Phenix

Estimating uncertainty in models by repetition of model-building

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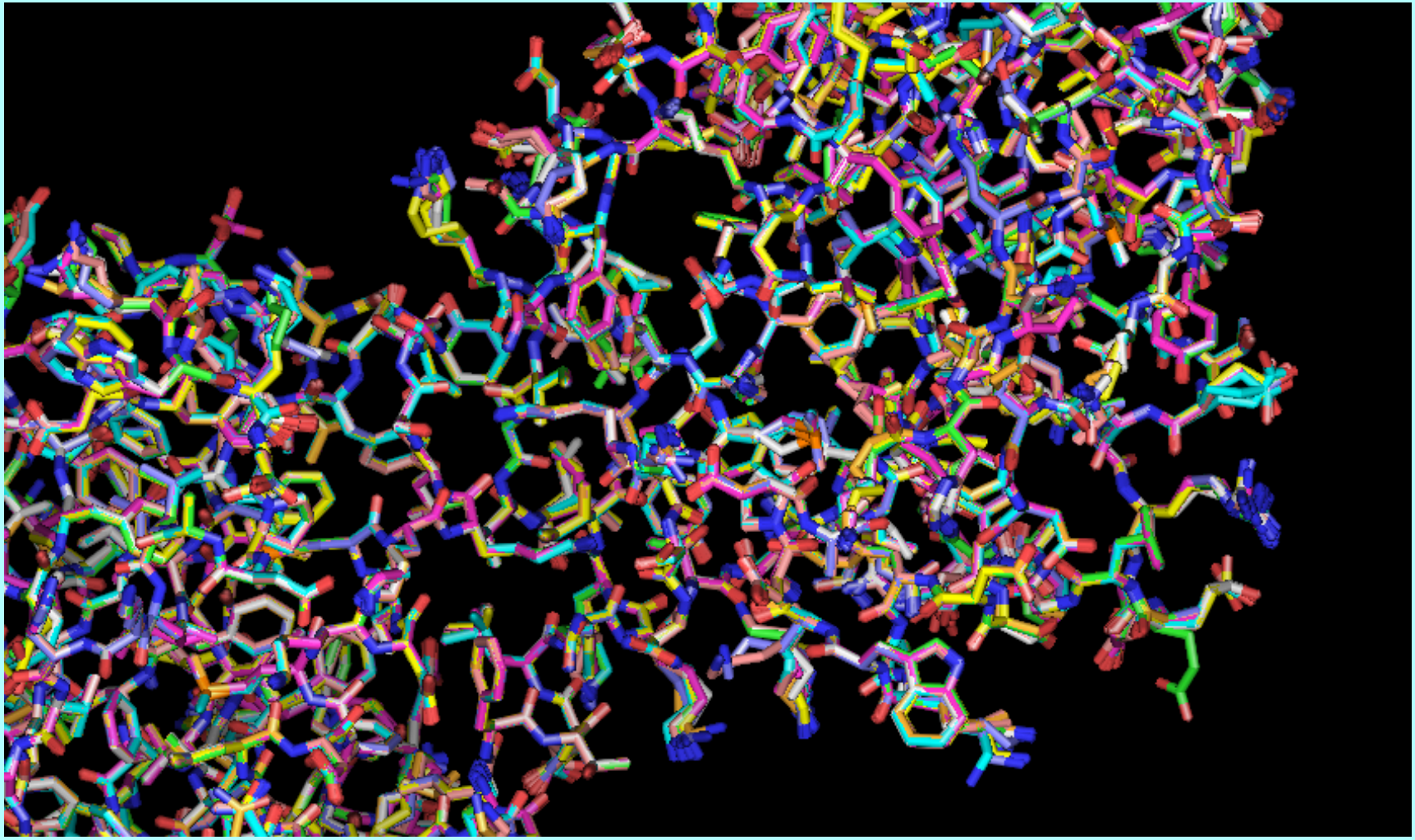
Multiple-model representation of uncertainties

