

*Phenix Workshop UTMB
October 2025*

Using Predicted models in Phenix (cryo-EM)



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Outline

1. About AlphaFold predictions
2. Using predicted models in cryo-EM
 - Docking
 - Model completion
 - Reference model restraints
3. Automated workflow:
Iterating prediction and model building

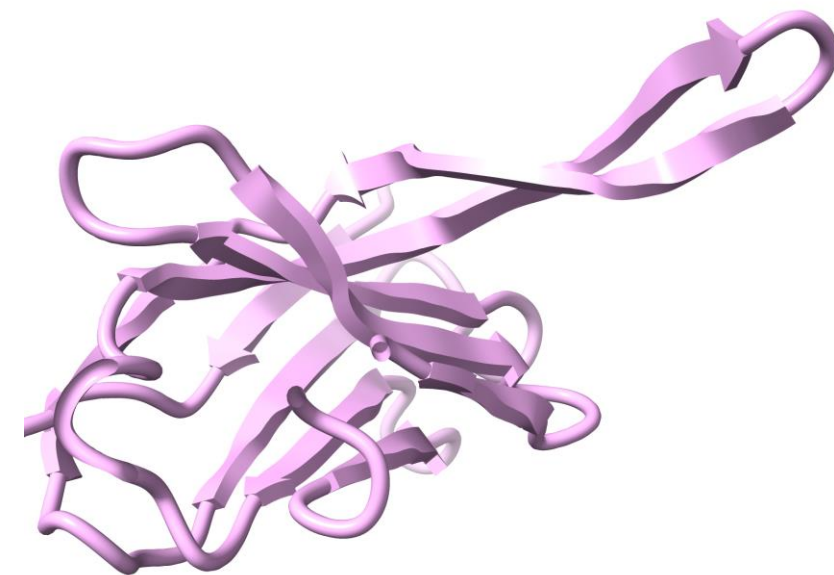
Part 1

About AlphaFold predictions

Predicting models with AlphaFold



EVQLVESGGGLVQPGGSLRLSCAASGFTN**I**YSS**S**IHWVRQAPGKGLEWVAYI
.....**F**.....**M**.....Q.....
.....K.....**Y**.....**L**.....A.....
.....A.....V.....
.....A.....
.....**L**.....**V**.....E.....
.....A.....Q.....



Sequence

Multiple sequence alignment

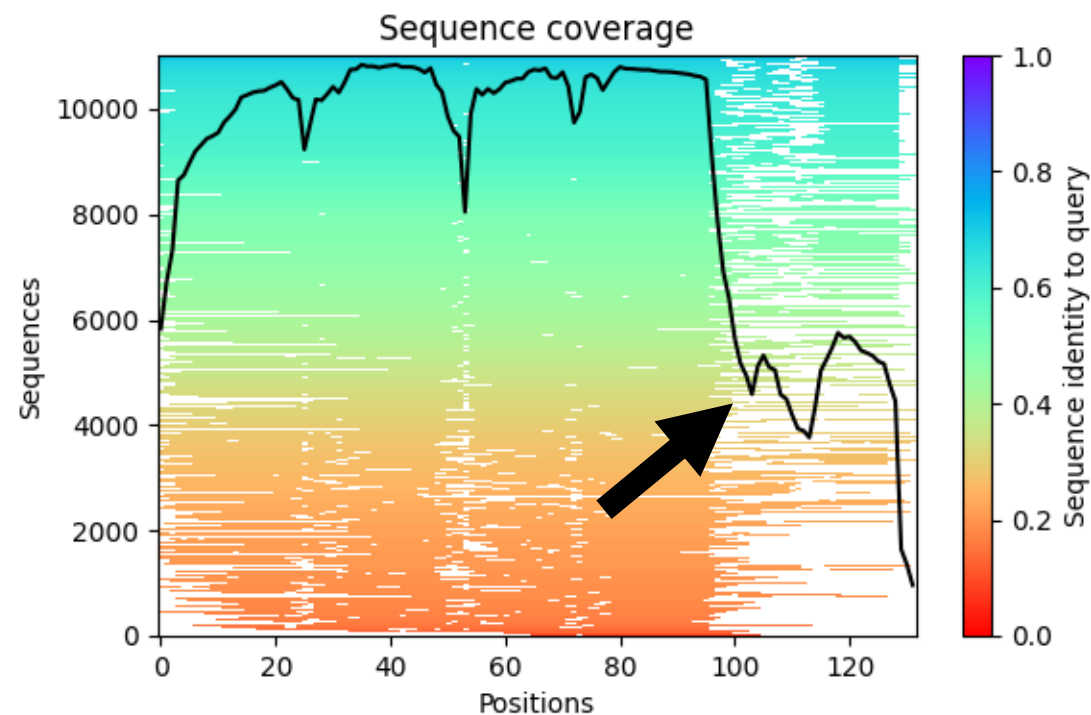
3D prediction

Predictions come with confidence measures

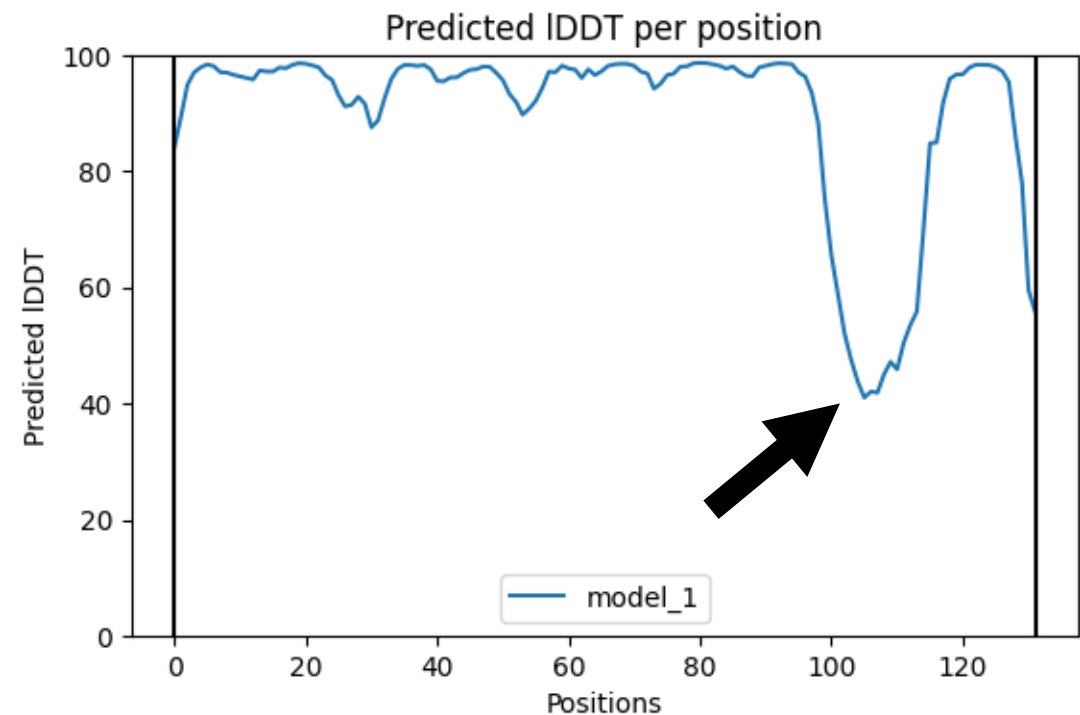
1. pLDDt (predicted Local Distance Difference Test)

- pLDDt identifies where errors are more likely.
- Per-residue confidence measure.
- Scales from 0 – 100 (pLDDt > 90: predicted with high accuracy).

Sequence coverage



Confidence



7mjs (3 Å, EMDB 23883)

Residues 1-100

Residues 100-120

Data from 7mjs, Cater, R.J., et al. (2021). Nature 595, 315–319

Predictions come with confidence measures

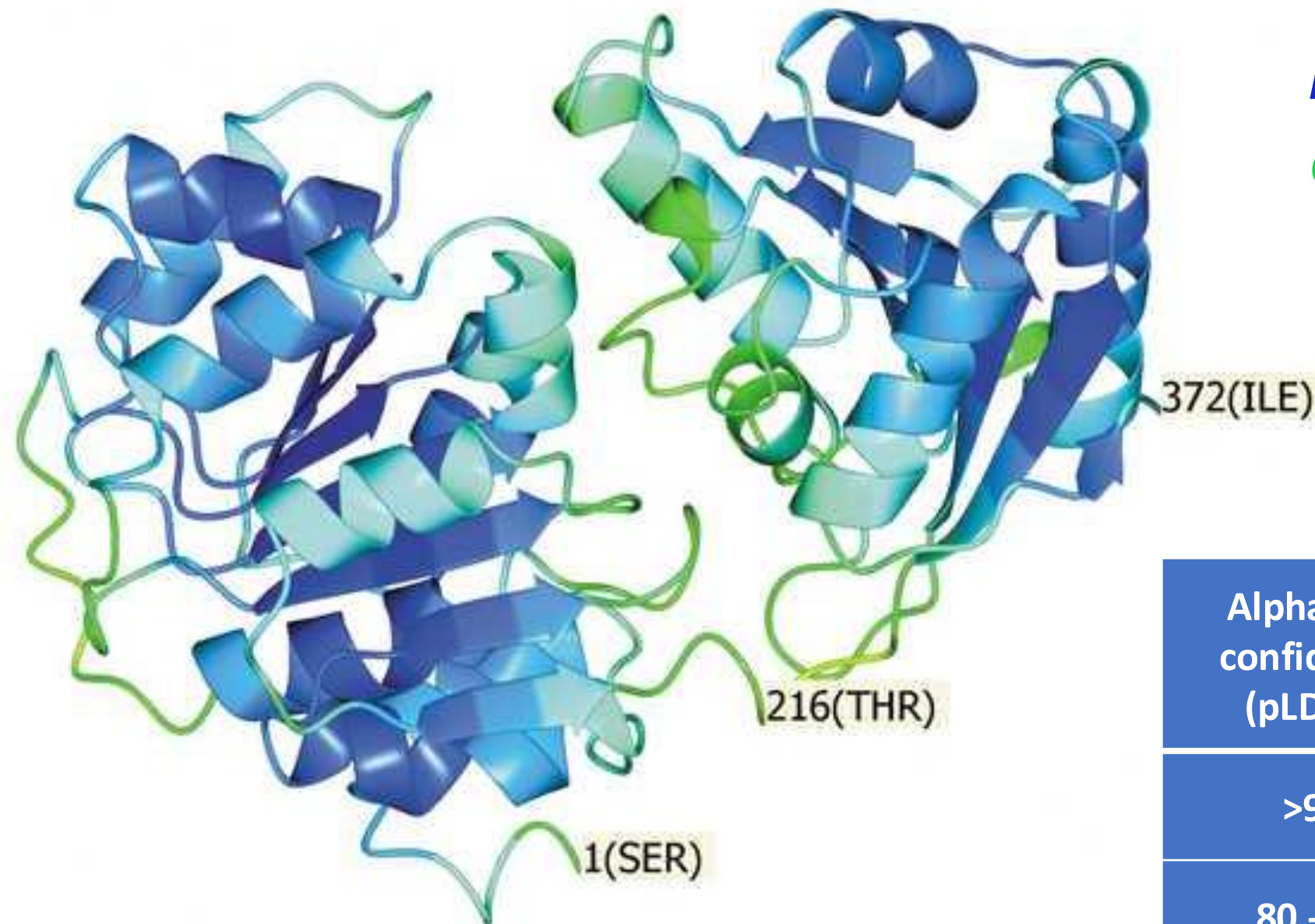
1. pLDDt (predicted Local Distance Difference Test)

- pLDDt identifies where errors are more likely.
- Per-residue confidence measure.
- Scales from 0 – 100 (pLDDt > 90: predicted with high accuracy).

AlphaFold confidence (pLDDT)	Median prediction error (Å)	Percentage with error over 2 Å
>90	0.6	10
80 - 90	1.1	22
70 - 80	1.5	33
<70	3.5	77

Predictions come with confidence measures

1. pLDDt (predicted Local Distance Difference Test)



Blue: pLDDt > 90

Green: pLDDt 80 - 90

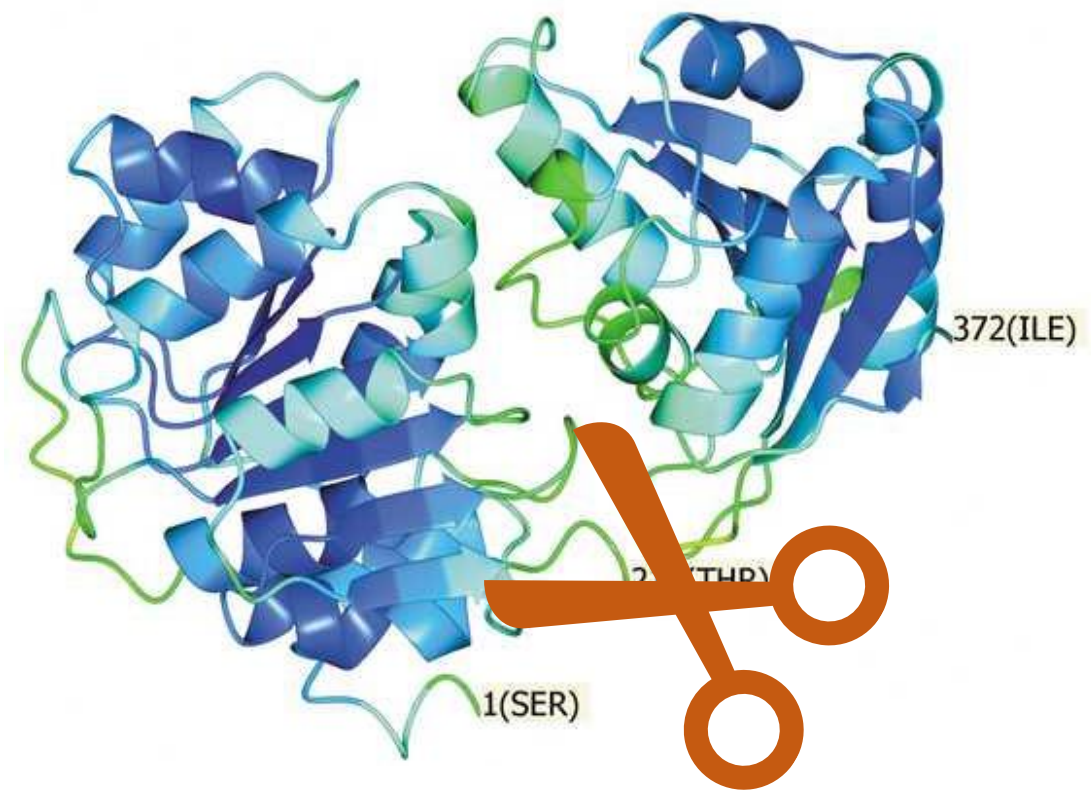
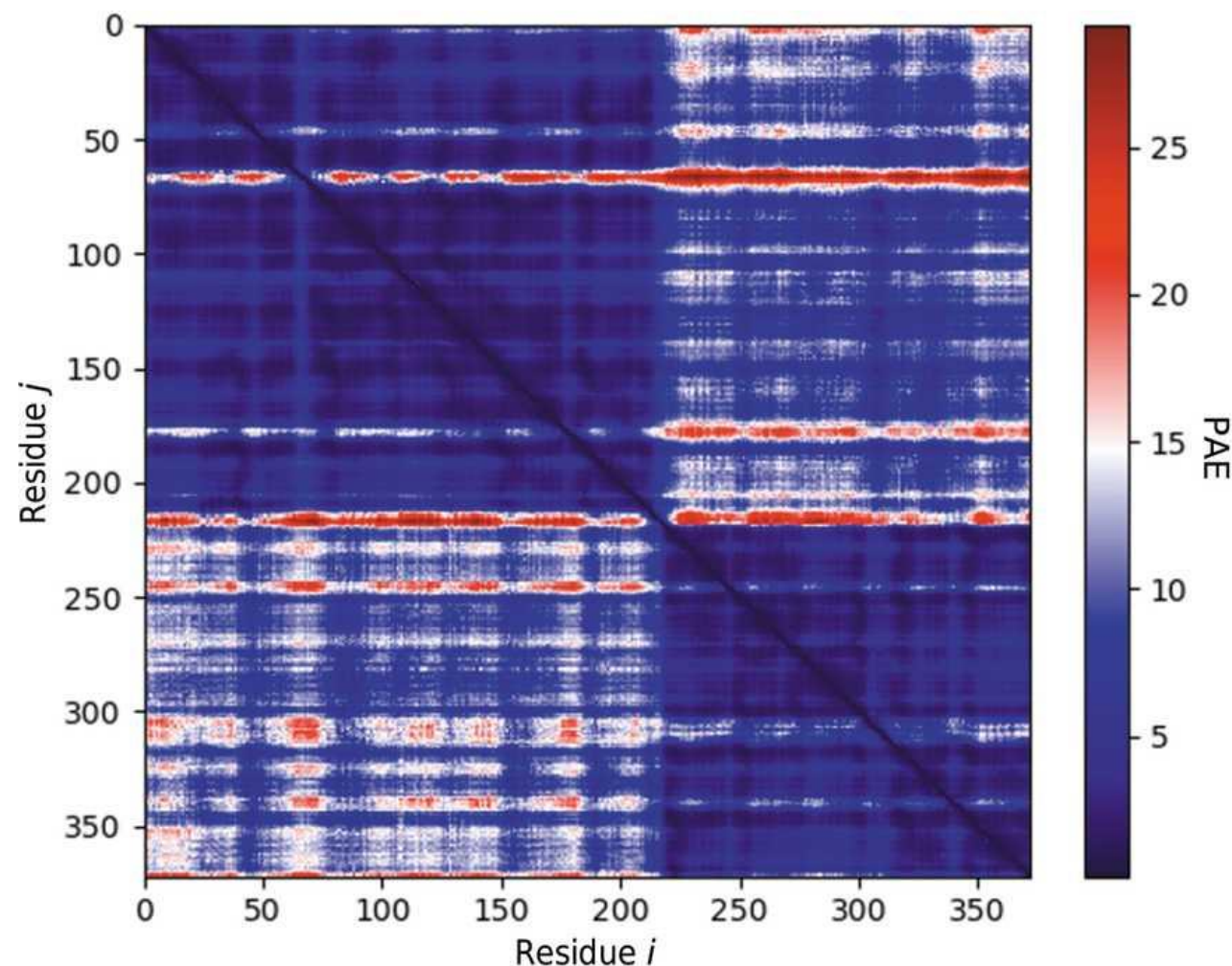
AlphaFold prediction for RNA helicase
(PDB entry 6L5L)

AlphaFold confidence (pLDDT)	Median prediction error (Å)	Percentage with error over 2 Å
>90	0.6	10
80 - 90	1.1	22
70 - 80	1.5	33
<70	3.5	77

Predictions come with confidence measures

2. Predicted aligned error (PAE)

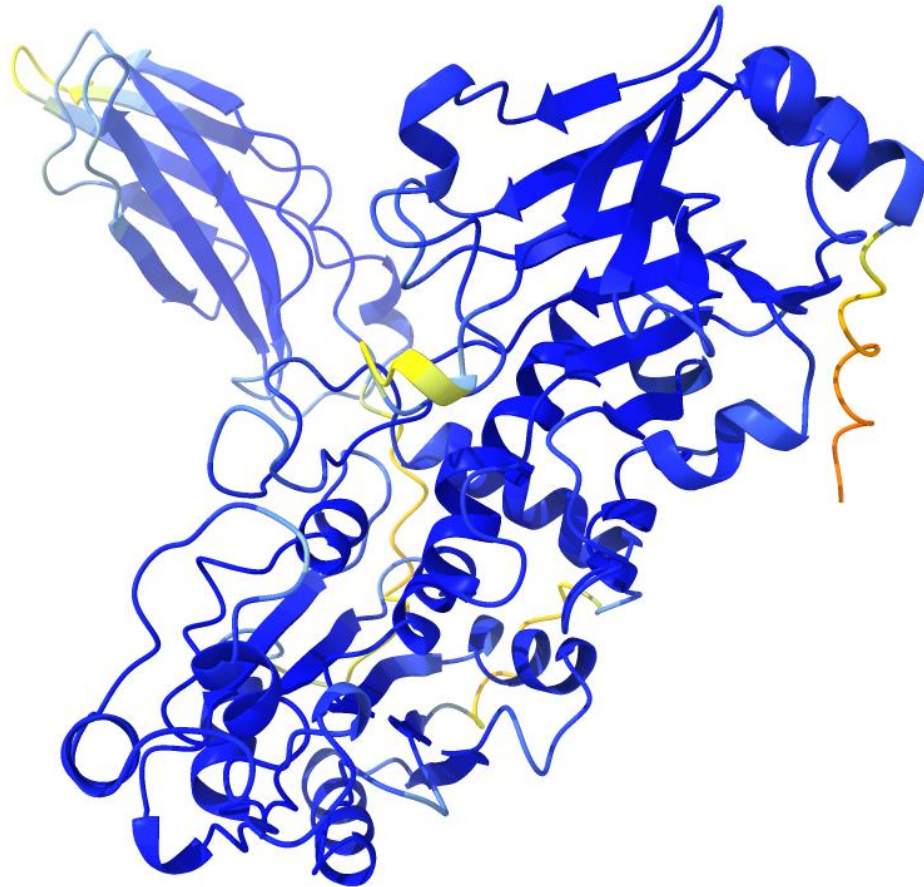
- Certainty of relative positions between two residues.
- Identifies accurately-predicted domains.
- Dark blue: uncertainty in relative positions $< 5 \text{ \AA}$.



- Suggests 2 domains

Using predicted models: B-factors

Color by pLDDT



Color by B-factor



high pLDDT (high confidence)

low pLDDT (low confidence, uncertain)



high B-factor (disordered, uncertain)

low B-factor (ordered)

Using predicted models: B-factors

high pLDDT (high confidence)

low pLDDT (low confidence, uncertain)



high B-factor (disordered, uncertain)

low B-factor (ordered)

B-factor may be used in downstream calculations, e.g. to calculate weights for docking. Residues with high B-factors are downweighed.

