

# Evaluation of model refinement in CASP14

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## Abstract

We report here an assessment of the model refinement category of the 14th round of Critical Assessment of Structure Prediction (CASP14). As before, predictors submitted up to five ranked refinements, along with associated residue-level error estimates, for targets that had a wide range of starting quality. The ability of groups to accurately rank their submissions and to predict coordinate error varied widely. Overall only four groups out-performed a “naïve predictor” corresponding to resubmission of the starting model. Among the top groups there are interesting differences of approach and in the spread of improvements seen: some methods are more conservative, others more adventurous. Some targets were “double-barrelled” for which predictors were offered a high-quality AlphaFold 2 (AF2)-derived prediction alongside another of lower quality. The AF2-derived models were largely unimprovable, their apparent errors being found to reside very largely at domain and, especially, crystal lattice contacts. Refinement is shown to have a mixed impact overall on structure-based function annotation methods to predict nucleic acid binding, spot catalytic sites and dock protein structures.

## Hosted file

Final-CASP14 refinement for submission.pdf available at <https://authorea.com/users/411883/articles/520766-evaluation-of-model-refinement-in-casp14>