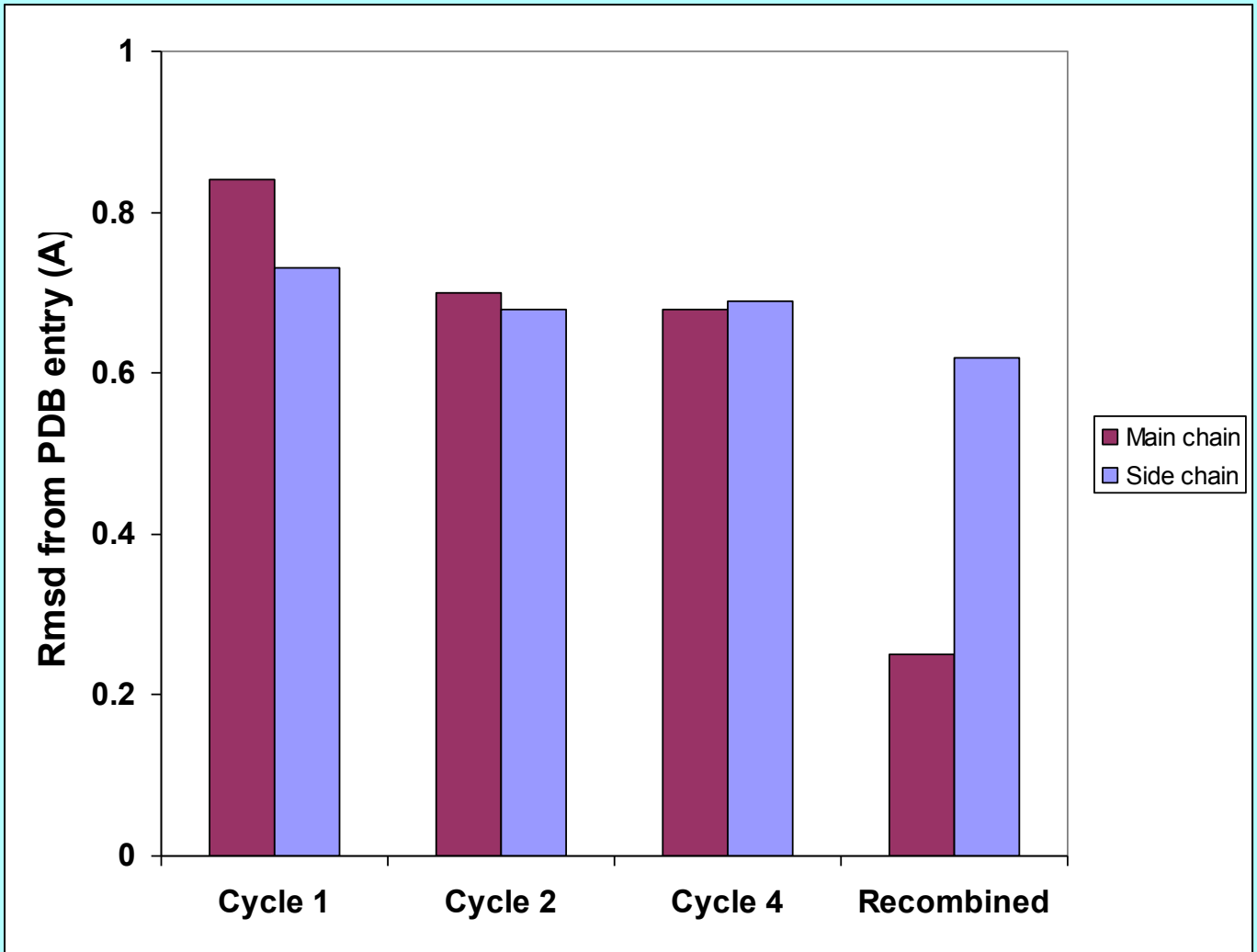
20 models built for 1CQP, no waters, Dmin=2.6 A R=0.19-0.20; Rfree=0.26-0.27

