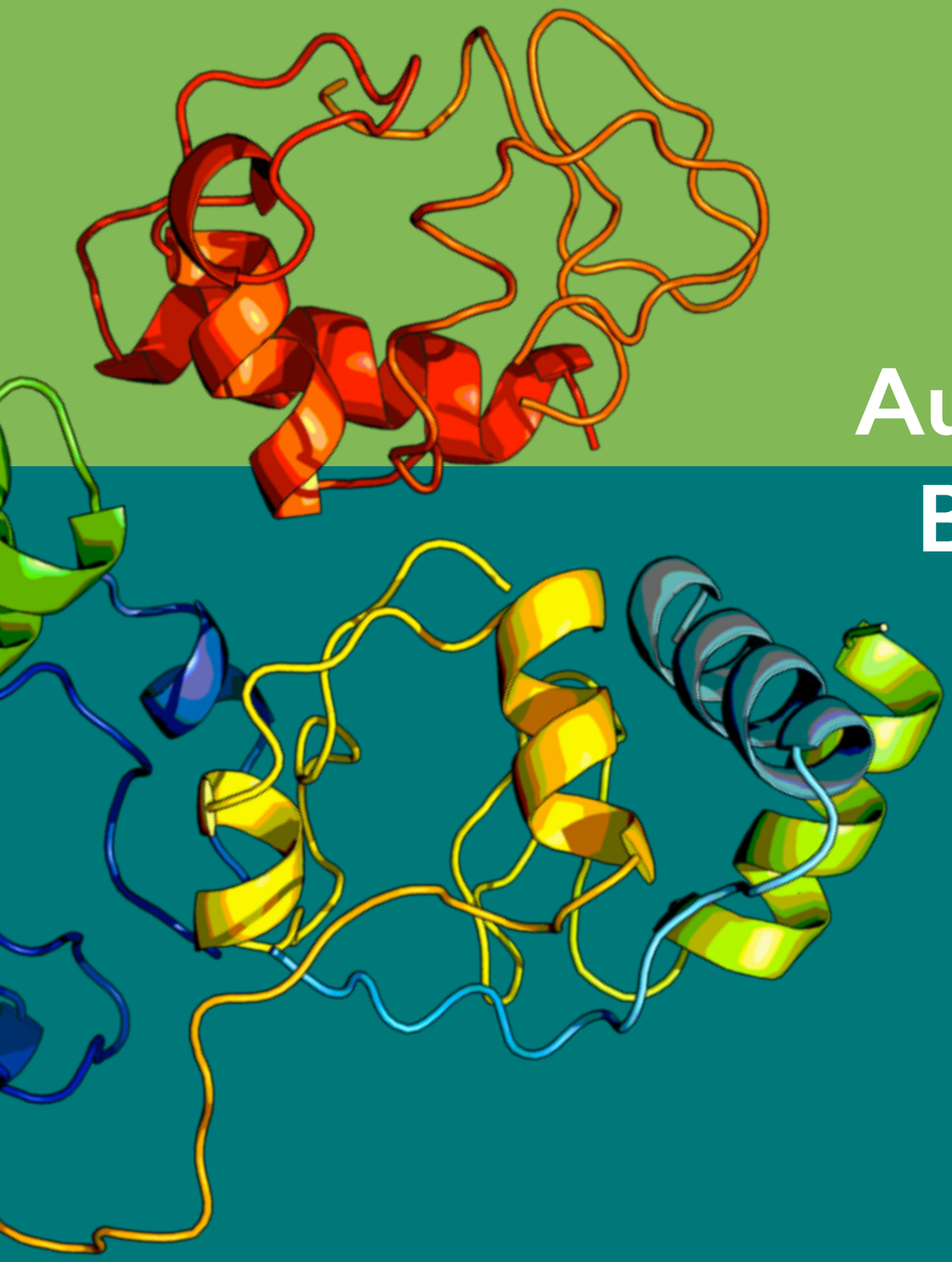
Joana Pereira
Lamzin Group
EMBL Hamburg, Germany



Automated Protein Model Building with ARP/wARP

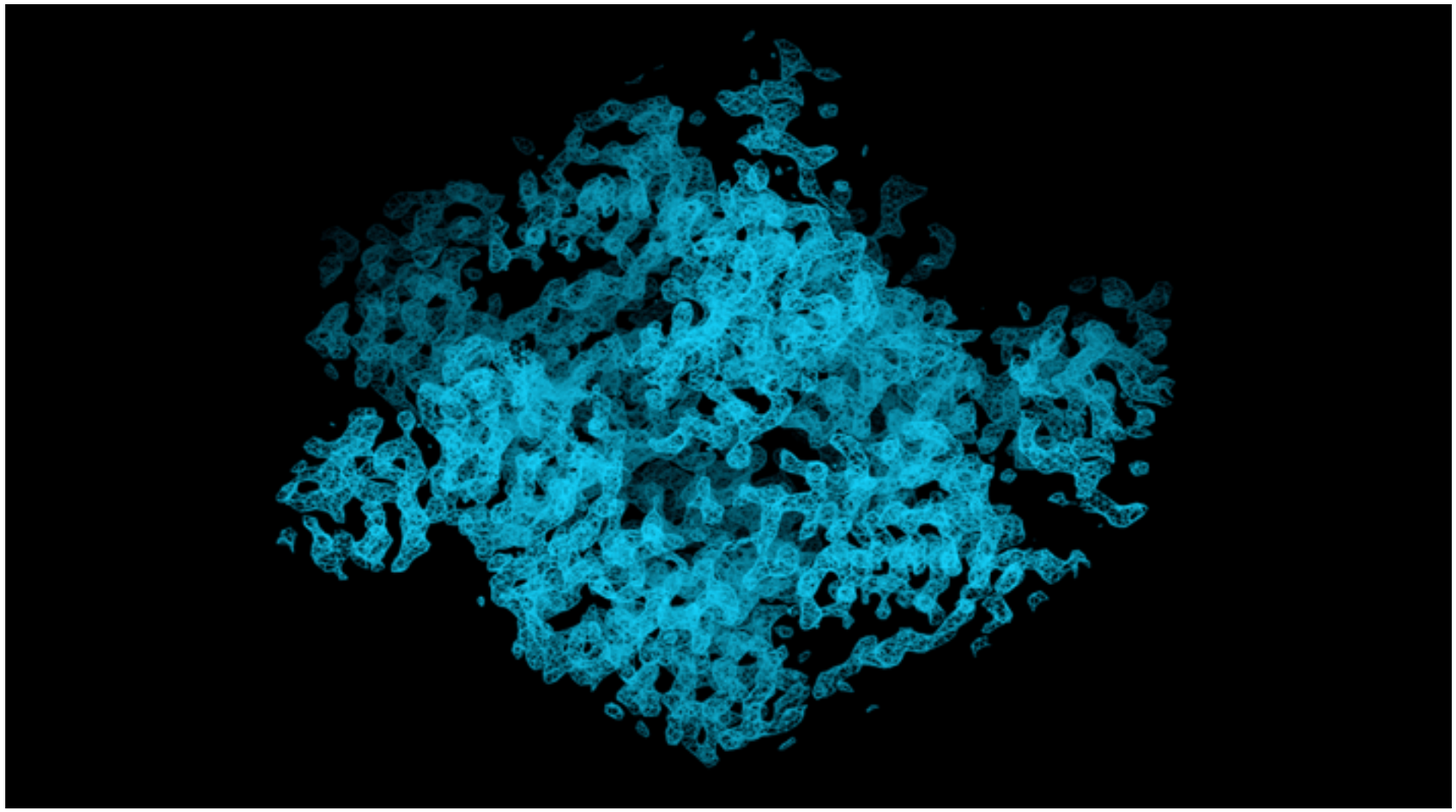
(and nucleic acids too)

EMBL 40 YEARS | 1974–2014

ARP wARP 7.5

Electron density map:
the ultimate result of a crystallography experiment

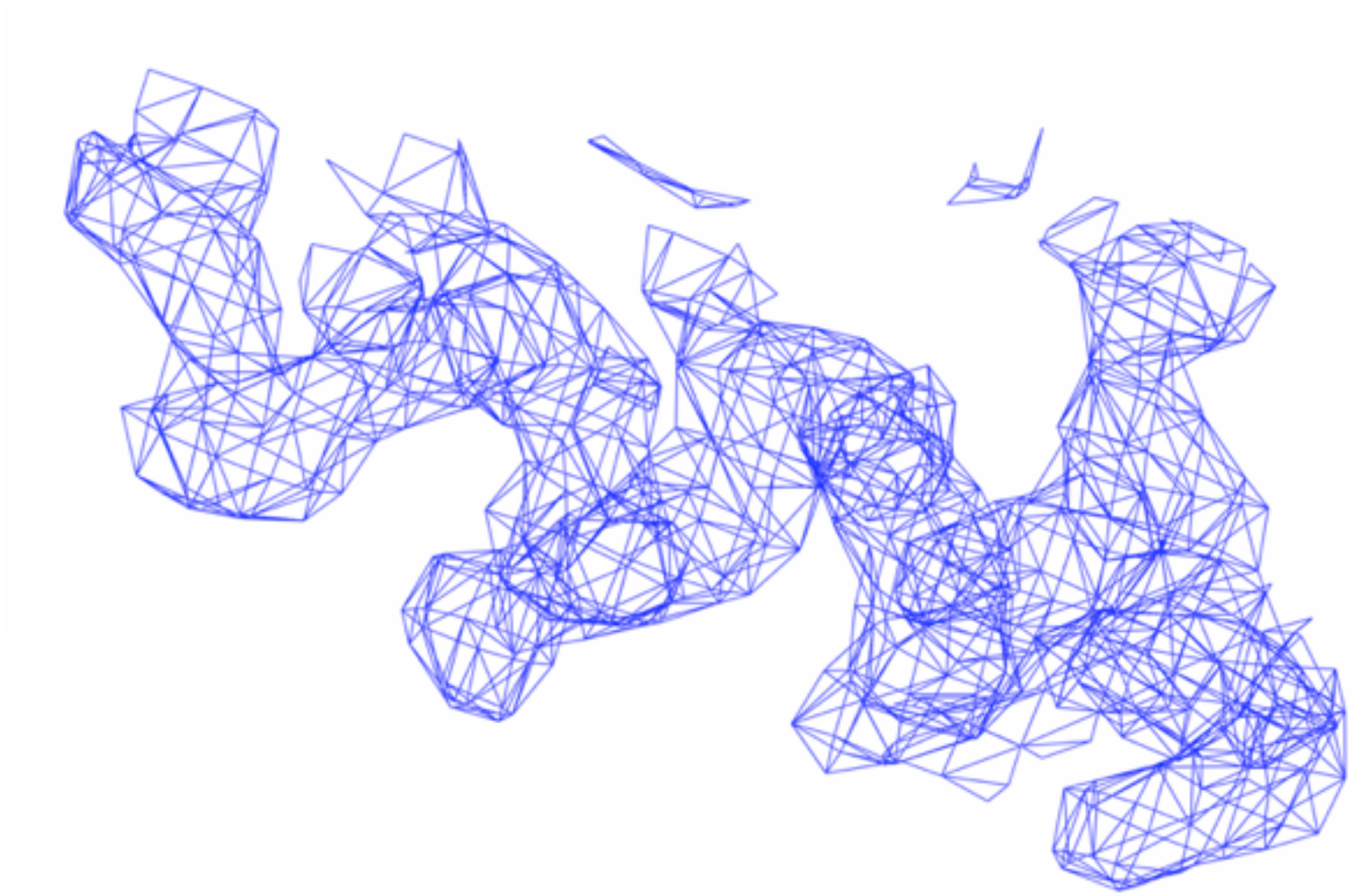
How would you do to interpret this map?



Building a molecular model from the electron density map calls for automation, it can take a long time when done by hand!

Methods for electron density map interpretation

Skeletonisation: tracing the path of the macromolecular chain using the connectivity of regions of high electron density



It gives a picture of how one can connect the electron density and where the main chain may run.

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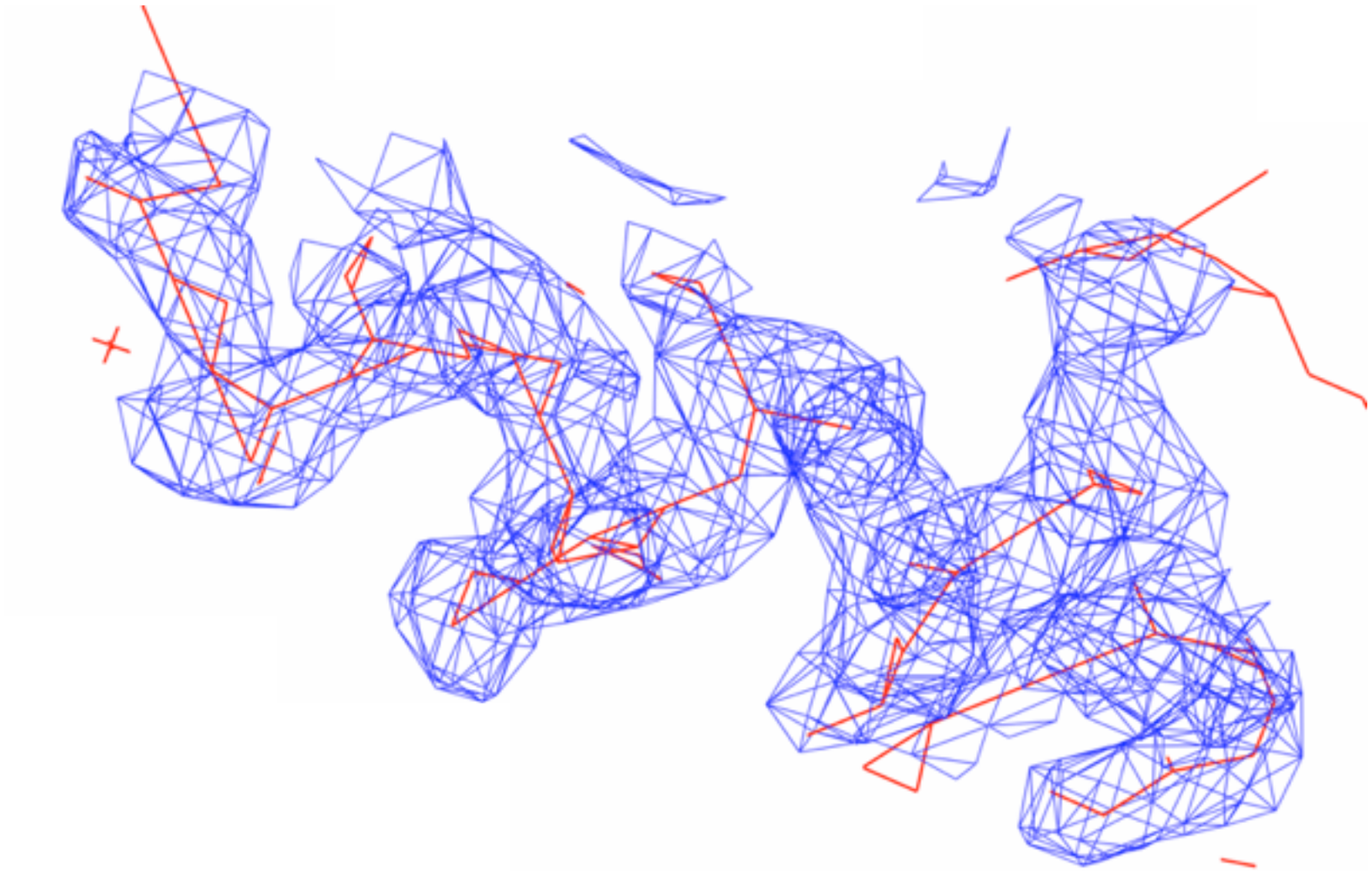

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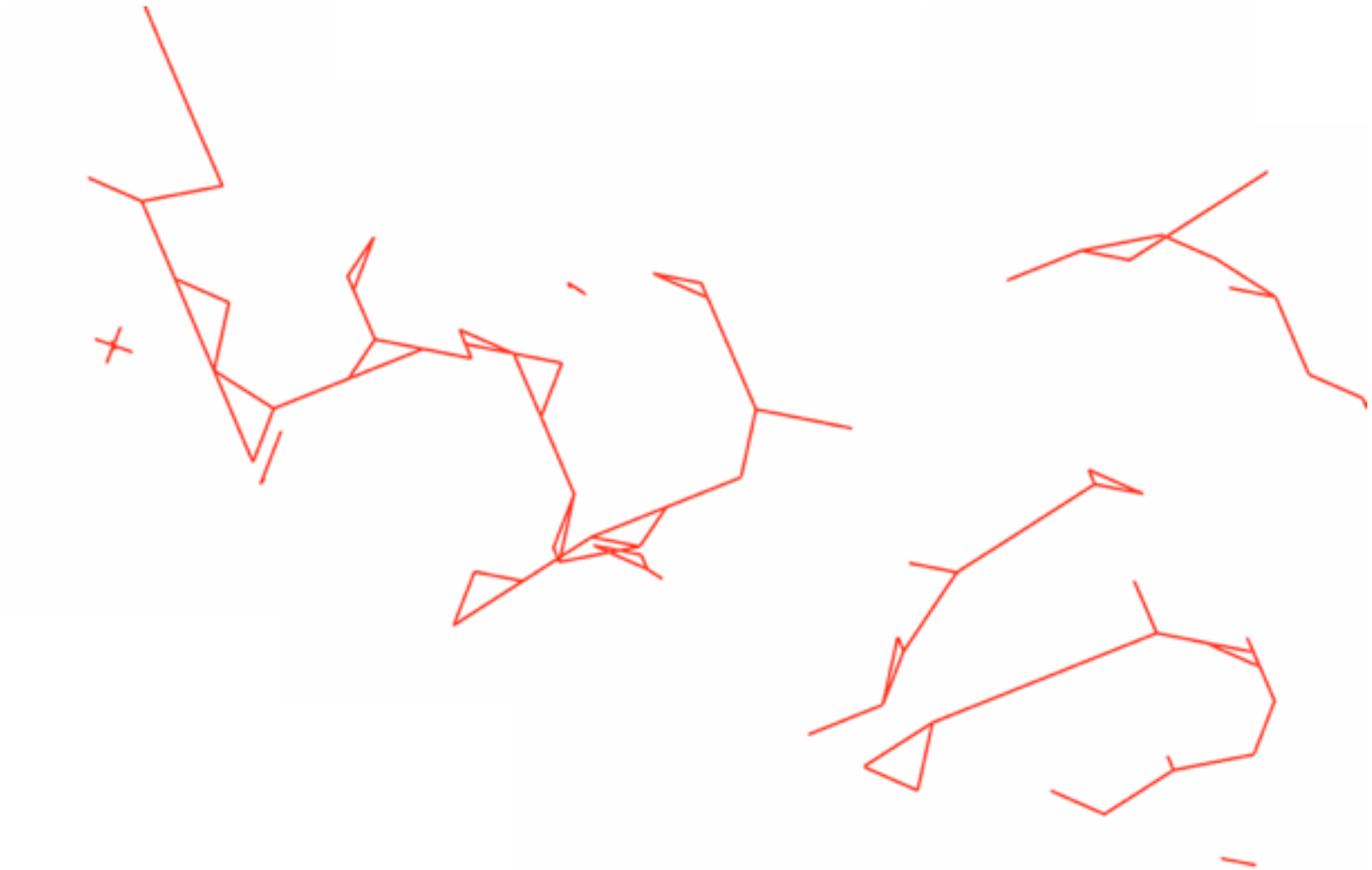

