments and benchmarking multiple sequence alignment methods. We tested the iRMSD score on 6 established multiple sequence alignment packages and found the results to be consistent with those obtained using an established reference alignment collection like Prefab.

AVAILABILITY: The iRMSD is part of the T-Coffee package and is distributed as an open source freeware (<http://www.tcoffee.org/>).