The variation among models is a lower bound on their uncertainty

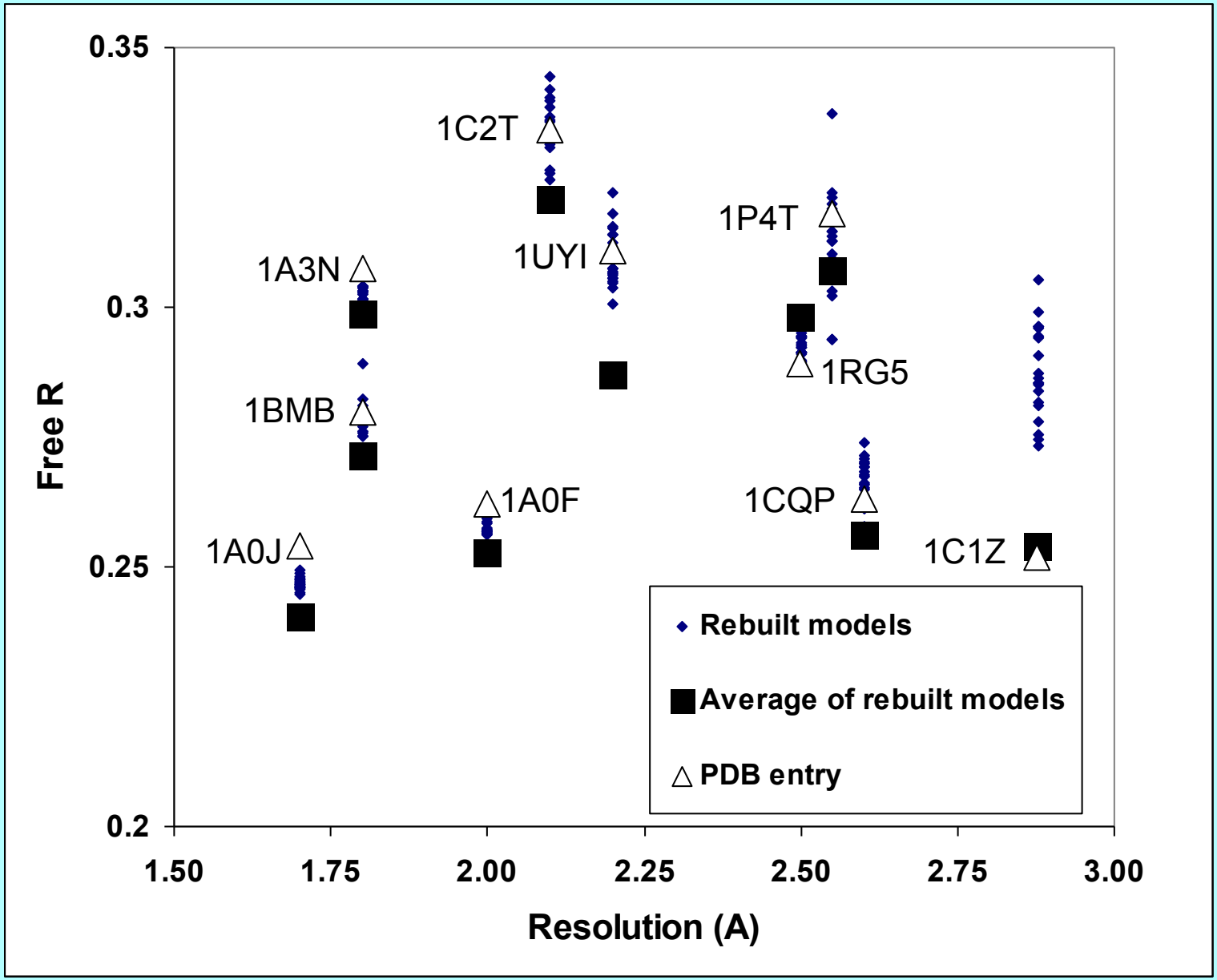


Rebuilding a model from PDB with PHENIX

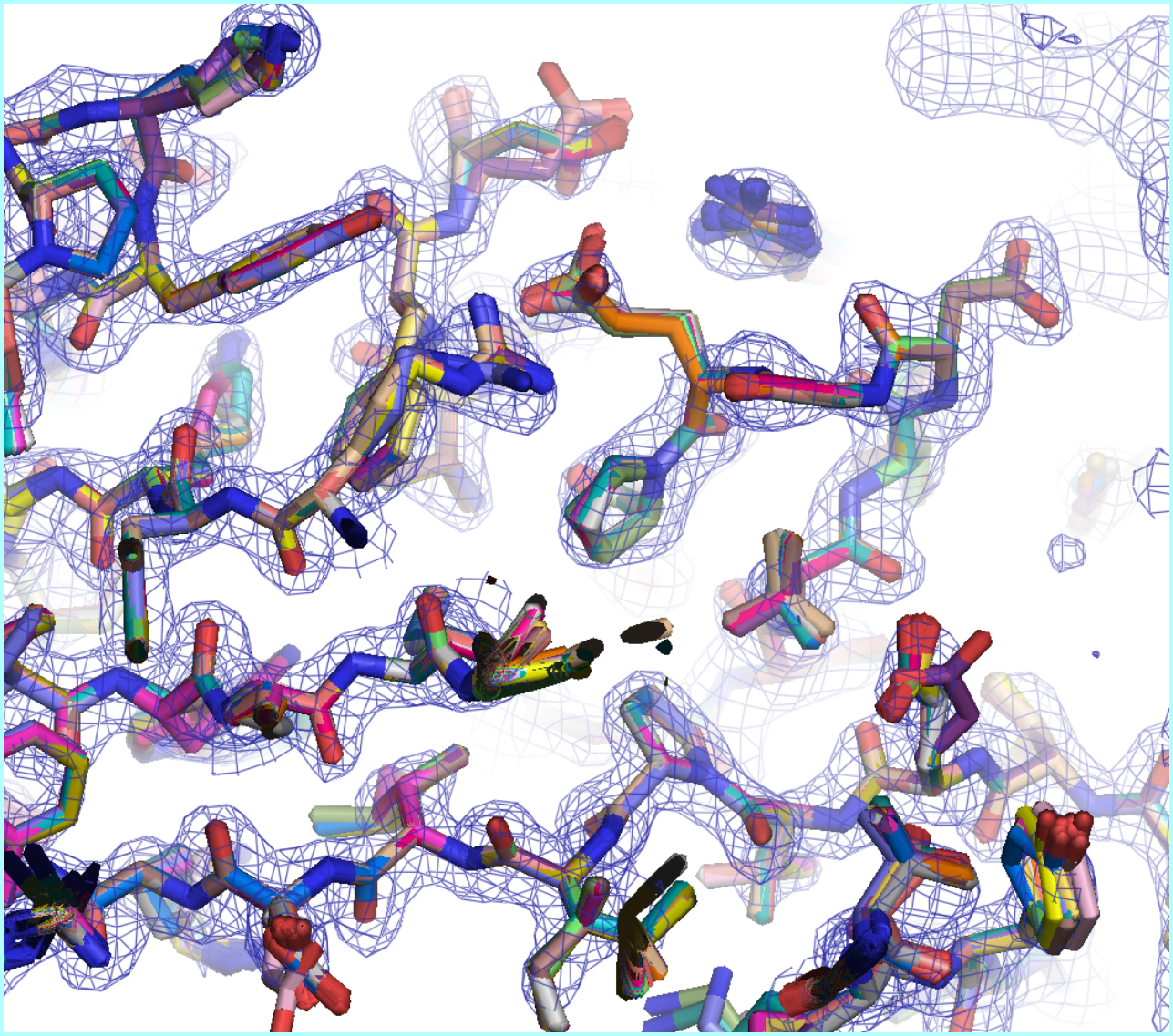
1. Remove waters, ligands
2. Rebuild model with random seed
3. Five cycles of rebuilding in place (rebuild, refine, density modify)
4. Recombine best parts of 5 models and refine to yield final model