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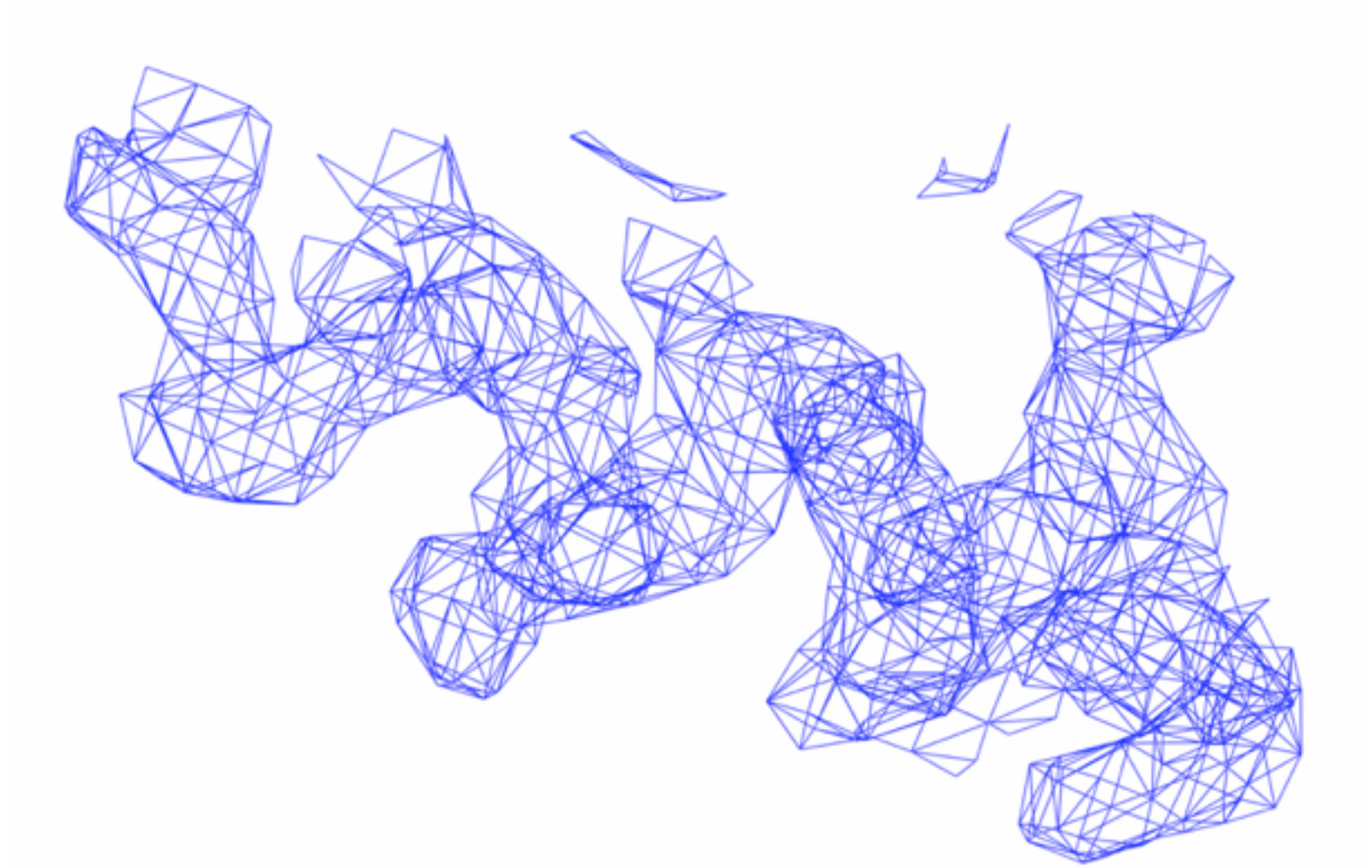
Secondary structure templates: using penta-alanine templates in ideal α-helix and β-sheet conformations to find secondary structure elements in the density



It shows where we can find the secondary structure elements and then one has to try to connect them.

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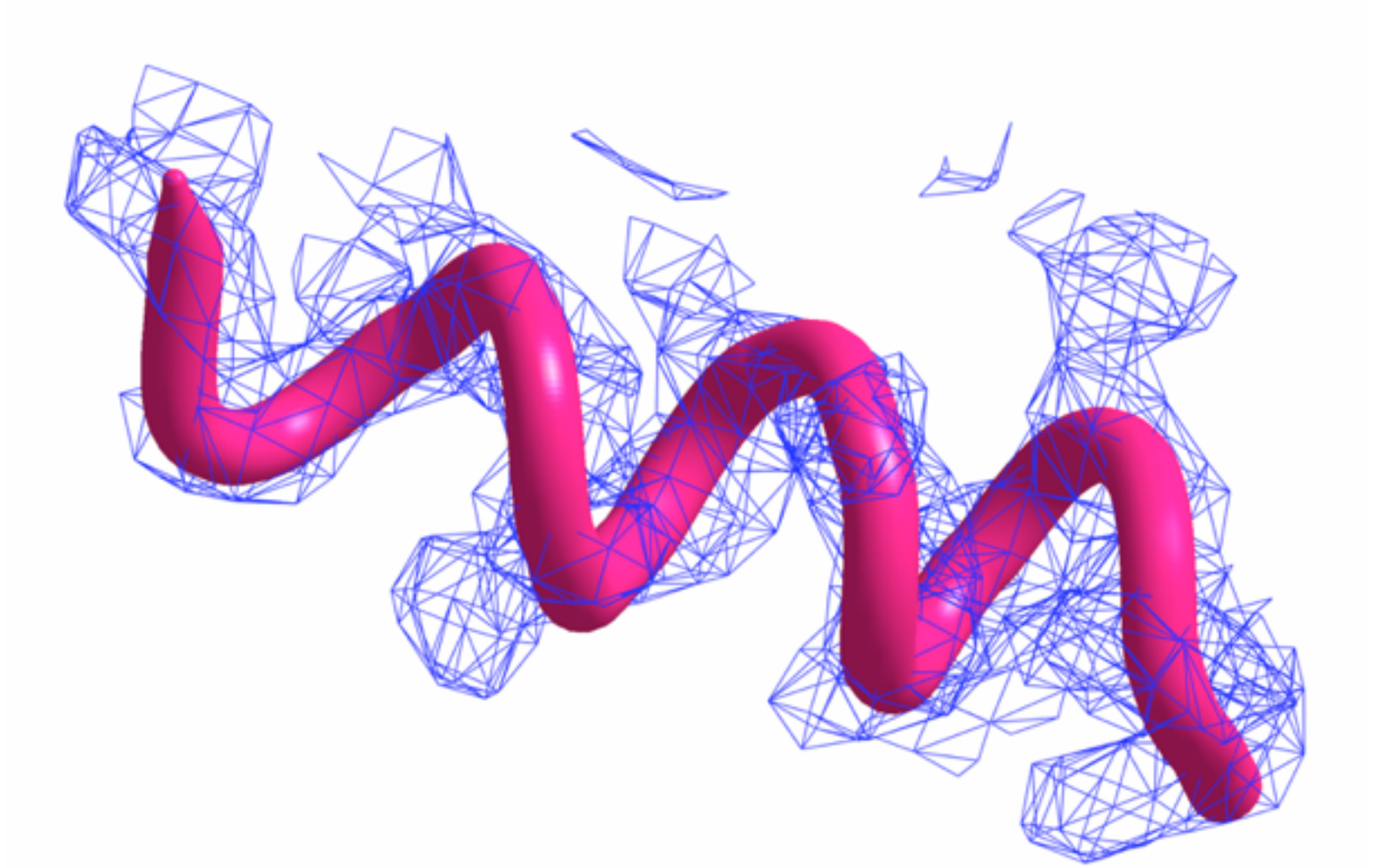

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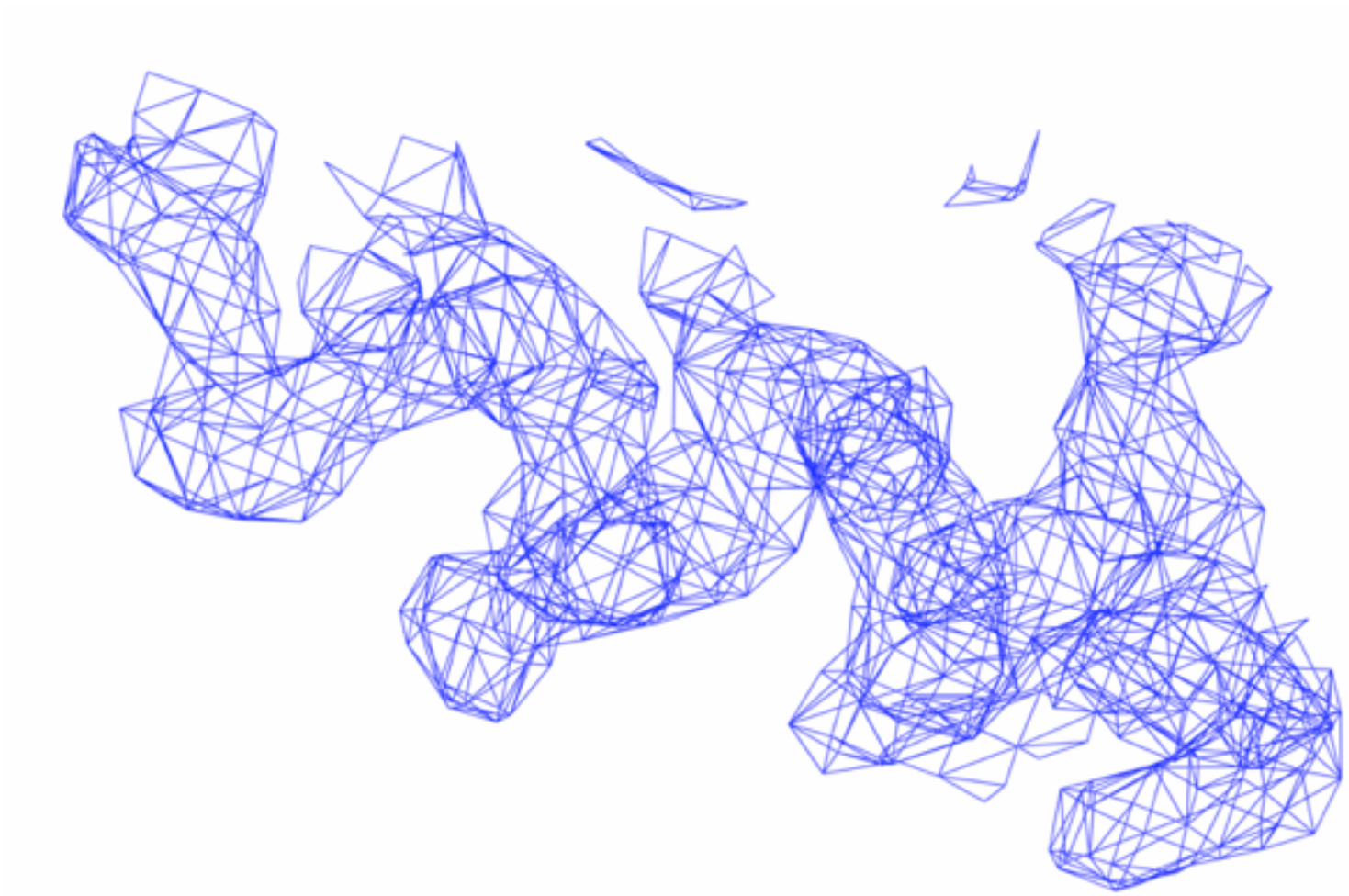

Searching for free atoms in possible Cα positions, the main chain can be found.

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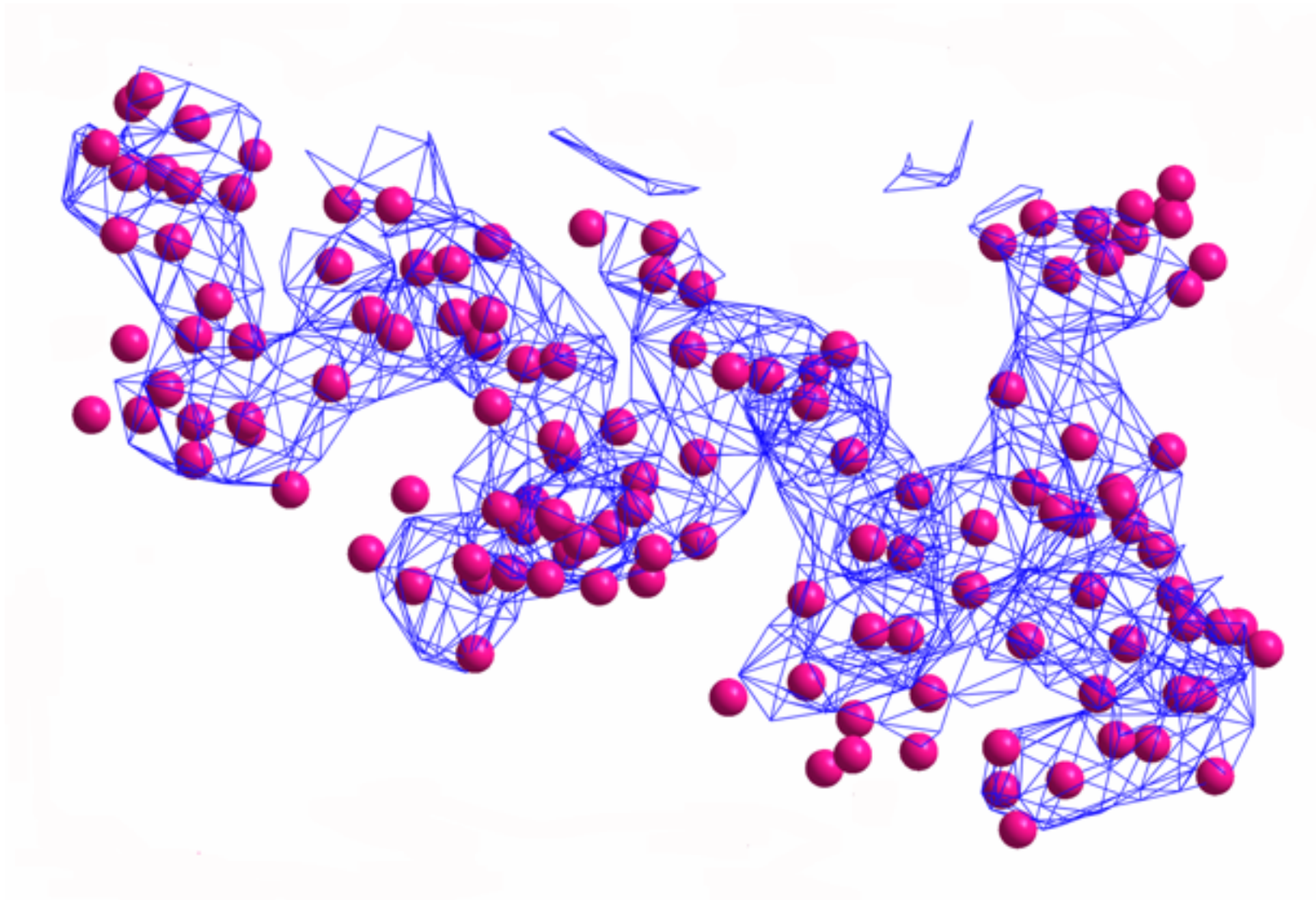

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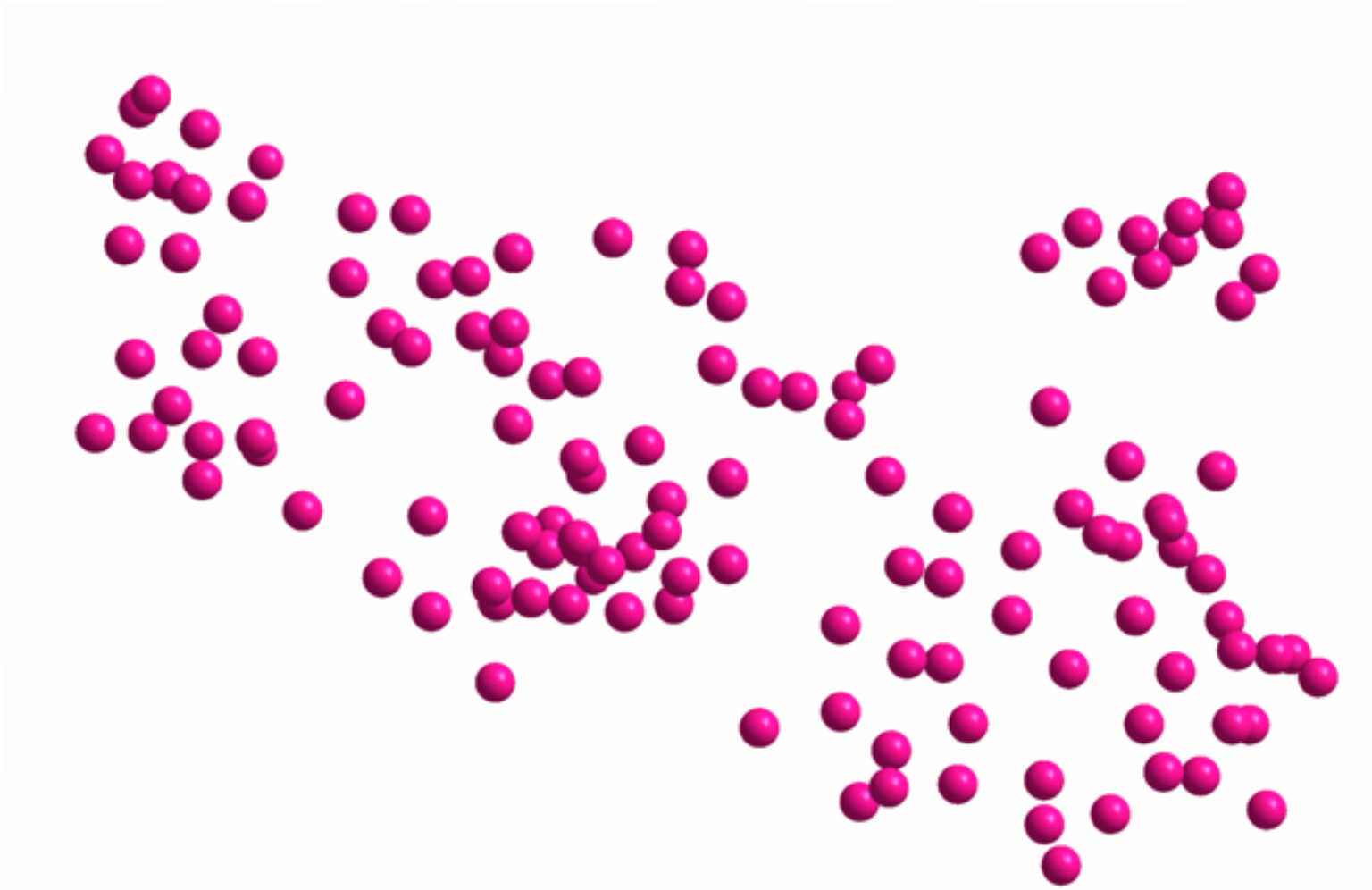