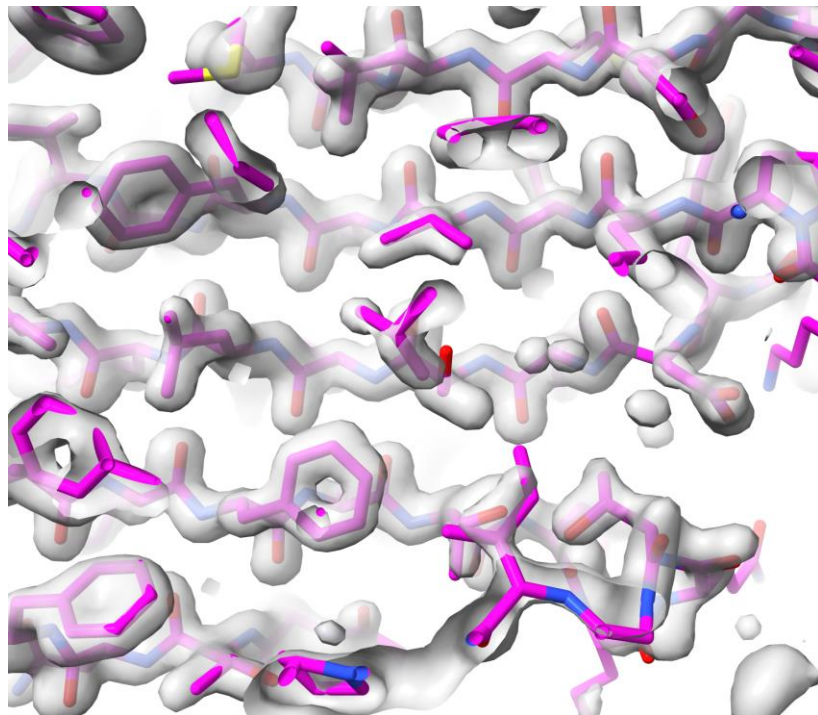
→ Convert pLDDT to pseudo B-factors.

$$\Delta = 1.5 \exp[4(0.7 - \text{pLDDT})]$$

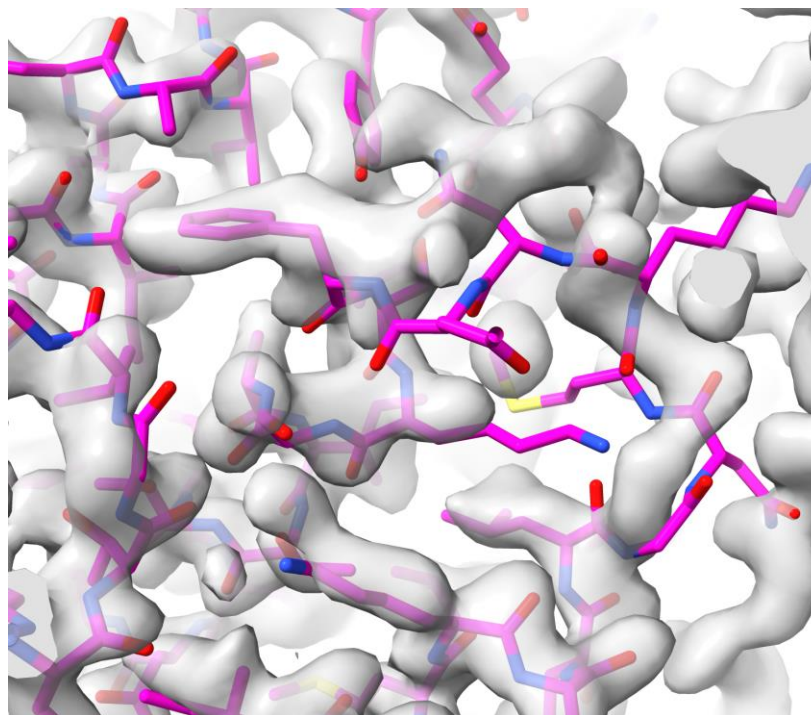
$$B = \frac{8\pi^2 \Delta^2}{3}$$

AlphaFold predictions are great hypotheses

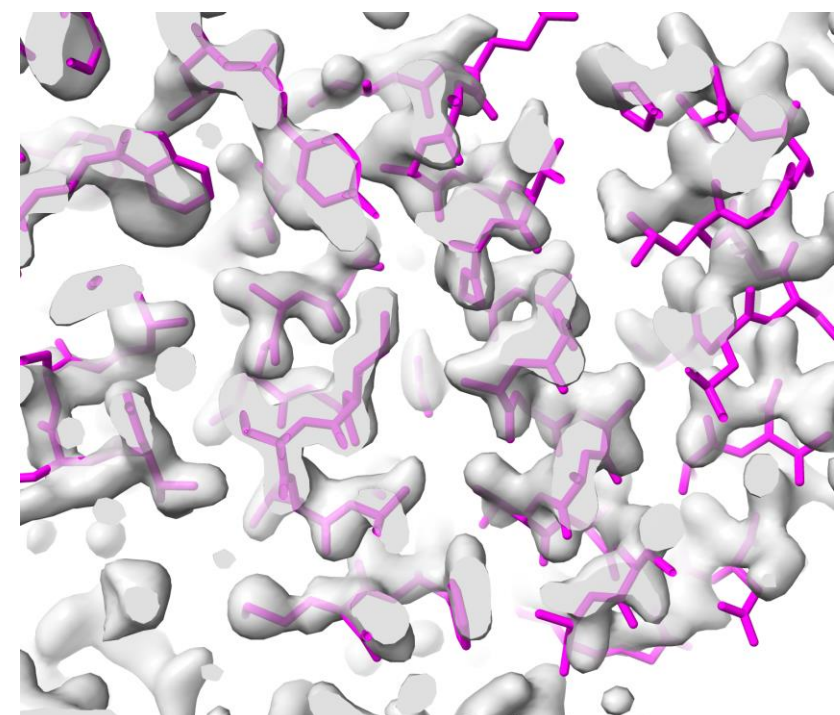
AlphaFold models
can be....



Awesome



Wrong



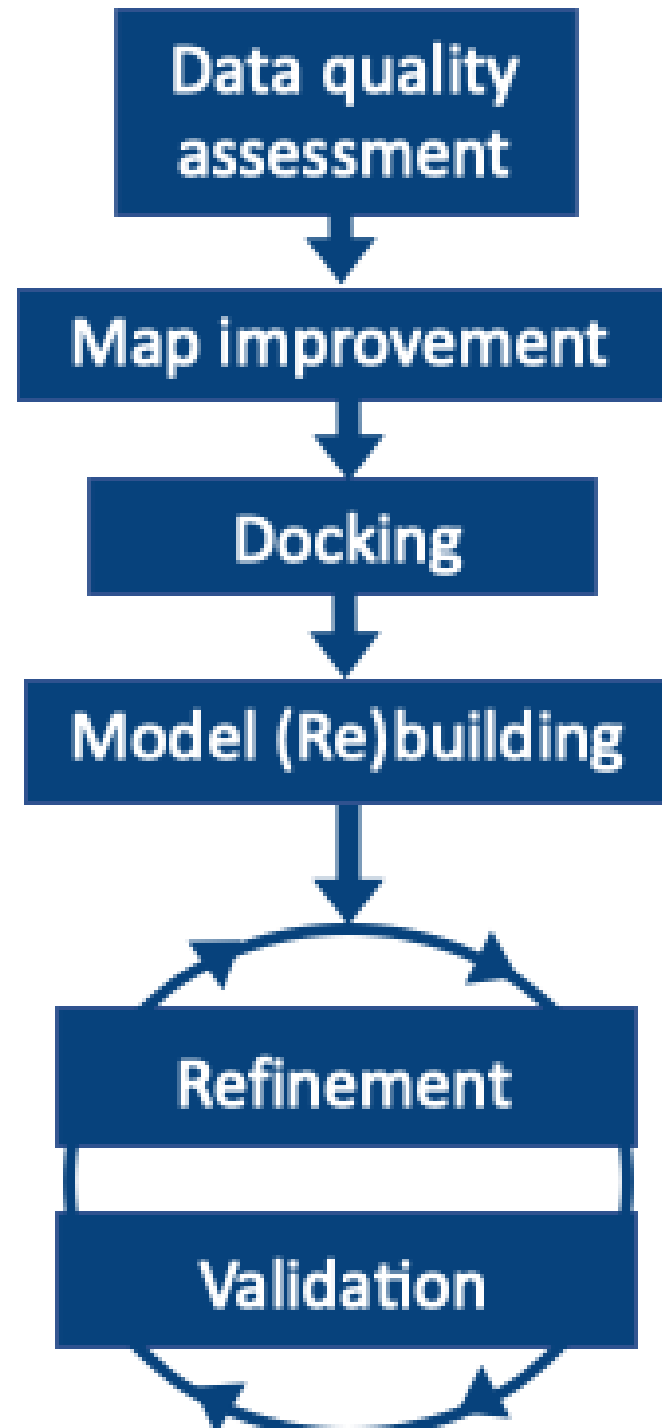
Distorted

Part 2

Using predicted models in Phenix

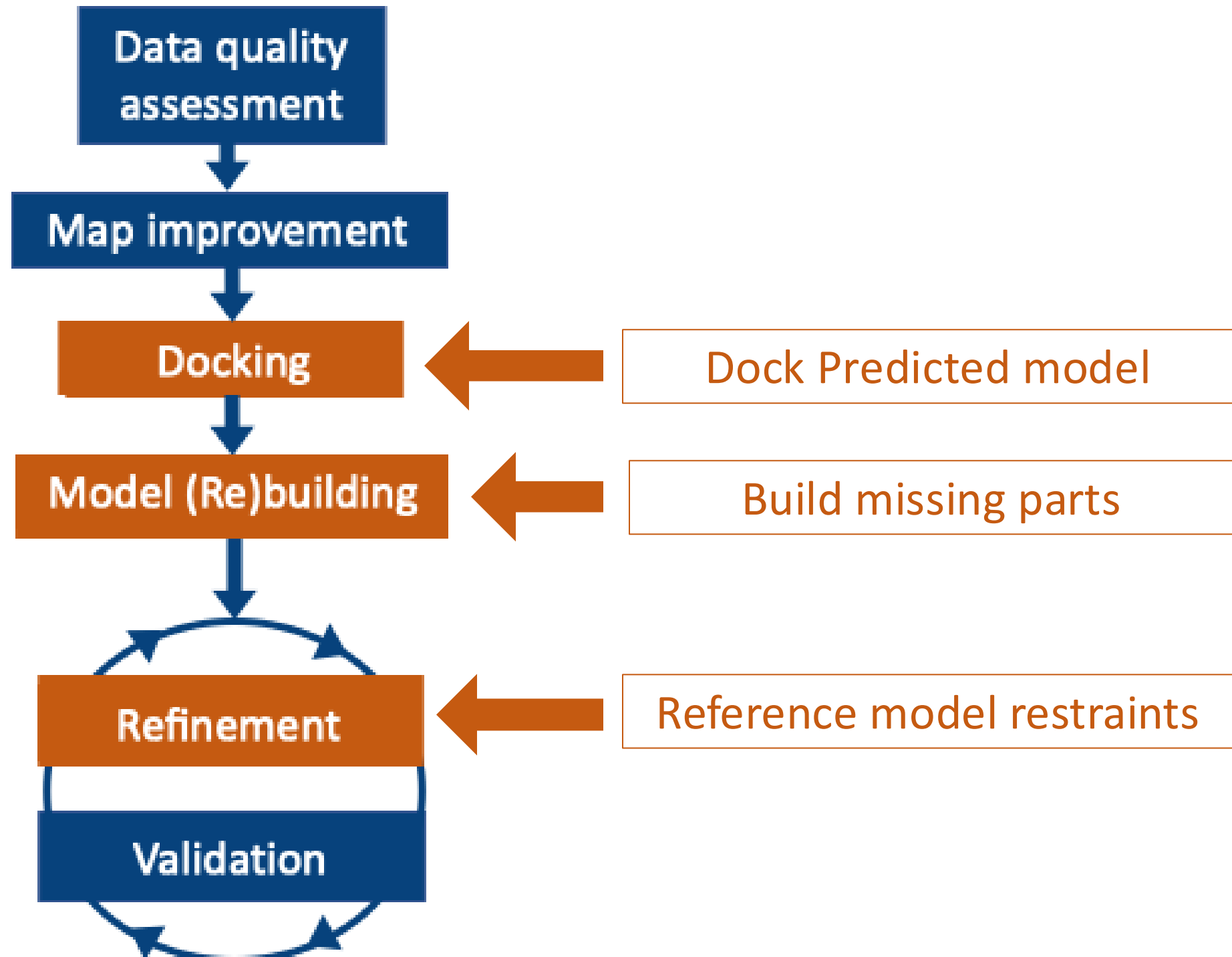
What can predicted models be used for?

Incorporate predictions into the typical cryo-EM workflow.

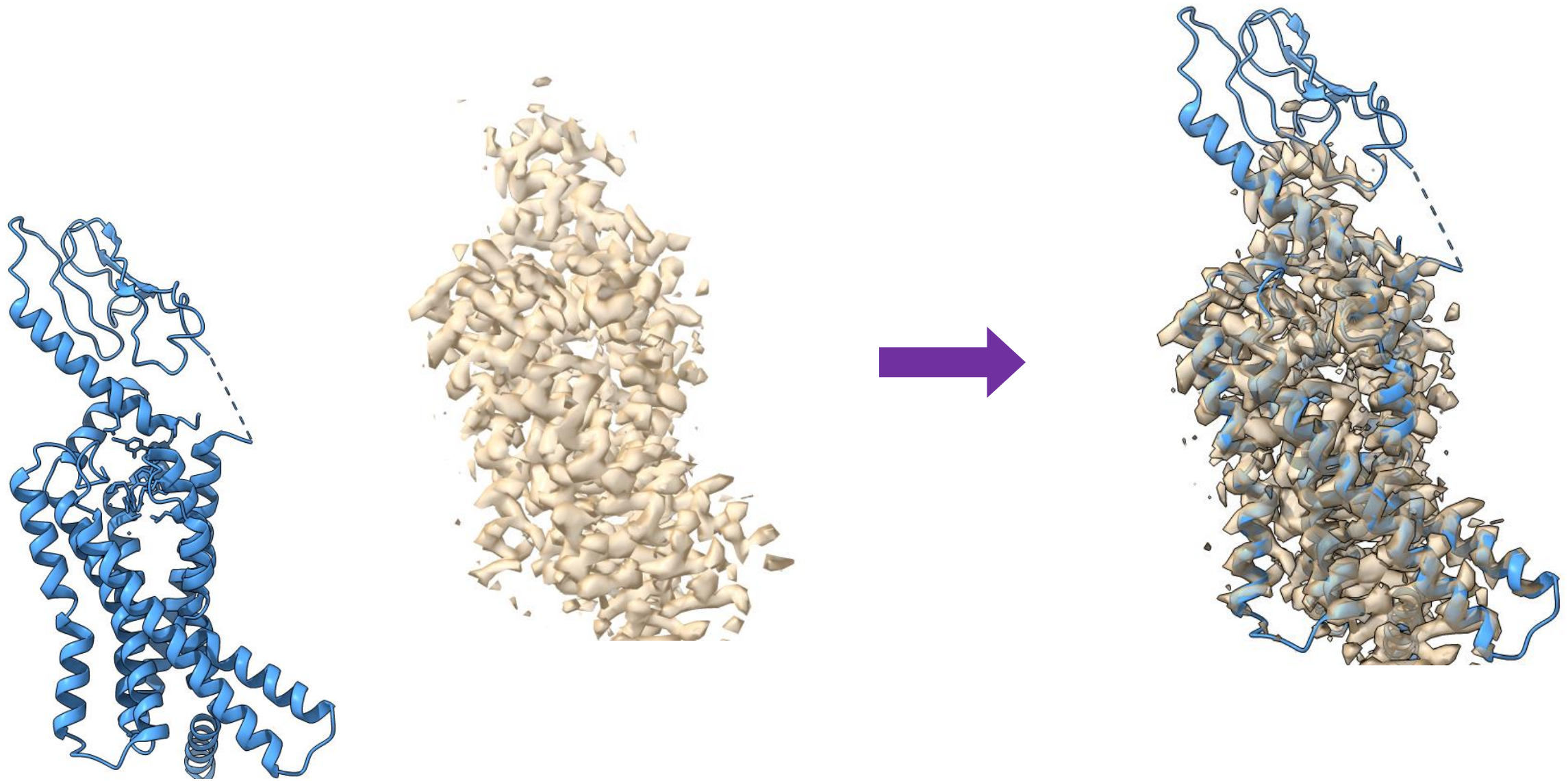


What can predicted models be used for?

Incorporate predictions into the typical cryo-EM workflow.



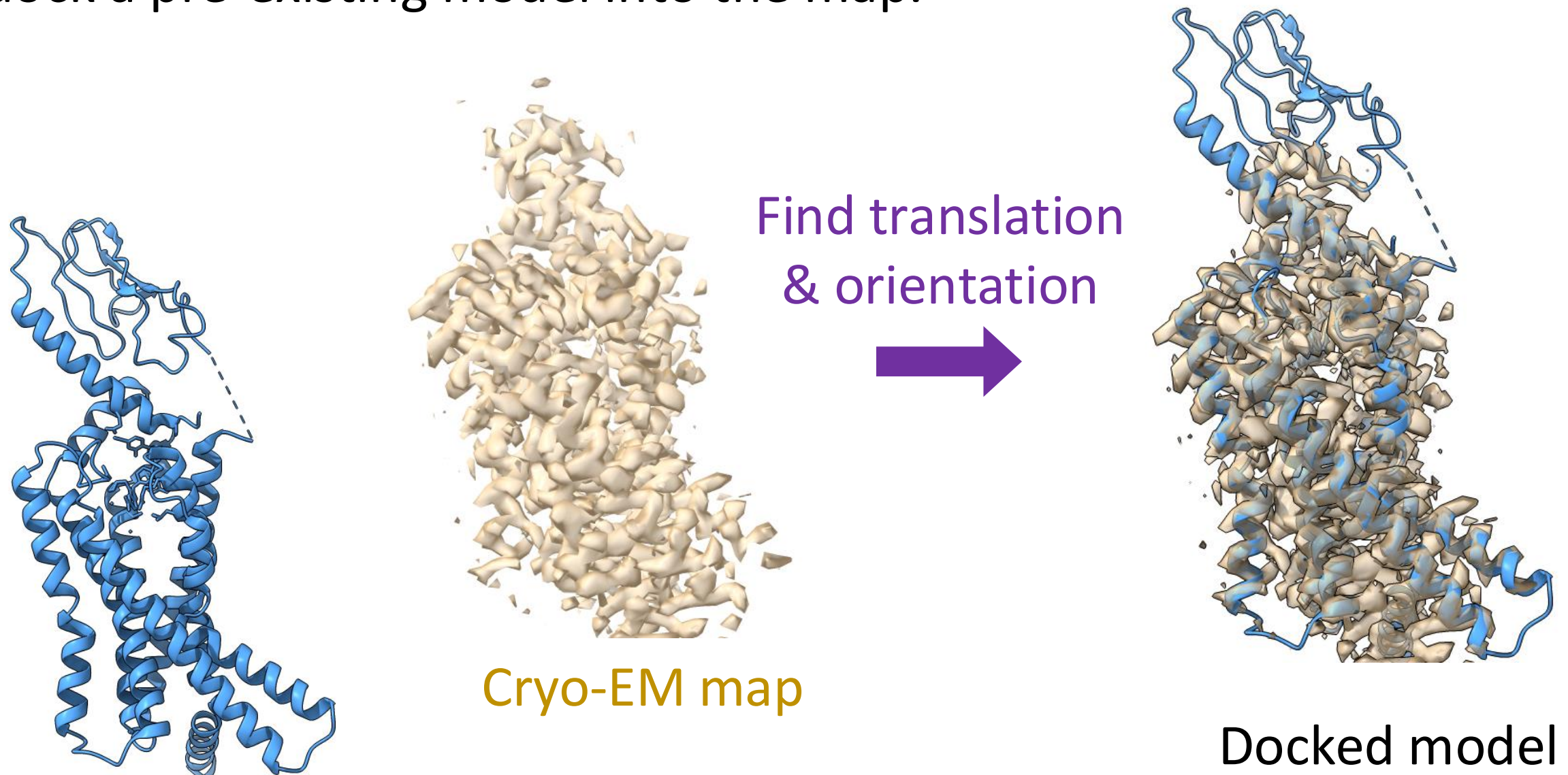
1. Use a prediction for cryo-EM docking



1. Use a prediction for cryo-EM docking

Cryo-EM maps typically lack the necessary resolution and quality for *ab initio* model building.

→ dock a pre-existing model into the map.



Model assumed to look like
the sample.

Use a predicted model for cryo-EM docking

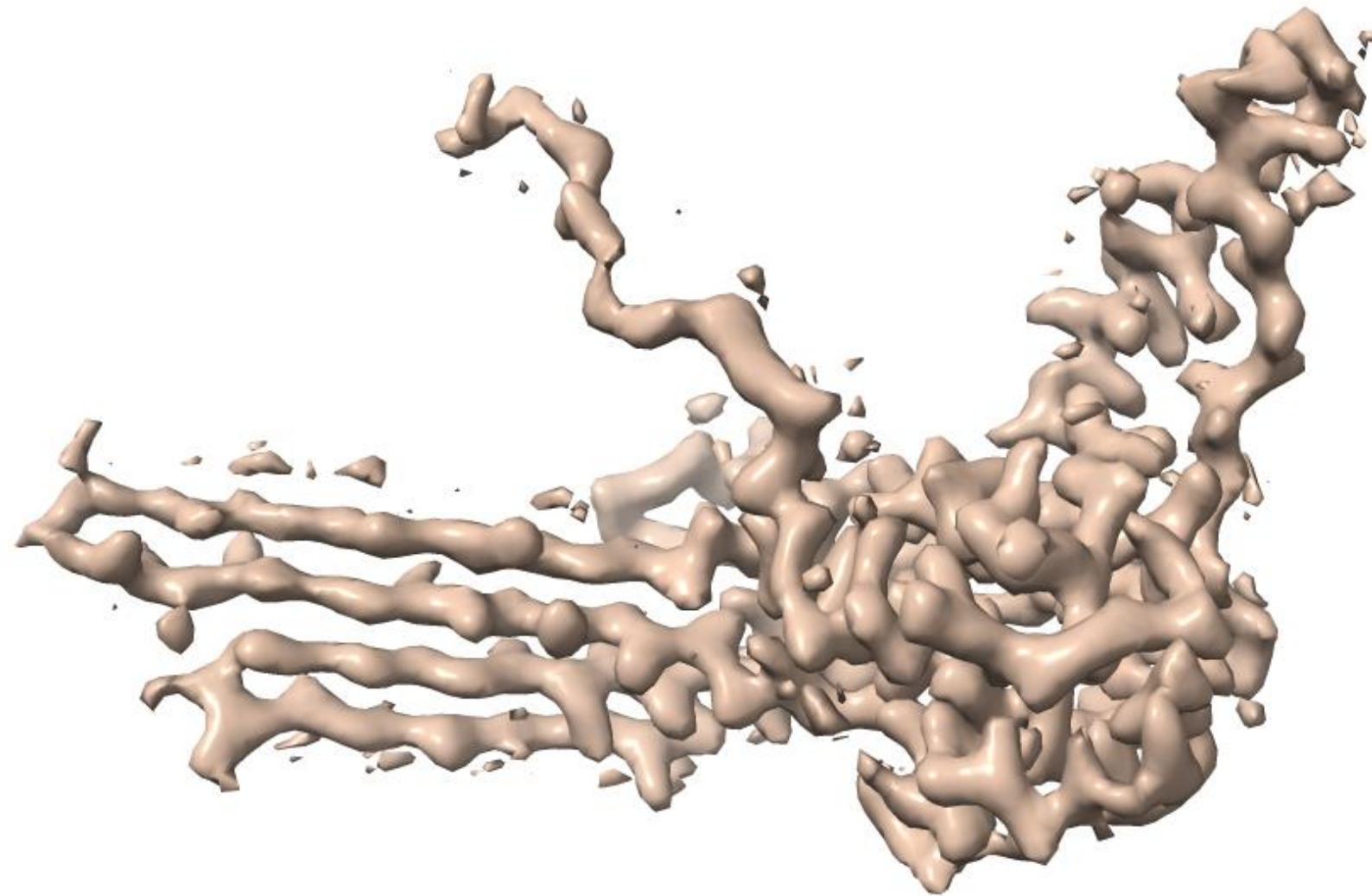
Example:

Cryo-EM map (30160 – 7brm)

