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Title:
CASP-SAXS: Comparison of protein structure predictions and crystal structures to experimental Small Angle X-ray Scattering data.

Abstract:
Machine learning algorithms have transformed protein structural biology. However, how well do these predictions truly solve the protein folding problem and match biologically-relevant protein conformations in solution? Here, we examined three CASP14 targets and collected Small Angle X-ray Scattering Data, in collaboration with the CASP14 participating crystallographers. We compared CASP14 predictions and crystal structures, with the SAXS data. We found in all cases that although AlphaFold2 indeed accurately predicted the crystal structures, both AlphaFold2 and the crystal structures did not match the solution conformations. This analysis both shows the power of structure prediction, but also its current limitations and the need for efficient, experimental validation of conformations in solution.