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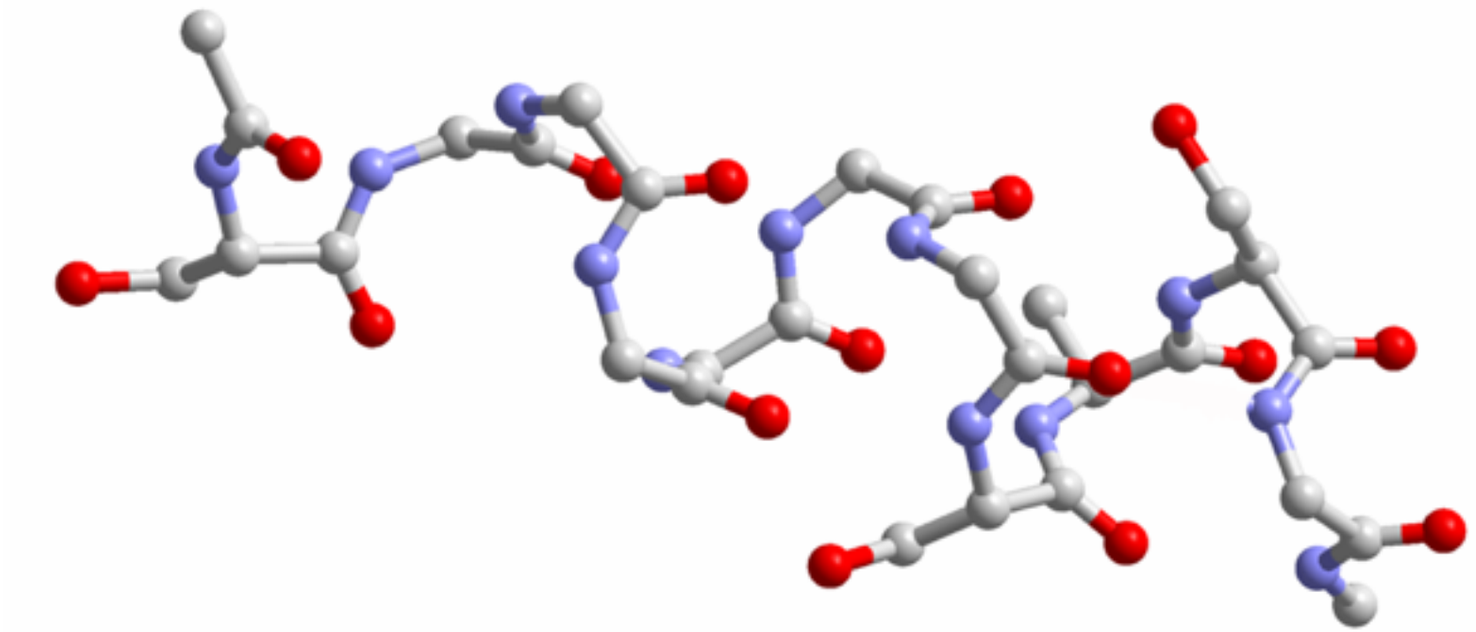

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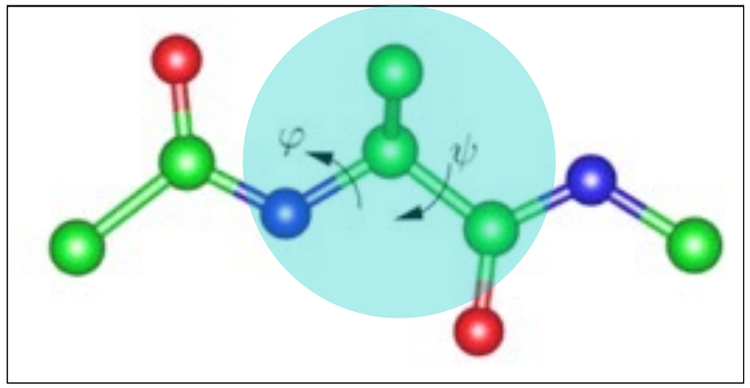
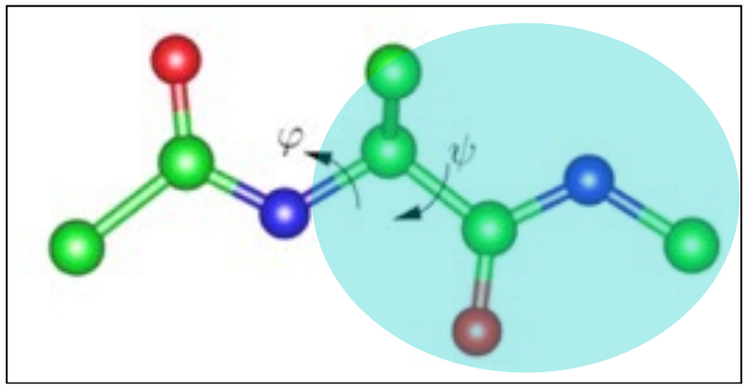
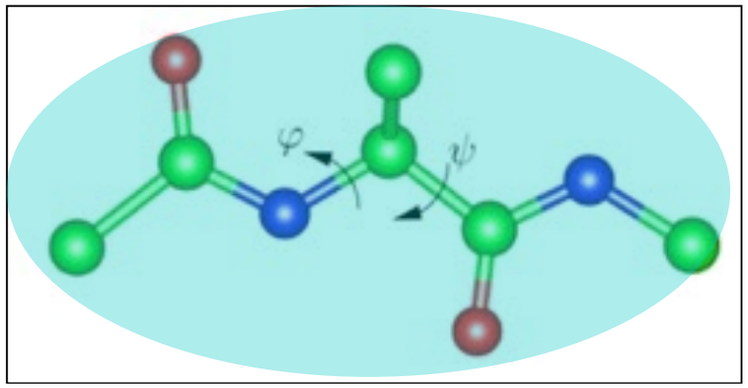
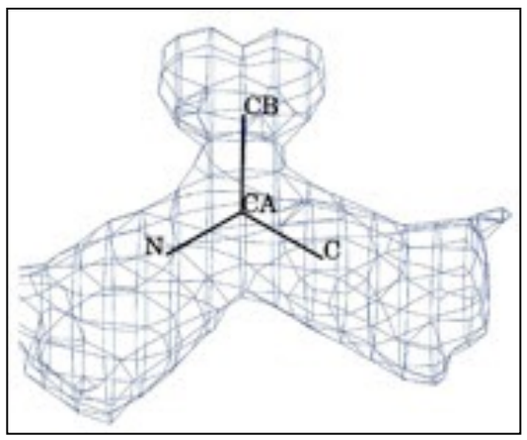
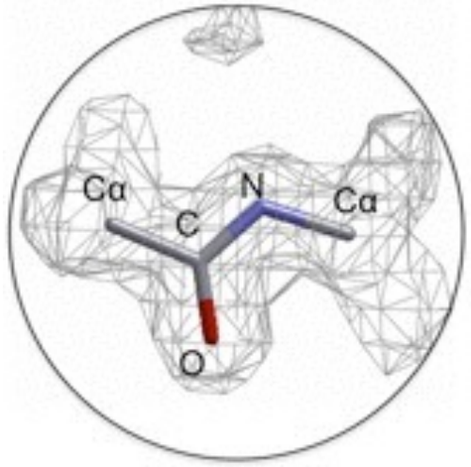
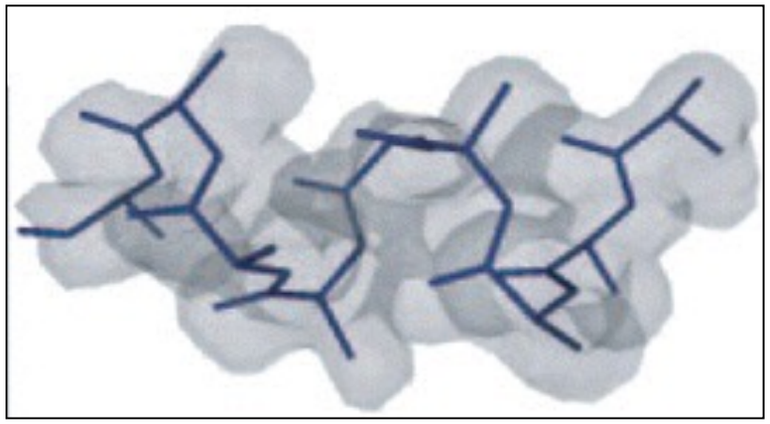
Methods for automated model building

Most current methods search for different patterns that are then used to build and extend a main chain:



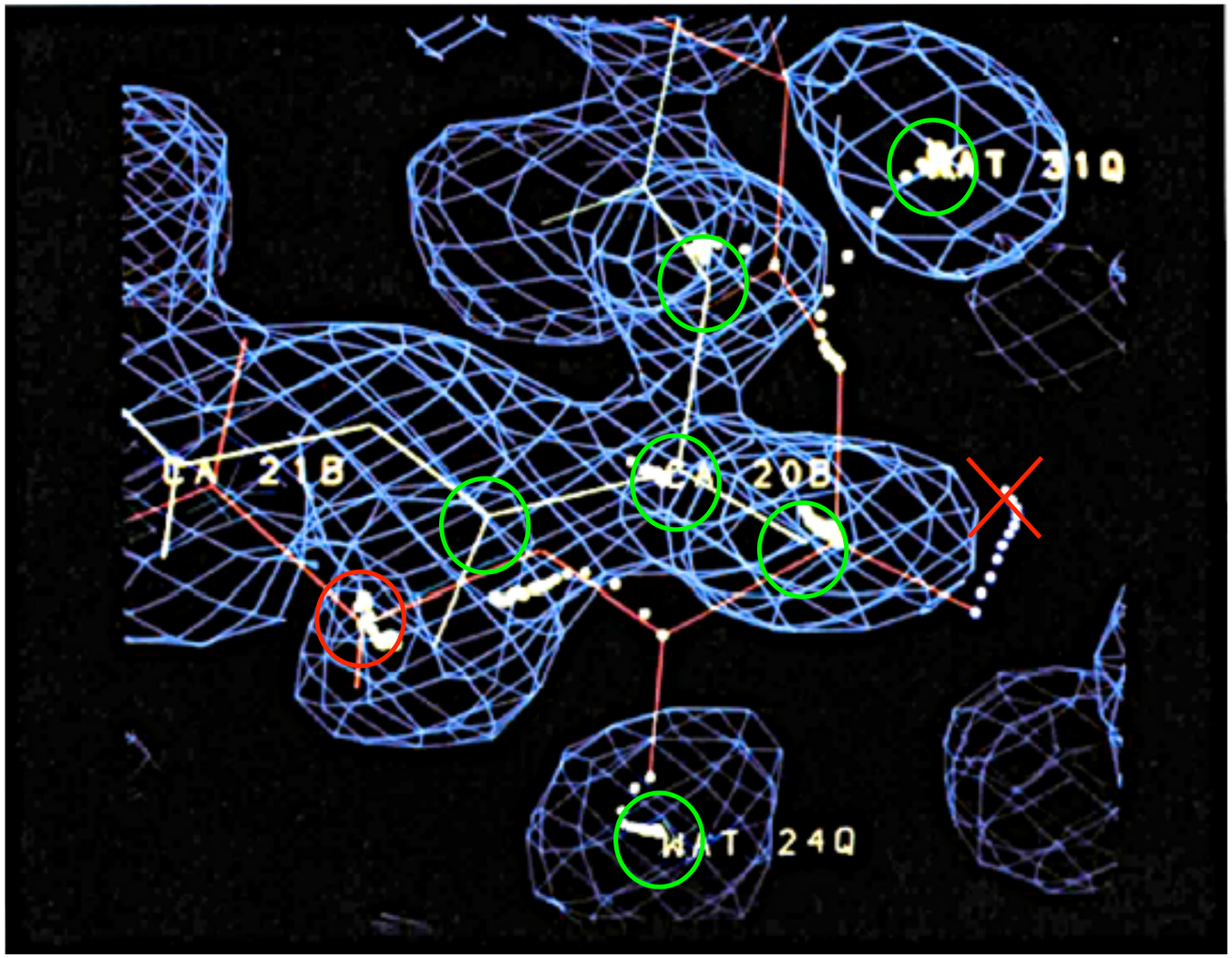




TEXTAL / Buccaneer	ARP/wARP	RESOLVE / ACMI
Cα	(Di-) Peptides	Fragments

ARP/wARP

Developed in Hamburg by the Lamzin group, it is:

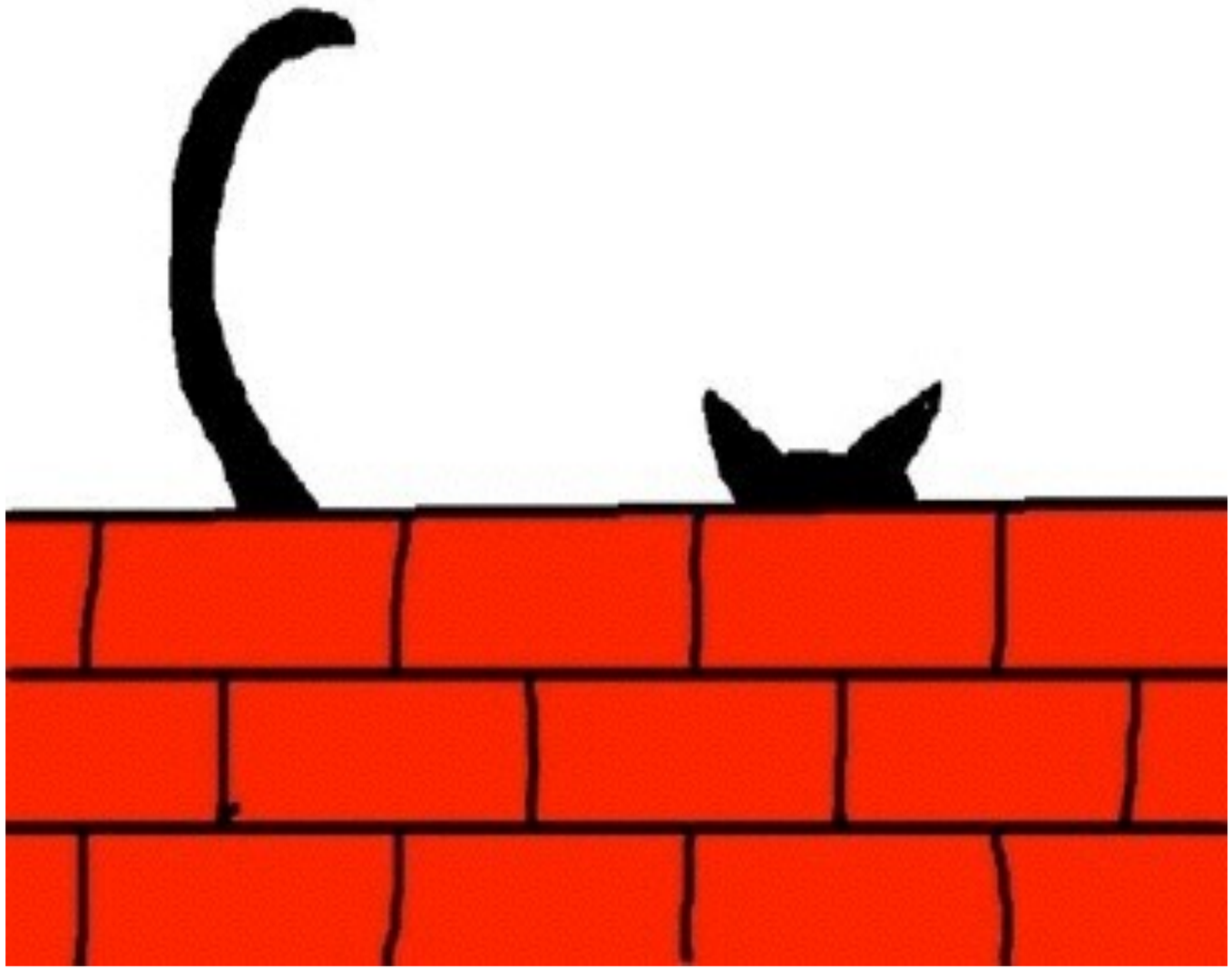


- one of the leading **MX** software projects
- used to build structures of **proteins**, **nucleotides**, **ligands** and their **complexes**
- making use of pattern recognition to build **models** from MX **electron density maps**

Lamzin, V.S. & Wilson, K.S. (1993) Automated refinement of protein models. *Acta Cryst.* **D49**, 129-147.

Pattern Recognition

It allows the transformation (reduction) of information from **signals** to **meaning** given **a *priori* available knowledge:**