3.6 Å

```
>chain ' A'  
XXXXXXXXXXXXXXXXCLTAPPKEAARPTLMPRAQSYKDLTHLPAP  
TGKIFVSVYNIQDETQQFKPYPASNFSTAVPQSATAMLVTALKDS  
RWFIPLERQGLQNLLNERKIIRAAQENGTVAINNRIPLQSLTAAN  
IMVEGSIIGYESNVKSGGVGARYFGIGADTQYQLDQIAVNLRVWN  
VSTGEILSSVNTSKTILSYEVQAGVFRFIDYQRLLEGEVGYTSNE  
PVMLCLMSAIETGVIFLINDGIDRGLWDLQNKAERQNDILVKYRH  
MS
```

sequence

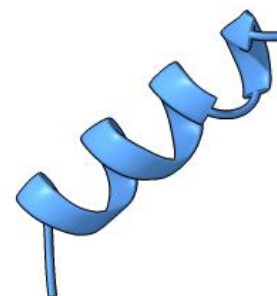
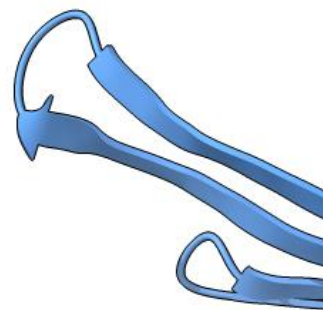
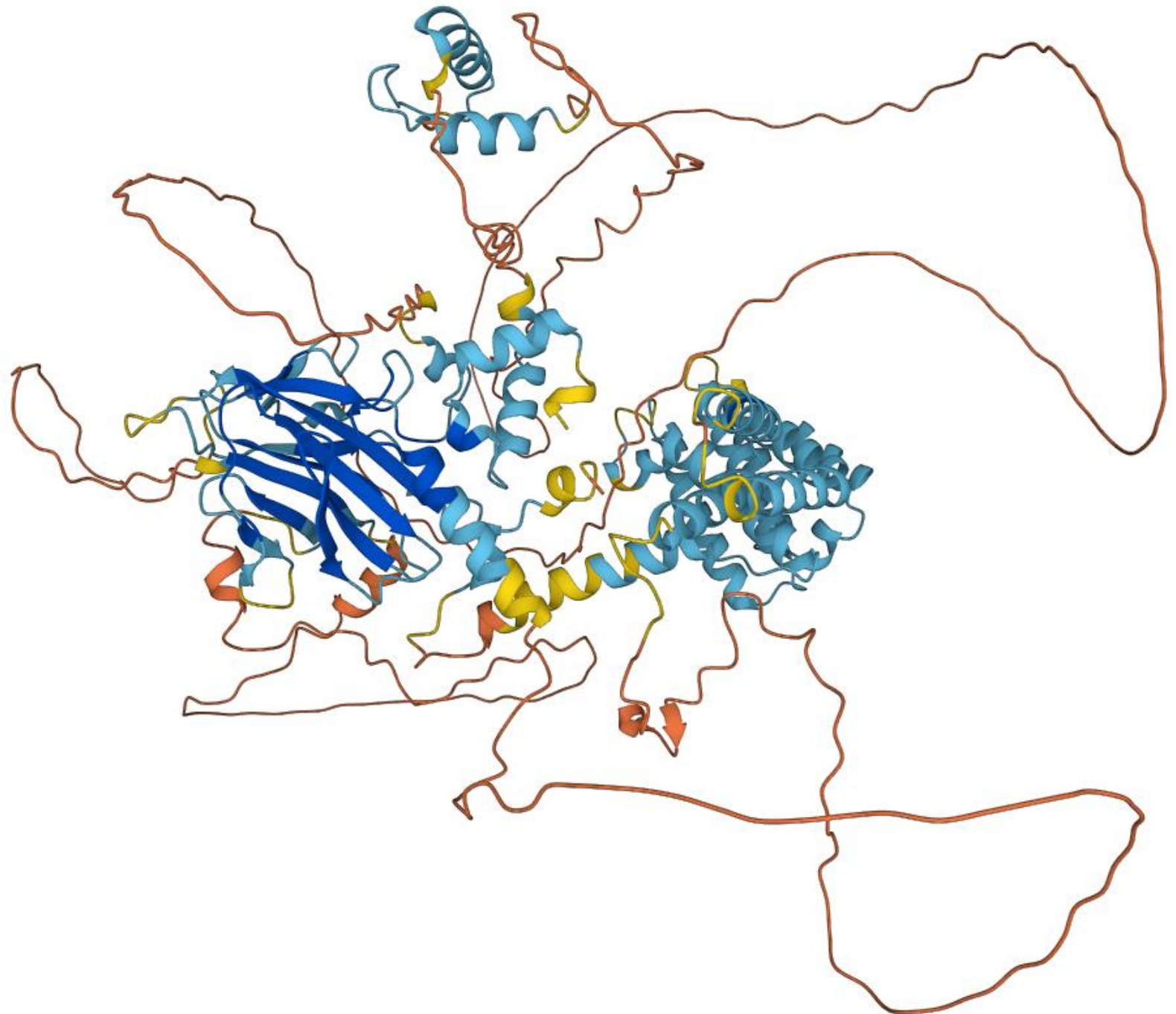


cryo-EM map

Get a prediction

sequence

```
>chain ' A'  
XXXXXXXXXXXXXXXXXCLTAPPKEAARPTLMPRAQSYKDLTHLPAP  
TGKIFVLSVNTADETGAEKDYBACNEETAUDGATAMLVTAIYDC  
RWFIP  
IMVEG  
VSTGE  
PVMLC  
MS
```

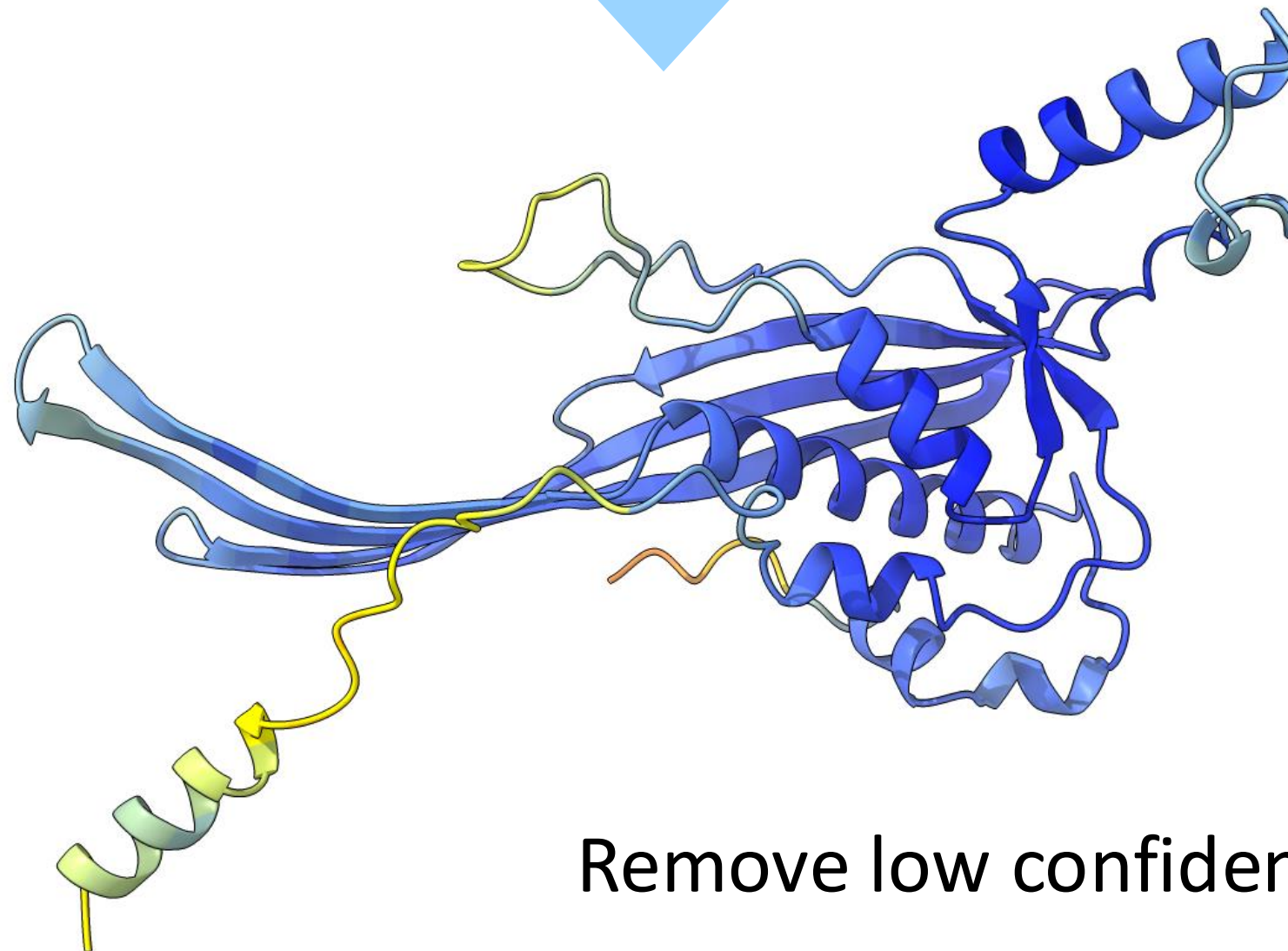
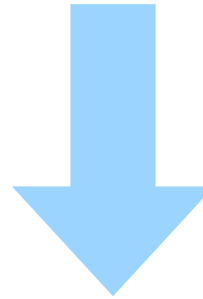


AlphaFold
model

Process prediction

sequence

```
>chain ' A'  
XXXXXXXXXXXXXXXXXCLTAPPKEAARPTLMPRAQSYKDLTHLPAP  
TGKIFVSVYNIQDETGQFKPYPASNFSTAVPQSATAMLVTALKDS  
RWFIPLERQGLQNLLNERKIIRAAQENGTVAINNRIPQLSLTAAN  
IMVEGSIIGYESNVKSGGVGARYFGIGADTQYQLDQIAVNLRVVN  
VSTGEILSSVNTSKTILSYEVQAGVFRFIDYQRLLEGEVGYTSNE  
PVMLCLMSAIETGVIFLINDGIDRGLWDLQNKAERQNDILVKYRH  
MS
```



AlphaFold
model

Remove low confidence parts

Process prediction

AlphaFold: Predicted models with Crystals or Cryo-EM



How to use AlphaFold in Phenix

Documentation for using AlphaFold2 models in Phenix



AlphaFold model prediction

Predict the chains in a sequence file with AlphaFold



Process Predicted Model

Replace B-factor field in model and optionally split into domains



Predict and Build: Crystallography

Iterative AlphaFold prediction, MR/docking, and rebuilding

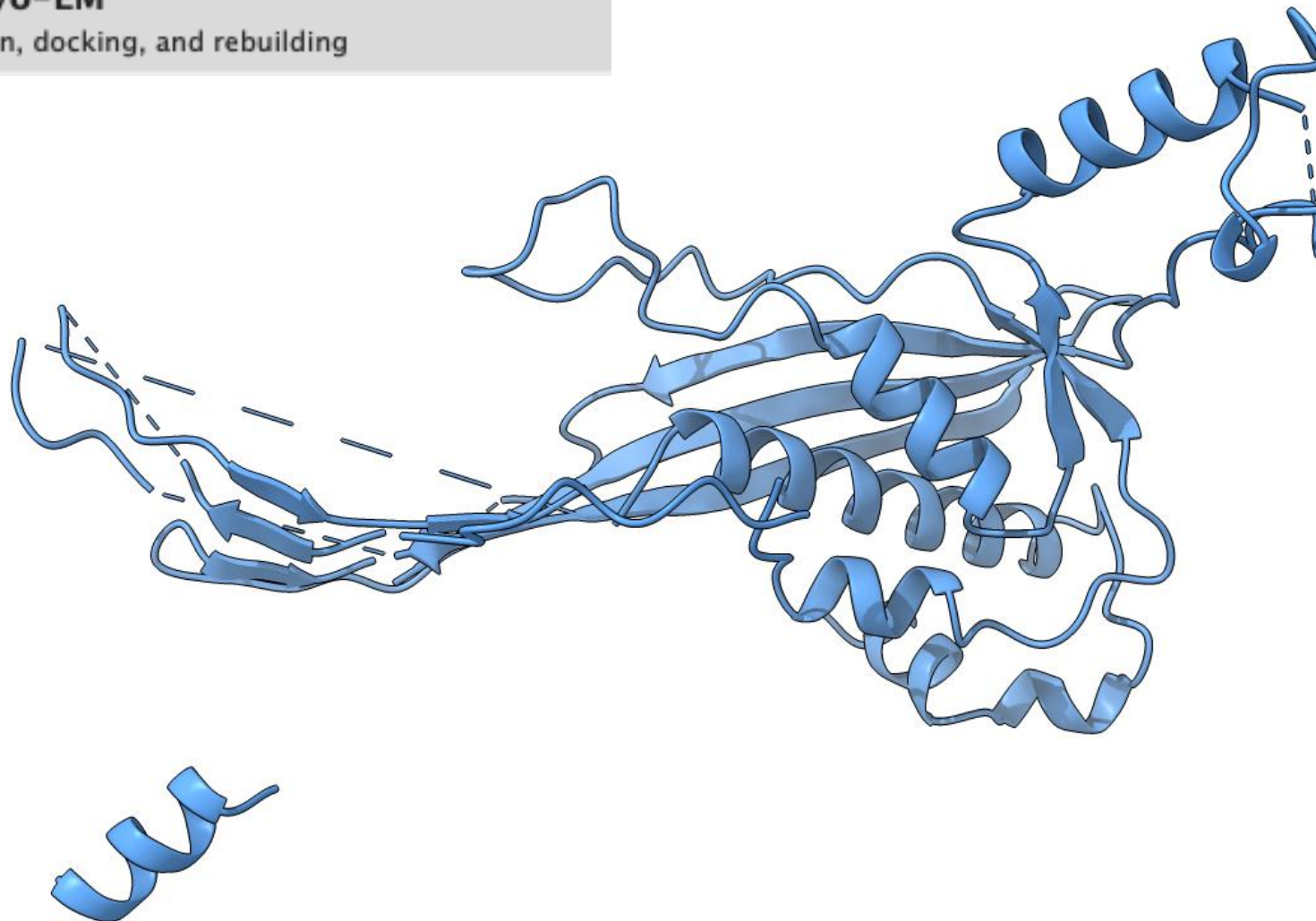


Predict and Build: Cryo-EM

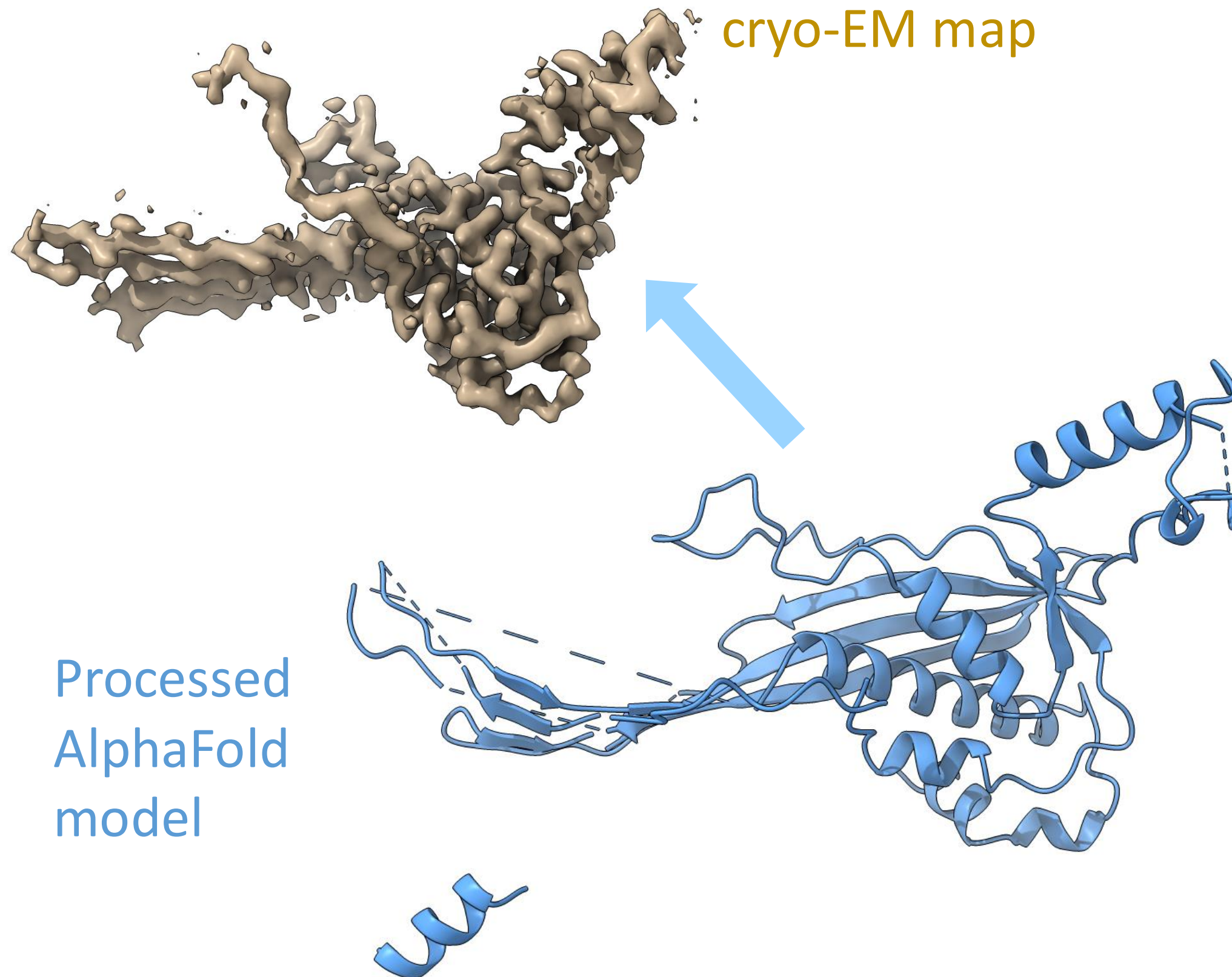
Iterative AlphaFold prediction, docking, and rebuilding

`phenix.process_predicted_model`

Processed
AlphaFold
model



Dock processed model



Docking in Phenix

Dock in map (T. Terwilliger)

The screenshot displays the Phenix software interface. The top toolbar includes icons for Quit, Preferences, Help, Citations, ChimeraX, Coot, PyMOL, KING, Tools, Help, and Chat. The main window is divided into two panes. The left pane, titled 'Projects', shows a table of project entries with columns for ID, Last modified, # of jobs, and R-free. The right pane, titled 'Validation', lists various actions. The 'Docking and model building' section is highlighted with an orange circle, and the 'Dock in map' option is specifically highlighted with a blue arrow.

Projects

Show group: All groups Manage...

Select Delete New project Import project Settings

ID	Last modified	# of jobs	R-free
apoferritin_chim...	Oct 14 2025 05:26 ...	4	---
✓ tst_fit_loops	Oct 14 2025 04:22 ...	26	---
AF_POMGNT2	Oct 01 2025 08:59 ...	15	---
apoferritin_den...	Oct 01 2025 08:36 ...	8	---
apoferritin_mod...	Sep 05 2025 01:40 ...	0	---
apoferritin_den...	Sep 05 2025 01:15 ...	1	---
tests	Jul 29 2025 04:39 ...	105	0.2650
groel_dock_refi...	Jul 09 2025 12:56 ...	5	---
test_ligand	Jul 08 2025 04:19 ...	3	0.2638
rnase-s	Jul 08 2025 03:37 ...	3	0.2555
b-CA-mr	Jul 06 2025 08:43 ...	5	---
1j4r_xtriage	Jul 06 2025 03:00 ...	3	---

Validation

- Map and structure factor calculation
- Map comparison and analysis
- Cryo-EM**
 - Map analysis and manipulation
 - Map improvement
 - Docking and model building
 - EM Placement (dock model with likelihood target)
Dock one model into a cryo-EM map
 - Dock in map**
Dock models into cryo-EM map
 - Predict and Build: Cryo-EM
Iterative AlphaFold prediction, docking, and rebuilding
 - Map to Model
Model-building into cryo-EM and low-resolution maps
 - Sequence From Map
Determine a sequence from a map
 - Fit Loops
Fit missing loops in a model
 - Rebuild a model in place
Adjust a model to match a map without changing atoms or connectivity
 - Douse (Add waters)

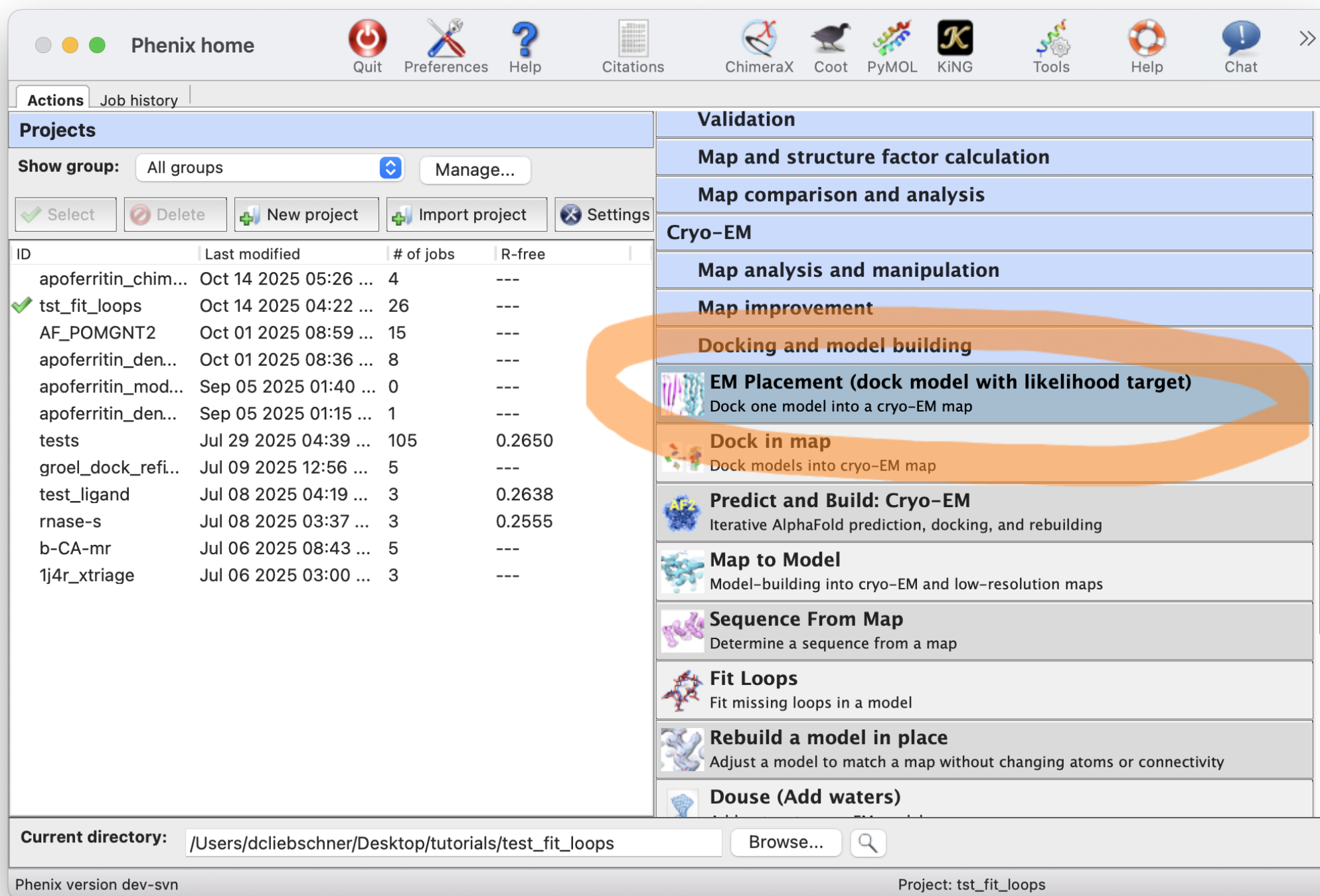
Current directory: /Users/dcliebschner/Desktop/tutorials/test_fit_loops Browse...

