

# Flexible structural protein alignment by a sequence of local transformations. Additional Example

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For paper limitations, the following example was not included in the main paper. It shows that the similarity between two different proteins could need relative motion for some parts beyond what traditional RMSD-based structure alignment tools allow.

The example is the pair of Type I PLP-dependent aspartate aminotransferase-like domains 1c4kA2 and 1cj0B2 (CATH 3.40.640.10). ProtDeform aligns 211 of the 313 and 271 sites, respectively, including the 3-layer (aba) sandwich. The alignment has a RMSD of 4.4 and an lRMSD of 2.8. As shown in Figure 1, one part of 1cj0B2 is rotated with respect to the main part.

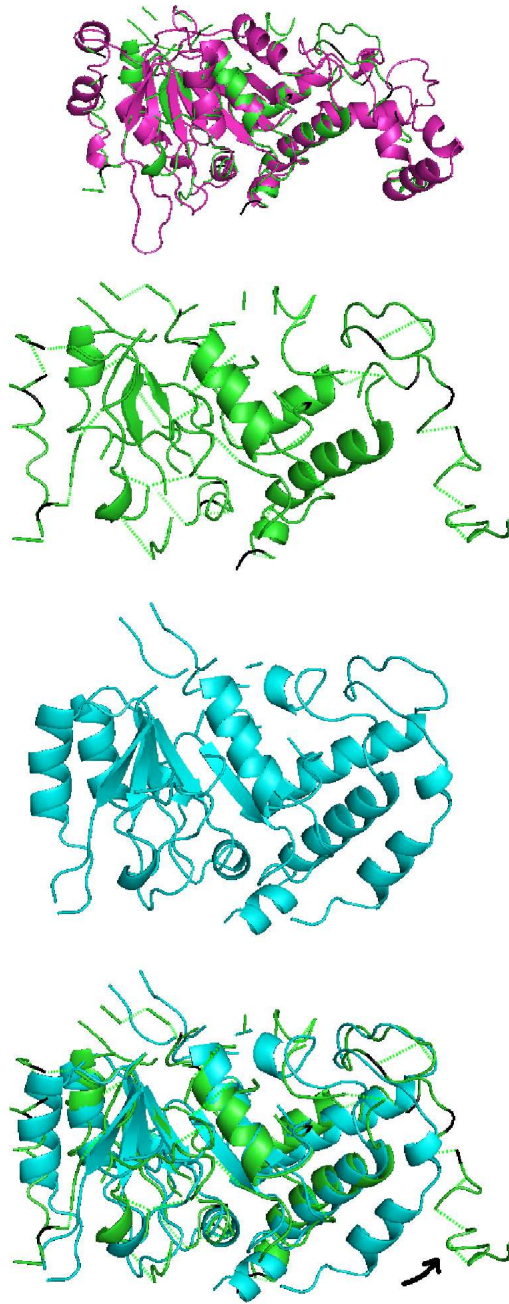


Figure 1: From top to bottom: First, alignment of the deformed domain 1c0B2 (green) and 1c4kA2 (red). Second, the same domain 1c0B2 deformed. Third, the same domain 1c0B2 without deformation. Forth, superposition of the rigid (green) and the deformed<sub>2</sub> (blue) domains; the arrow shows the local rotation.