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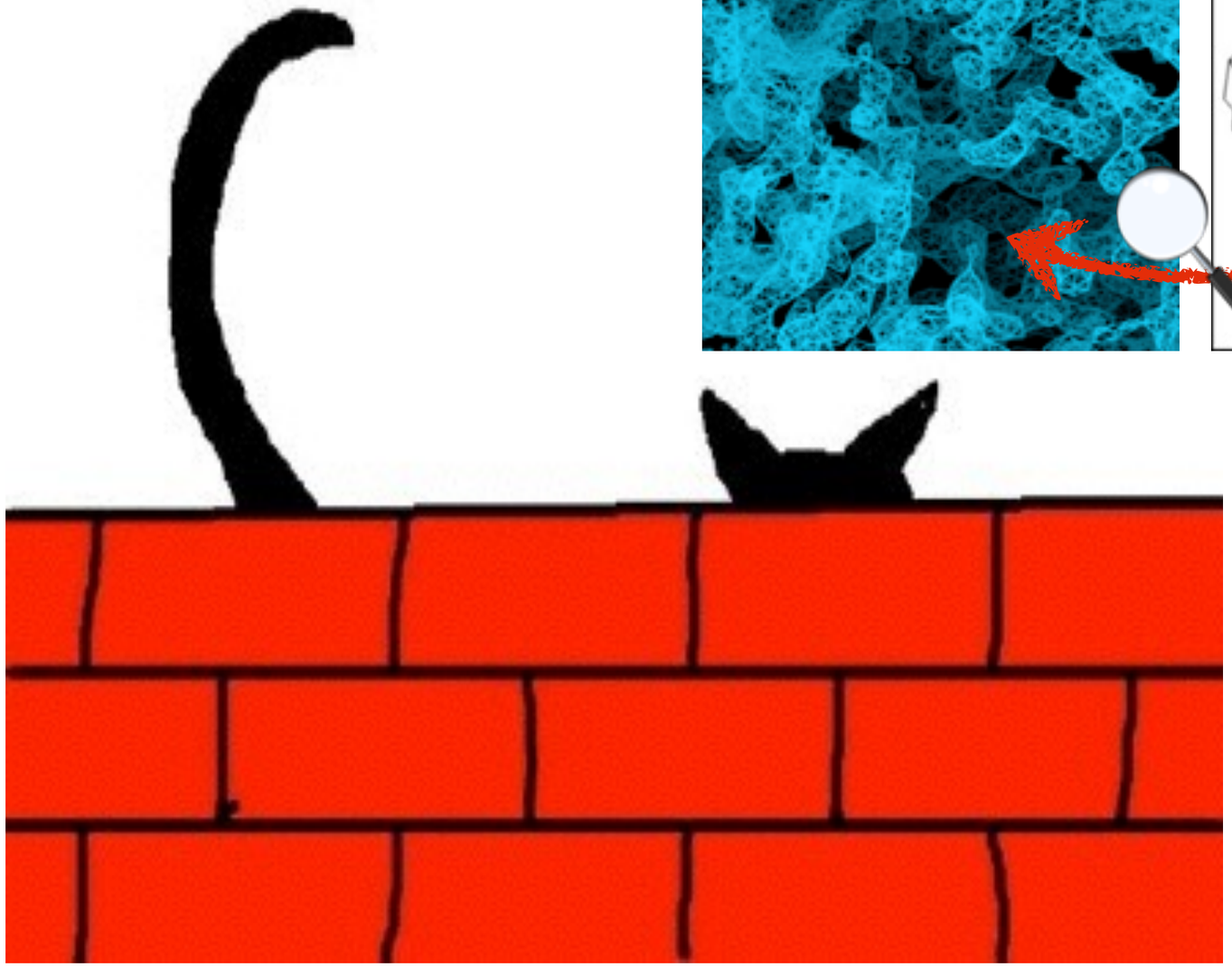
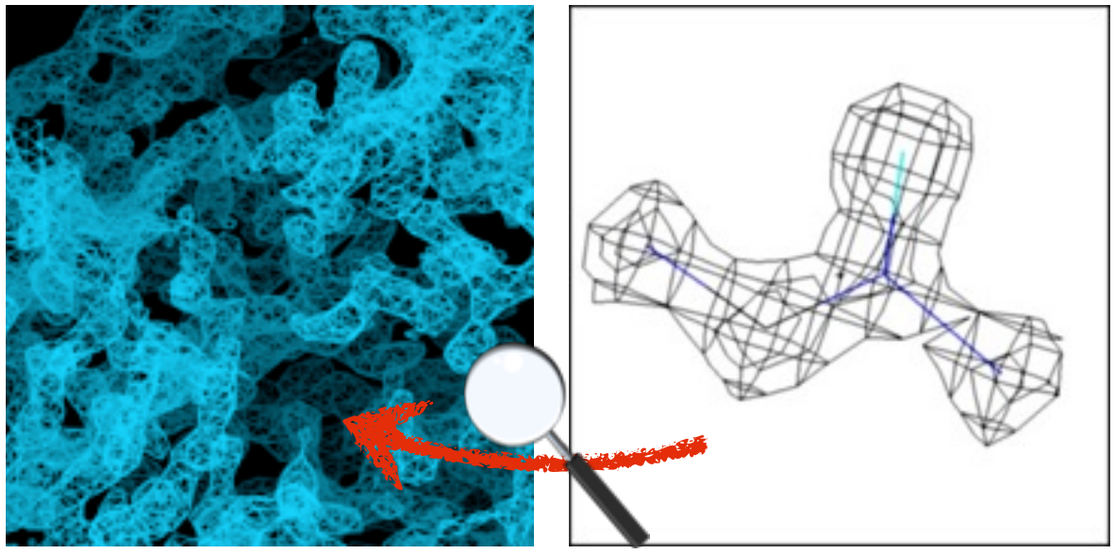
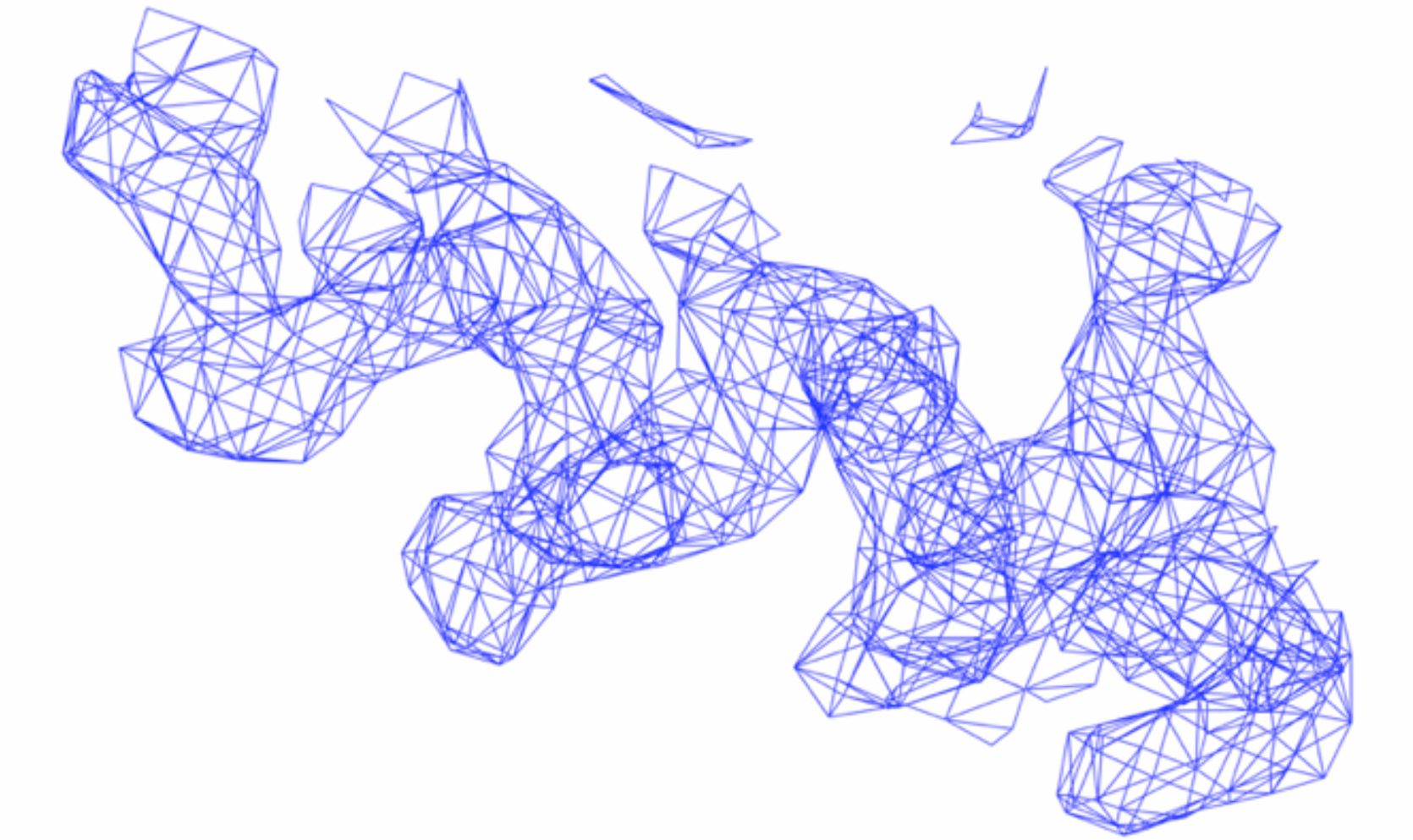




The initial model

Given an electron density map and the protein sequence, ARP/wARP describes the electron density map as a set of free atoms without chemical identity:



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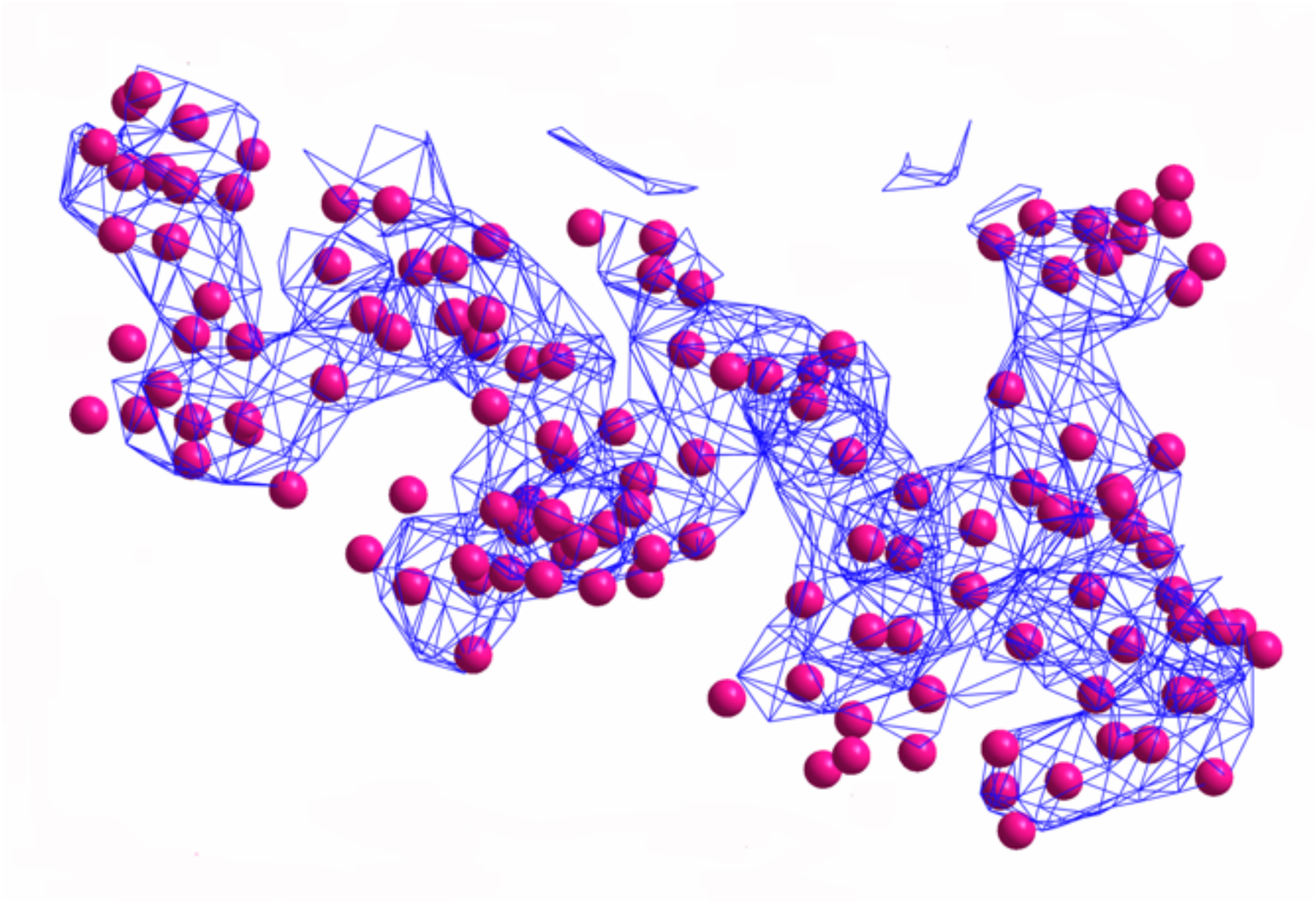

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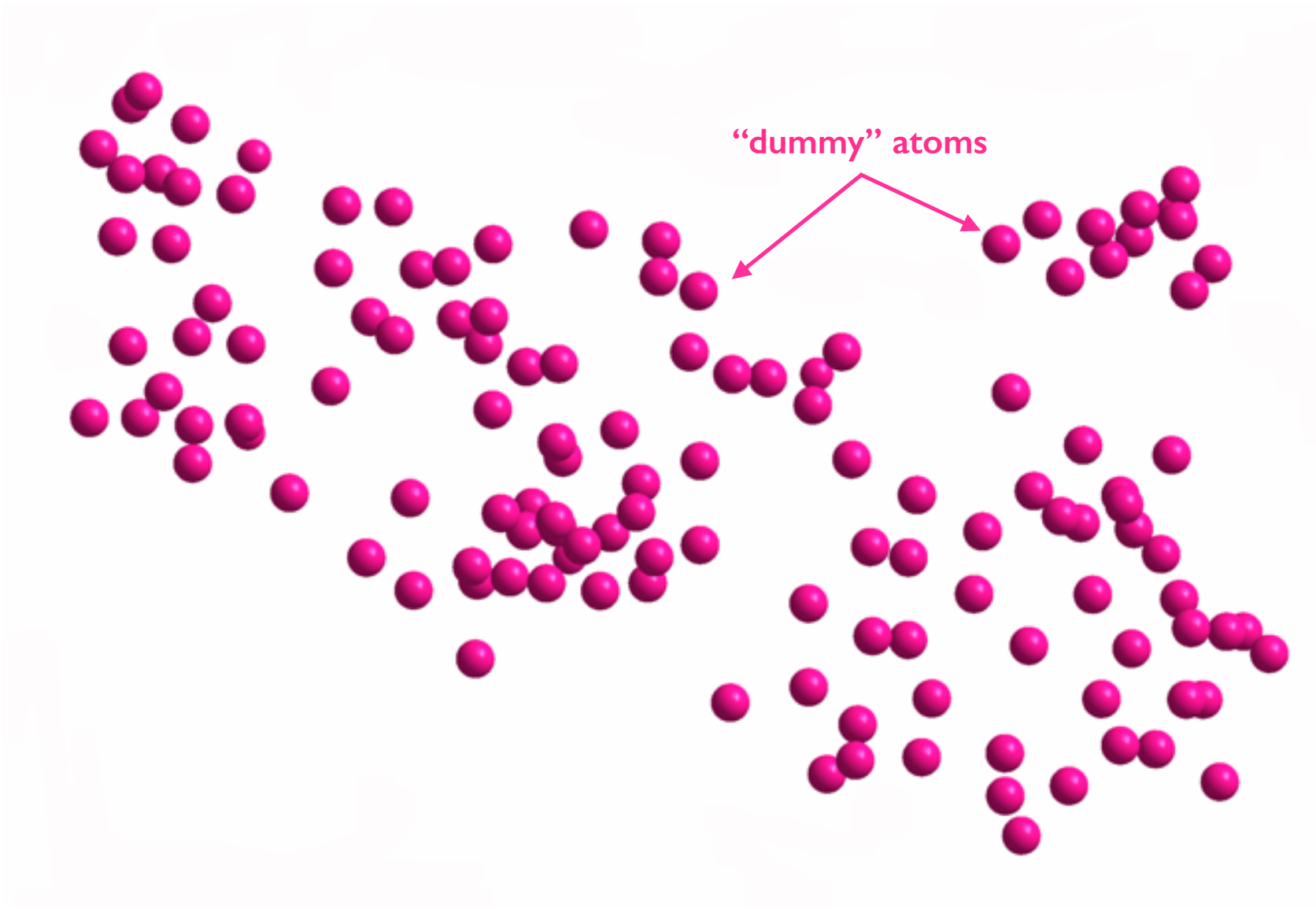

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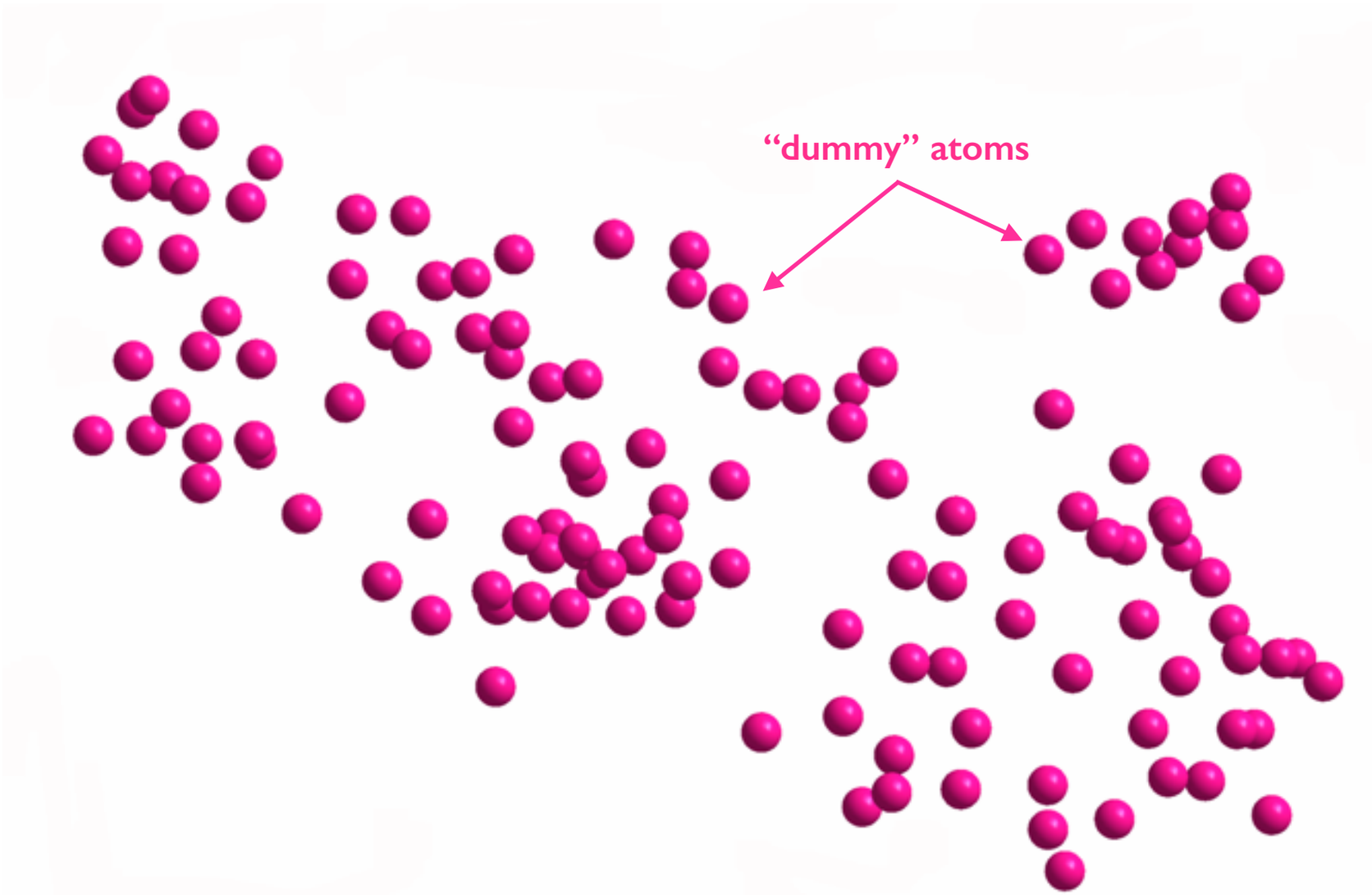
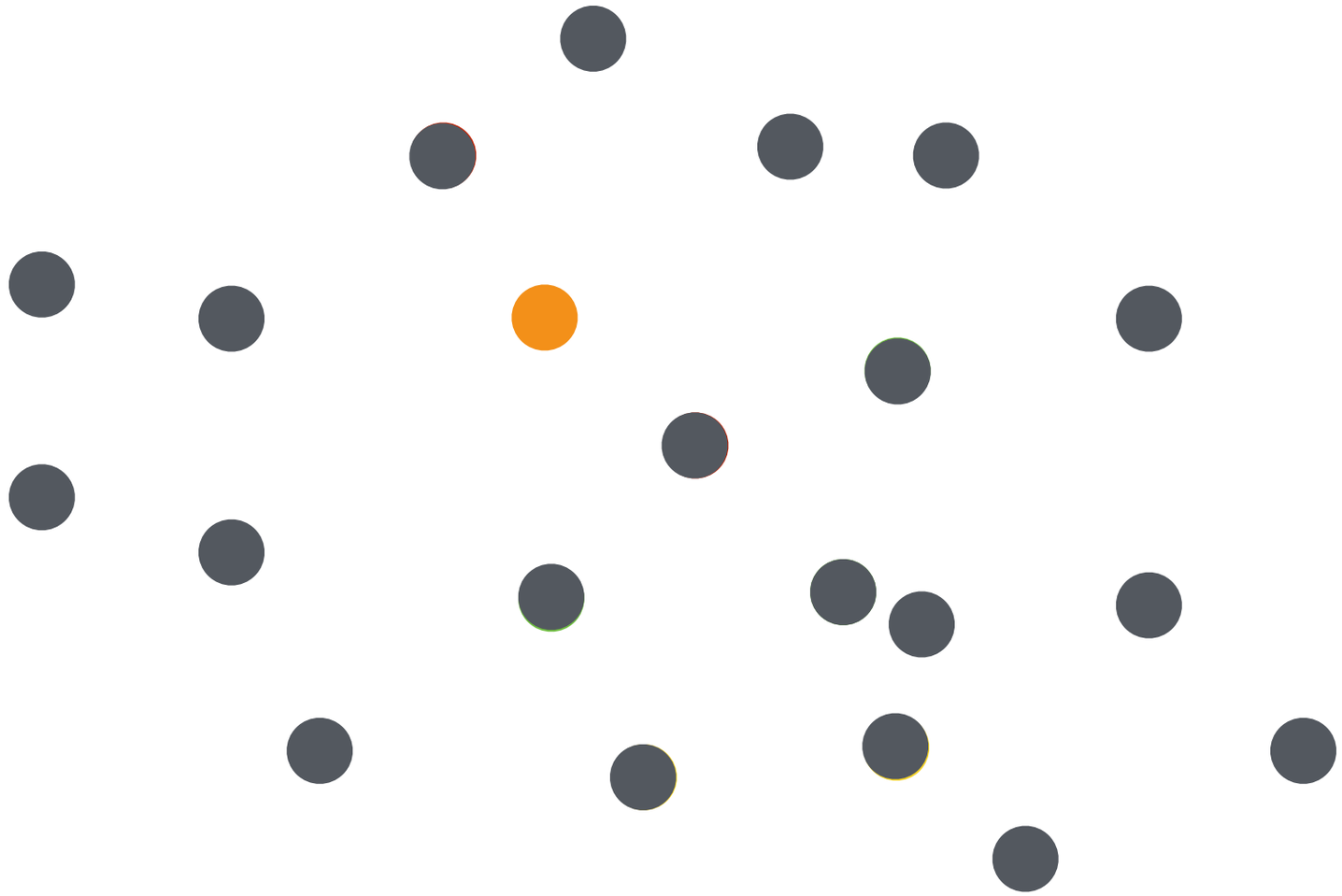


How to connect the free atoms?