Phenix version dev-svn Project: tst_fit_loops

Docking in Phenix

Likelihood-based EM docking (R. Read)

- Use likelihood scores to dock a model into a map
- Works at low resolution (8.5 Å)



The screenshot displays the Phenix home web interface. The top navigation bar includes links for Quit, Preferences, Help, Citations, ChimeraX, Coot, PyMOL, KING, Tools, Help, and Chat. The main content area is divided into two panels. The left panel, titled 'Projects', shows a table of projects with columns for ID, Last modified, # of jobs, and R-free. The right panel, titled 'Validation', lists various actions. The 'Docking and model building' section is highlighted with an orange oval, containing the following items:

- EM Placement (dock model with likelihood target)**: Dock one model into a cryo-EM map
- Dock in map**: Dock models into cryo-EM map
- Predict and Build: Cryo-EM**: Iterative AlphaFold prediction, docking, and rebuilding
- Map to Model**: Model-building into cryo-EM and low-resolution maps
- Sequence From Map**: Determine a sequence from a map
- Fit Loops**: Fit missing loops in a model
- Rebuild a model in place**: Adjust a model to match a map without changing atoms or connectivity
- Douse (Add waters)**

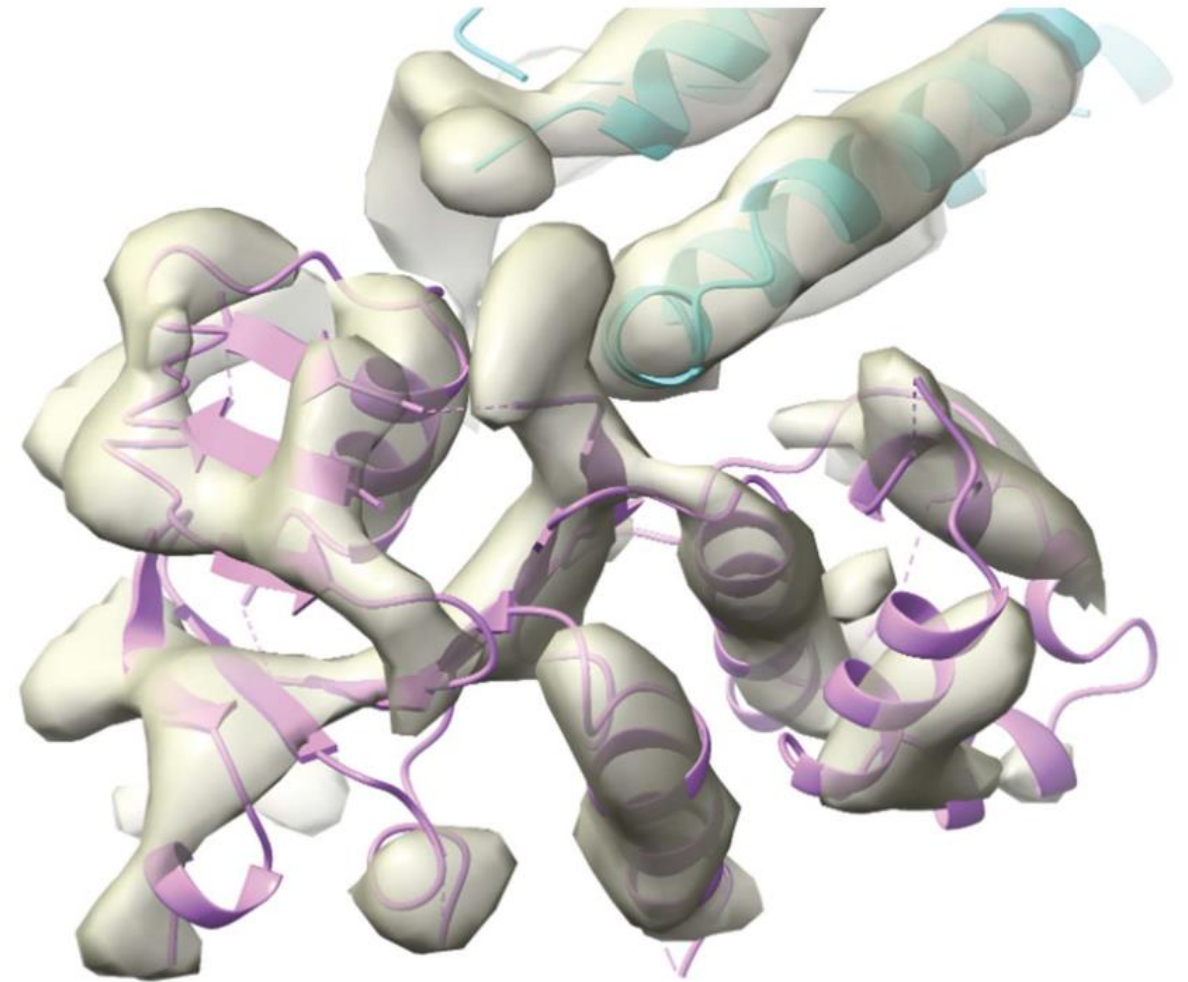
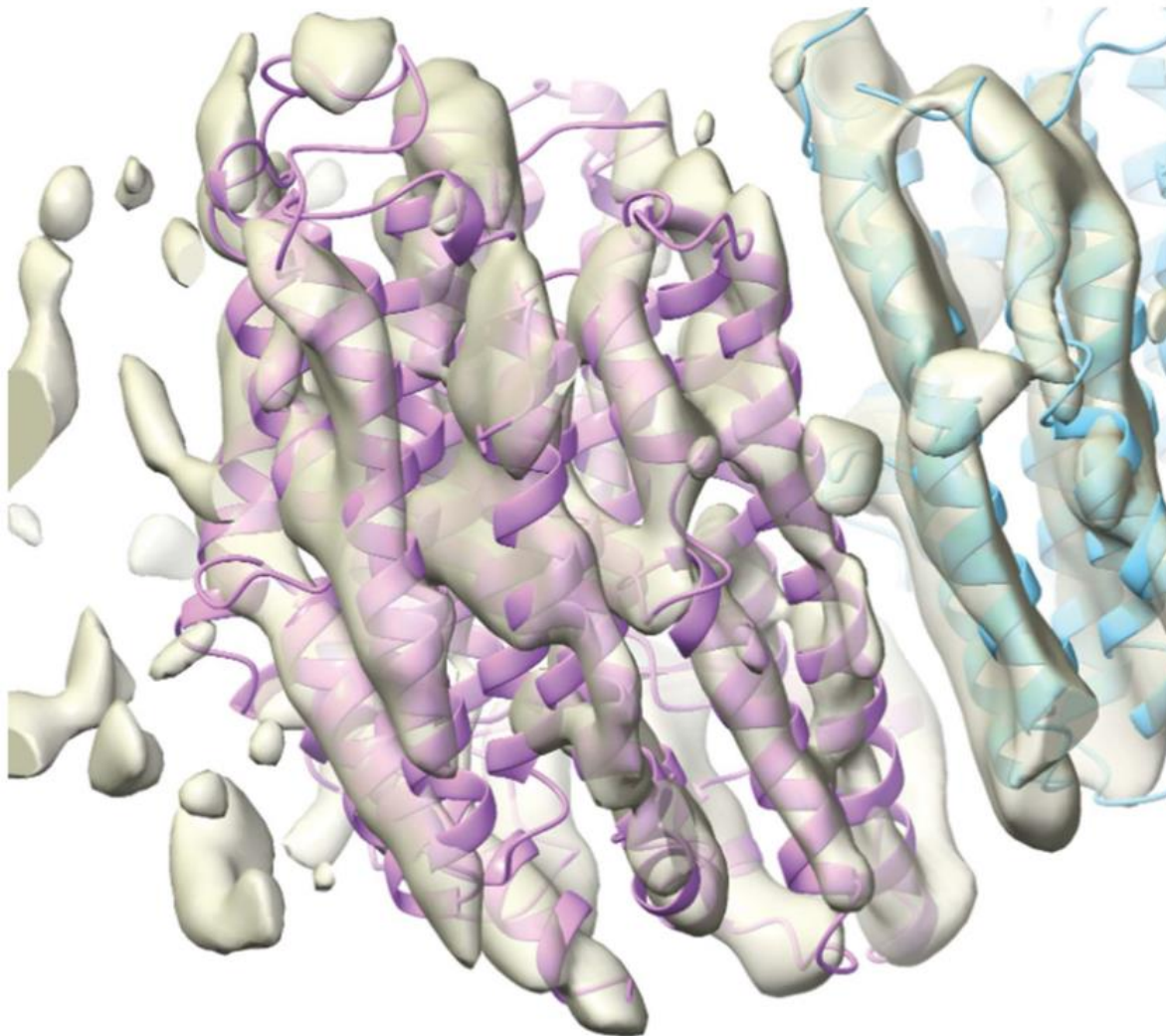
The 'Current directory' is set to /Users/dcliebschner/Desktop/tutorials/test_fit_loops. The Phenix version is dev-svn, and the current project is tst_fit_loops.

ID	Last modified	# of jobs	R-free
apoferritin_chim...	Oct 14 2025 05:26 ...	4	---
✓ tst_fit_loops	Oct 14 2025 04:22 ...	26	---
AF_POMGNT2	Oct 01 2025 08:59 ...	15	---
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apoferritin_mod...	Sep 05 2025 01:40 ...	0	---
apoferritin_den...	Sep 05 2025 01:15 ...	1	---
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1j4r_xtriage	Jul 06 2025 03:00 ...	3	---

Docking in Phenix

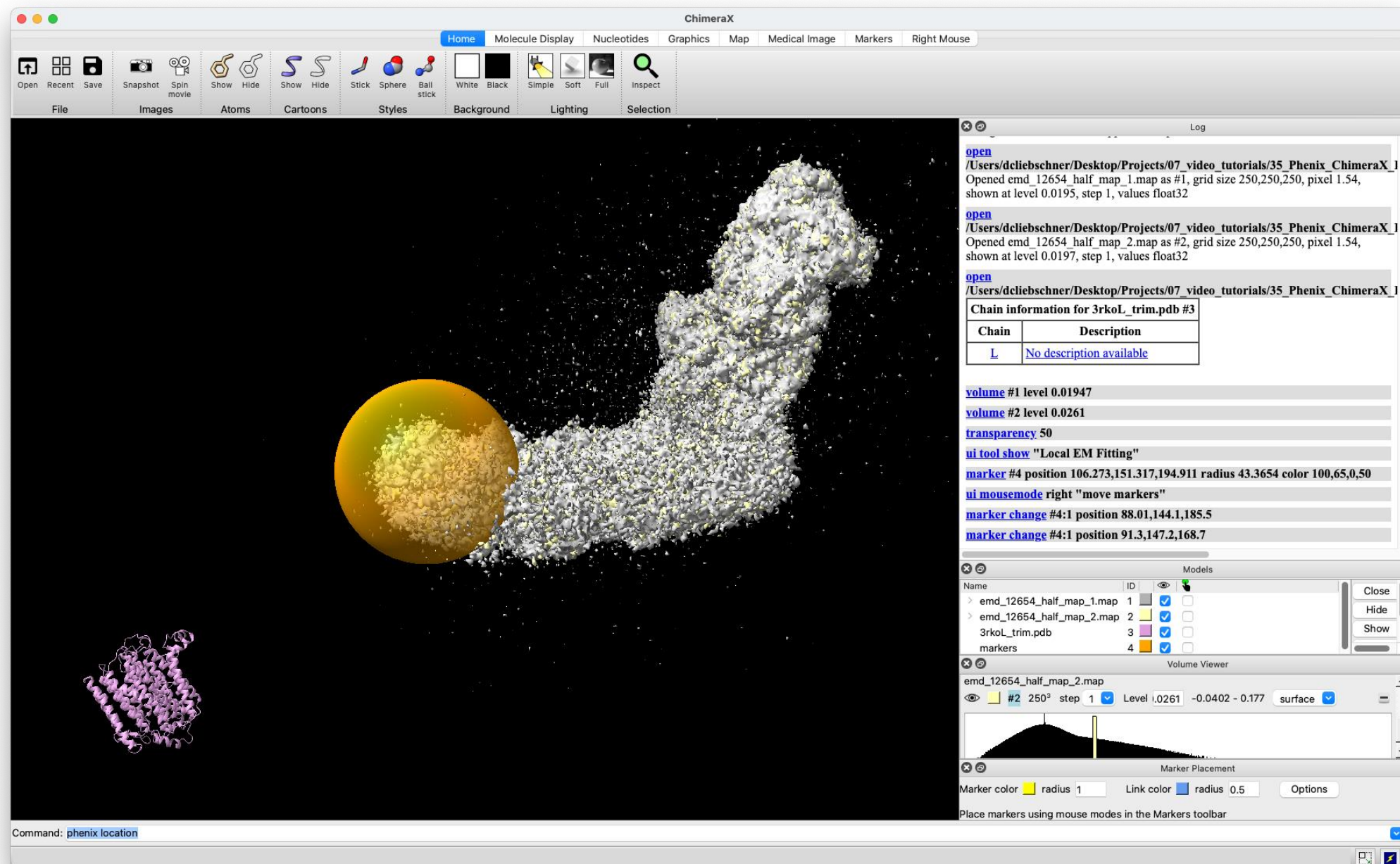
Likelihood-based EM docking (R. Read)

- Use likelihood scores to dock a model into a map
- Works at low resolution (8.5 Å)

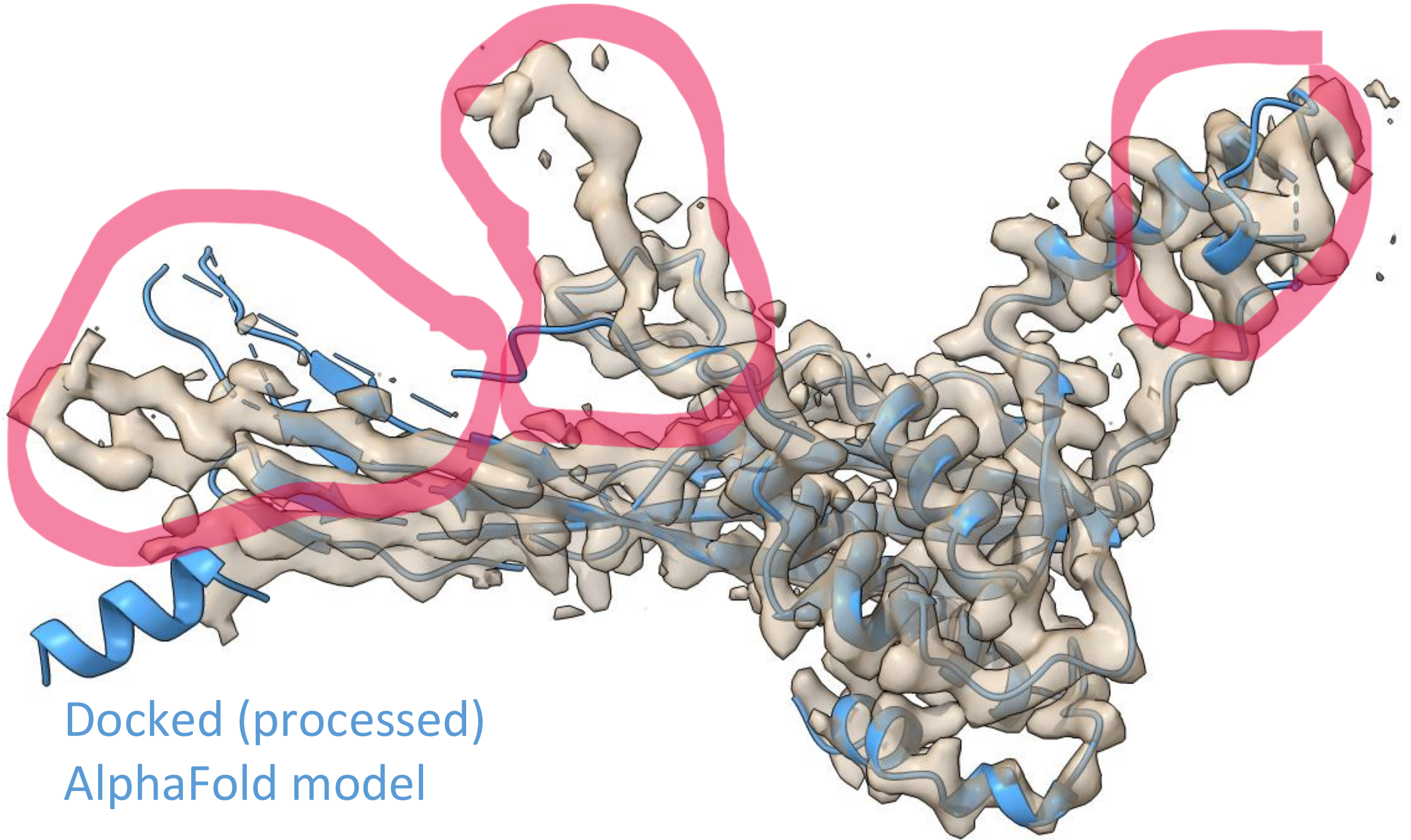


Docking in Phenix/ChimeraX

- Likelihood-based docking can be done via ChimeraX.
- Can select the region into which the model should be docked.



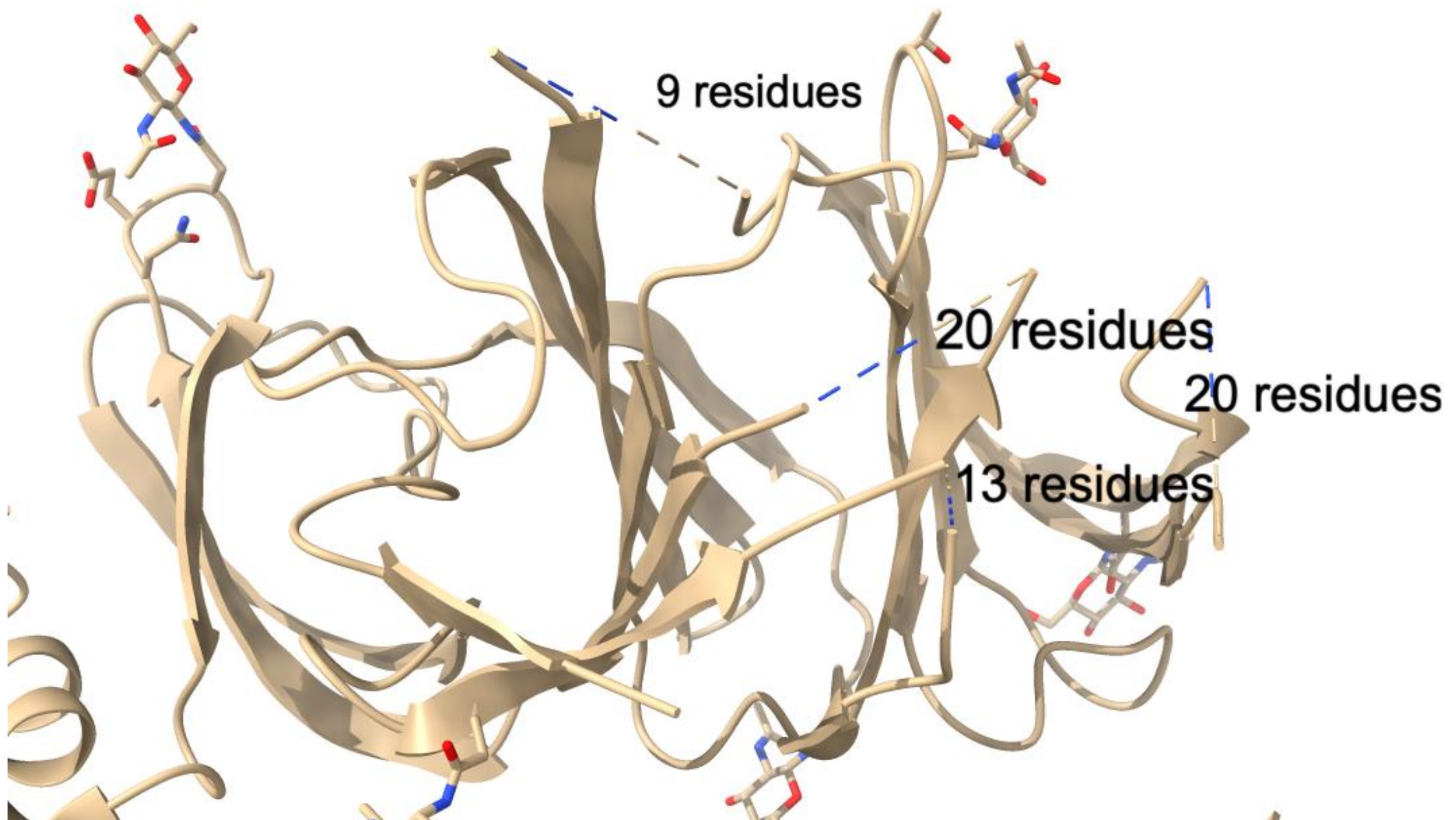
Dock processed model



Docked (processed)
AlphaFold model

Some parts don't fit into the map

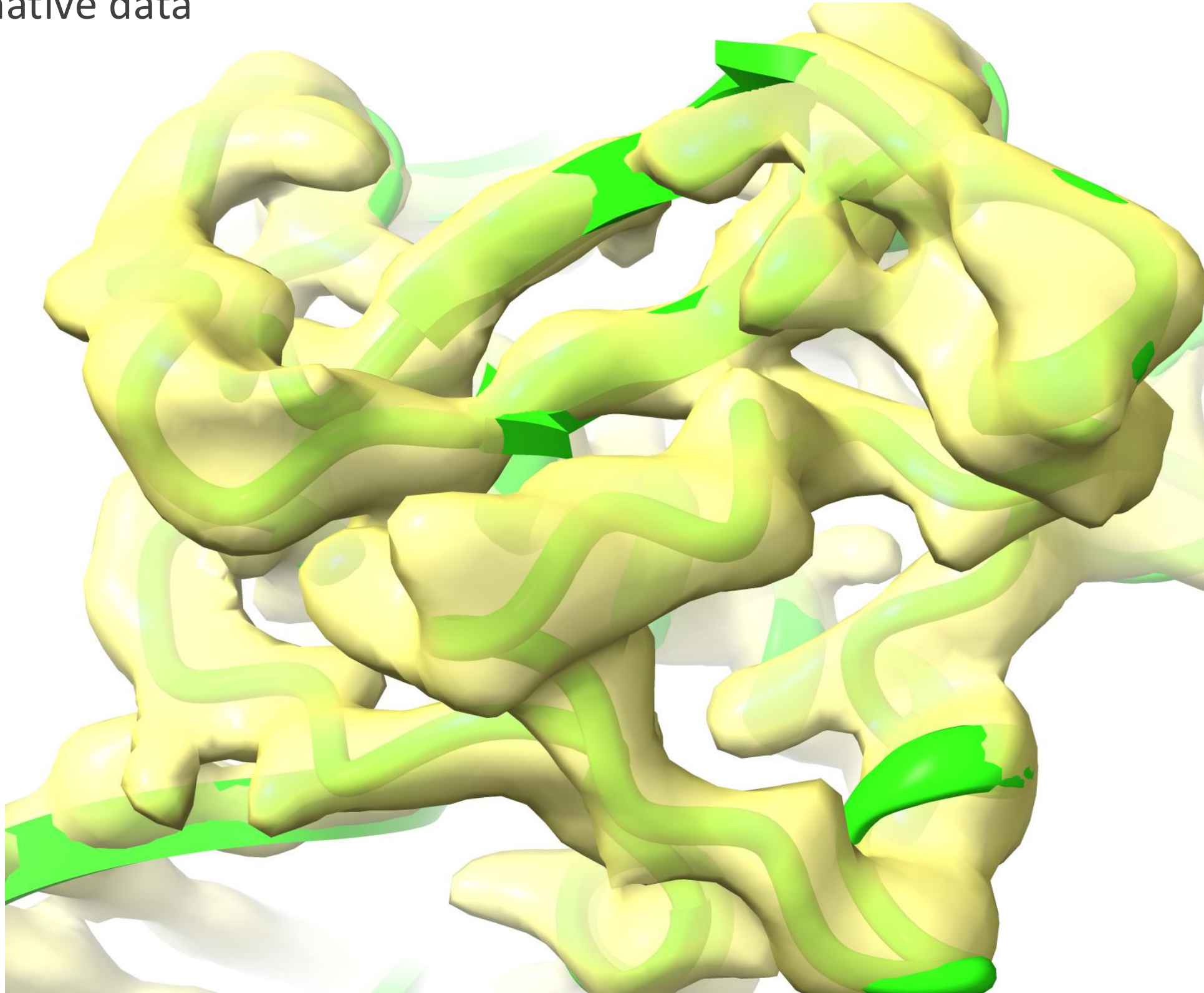
2. Use a prediction to complete a model



Use predicted model as hypothesis for missing parts.

Can AF predictions help if the structure is already solved?

Repressor-DNA complex, solved with 2.6 Å SeMet SAD data & refined against 3.1 Å native data



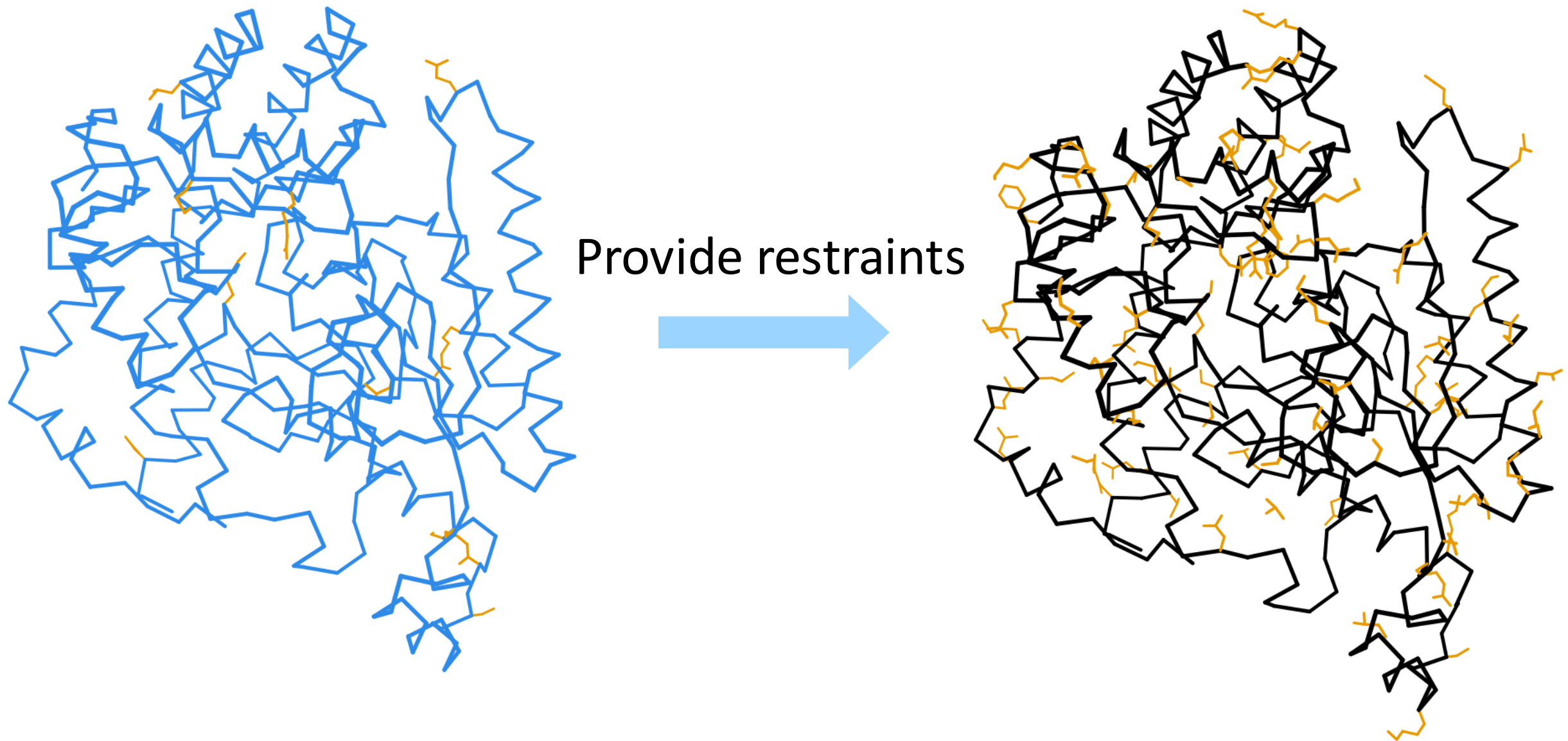
*Before AlphaFold,
 $R/R_{\text{free}} = 0.27/0.29$*

*AlphaFold model:
A **hypothesis** about
this structure*

*After AlphaFold,
 $R/R_{\text{free}} = 0.21/0.24$
(it was a good
hypothesis)*

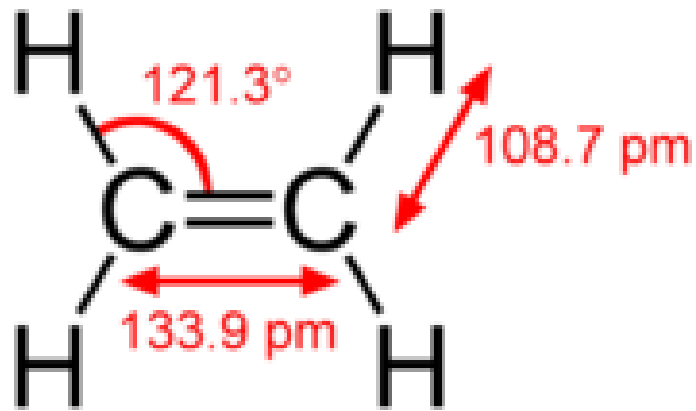
*Jamie Wallen, Western
Carolina University*

3. Use a prediction as reference model



Restraints: *a priori* knowledge

- Restraints increase the number of observations.
- Restraints modify the target function by creating relationships between independent parameters.
- **Example:** restrained bond lengths



- the coordinates of the two atoms are independent
- restraint keeps their distance within a certain target value
- imposes a penalty if it deviates too much.