Building 20 models for each of 10 structures

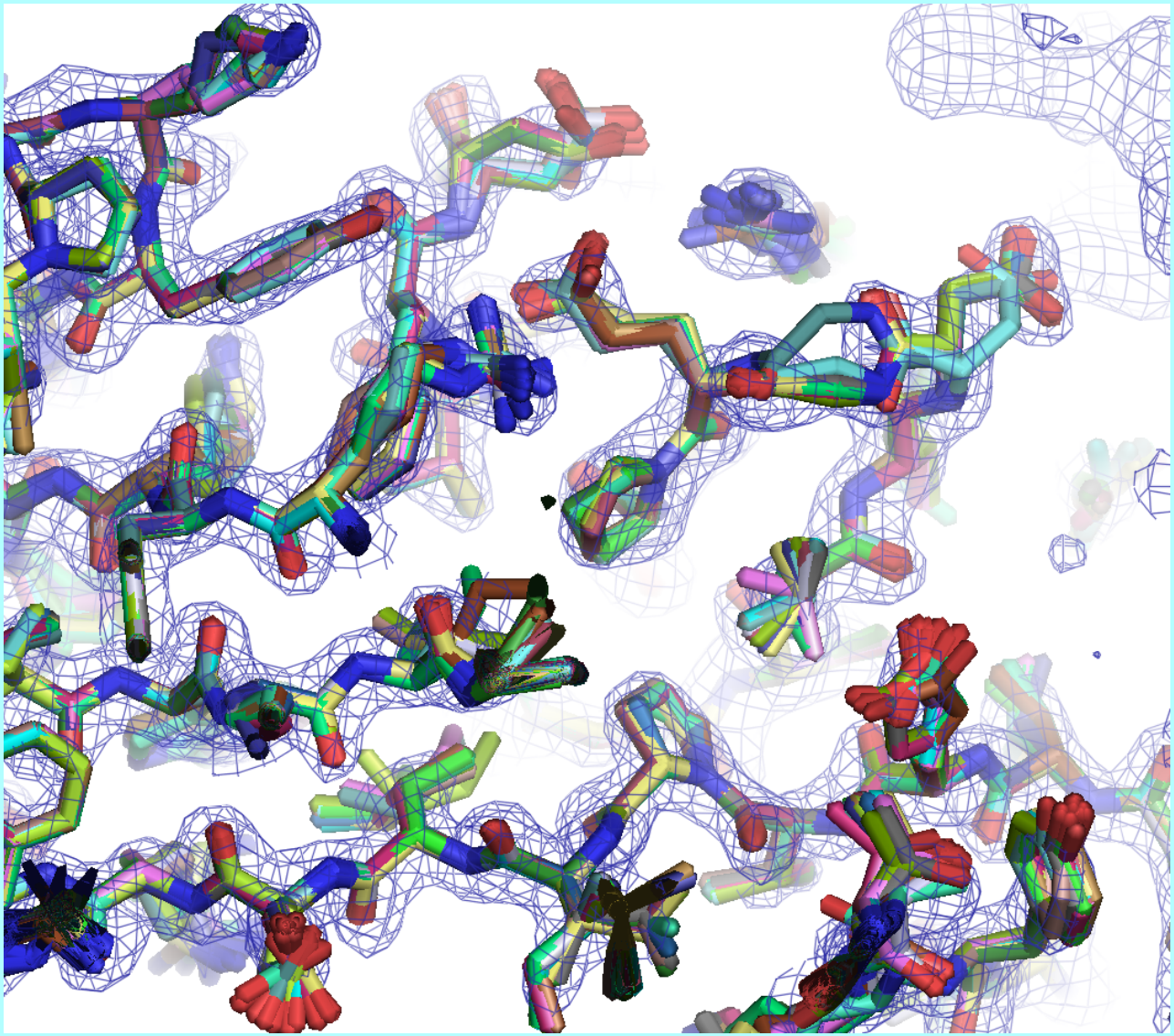


What does the RMSD among models tell us?



