Figure S3: Investigating Cα distance based scoring approaches in the context of automated evaluations

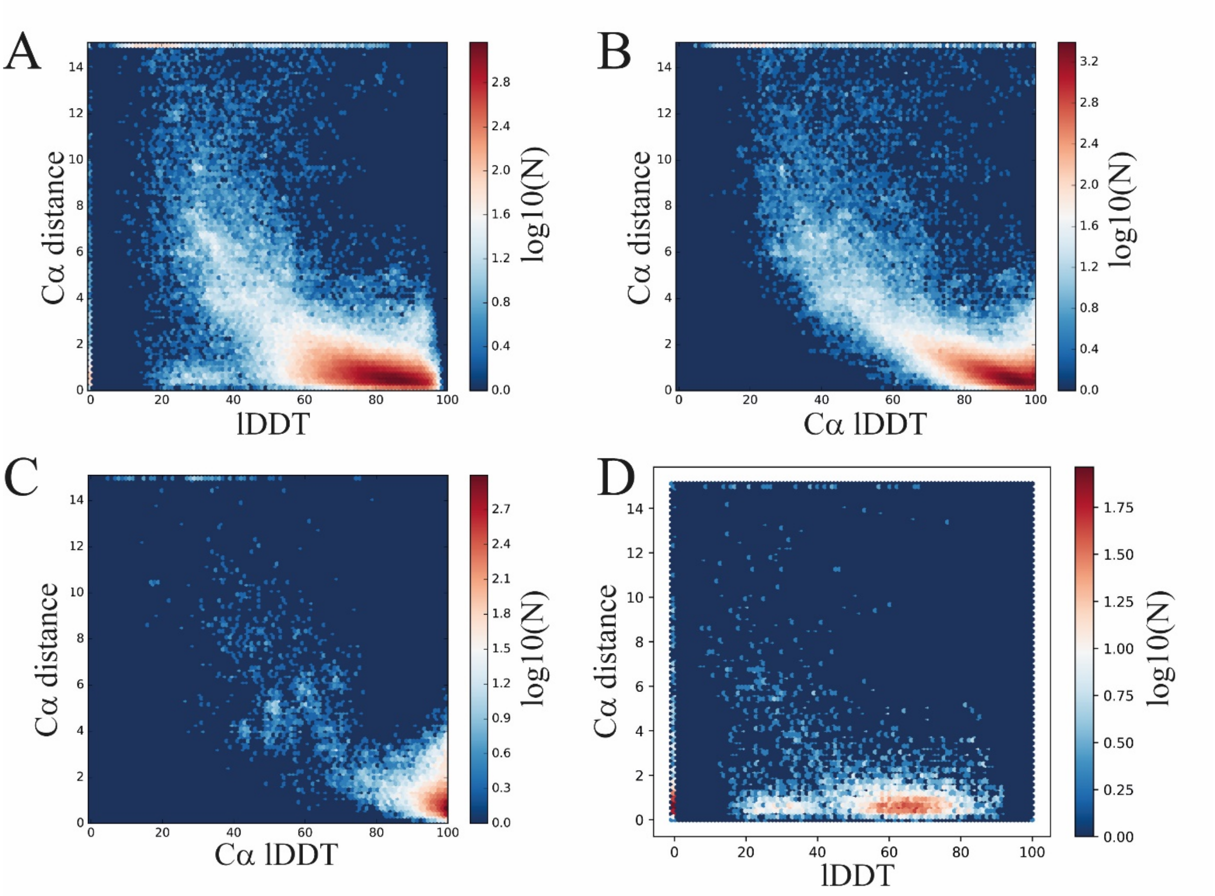

Figure S3 Evaluating high quality models based on a superposition-dependent global score in the context of fully automated evaluations: We were in particular focusing on robustly assessing domain orientations and have, thus, selected a subset of CASP12 models with GDT-TS > 80, resulting in a total of 901 of originally 10771 models on which we have carried out further analysis. The results emphasize the need for a sensitive superposition-independent score. We have exemplarily employed lDDT, an all-atom score accounting for low quality sidechain orientations and stereochemical violations.

Panel A *- even for models exhibiting a high GDT-TS, a low Cα distance does not imply a high per-residue lDDT score. Observed lDDT scores are smeared out over a wide range, from around 20 to close to 100, please note the outliers with lDDT scores of 0, resulting from excluded sidechain atoms by the stereochemistry filter (see Panel D).* ***Panel B*** *- Calculating the lDDT score based on Cα atoms, the correlation with Cα distances improves. Low scores due to sidechains aberrations disappear (lDDT between 20 and 40 with Cα distances below 2 Å).* ***Panel C*** *- Increased Cα distances are observed for the 71 models of target T0903 (pdb id 5a7d) stemming from minor twisting motions based on a superposition based analysis. Yet these minor discrepancies do not account for the poor match in panel A, which are most likely arising from sidechains that are either badly modelled or stereochemically problematic.* ***Panel D*** *– Reduced lDDT scores are observed in 30 models of tertiary structure prediction server TS421. Residues with large stereochemical deviations and physically impossible close contacts are assigned low scores by lDDT.*