Reference Model Restraints

Concept

- Use a related model to generate a set of **torsion restraints**.
- Restrain **each torsion angle** in the working model to the corresponding torsion angle in the reference model.
- Allows for structural differences.

When to use

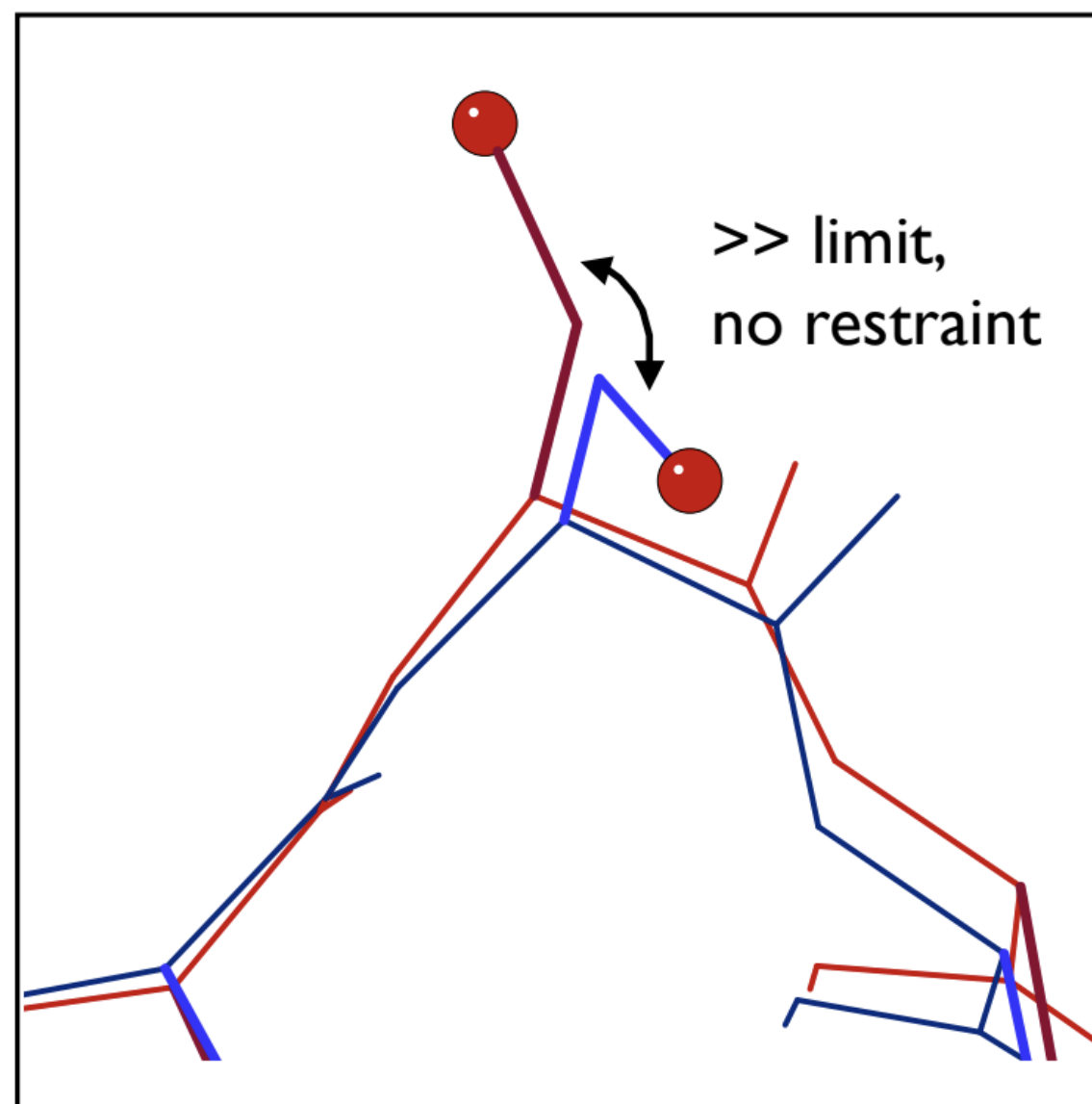
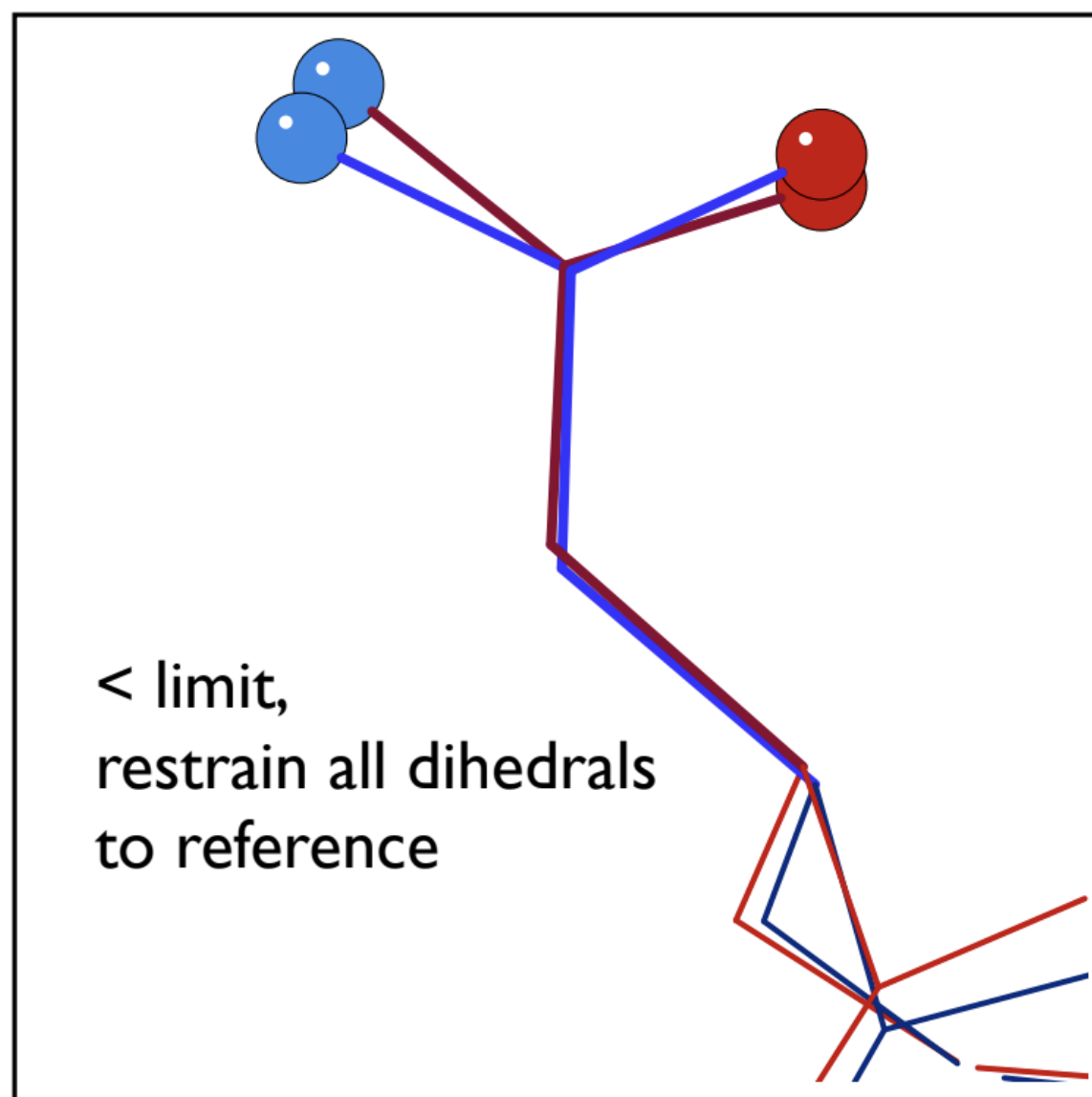
Low resolution (worse than 3Å).

If no high resolution homologue available, could use AF model for reference model (AF models have good geometry).

Reference Model Restraints

The 'limit' parameter

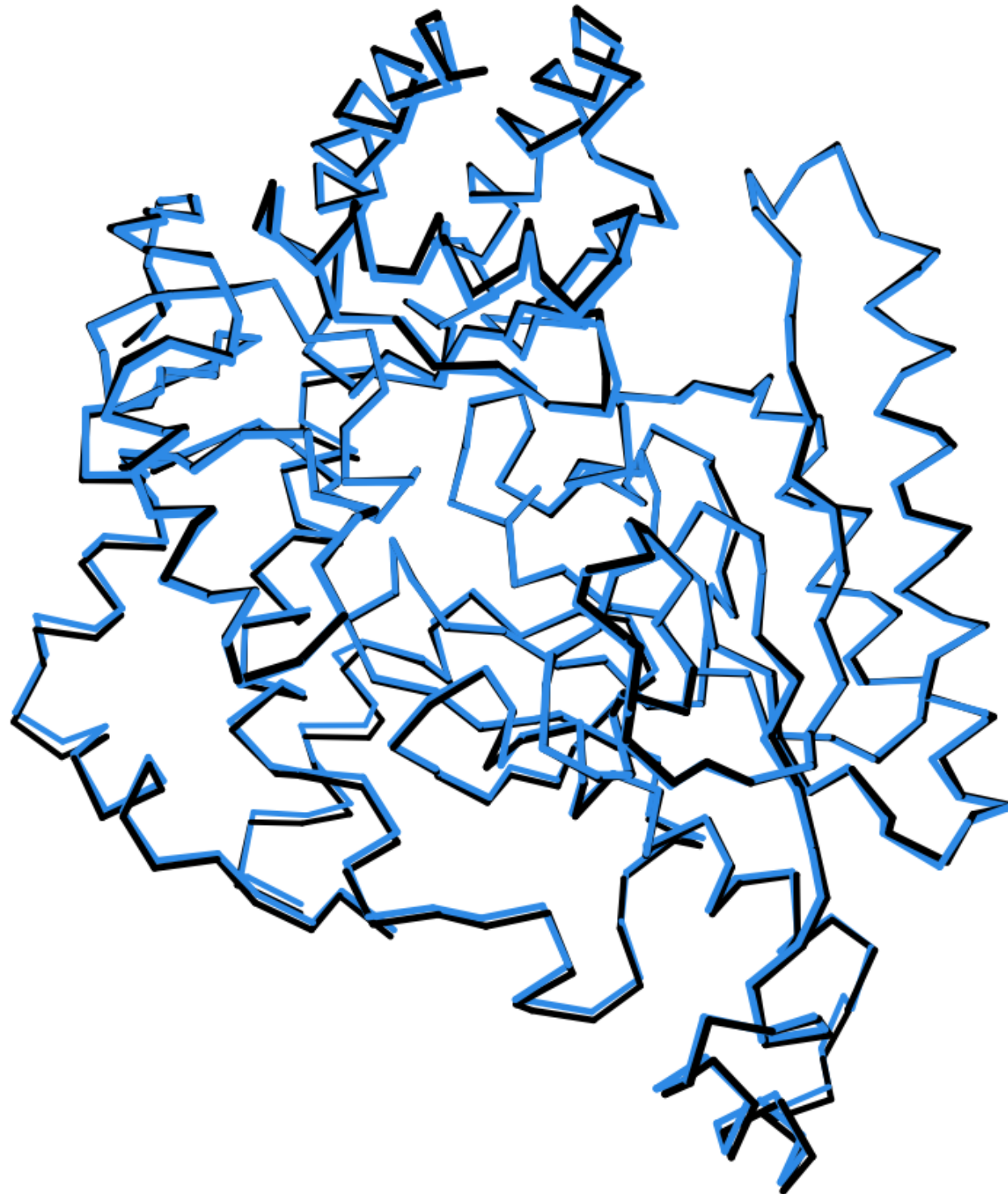
default: limit = 15.0°



Reference model Restraints: example

1GTX: 3.0 Å

1OHV: 2.3 Å



4-aminobutyrate-aminotransferase

Reference model Restraints: example



1OHV: 2.3 Å



1GTX: 3.0 Å

4-aminobutyrate-aminotransferase

Reference model Restraints

How to use

Supply a reference model in phenix.real_space_refine; check the corresponding box.

(Oleg Sobolev: working on finding reference model automatically)

The screenshot displays the 'phenix.real_space_refine' application window. The 'Input/Output' tab is selected, and the 'Refinement Settings' sub-tab is active. In the 'Input' section, a table lists files for refinement. The 'Data type' column has three entries: 'Model file', 'Reference model' (circled in orange), and 'MTZ file'. Below the table are buttons for 'Add file', 'Remove file', and 'Modify file data type...'. The 'Resolution' field is empty, and the 'Map coefficients label' is set to '-...'. The 'Ignore symmetry conflicts' checkbox is unchecked. In the 'Output' section, the 'Prefix' field is empty, and the 'Write initial geo file', 'Write final geo file', 'Write all states', and 'Run validation' checkboxes are all checked. The 'Refinement Settings' sub-tab contains various options. The 'Strategy' section includes checkboxes for 'minimization_global' (checked), 'rigid_body' (unchecked), 'local_grid_search' (checked), 'morphing' (unchecked), 'simulated_annealing' (unchecked), 'adp' (checked), 'occupancy' (checked), and 'nqh_flips' (checked). The 'Max iterations' is set to 100, 'Macro cycles' to 5, 'Target bonds rmsd' to 0.01, and 'Target angles rmsd' to 1.0. The 'Use secondary structure restraints' checkbox is checked, and 'Ncs constraints' is unchecked. The 'Strategy Options' section shows 'Morphing' set to 'first' and 'Simulated annealing' set to 'once'. The 'Reference model restraints' checkbox is checked and circled in orange. The 'Other Options' section includes 'Scattering table' set to 'electron', 'Weight' set to 1, 'Resolution factor' set to 0.25, 'Nproc' set to 1, and 'Random seed' set to 0. The 'Ramachandran restraints' checkbox is checked, 'Refine ncs operators' is unchecked, and 'Show per residue' is checked. At the bottom, there are buttons for 'Model interpretation...', 'Rotamers...', 'Automatic linking...', and 'All parameters...'.

Real-space refinement (Project: 7rpq_AF_reference_m...)

Input/Output | Refinement Settings

By default real-space refinement applies Ramachandran restraints to the model to maintain good stereochemistry. However, if your input model contains Ramachandran outliers these restraints may lead to a non-optimal local geometry, which will require other validation metrics to detect, such as CABLAM and the Rama-Z score. We recommend that you manually fix these outliers before running real-space refinement.

Job title :

Input

File path	Format	Data type
/Users/dcliebschner/Documents/7rpq_AF_reference...	PDB	Model file
/Users/dcliebschner/Documents/7rpq_AF_reference...	PDB	Reference model
/Users/dcliebschner/Documents/7rpq_AF_reference...	ccp4_mtz	MTZ file

Add file Remove file Modify file data type...

Resolution : Map coefficients label : -...

☐ Ignore symmetry conflicts

Output

Prefix :

☒ Write initial geo file ☐ Write final geo file ☐ Write all states ☒ Run validation

Refinement Settings

Strategy

☒ minimization_global ☐ rigid_body ☒ local_grid_search

Run : ☐ morphing ☐ simulated_annealing ☒ adp

☒ occupancy ☒ nqh_flips

Max iterations : 100 Macro cycles : 5

Target bonds rmsd : 0.01 Target angles rmsd : 1.0

Select Atoms ☒ Use secondary structure restraints ☐ Ncs constraints

Strategy Options

Morphing : first

Simulated annealing : once

☒ Reference model restraints

Options

Other Options

Scattering table : electron Weight : Resolution factor : 0.25

Nproc : 1 Random seed : 0

☒ Ramachandran restraints ☐ Refine ncs operators ☒ Show per residue

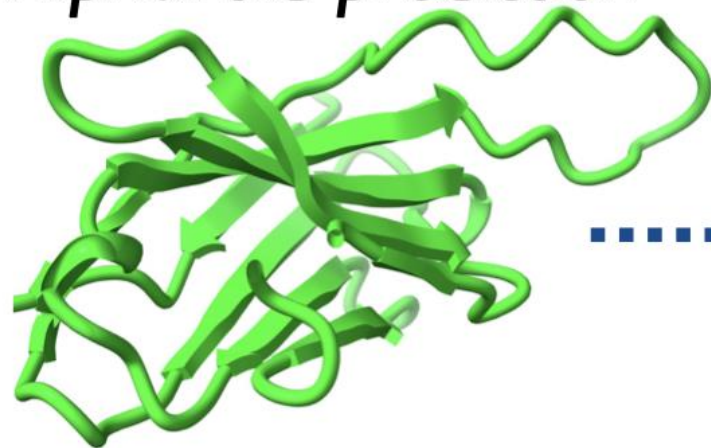
Model interpretation... Rotamers... Automatic linking... All parameters...

Use your working model to get a new AlphaFold prediction

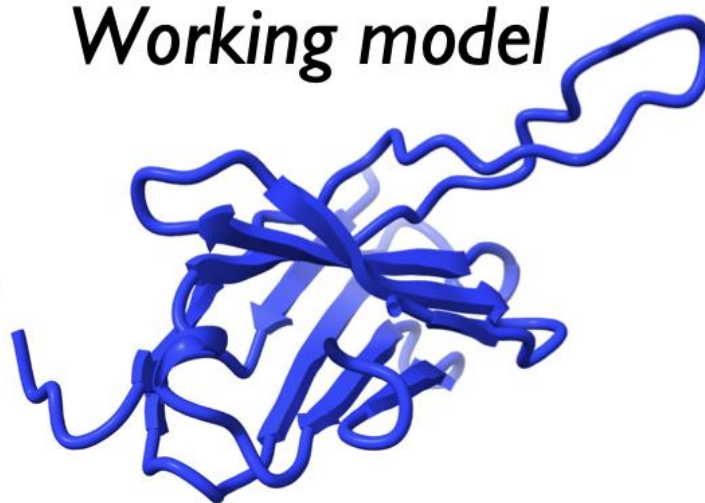
Why?

