Impact of AlphaFold on Structure Prediction of Protein Complexes: The CASP15-CAPRI Experiment

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Abstract

We present the results for CAPRI Round 54, the 5th joint CASP-CAPRI protein assembly prediction challenge. The Round offered 37 targets, including 14 homo-dimers, 3 homo-trimers, 13 hetero-dimers including 3 antibody-antigen complexes, and 7 large assemblies. On average ~70 CASP and CAPRI predictor groups, including more than 20 automatics servers, submitted models for each target. A total of 21941 models submitted by these groups and by 15 CAPRI scorer groups were evaluated using the CAPRI model quality measures and the DockQ score consolidating these measures. The prediction performance was quantified by a weighted score based on the number of models of acceptable quality or higher submitted by each group among their 5 best models. Results show substantial progress achieved across a significant fraction of the 60+ participating groups. High-quality models were produced for about 40% for the targets compared to 8% two years earlier, a remarkable improvement resulting from the wide use of the AlphaFold2 and AlphaFold-Multimer software. Creative use was made of the deep learning inference engines affording the sampling of a much larger number of models and enriching the multiple sequence alignments with sequences from various sources. Wide use was also made of the AlphaFold confidence metrics to rank models, permitting top performing groups to exceed the results of the public AlphaFold-Multimer version used as a yard stick. This notwithstanding, performance remained poor for complexes with antibodies and nanobodies, where evolutionary relationships between the binding partners are lacking, and for complexes featuring conformational flexibility, clearly indicating that the prediction of protein complexes remains a challenging problem.

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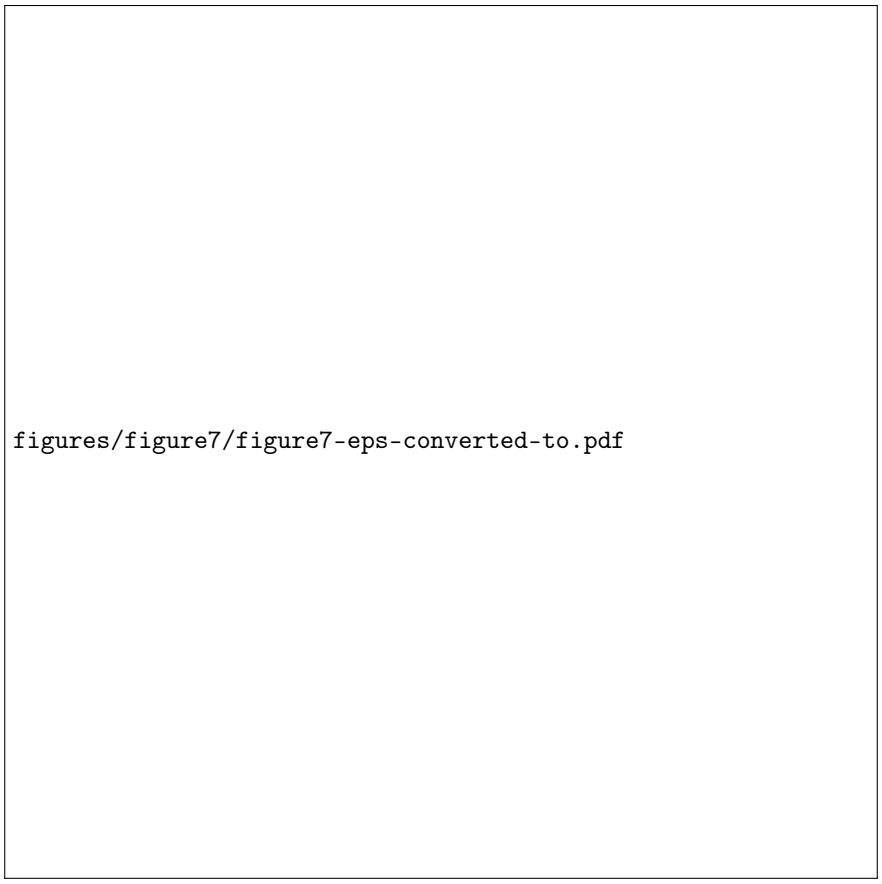

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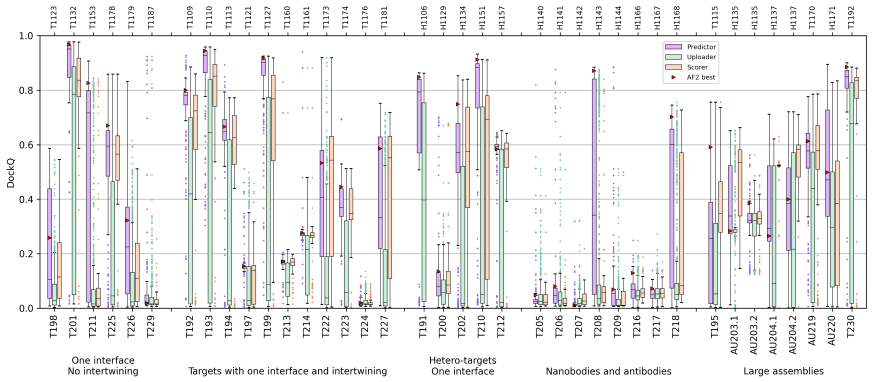

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