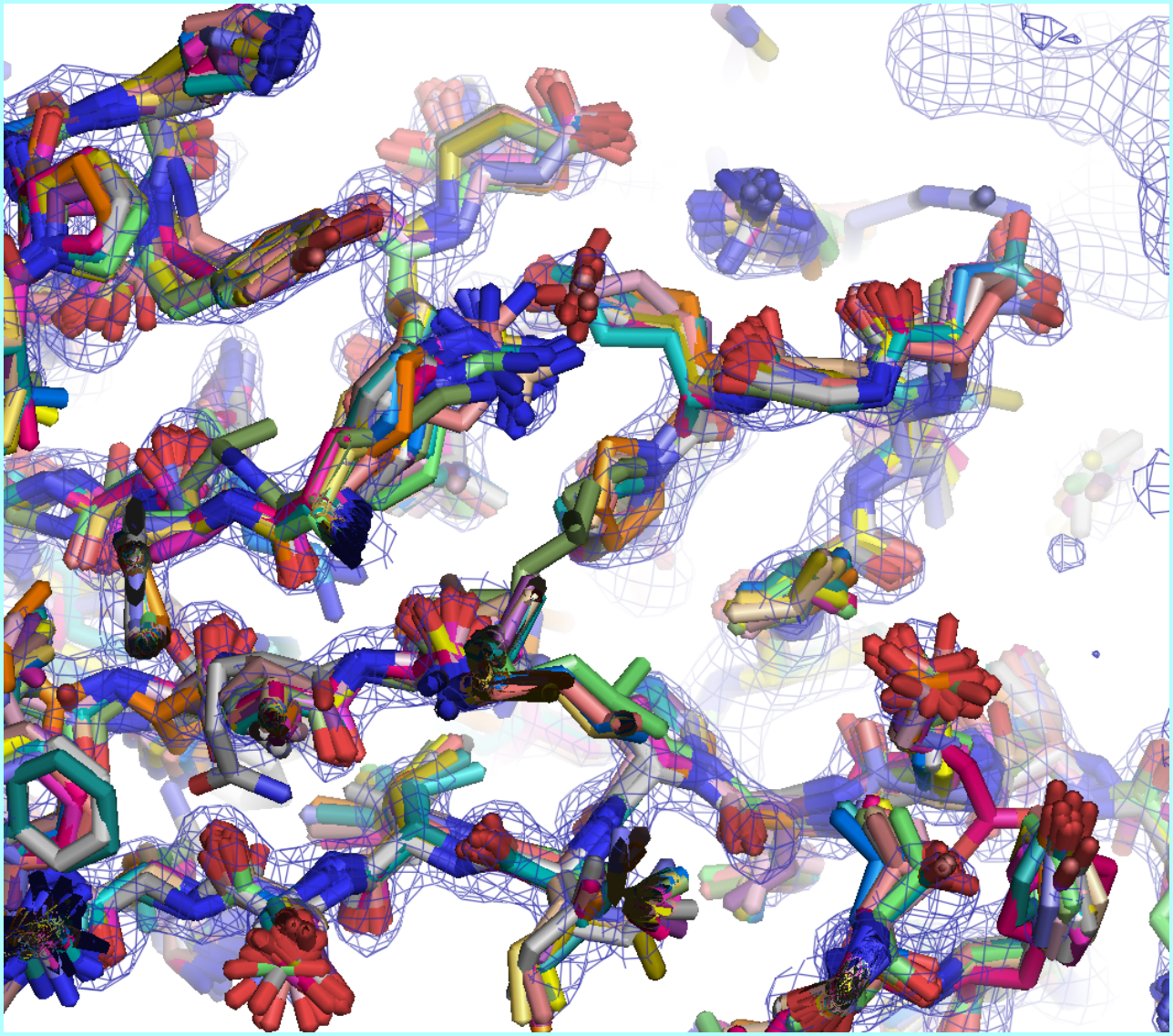
Rebuild model
20 times with
1.75 Å data

What does the RMSD among models tell us?