Because your new prediction might be better than your model

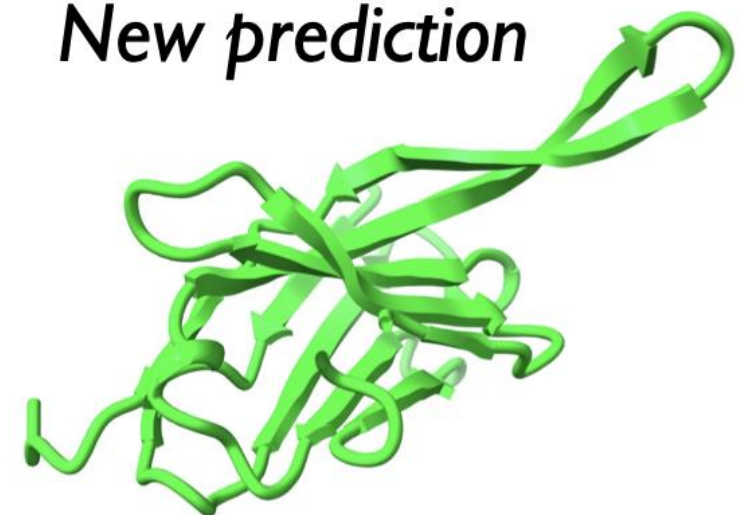
AlphaFold prediction



Working model



New prediction



Example: Fab heavy chain

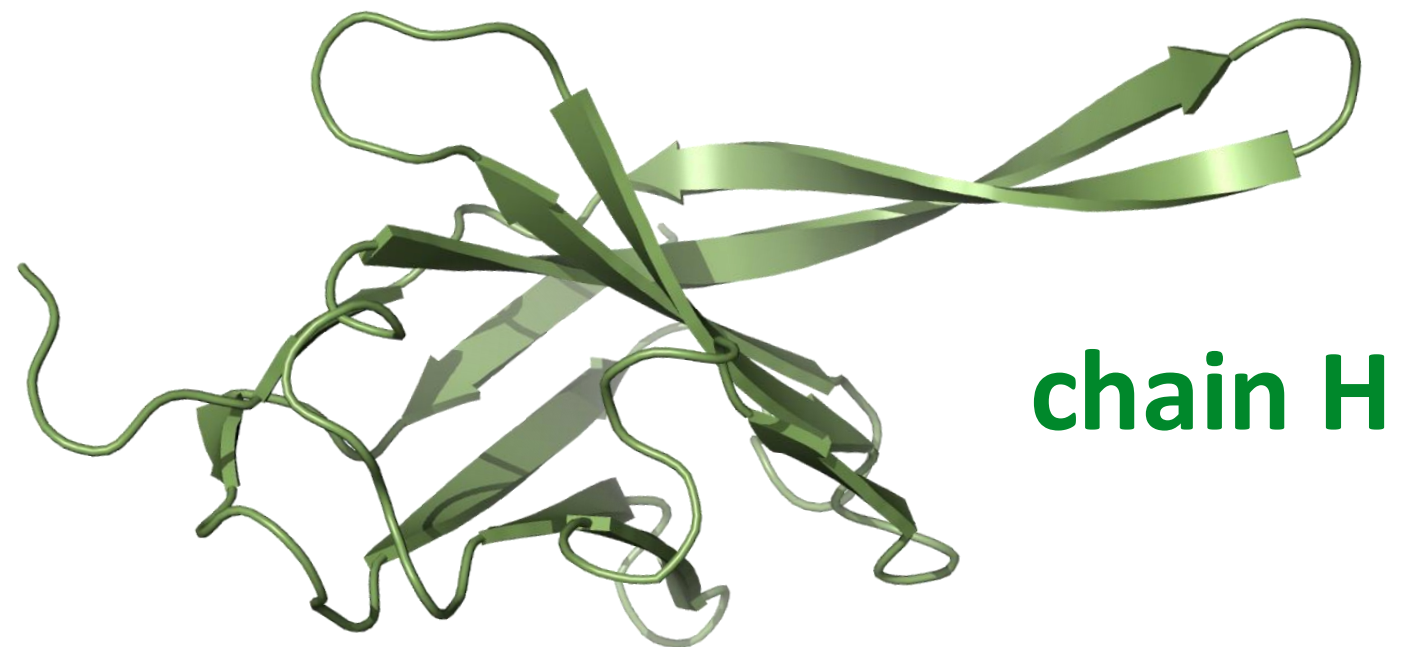
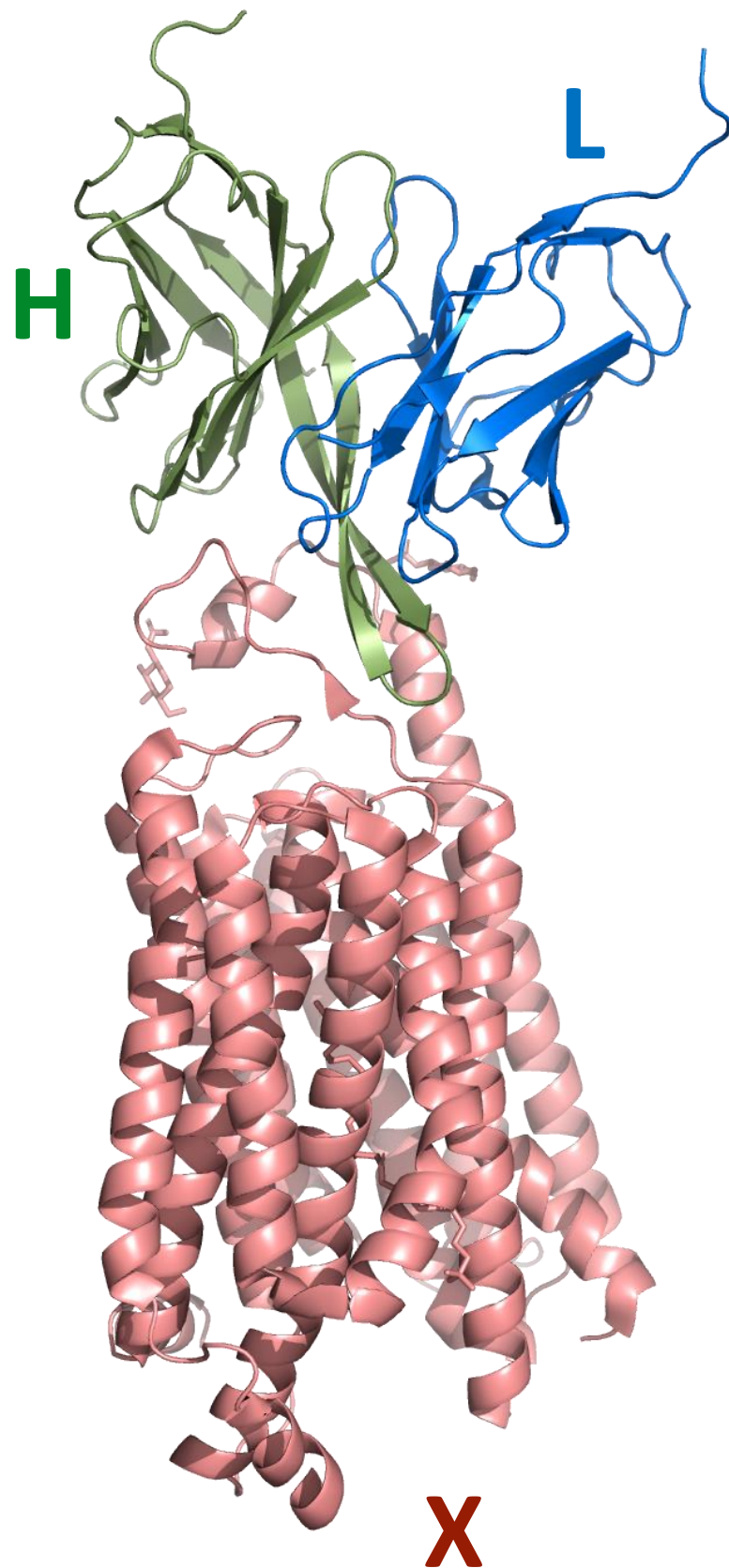
 **7MJS**

Single-Particle Cryo-EM Structure of Major Facilitator Superfamily Domain containing 2A in complex with LPC-18:3

PDB DOI: <https://doi.org/10.2210/pdb7MJS/pdb>

EM Map EMD-23883: [EMDB EMDDataResource](https://www.ebi.ac.uk/emdb/EMD-23883)

3.03 Å resolution

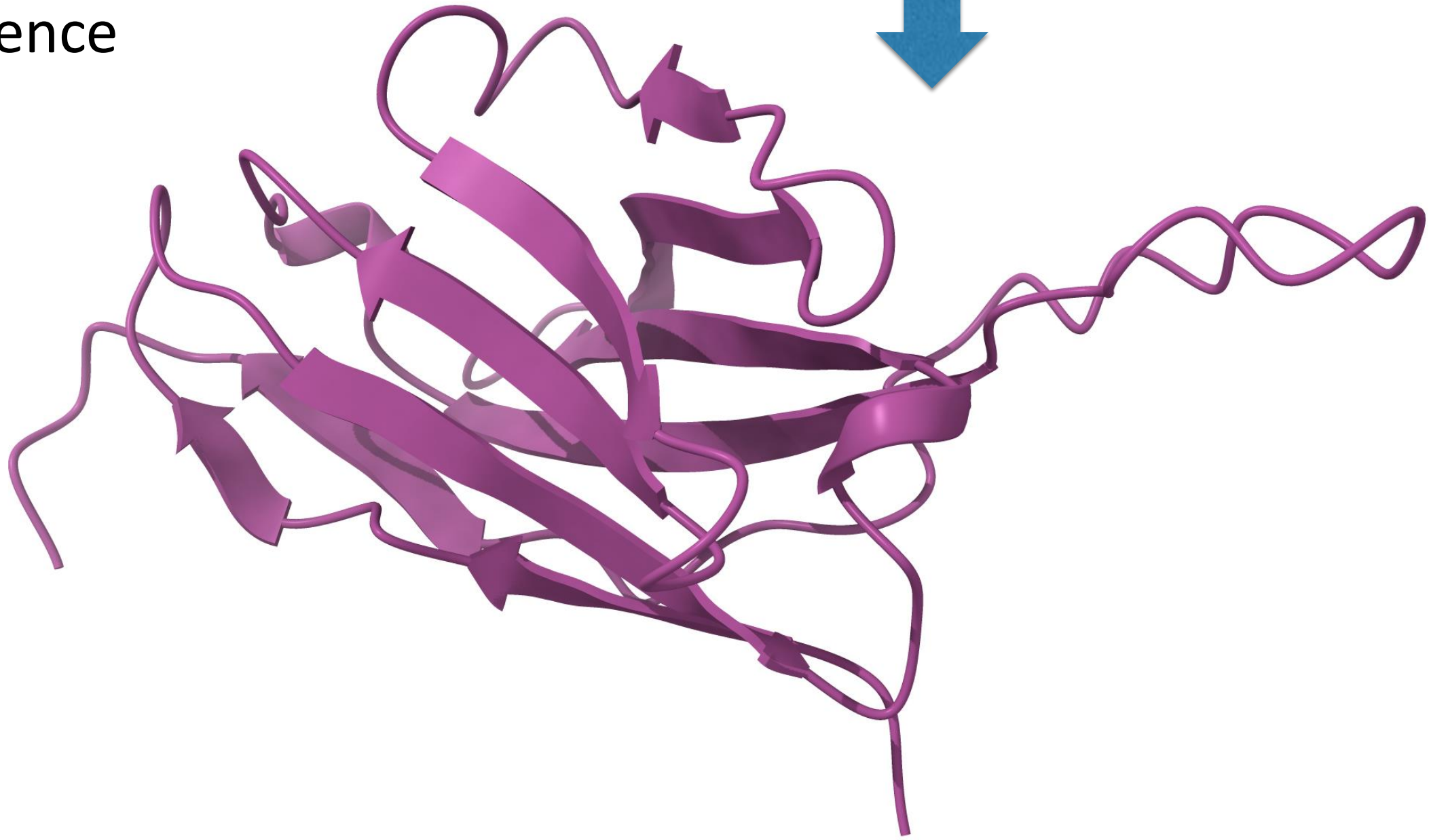


A loop that interacts with other chains is not correctly predicted.

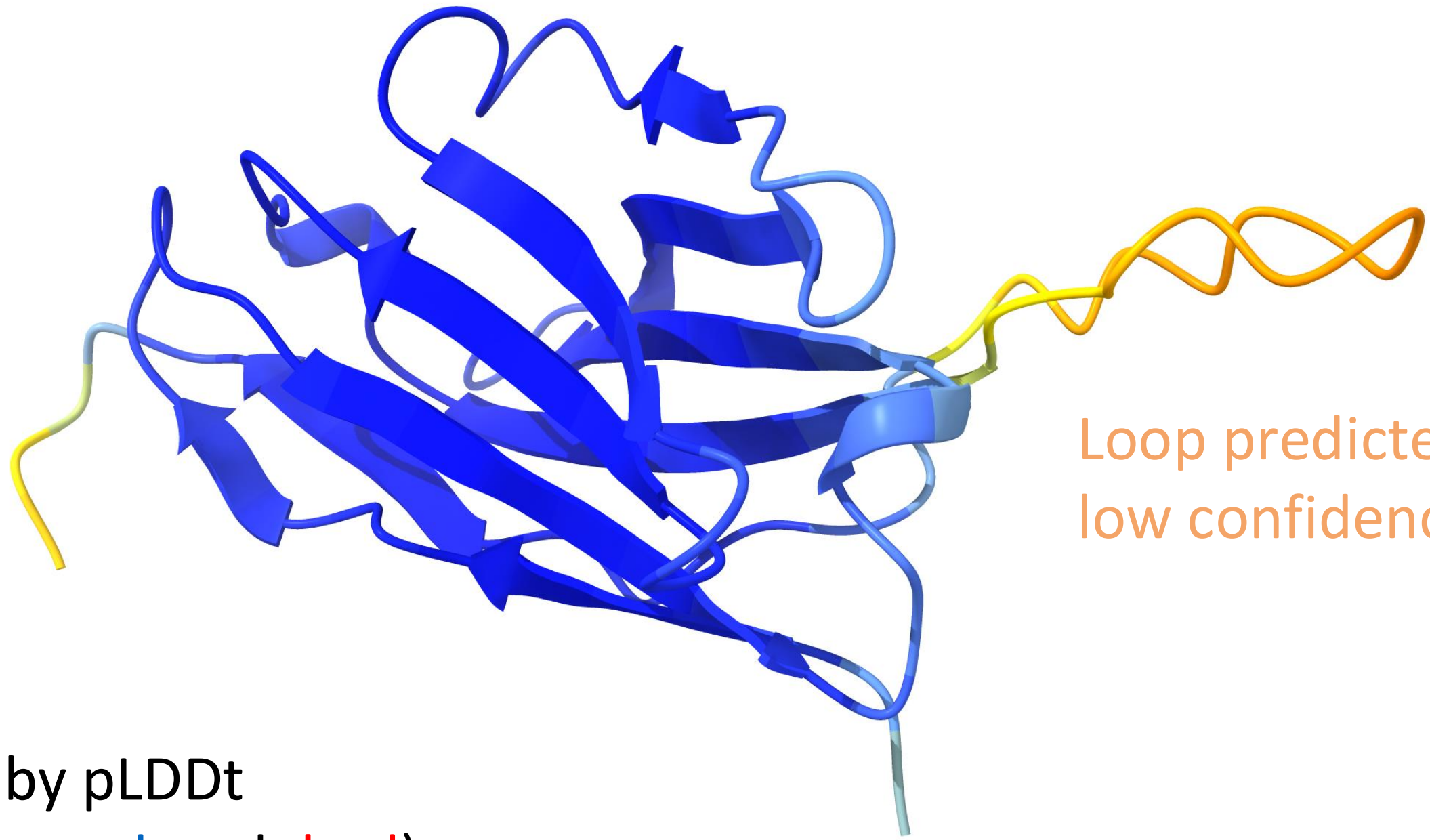
AF2 prediction of chain H

EVQLVESGGGLVQPGGSLRLSCAASGFNIYSSSIHWVRQ
APGKGLEWVAYIYSYSGYTSYADSVKGRFTISADTSKNTA
YLQMNSLRAEDTAVYYCARSLEYLYSSGYQYKWATGLDY
WGQGTLVTVSSAST

Sequence



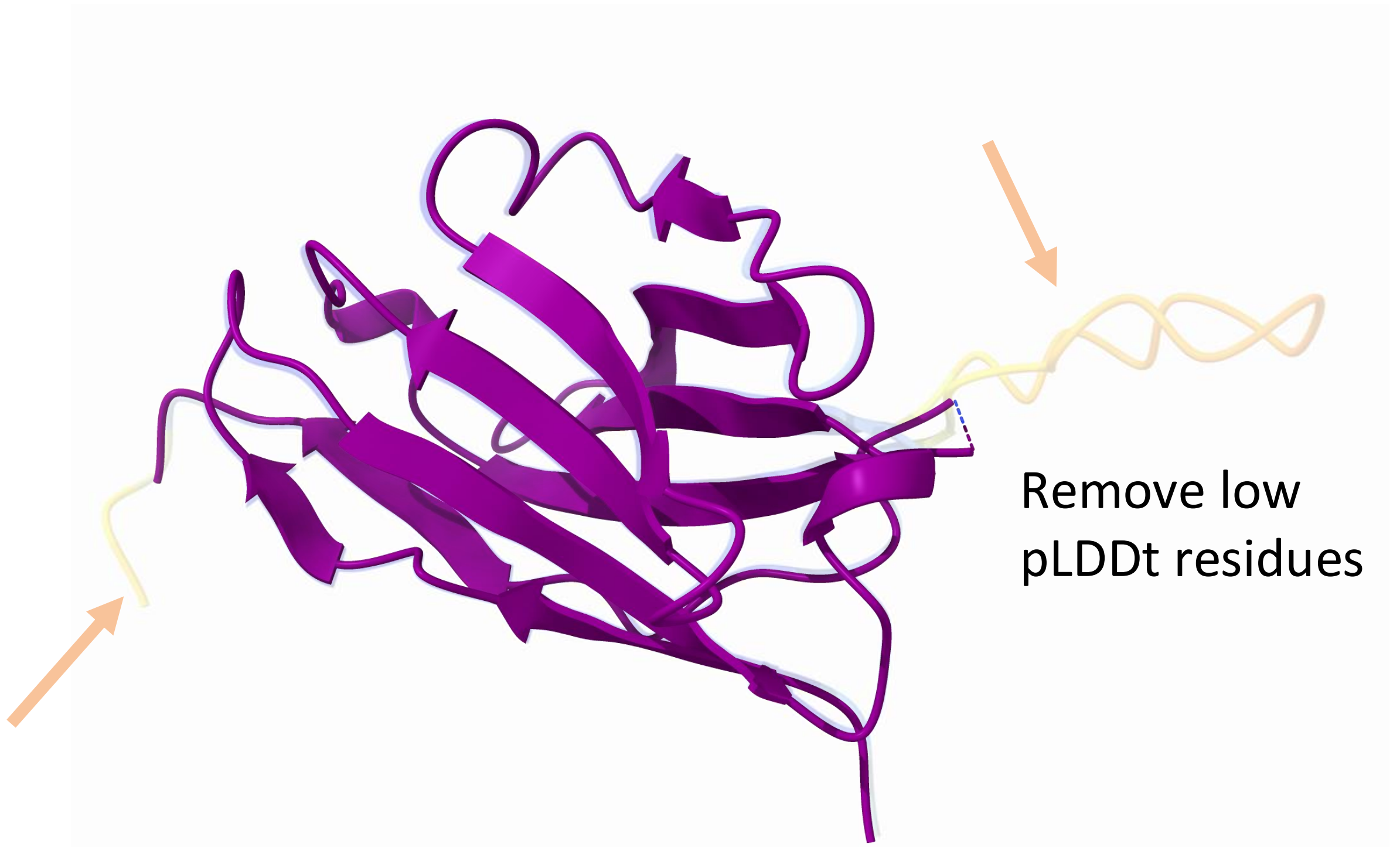
AF2 prediction of chain H



Loop predicted with
low confidence

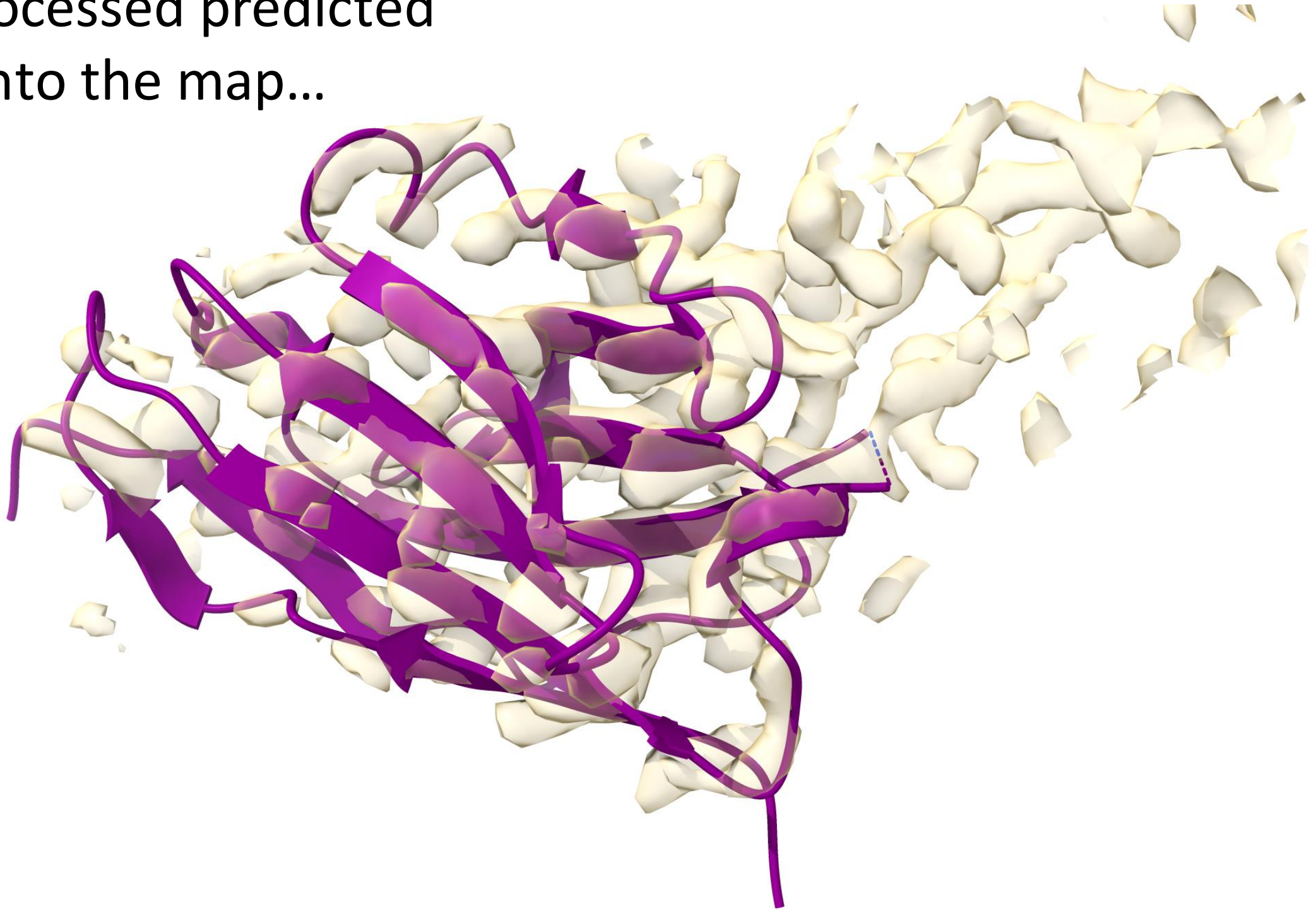
Color by pLDDt
(blue: good, red: bad)

Process AF2 prediction

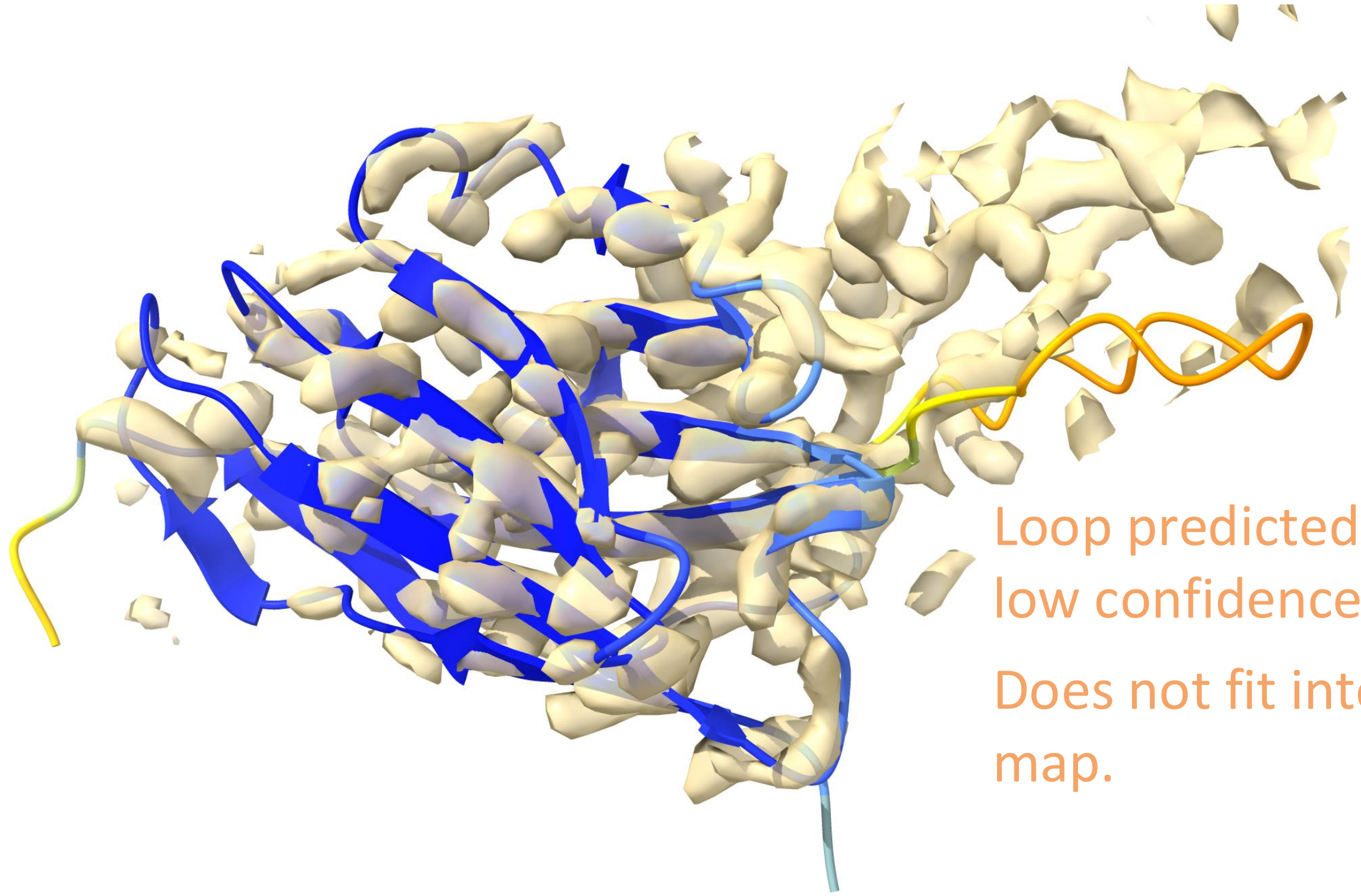


Dock processed model into the map

Dock processed predicted
model into the map...