Finding peptides

Free atoms at distances close to the ones observed in peptides are searched:



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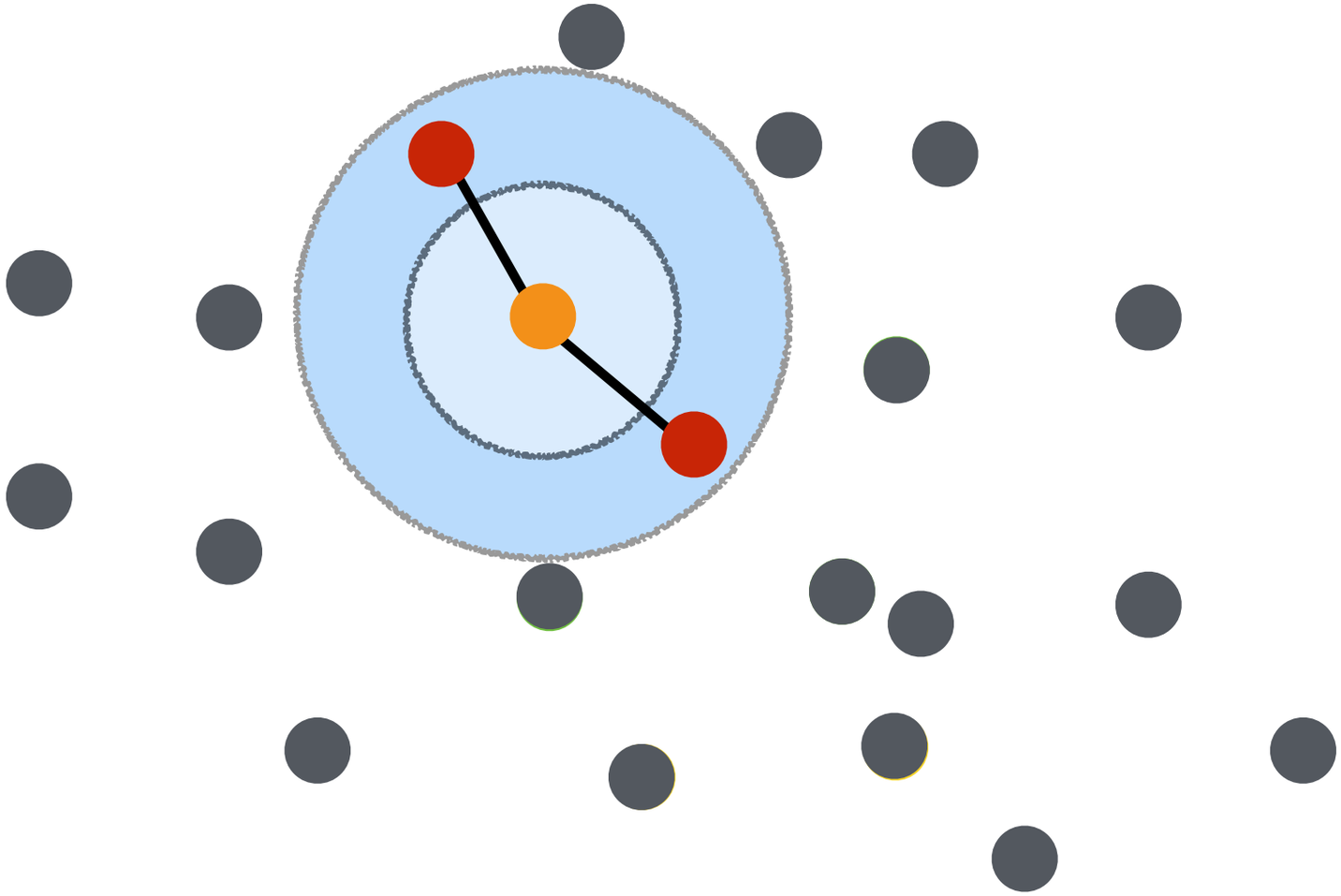
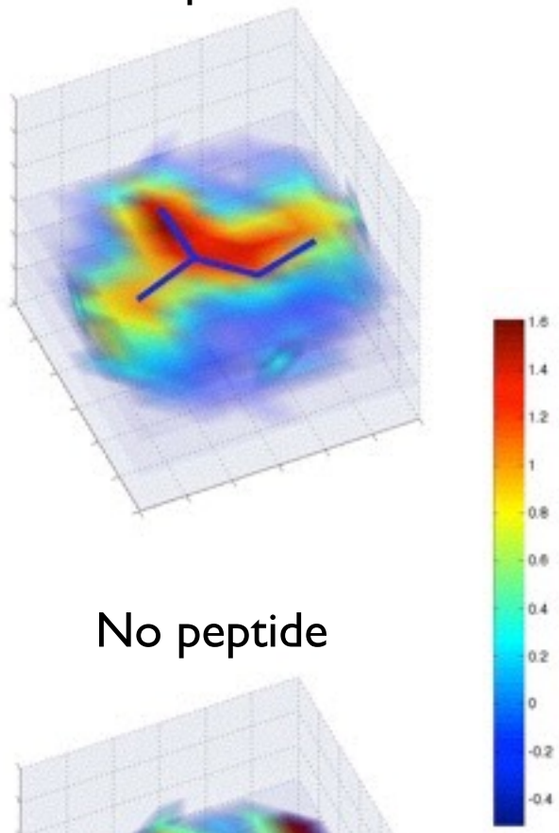
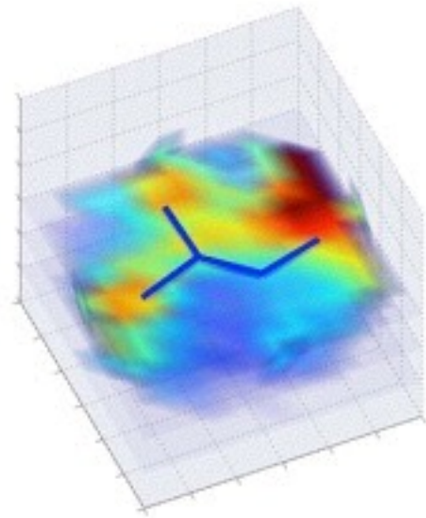


Peptide



No peptide



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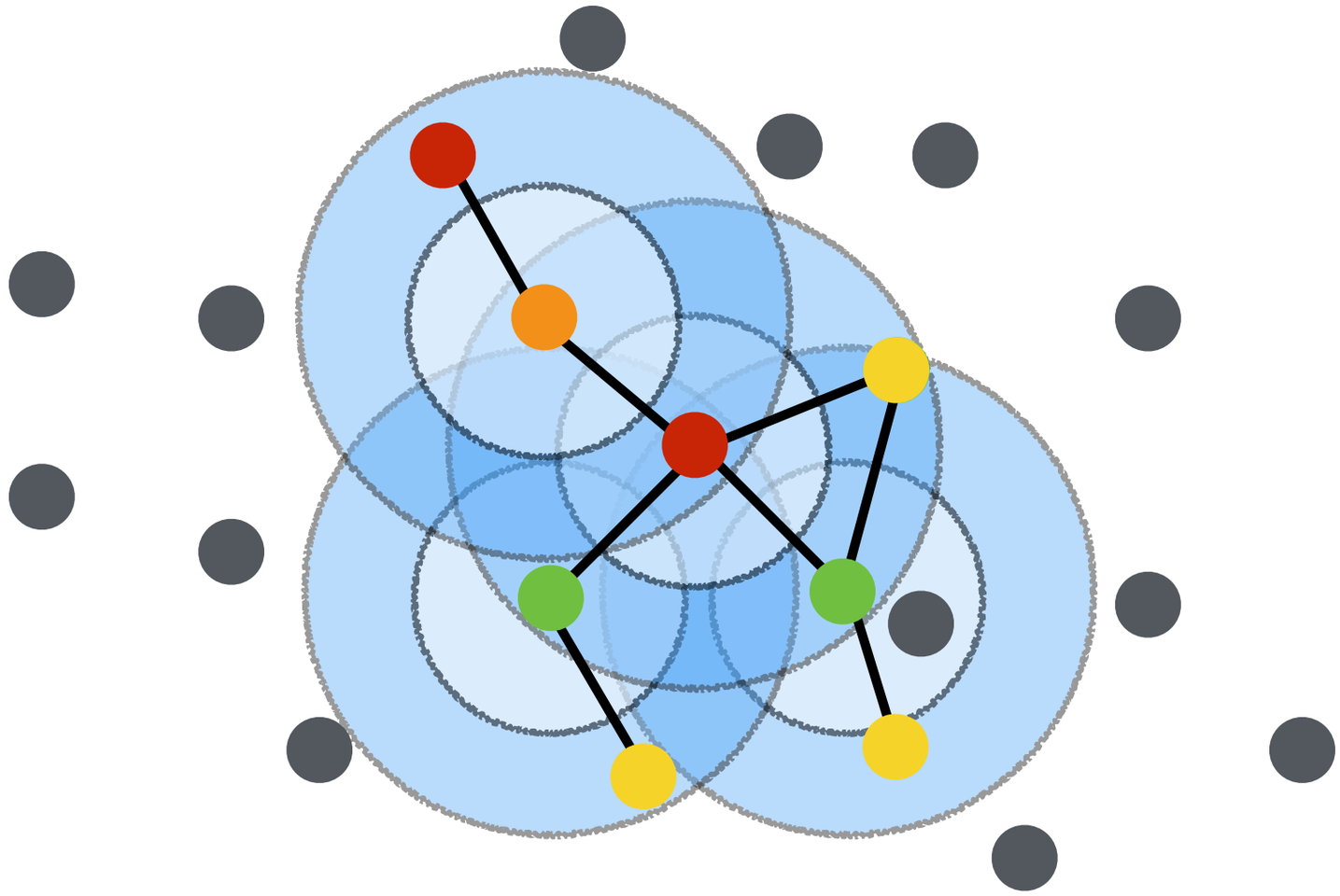

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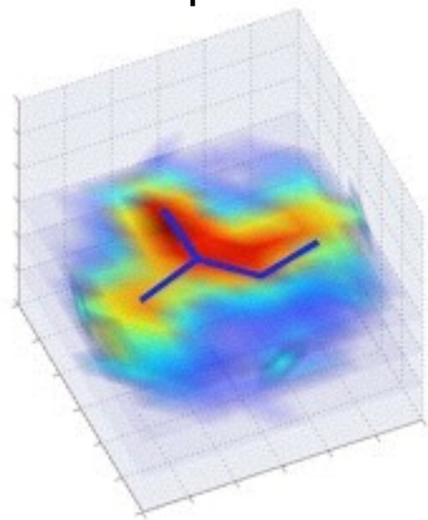

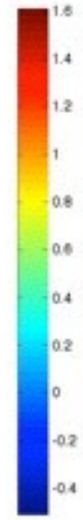

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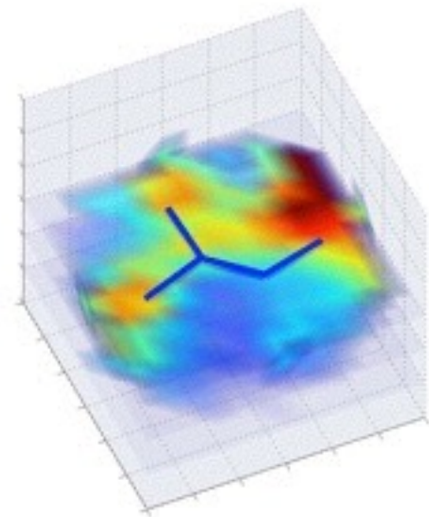

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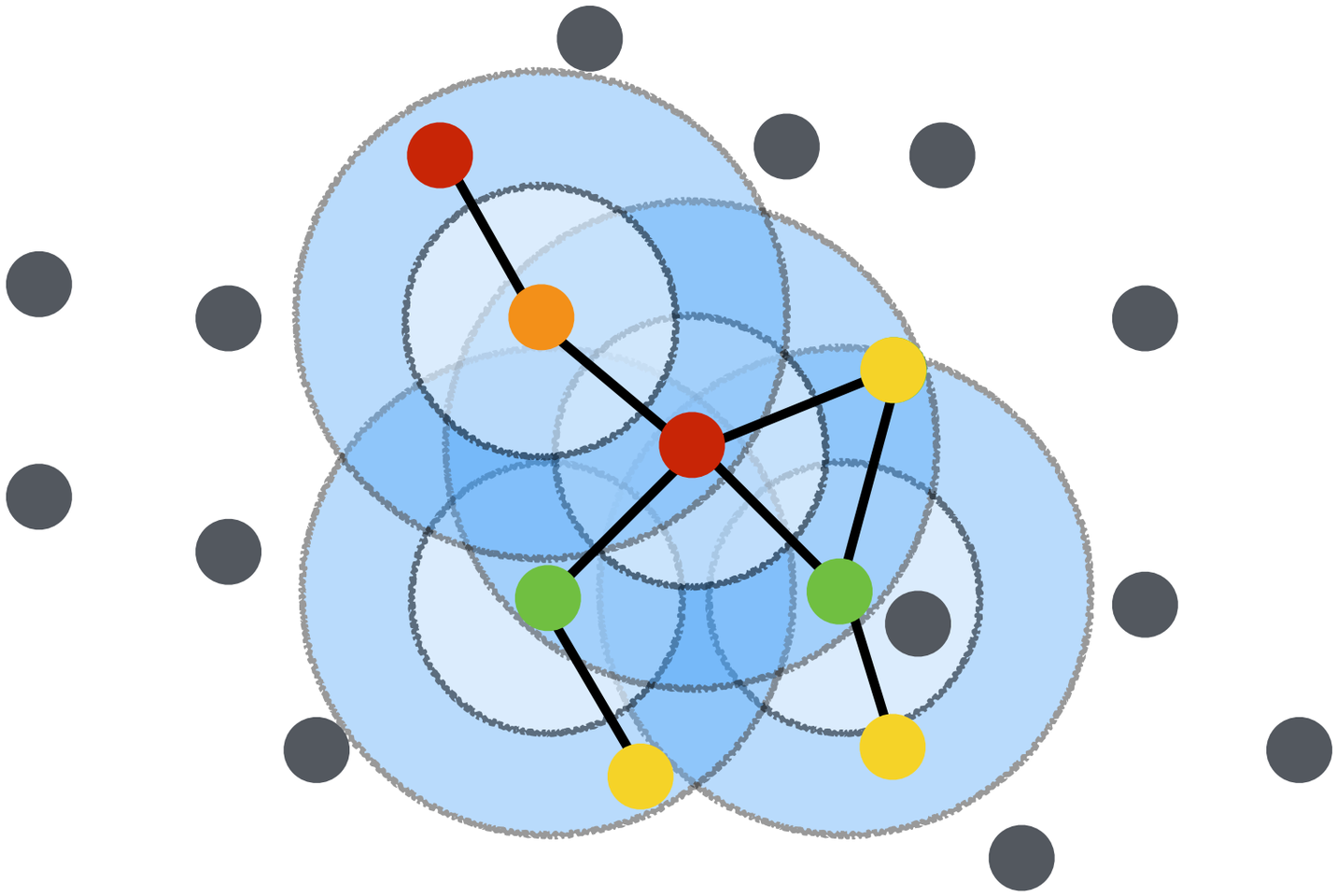

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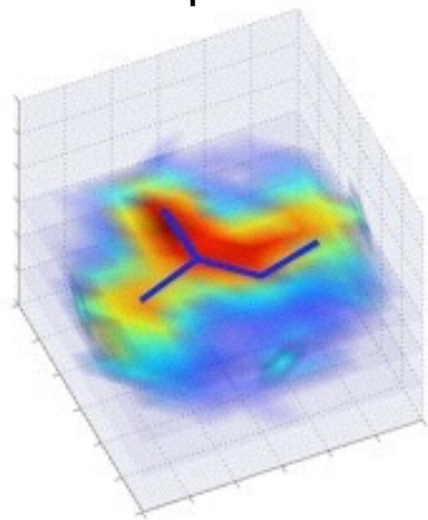

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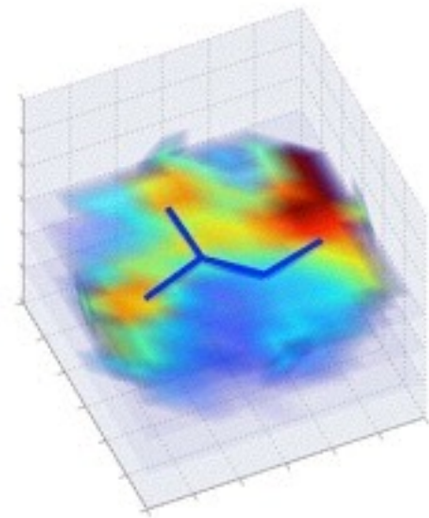
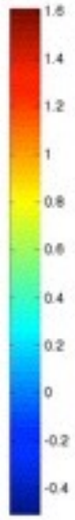
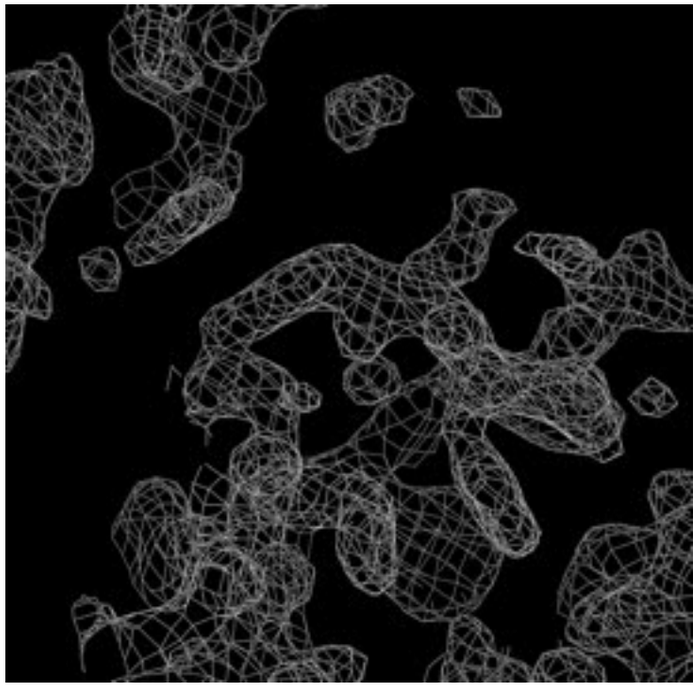
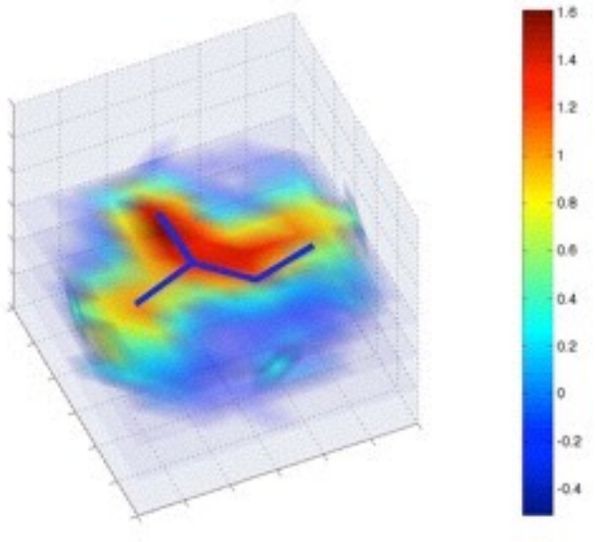




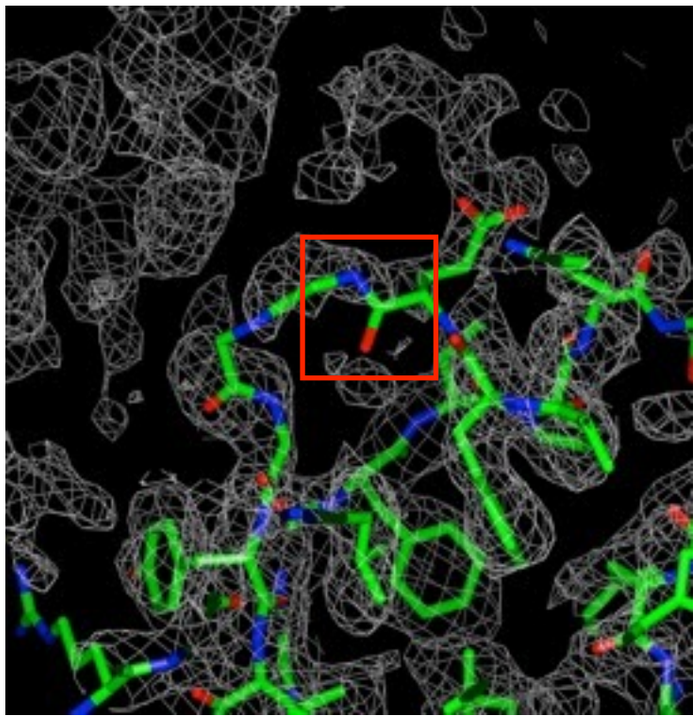
Peptides that share one Cα atom can be connected and dipeptides with correct conformation connected to build the longest fragment

Finding peptides

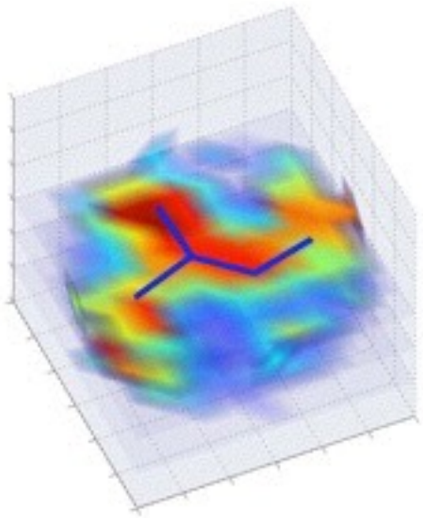




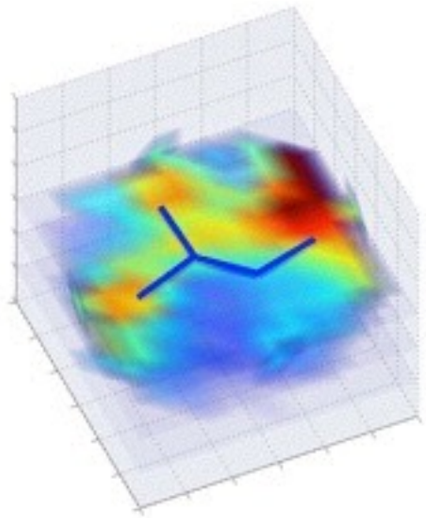
The task:
Separating **true** peptides
from **false** ones.