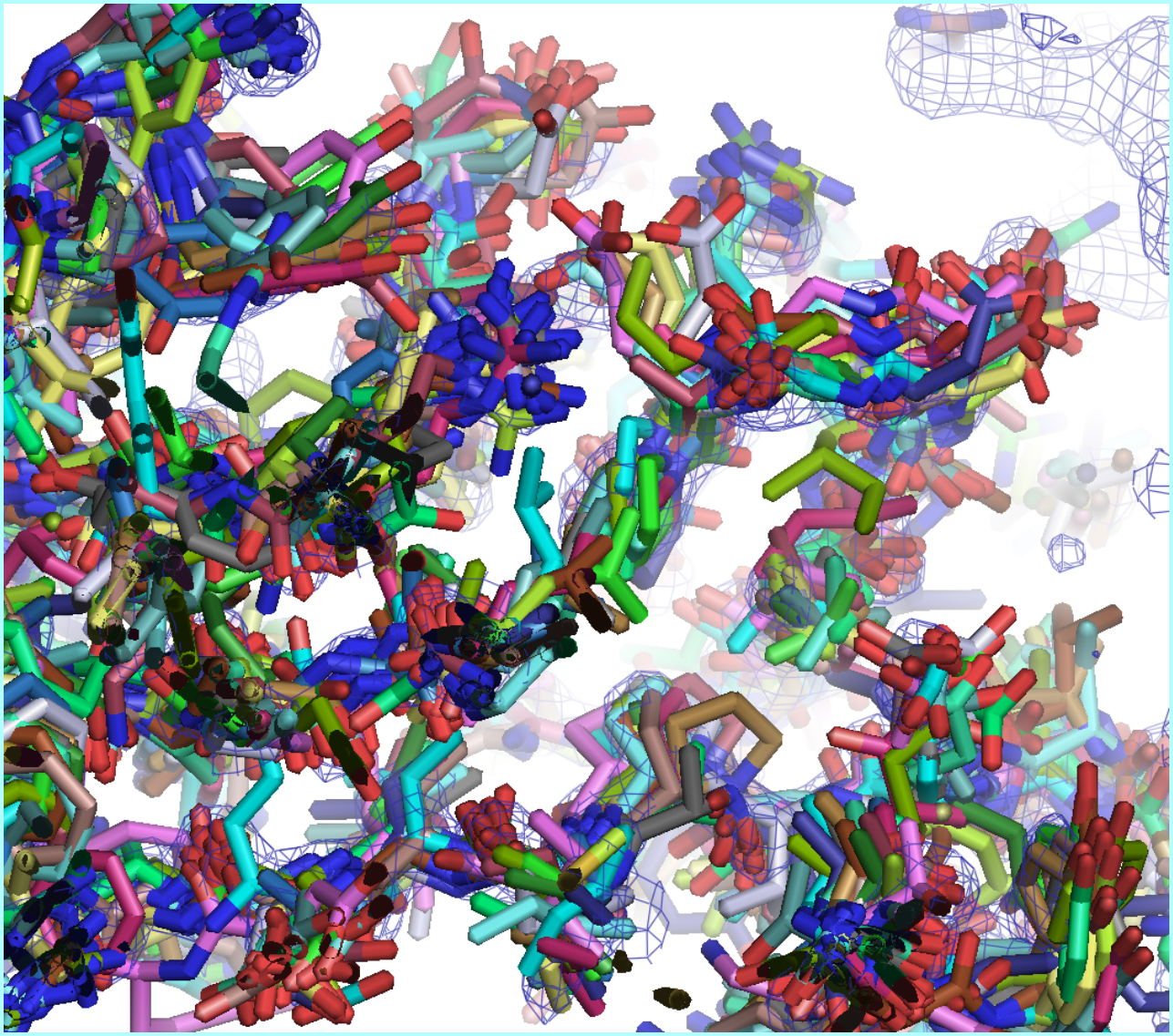
Rebuild model
20 times with 2.5
Å data

What does the RMSD among models tell us?



Rebuild model
20 times with 3.5
Å data

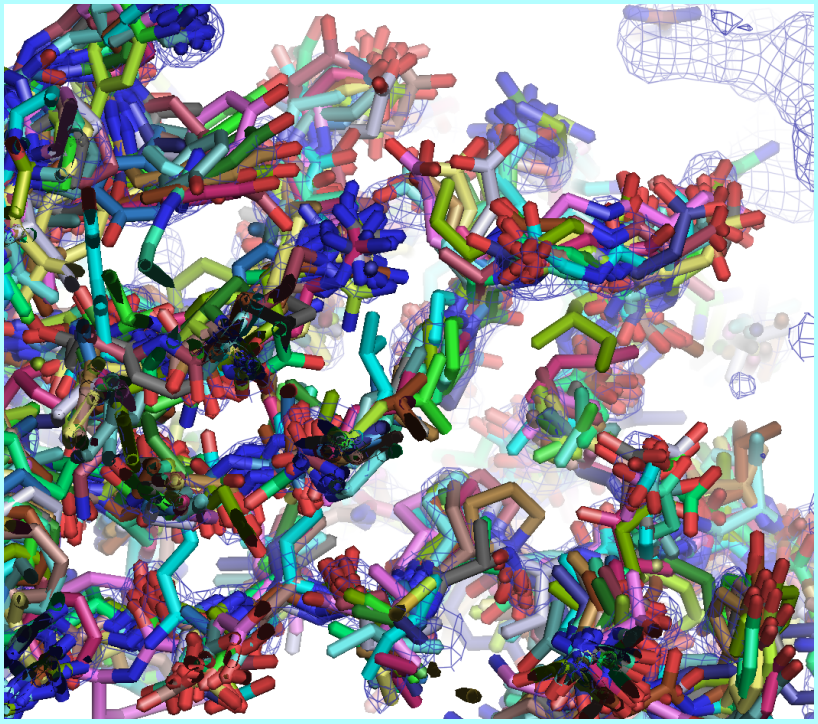
What does the RMSD among models tell us?



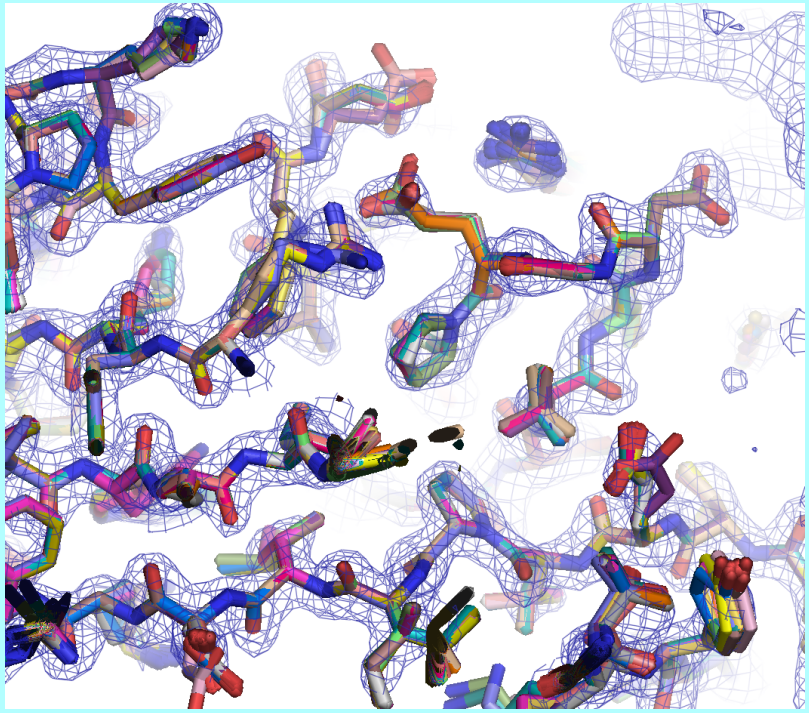
Rebuild model
20 times with 4.5
Å data

->The RMSD among models tells us (a lower bound on) the uncertainty in our models