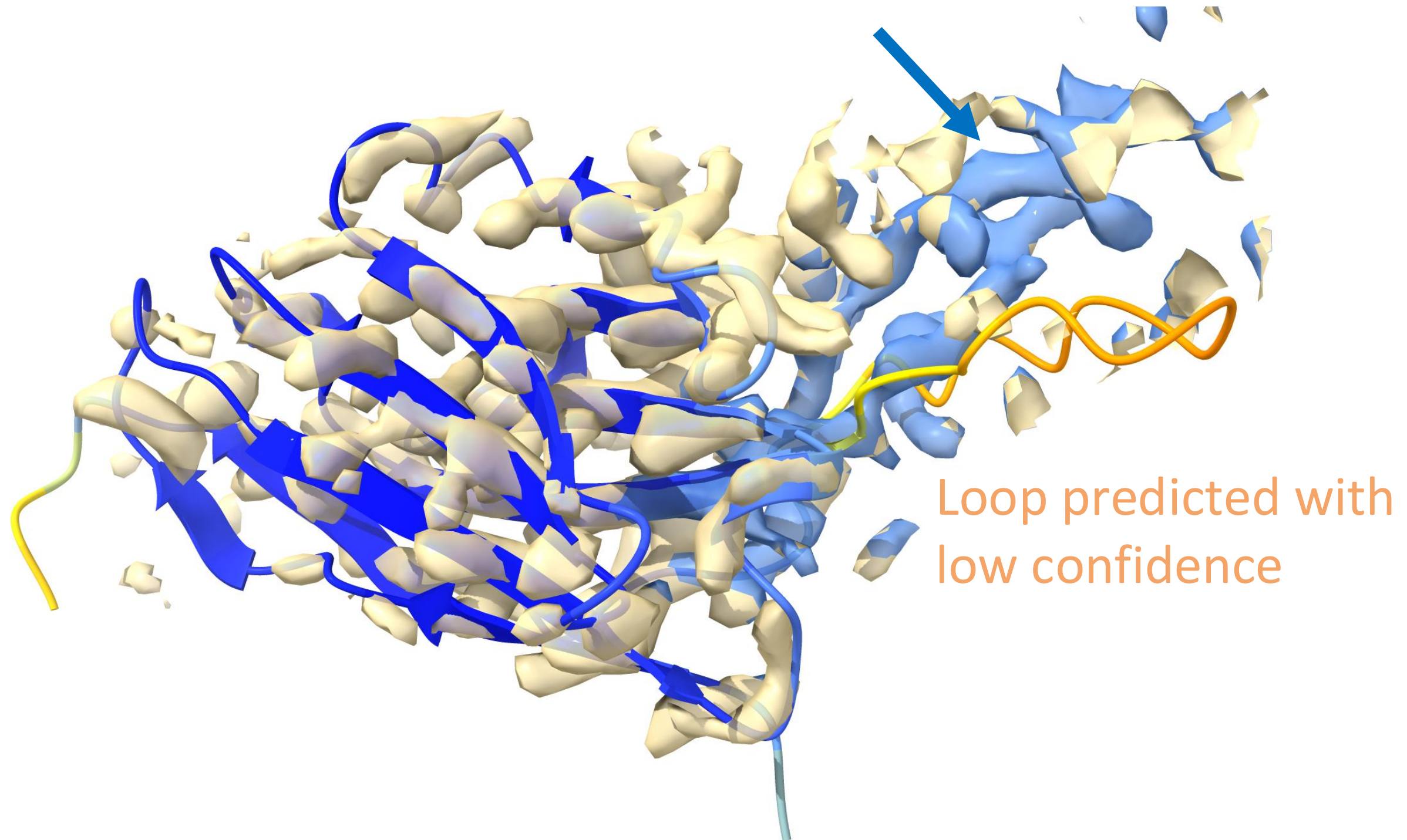
AF2 prediction of chain H



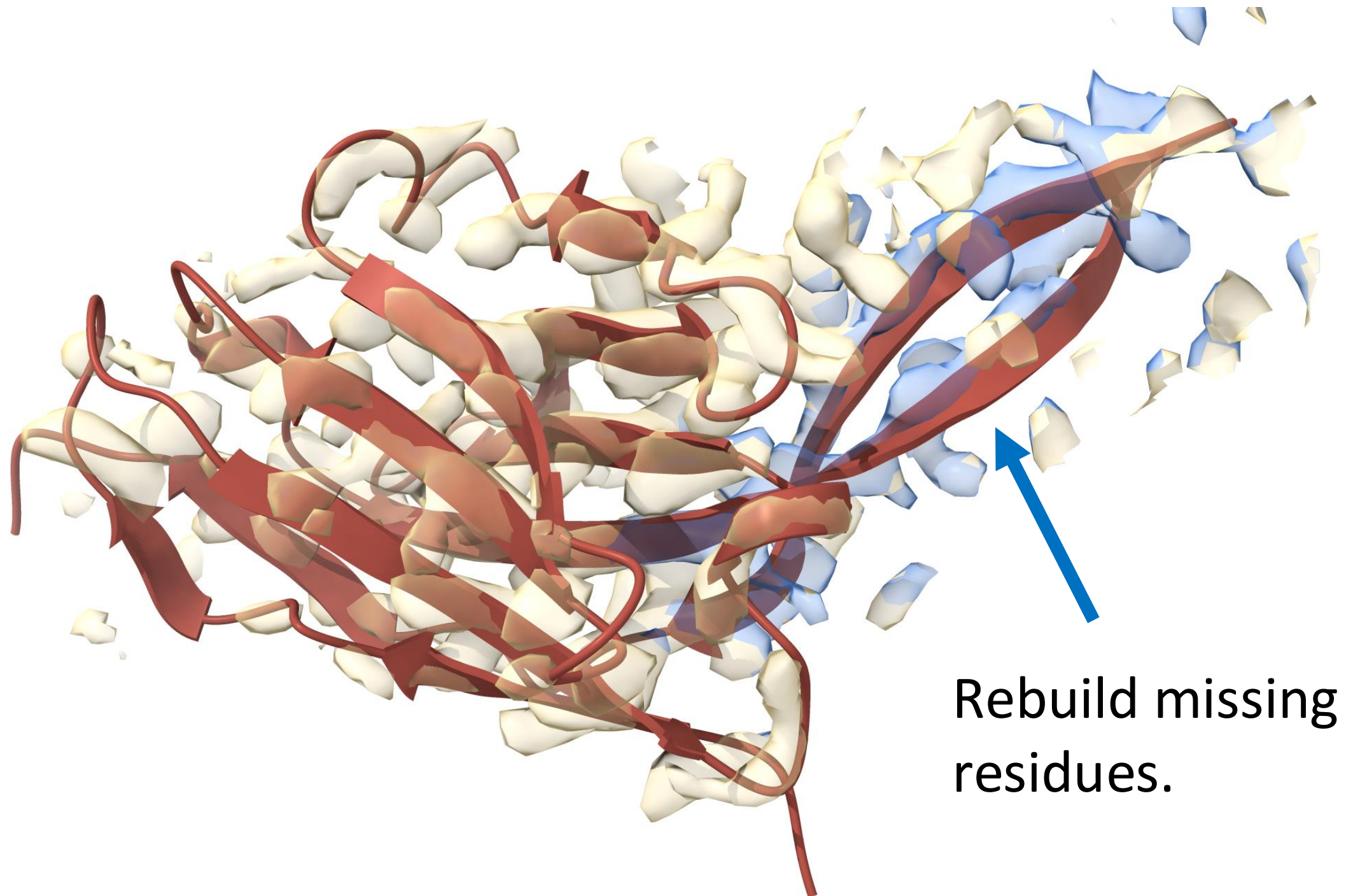
Loop predicted with
low confidence

Does not fit into
map.

AF2 prediction of chain H



Dock and rebuild model



Rebuild missing
residues.

“predicted-processed-docked-rebuilt” model

Make a new prediction

Sequence

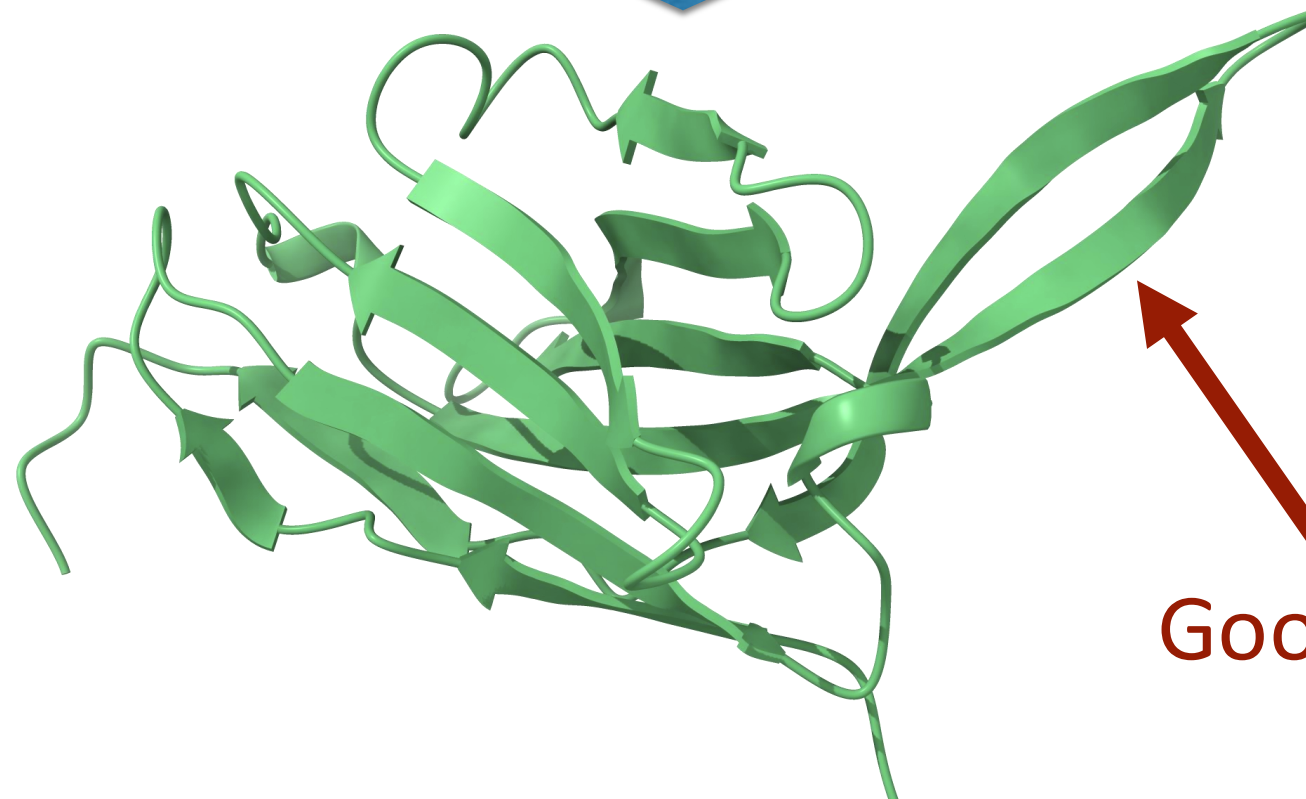
EVQLVESGGGLVQPGGSLRLSCAASGFNIYSSSIHWVRQ
APGKGLEWVAYIYSYSGYTSYADSVKGRFTISADTSKNTA
YLQMNSLRAEDTAVYYCARSLEYLYSSGYQYKWATGLDY
WGQGTLVTVSSAST

Template



Good loop

AlphaFold



Good loop

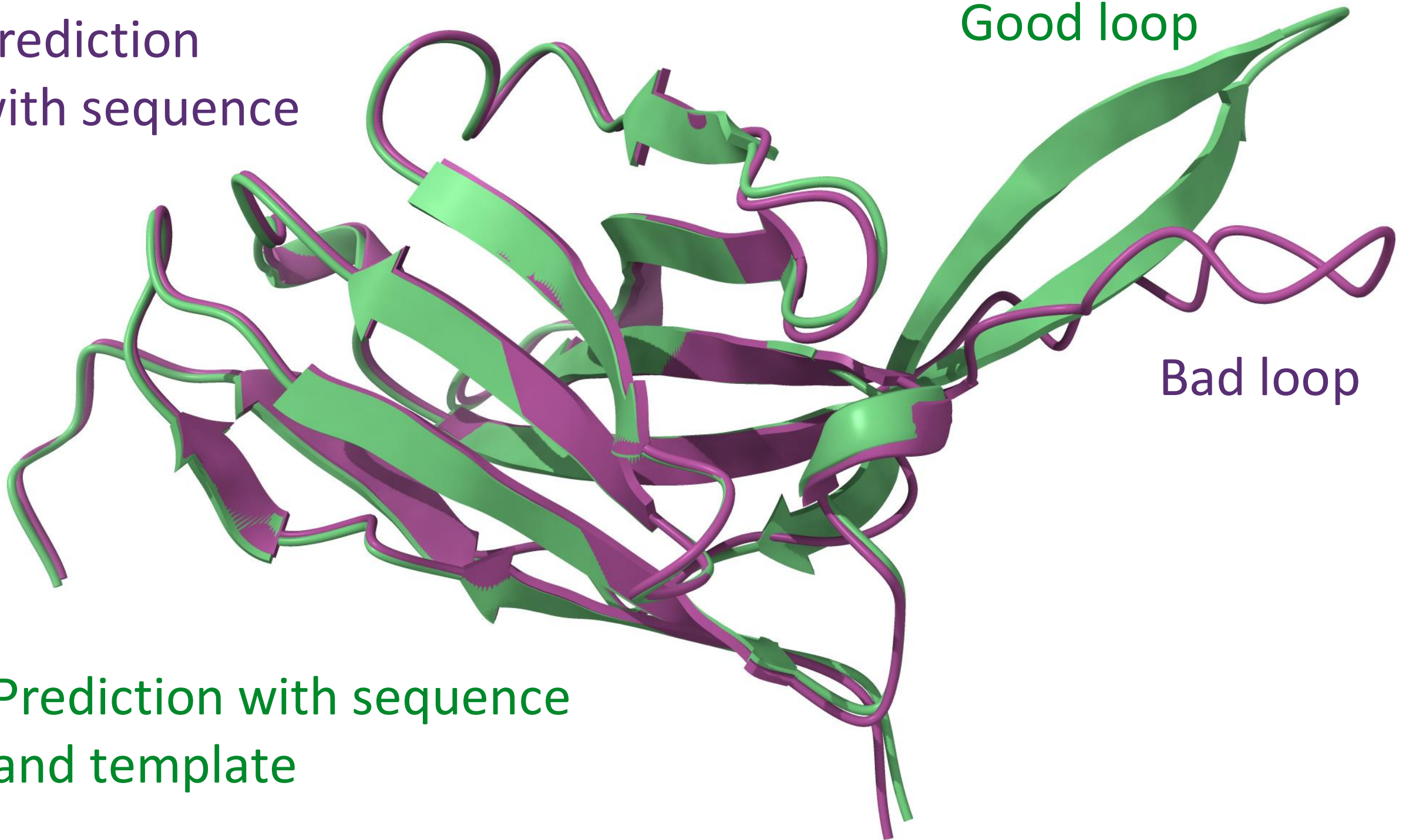
Using a template improves prediction

Prediction
with sequence

Good loop

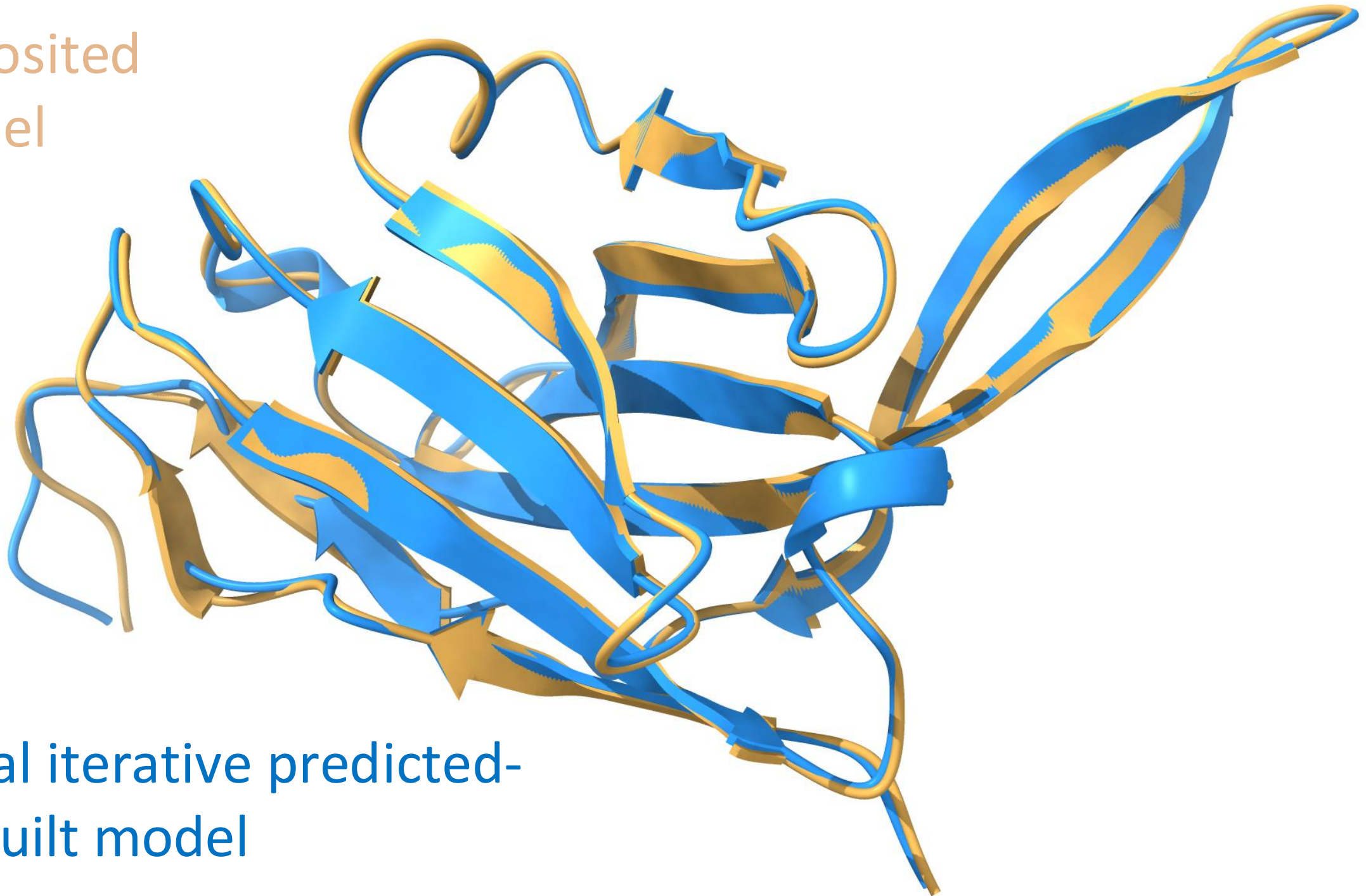
Bad loop

Prediction with sequence
and template



Iterate prediction and rebuilding

Deposited
model

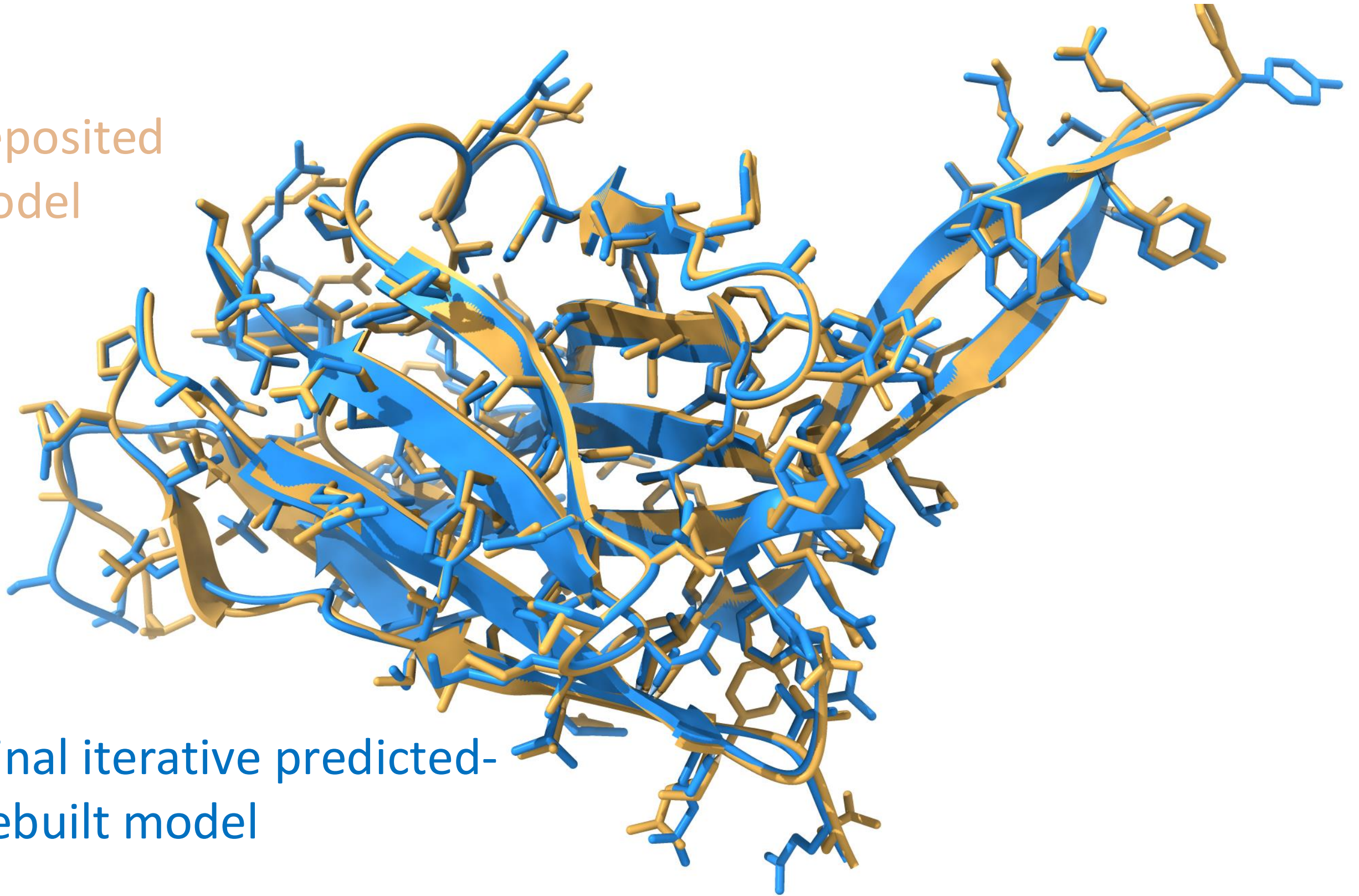


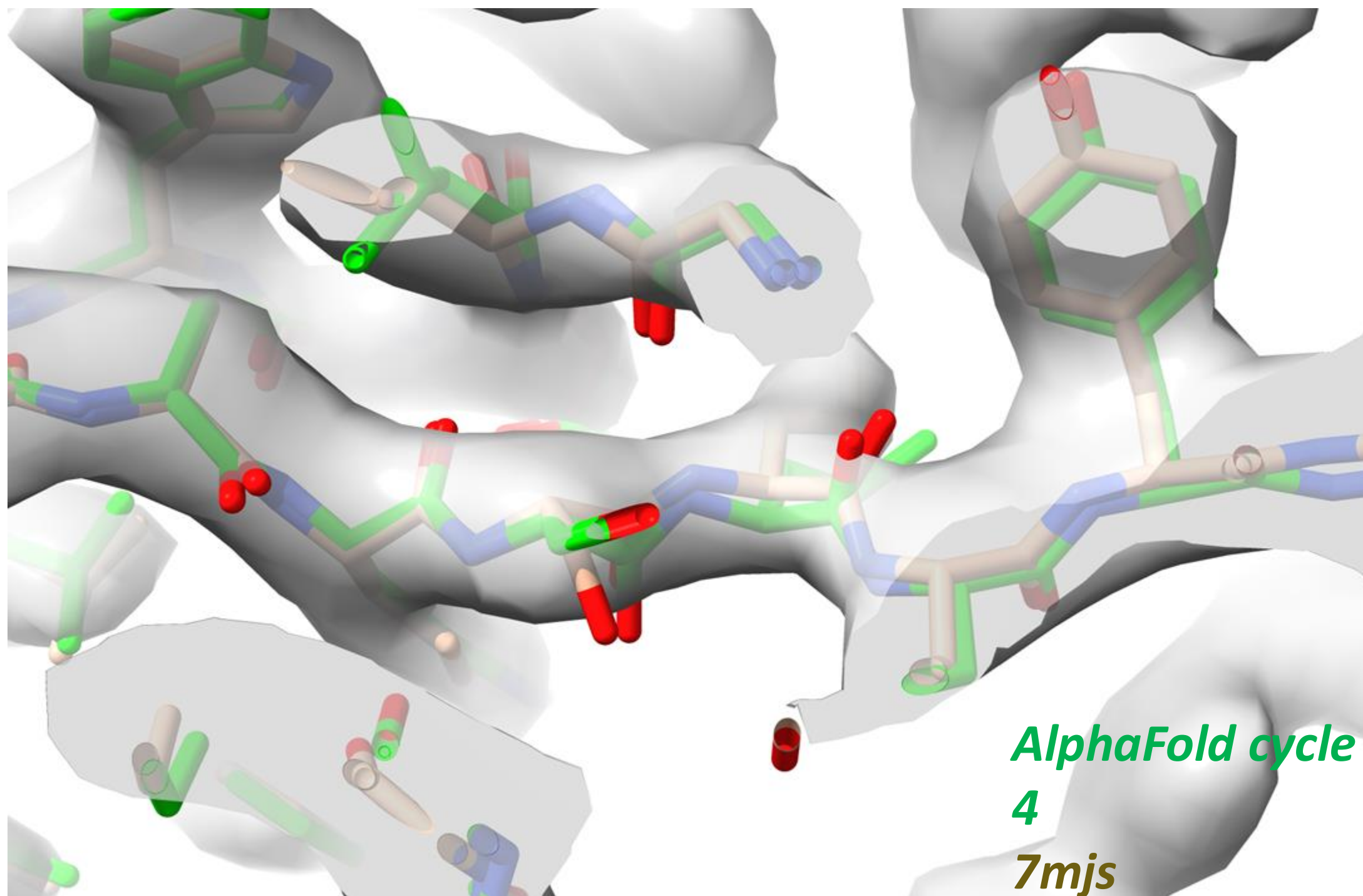
Final iterative predicted-
rebuilt model