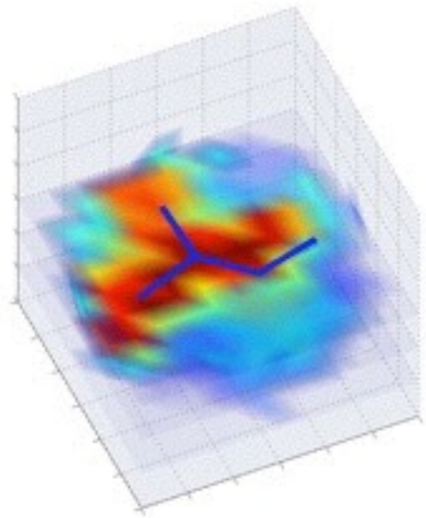
peptide
good fit



peptide
but poor fit



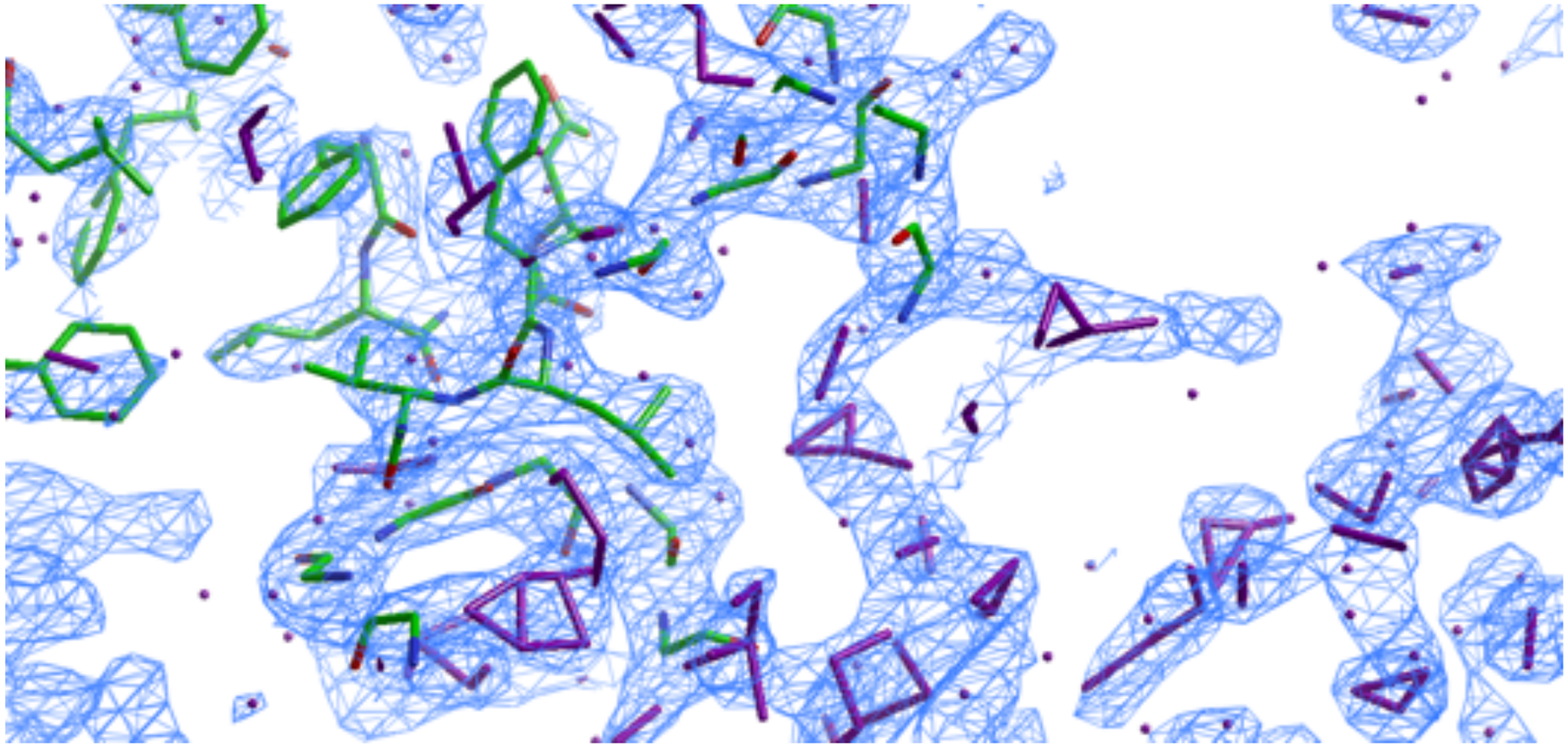
non-peptide
but good fit



The hybrid model

As only a small part of the initial free atoms model is now recognised as a putative protein, we have an hybrid model that combines 2 sources of information:

- **Chemical knowledge** from the partially built model
- **Free atoms** continue to describe the electron density



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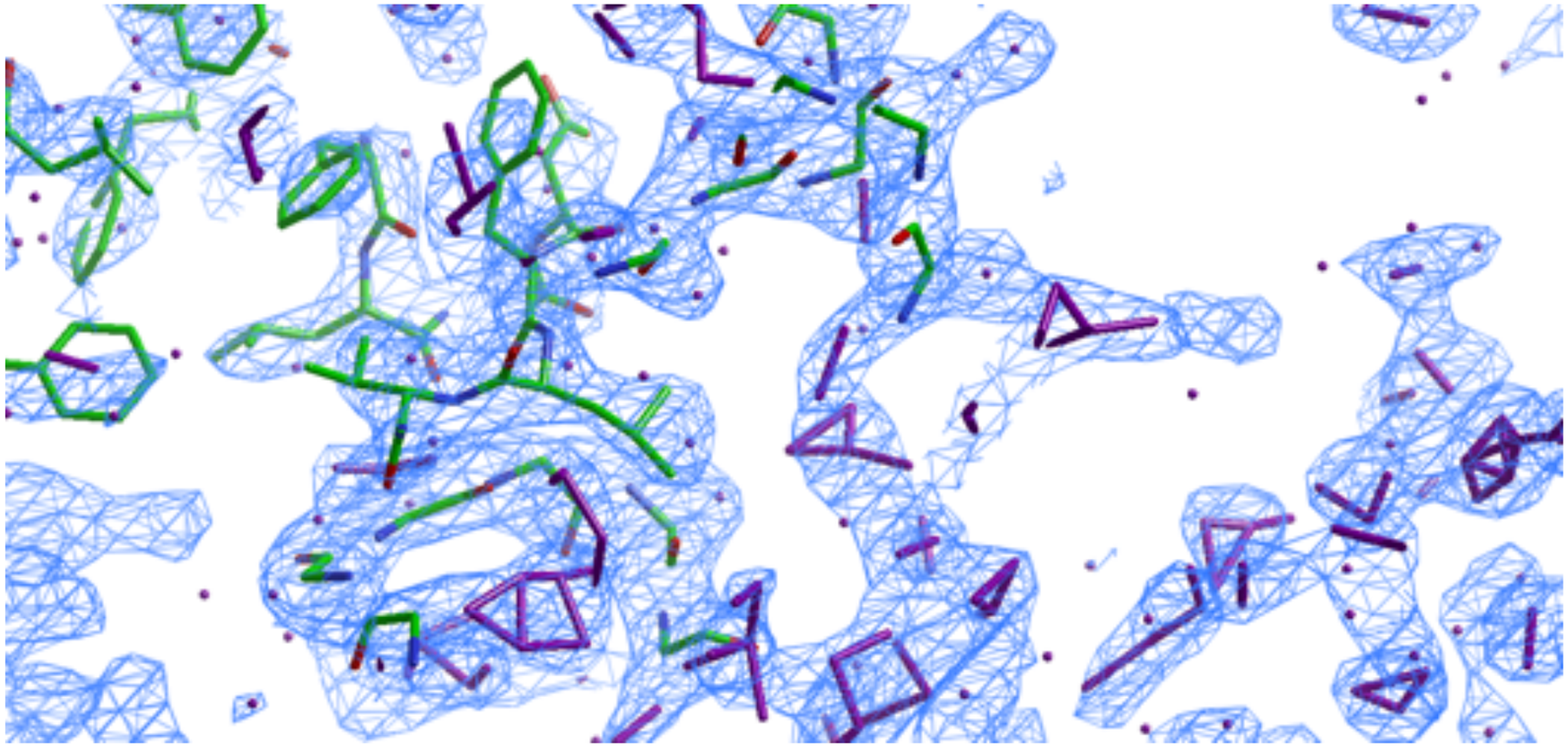

It can provide restraints for further **refinement**

Allows the improvement of the map and consequent better model building

Model update

As the density is improved by refinement, the model can be updated by removing and addition of atoms:

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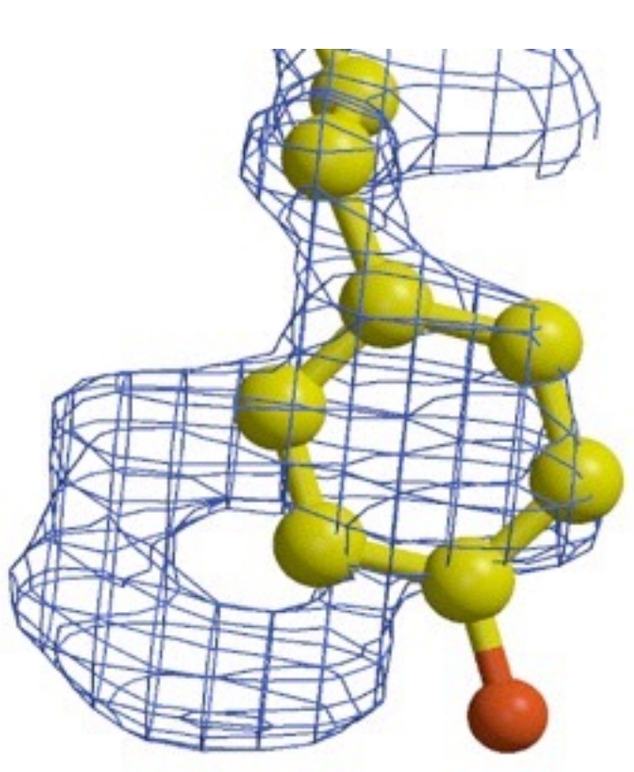
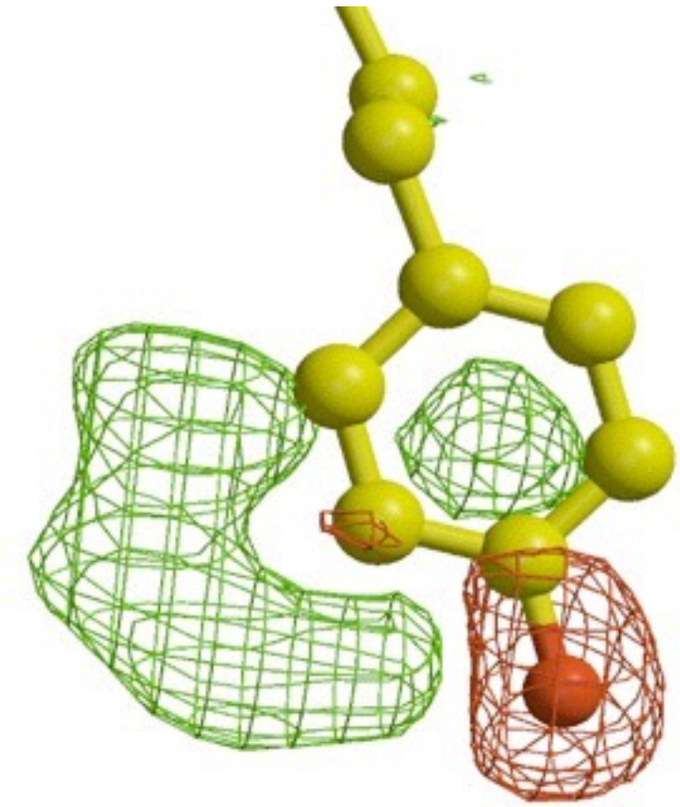


2Fo-Fc map

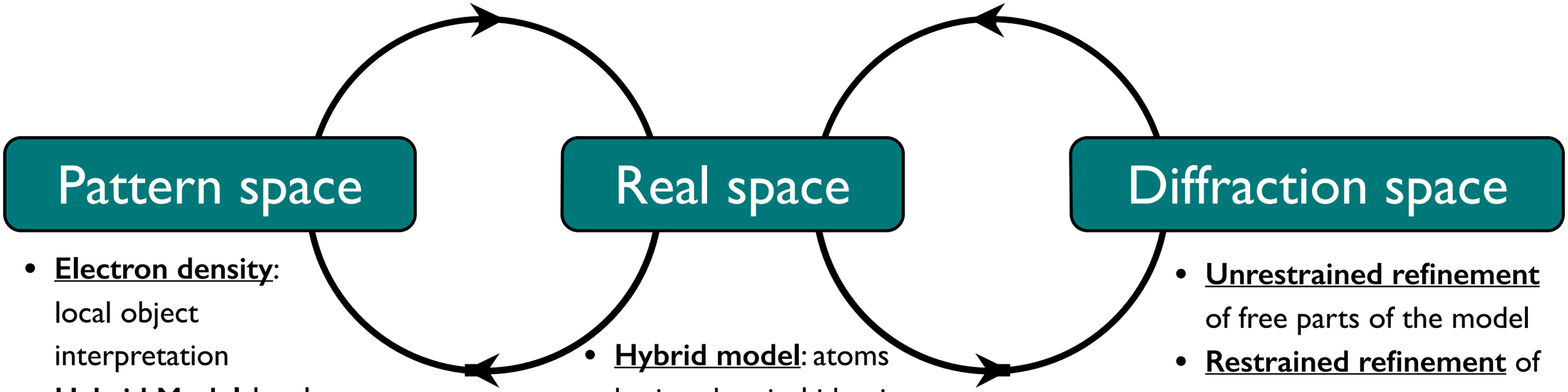


Fo-Fc map

```
ARP/wARP will be iterated with REFMAC5
50 refinement / model update cycles will be run in total.
Atoms will be removed below 1.0 sigma in 2mFoDFc map and added above 3.2 sigma in mFoDFc
map.
```

The fundamental ARP/wARP concept

ARP/wARP circulates between three spaces, forming a unified process of model building:



- **Electron density**: local object interpretation
- **Hybrid Model**: local motif interpretation

- **Hybrid model**: atoms having chemical identity and free atoms
- **Model update**: removing and adding parts of the model

- **Unrestrained refinement** of free parts of the model
- **Restrained refinement** of chemically assigned atoms

Scheme of restraints and free atoms are iteratively updated

Hybrid model is converging to the final model

ARP/wARP workflow

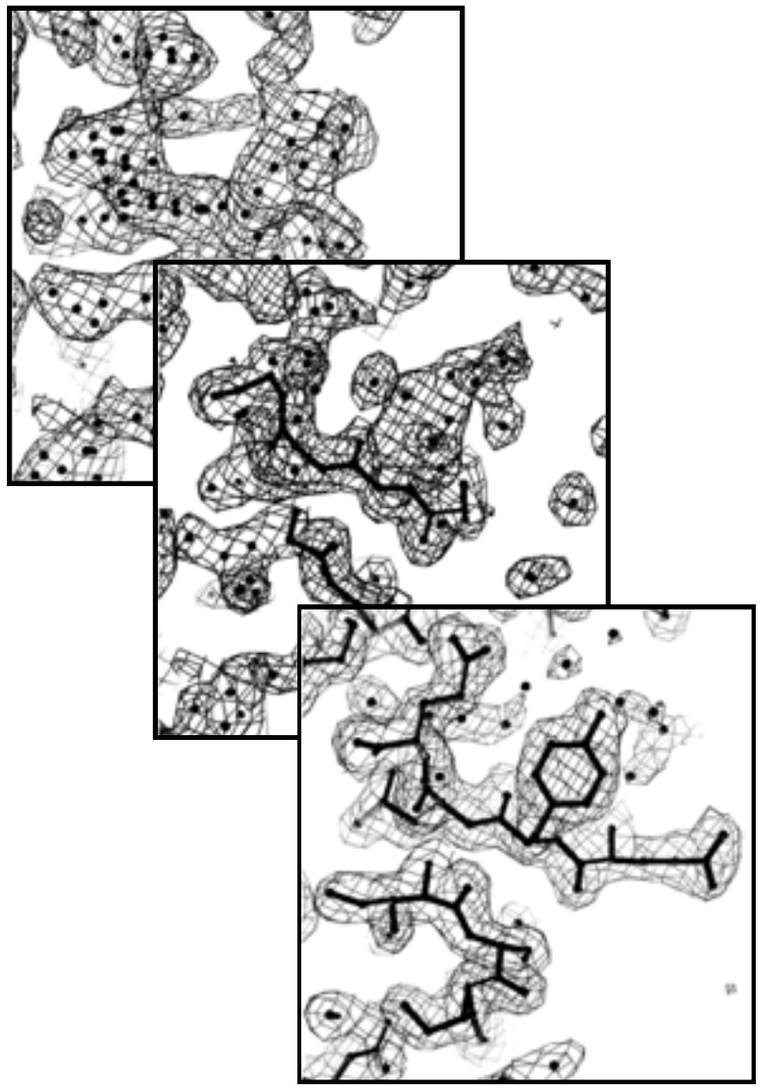
ARP/wARP iterates between main chain tracing, refinement and model update to build models that converge to the final model:

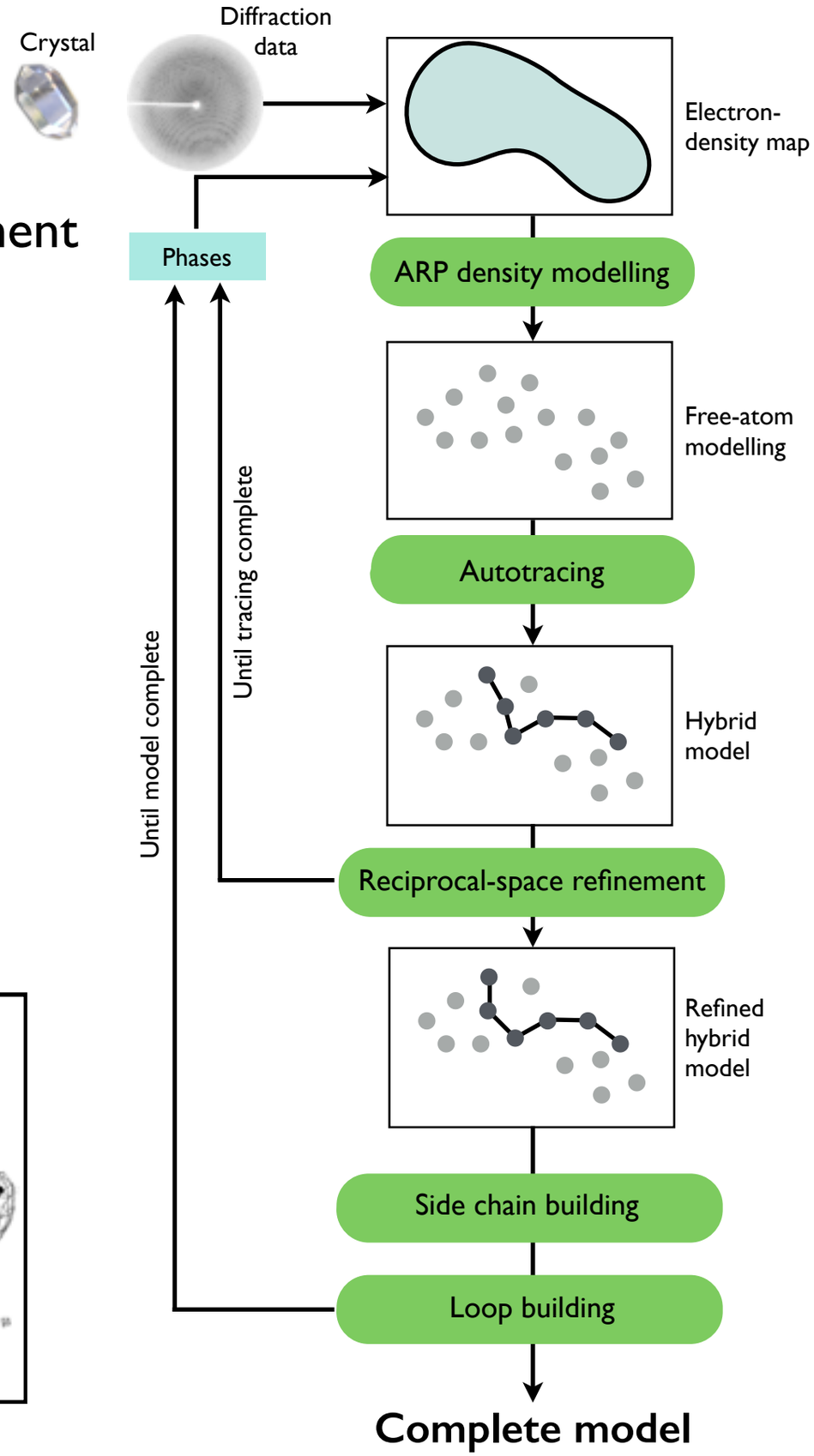
Free Atoms

Pattern Recognition

Hybrid Models

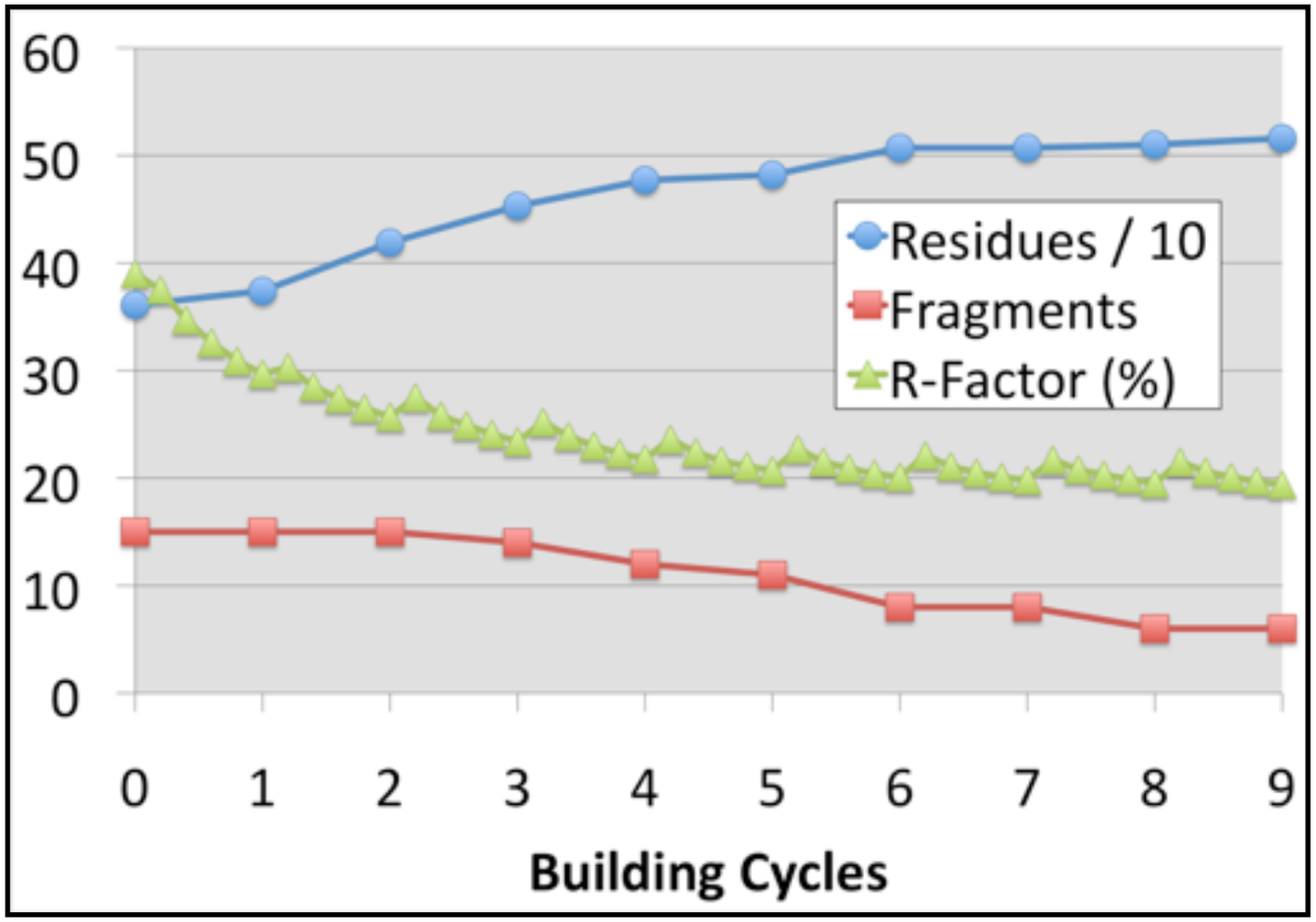
Iterations





ARP/wARP workflow

ARP/wARP iterates between main chain tracing, refinement and model update to build models that converge to the final model:



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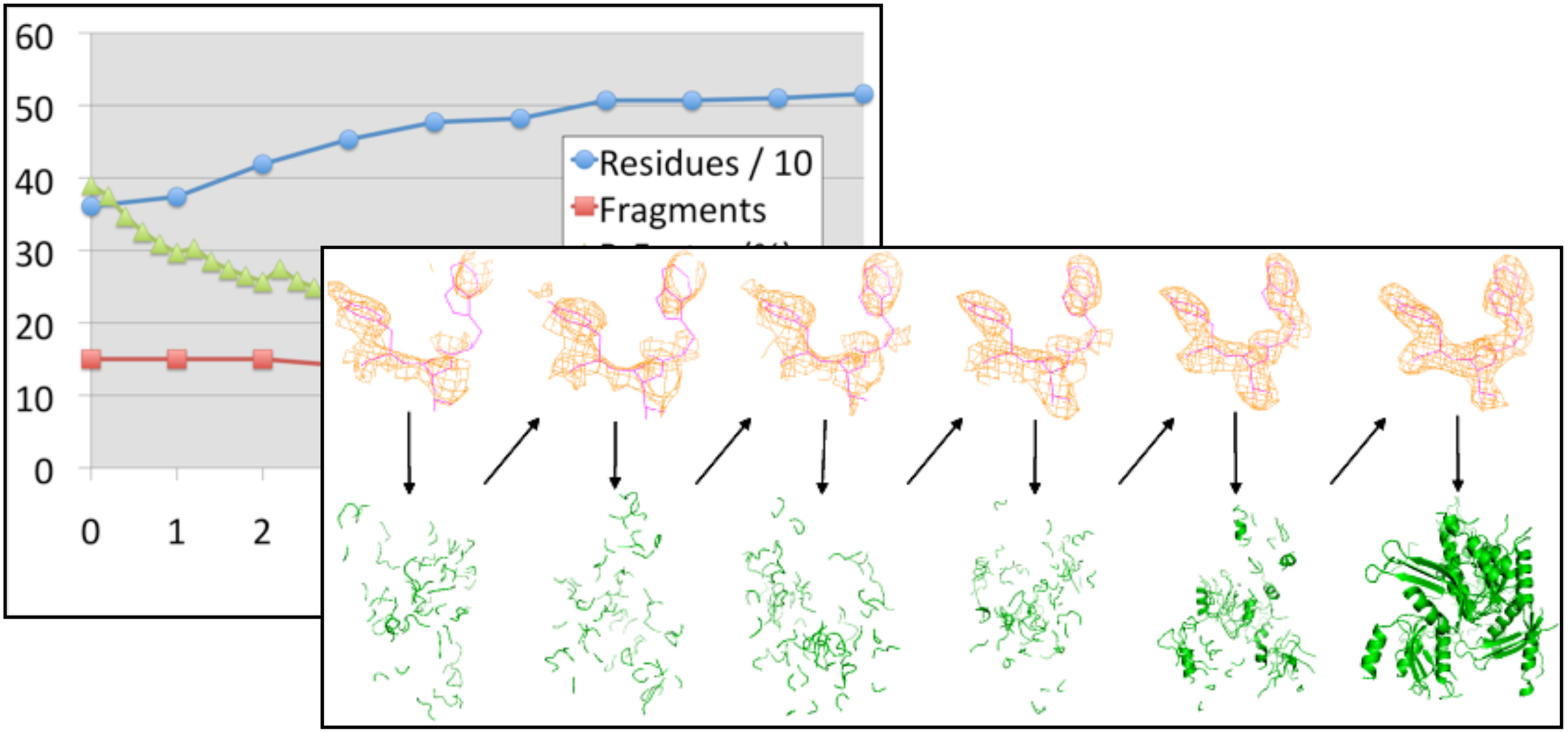
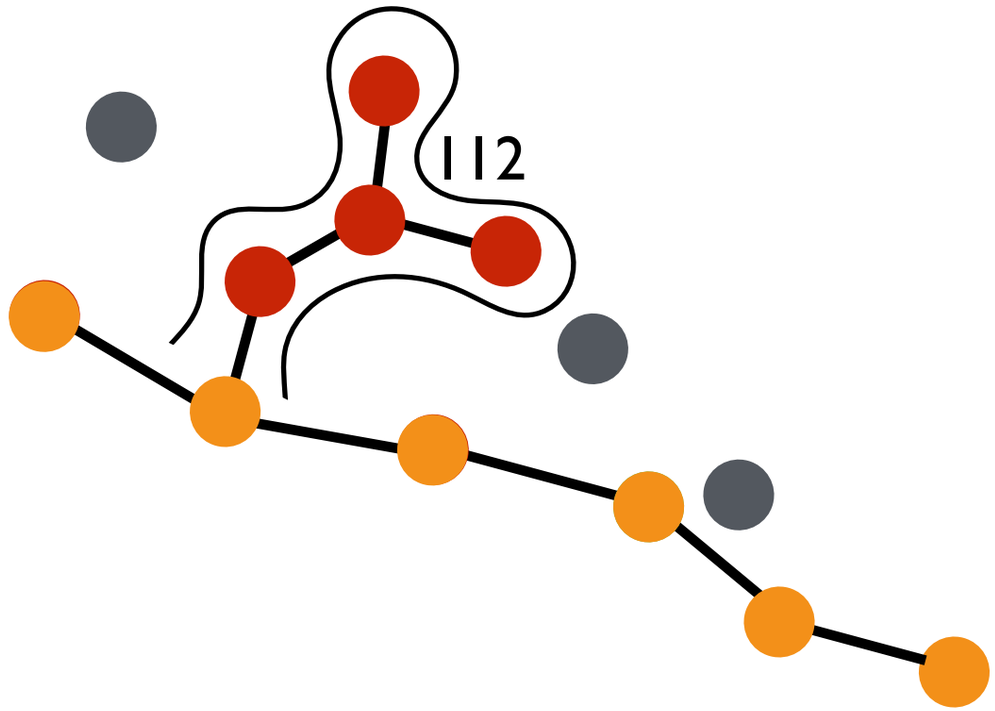


Sequence docking and side chain building

After main-chain tracing, one gets a set of main-chain fragments and the side chain-building module has to:

1. **Sequence docking** using connectivity vectors
   (e.g., serine "11", aspartate "112")

2. **Side chain building** using the Richardson's rotamer database



This allows the construction of loops!

Loop building

Even after a successful automated model-building run, some regions of known start, end, length and amino-acid sequence remain to be built, and ARP/wARP builds these **loops** by:

- Using **knowledge of angles** between anchors
- **Check with density** to see if modelled loops are valid

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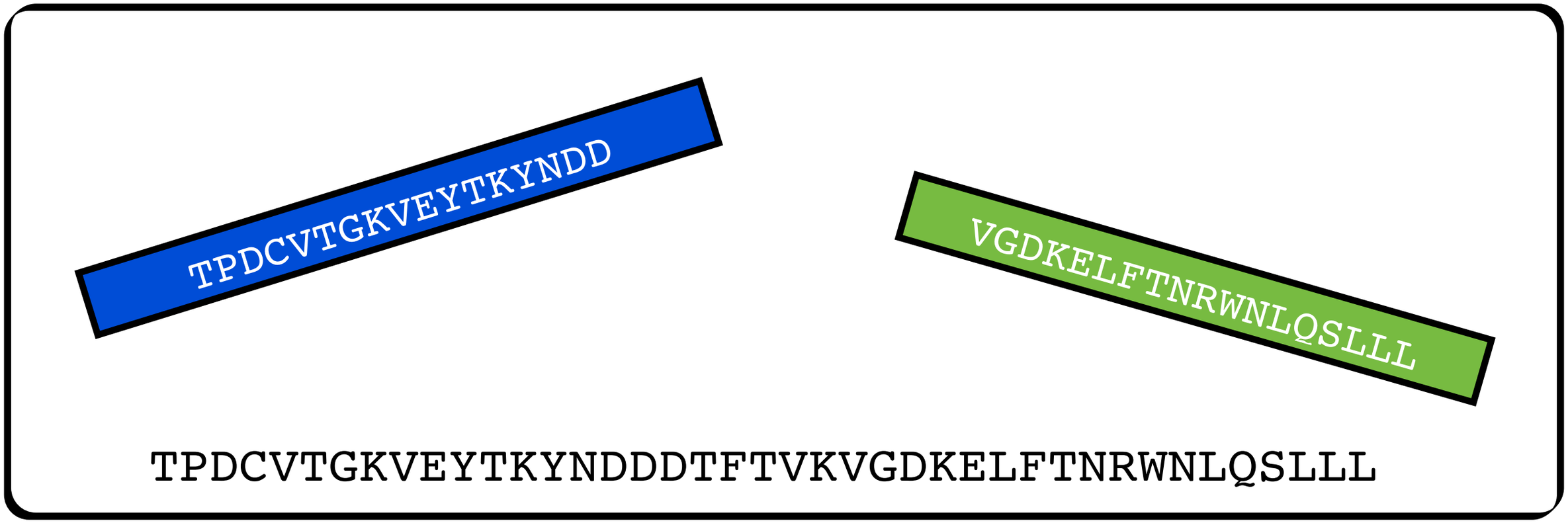

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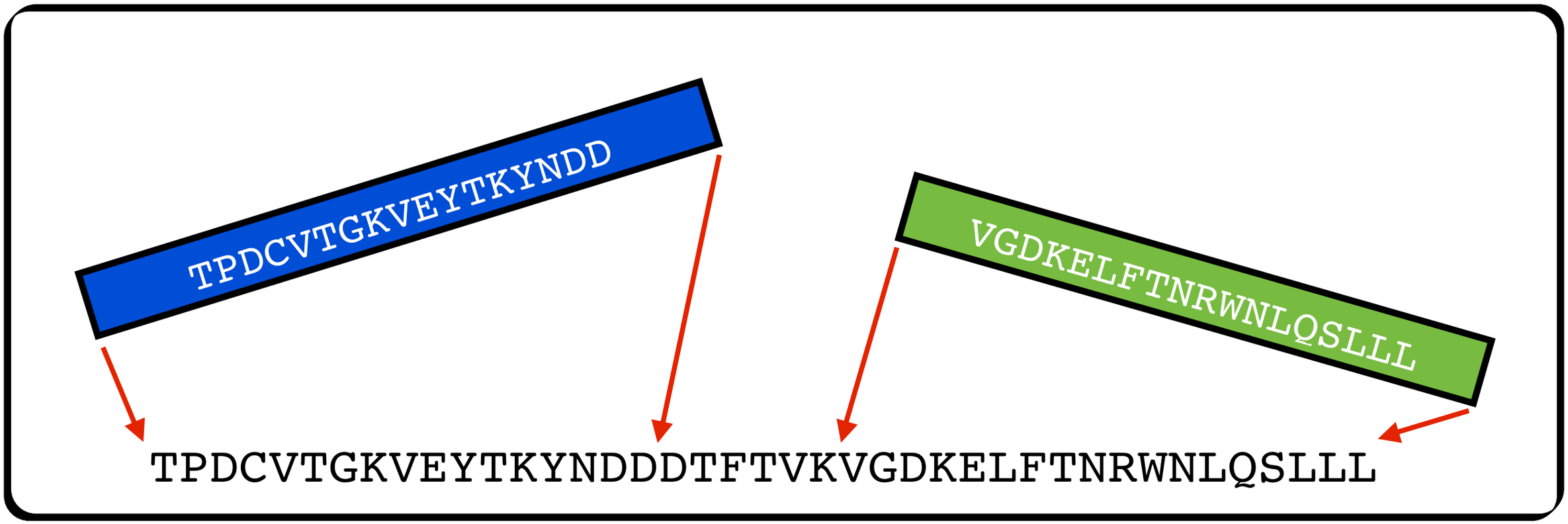