(It is not the RMSD of true structures in the crystal)



Rebuild with 4.5 Å data



Rebuild with 1.75 Å data

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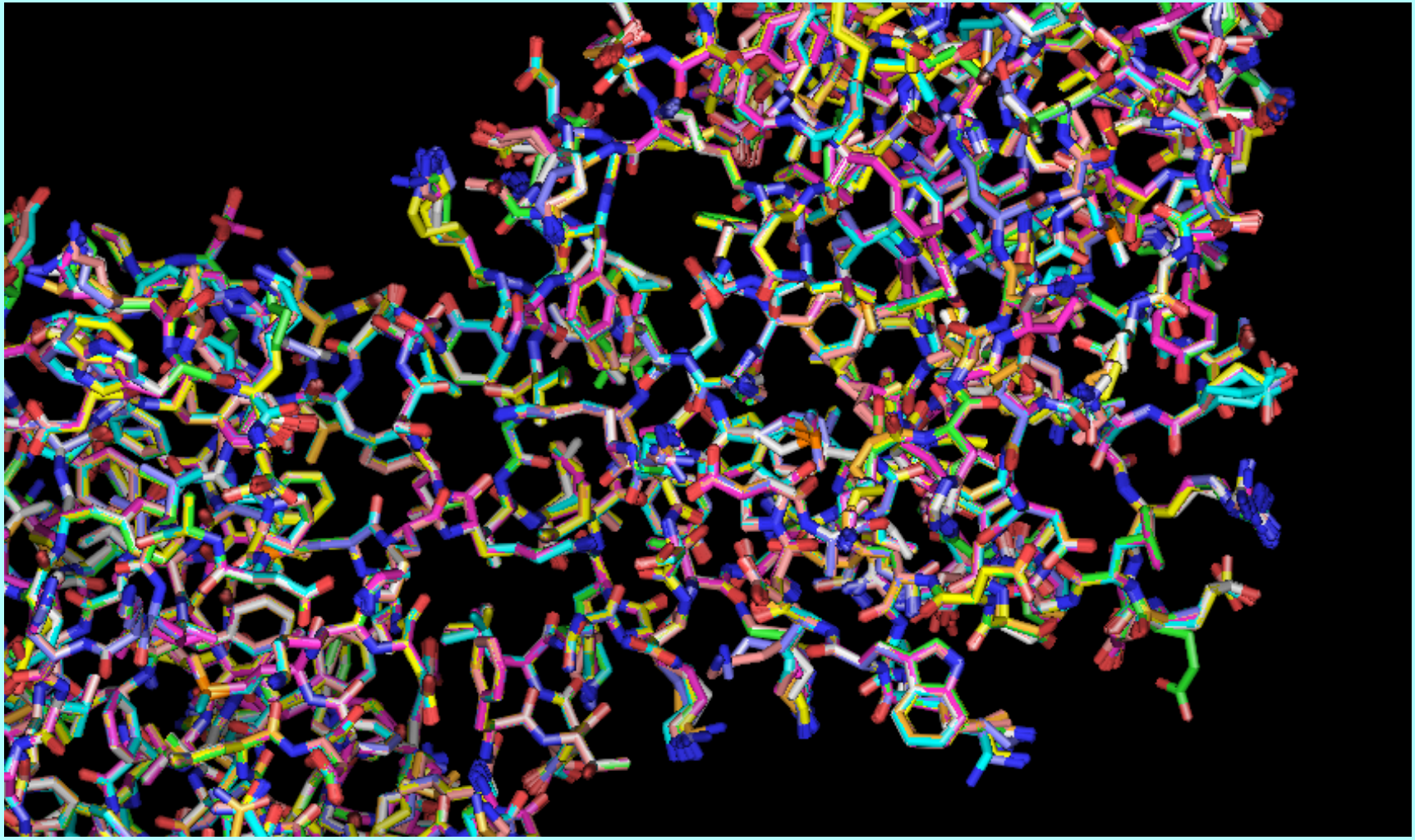

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