Iterate prediction and rebuilding

Deposited
model

Final iterative predicted-
rebuilt model



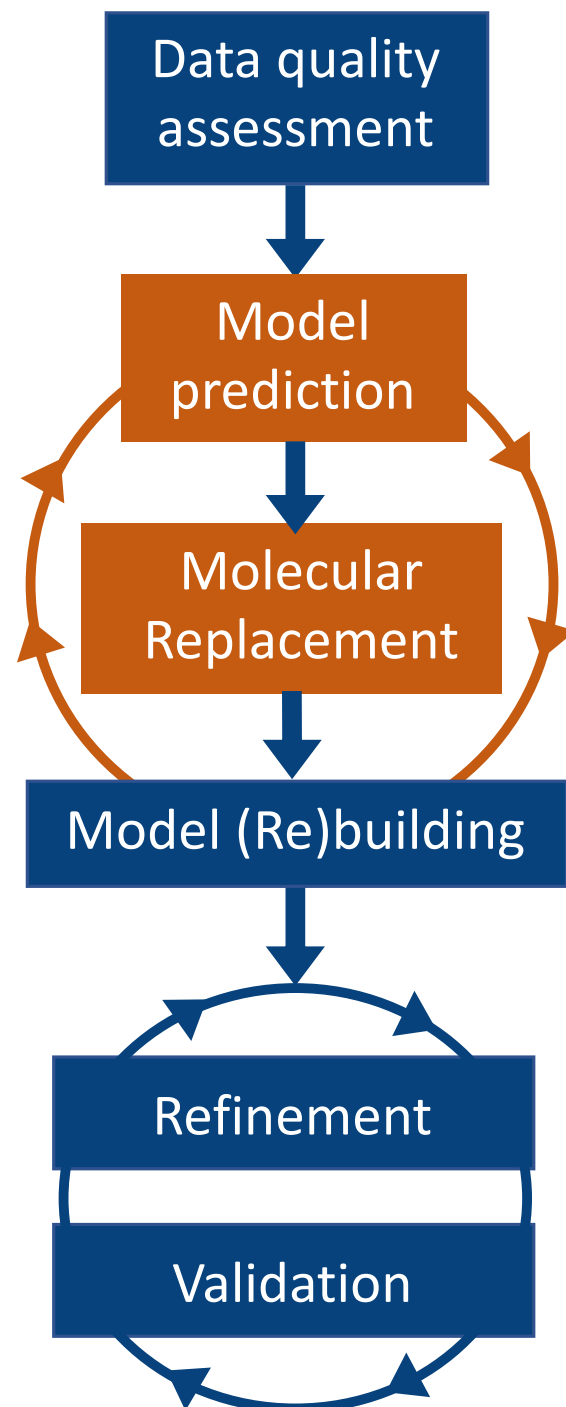


Data from 7mjs, Cater, R.J., et al. (2021). Nature 595, 315–319

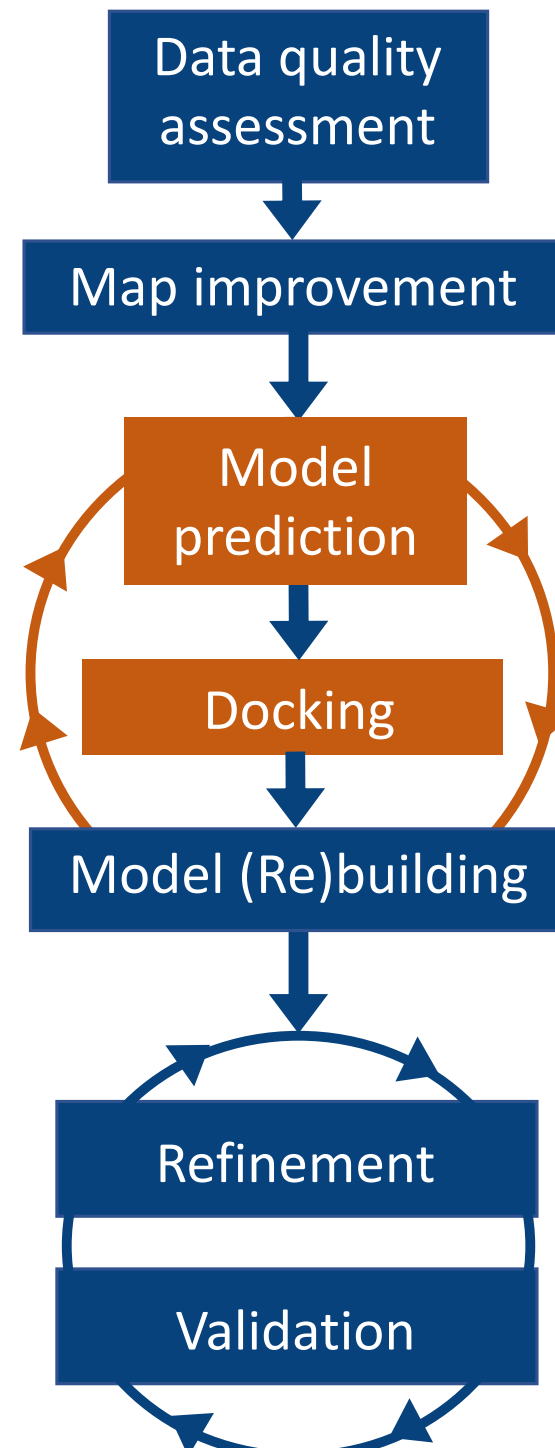
Using predicted models

Updated approach: Iterate prediction and model building

Crystallography

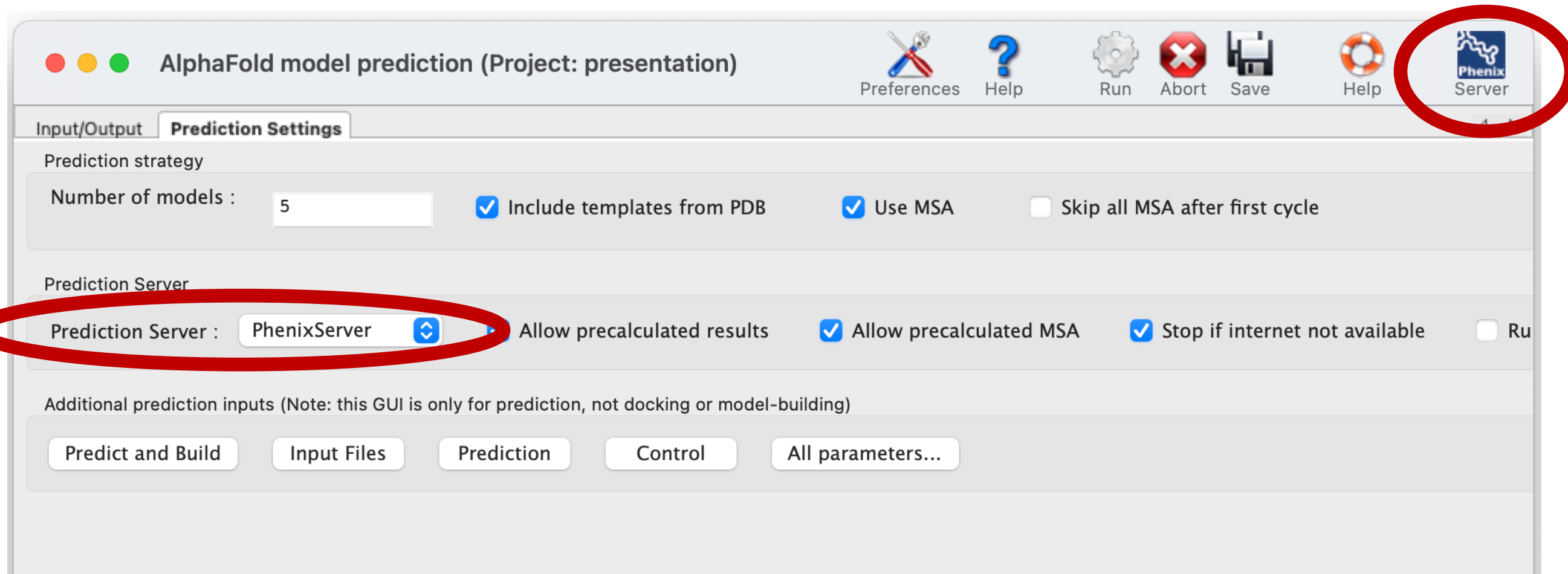


Cryo-EM

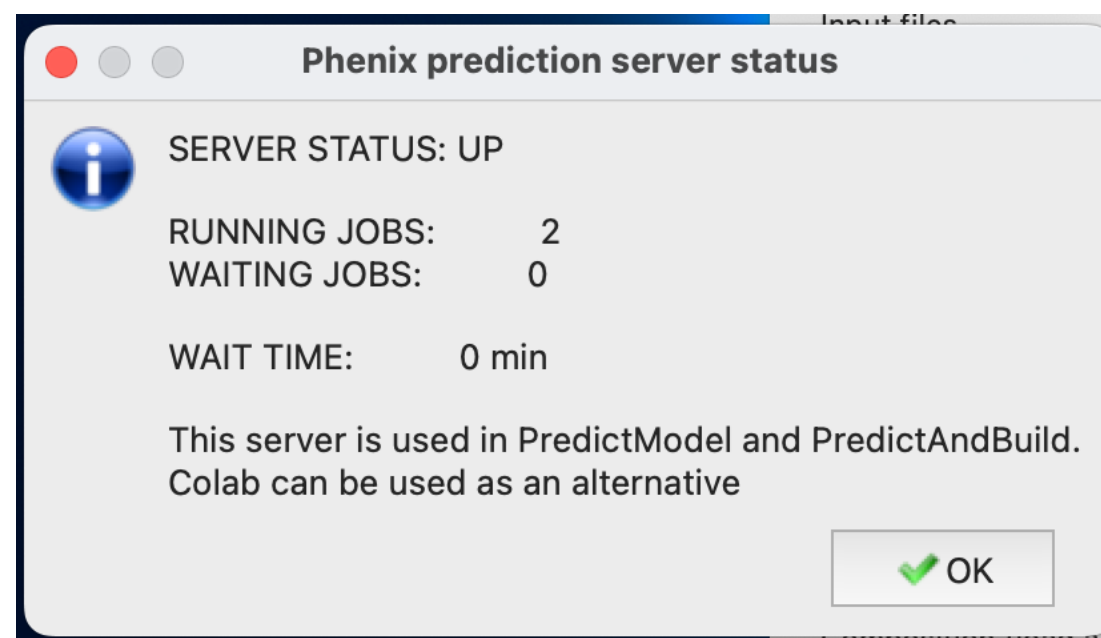




Phenix Server for running AlphaFold



No need for a local
AlphaFold installation



Process predicted model

Process Predicted Model (Project: 7rpq_AF_reference_model)

Preferences Help Run Abort Help

Configure

ProcessPredictedModel: Prepare predicted model for structure determination

Replace values in B-factor field with estimated B values.
Optionally remove low-confidence residues and split into domains.

Inputs: Model file (PDB, mmCIF)

Job title :

Input

Note: The B-value field in your model can be pLDDT, RMSD, or B

Predicted model : Browse...

Contents of B-value field for input models :

Optional input files

Output

Output file prefix (optional) :

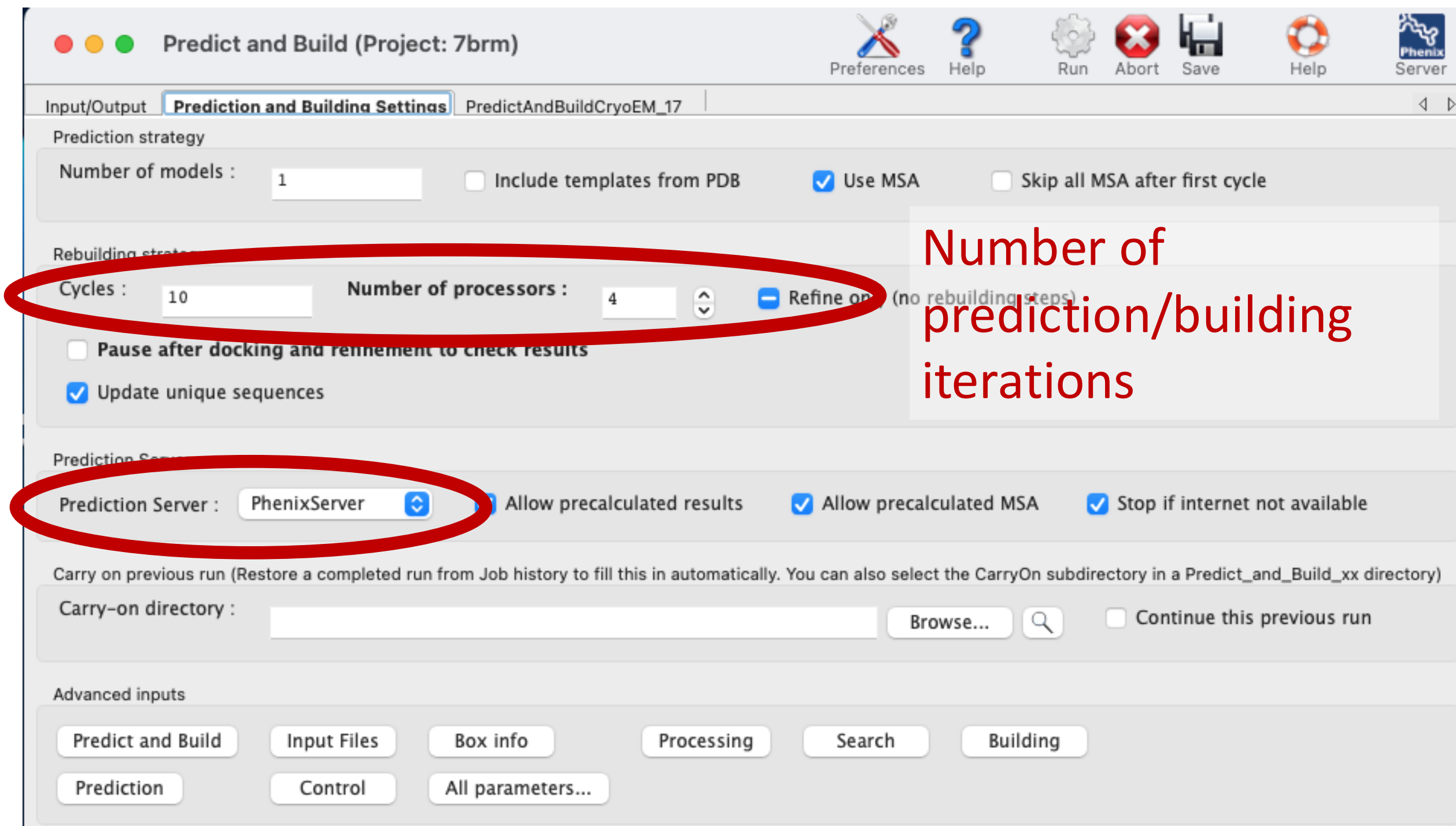
Options

☒ Remove low-confidence residues ☒ Split model into compact regions Maximum output B :

☒ Remove hydrogen ☐ Use only single-letter chain ID ☐ Maintain continuous chain

Processing options All parameters...

Iterate with Predict and Build



The screenshot shows the Phenix Predict and Build interface for project 7brm. The 'Prediction and Building Settings' tab is active. A red oval highlights the 'Cycles' field set to 10 and the 'Number of processors' field set to 4. A red oval also highlights the 'Prediction Server' dropdown menu, which is set to 'PhenixServer'. A red text box with the text 'Number of prediction/building iterations' points to the 'Cycles' field. The interface includes sections for Prediction strategy, Rebuilding strategy, Prediction Server, Carry-on directory, and Advanced inputs.

Predict and Build (Project: 7brm)

Input/Output **Prediction and Building Settings** PredictAndBuildCryoEM_17

Prediction strategy

Number of models : 1 ☐ Include templates from PDB ☒ Use MSA ☐ Skip all MSA after first cycle

Rebuilding strategy

Cycles : 10 Number of processors : 4 ☒ Refine on (no rebuilding steps)

☐ Pause after docking and refinement to check results

☒ Update unique sequences

Prediction Server

Prediction Server : PhenixServer ☒ Allow precalculated results ☒ Allow precalculated MSA ☒ Stop if internet not available

Carry on previous run (Restore a completed run from Job history to fill this in automatically. You can also select the CarryOn subdirectory in a Predict_and_Build_xx directory)

Carry-on directory : Browse... ☐ Continue this previous run

Advanced inputs

Predict and Build Input Files Box info Processing Search Building

Prediction Control All parameters...

Fully automatic – AF prediction, processing, building, refinement.

Strategy for structure determination

1. Predict your structure

Design your experiment accordingly

(choose experimental approach, consider trimming at domain boundaries)

2. Solve your structure

Cryo-EM: docking

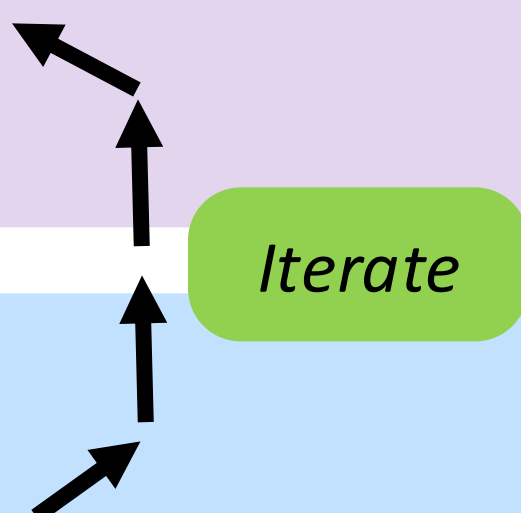
X-ray: MR; SAD

3. Update your prediction

Run AlphaFold again with your best model as a template

4. Improve your structure

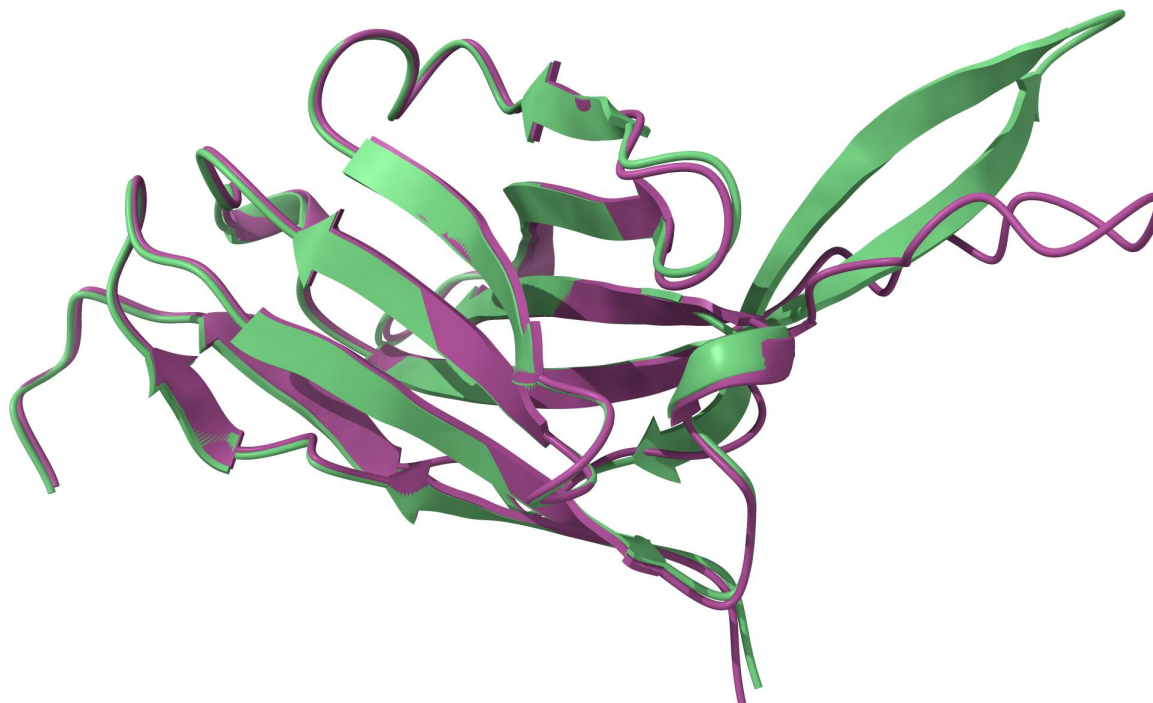
Use your new prediction as hypothesis, rebuild parts



Iterate

Summary

- AlphaFold models are great hypotheses.
- Can be used for cryo-EM docking (need to interpret the confidence measures), model completion, reference model restraints.
- Iterating prediction and model building can lead to improved models.
- Still need experiment to get a model that best explains the data.

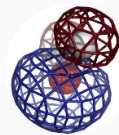


Further reading/material

Documentation:

<https://www.phenix-online.org/documentation/>

Phenix Tutorials



Phenix Tutorials

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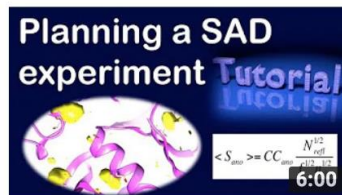
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ABOUT



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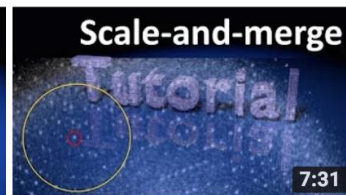
SORT BY



Simulate a SAD experiment with...



Automatic map interpretation with map_to_model



Scaling and merging anomalous data



Automated map sharpening with phenix.autosharpen

Video tutorials

<https://www.youtube.com/c/phenixtutorials>

Working with AlphaFold2, RoseTTAFold and other predicted models

You can use the predicted models from AlphaFold and other prediction software in Phenix. Using these models can be very helpful in structure determination because the models can be very accurate over much of their length and the models come with accuracy estimates that allow removal of poorly-predicted regions.

How to use predicted models in Phenix

Use [Predict_and_build](#) to incorporate predicted models in the structure solution workflow.

Predict_and_build generates predicted models and uses them to solve an X-ray structure by MR or to interpret a cryo-EM map. The tool then carries out iterative model rebuilding and prediction to improve the models. The iterative procedure allows creating more accurate predicted models than can be obtained with a simple prediction.

Predict and build can automatically generate a fairly accurate model starting from just a sequence file and either cryo-EM half-maps or X-ray data. Additionally, it provides morphed versions of unrefined predicted models that can be useful as reference models for refinement.

Other tools for using predicted models:

- [Overview](#): AlphaFold and Phenix
- [Processing](#) a predicted model
- [Docking](#) a processed predicted model in a cryo-EM map
- [Rebuilding](#) a docked predicted model in a cryo-EM map
- [Processing, docking and rebuilding](#) a predicted model in a cryo-EM map
- [Trimming overlapping parts](#) of models

Tom Terwilliger: AlphaFold changes everything

<https://youtu.be/ugMPYdPo8Bc?feature=shared>

The Project



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Dorothee Liebschner, Nigel
Moriarty, Billy Poon,
Christopher Schlicksup,
Oleg Sobolev



University of Cambridge

Randy Read, Airlie McCoy,
Alisia Fadini



Los Alamos National Laboratory New Mexico Consortium

Tom Terwilliger, Li-Wei Hung



UTHealth

Matt Baker



Duke University

Jane Richardson, Christopher
Williams, Vincent Chen



An NIH/NIGMS funded
Program Project

Liebschner D, *et al.*, Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in *Phenix*. Acta Cryst. 2019 **D75**:861–877