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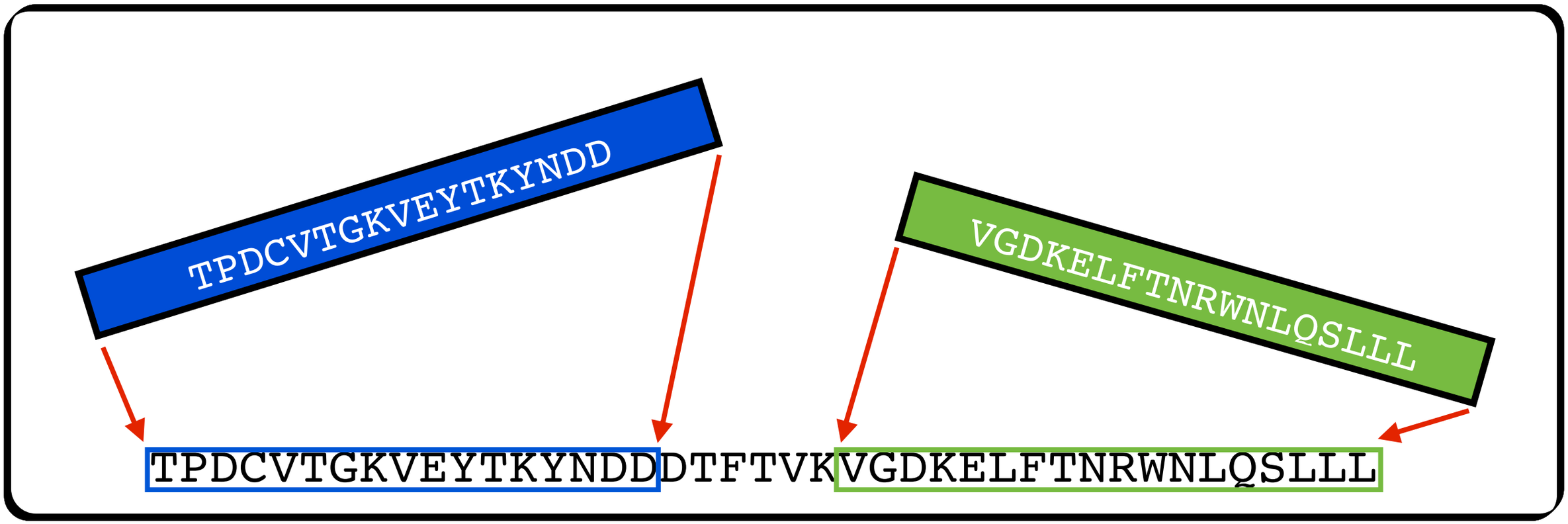

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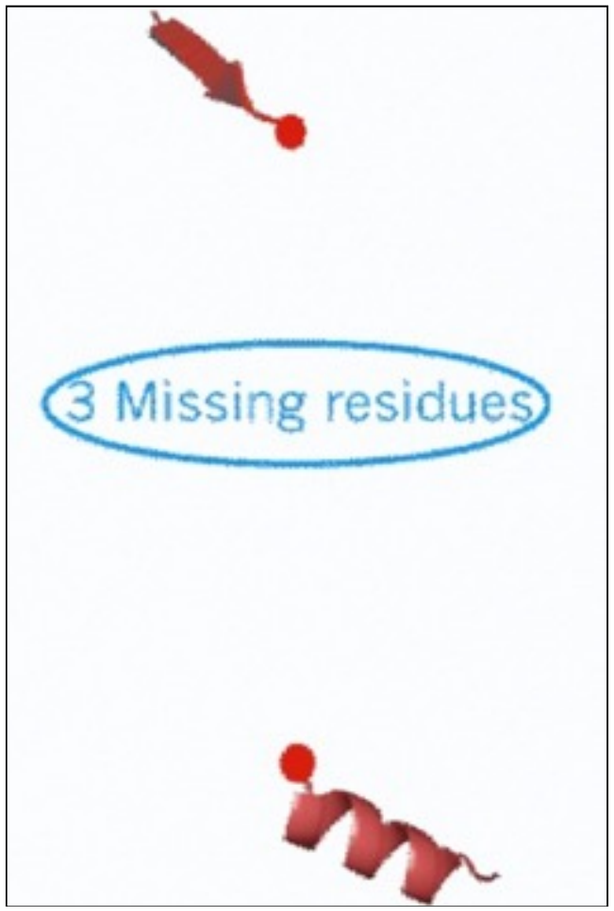
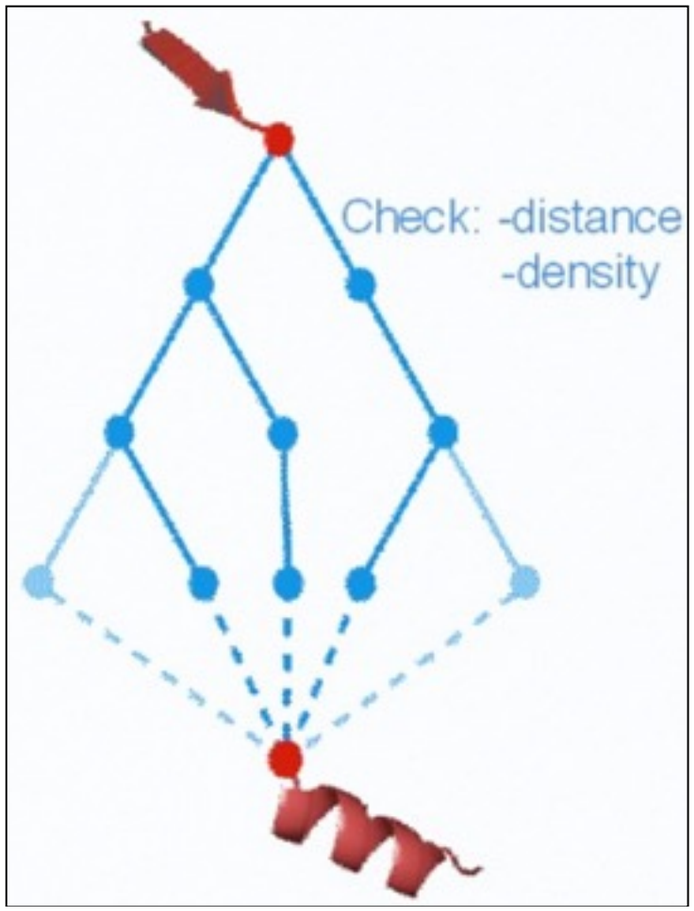
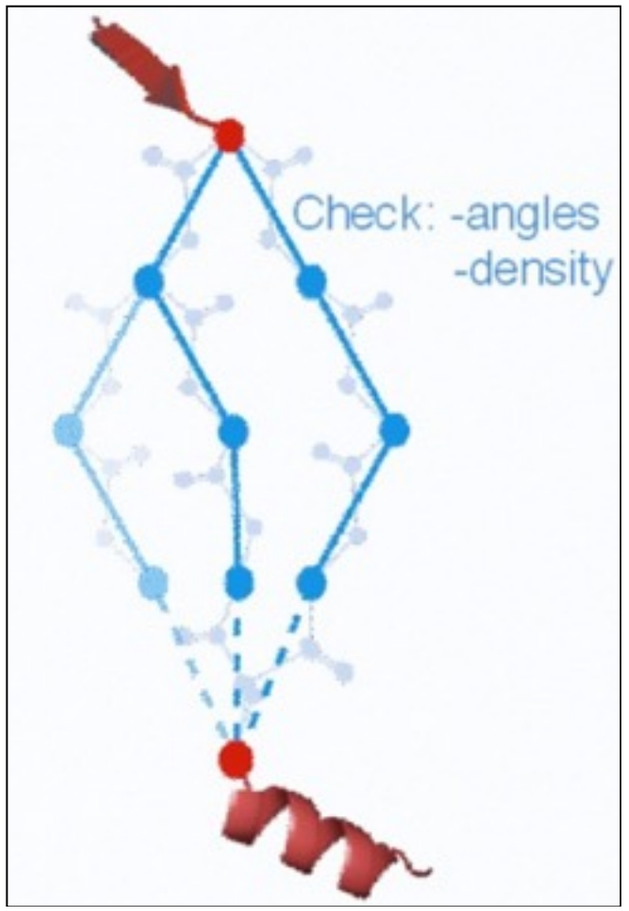
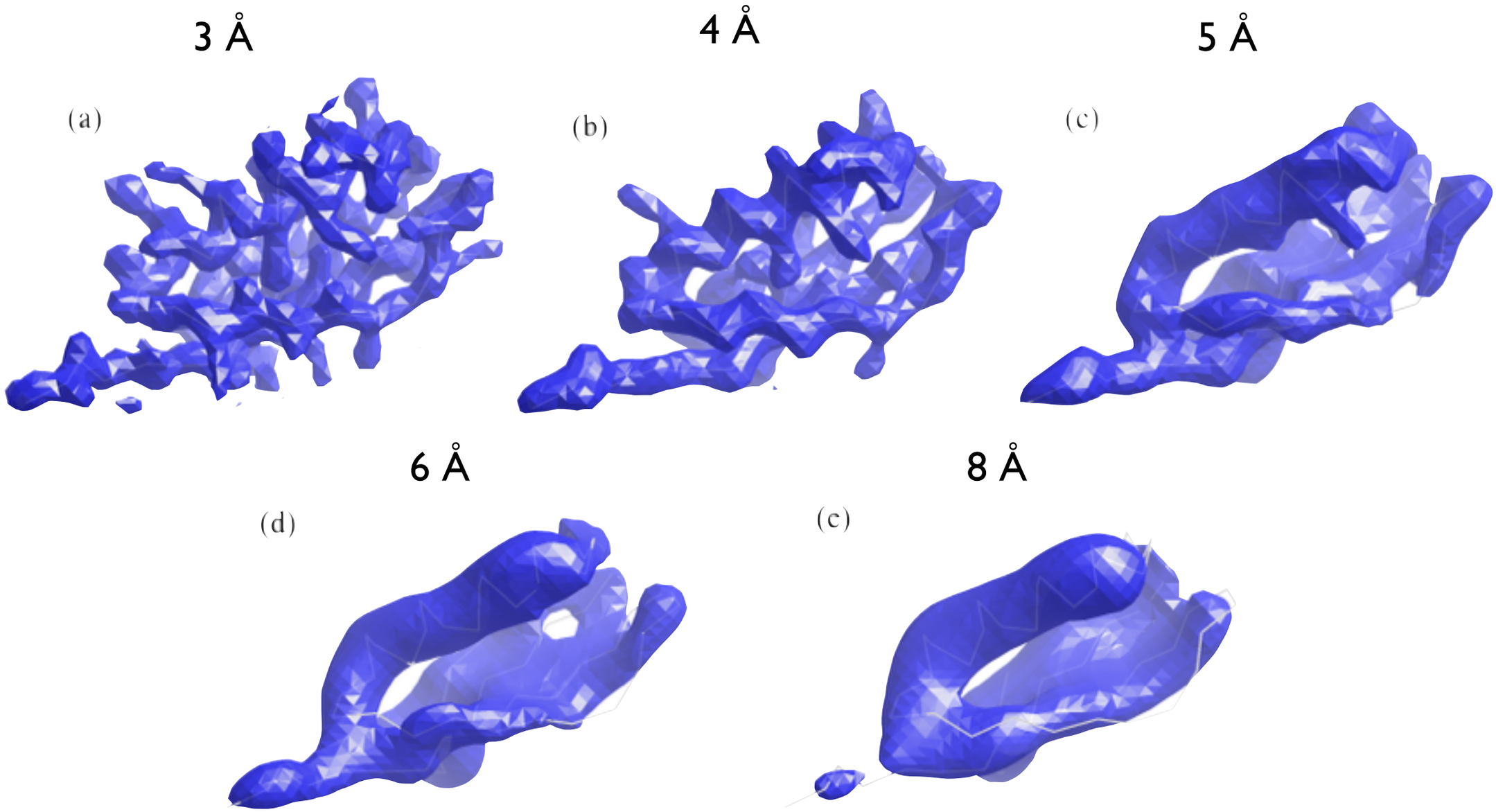






Low resolution as a limit

The primary factor determining the accuracy of an experimental protein structure is the **resolution of the X-ray data**:



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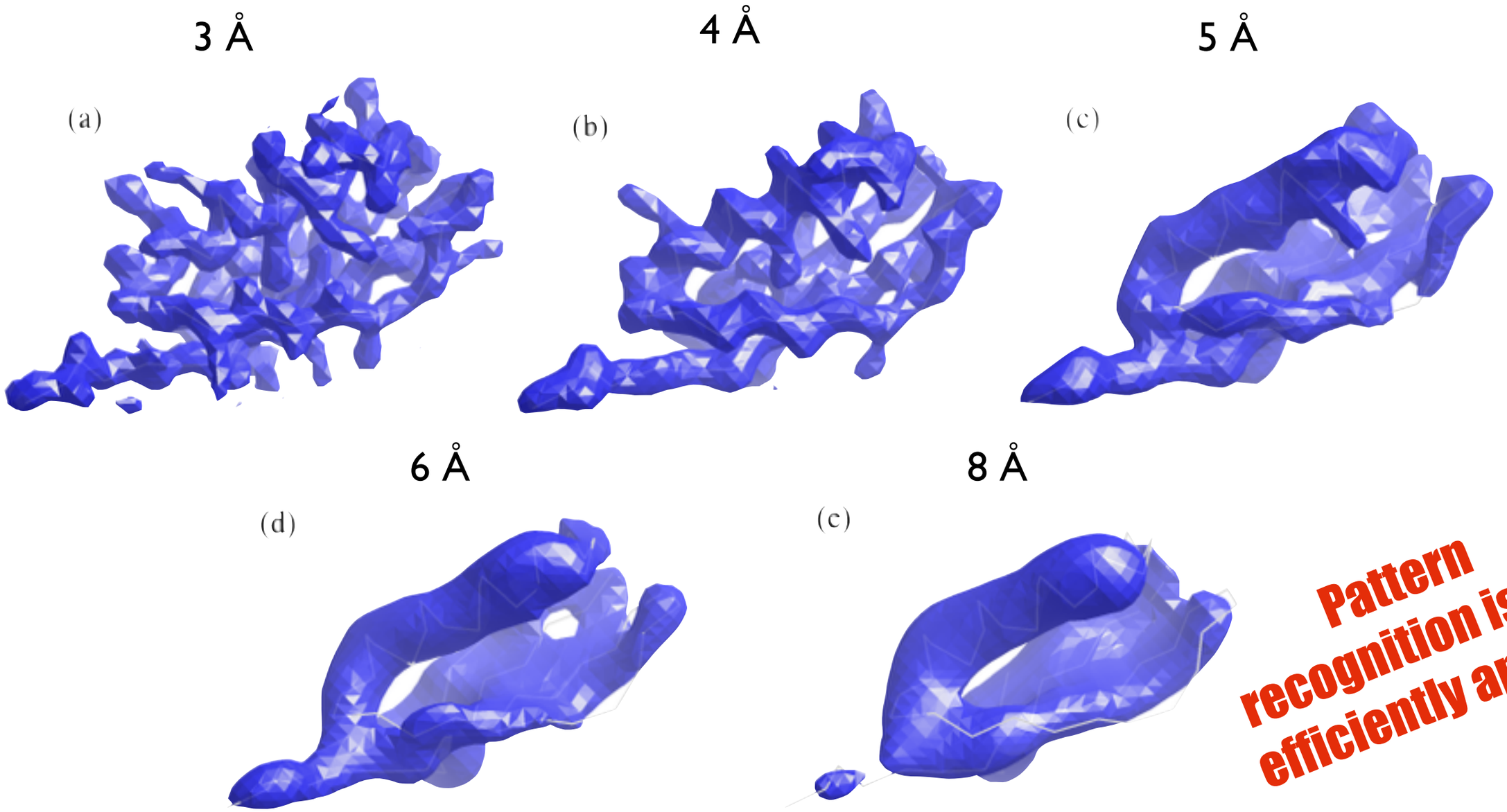


Pattern recognition is not efficiently applied

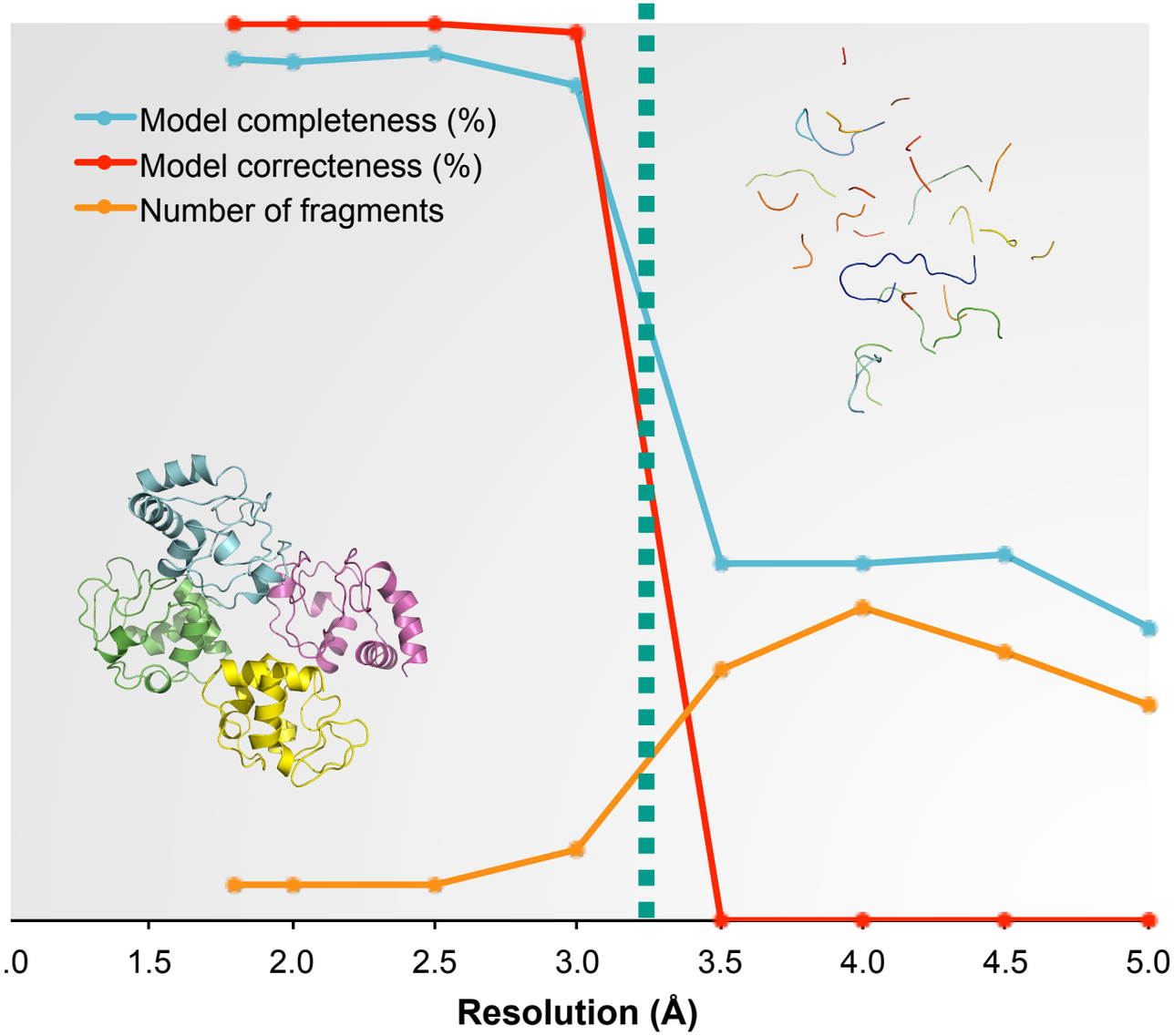
Low resolution as a limit

So what happens?

Hard to build main chain
Hard to find side chains

1.0 to 3.0 Å

Good quality final models



3.0 to 5.0 Å

Bad quality final models

ARP/wARP and resolution

Model building methods were historically developed for and work considerably better with high-resolution diffraction data:

Results from the ARP/wARP webservice (tracing performance)

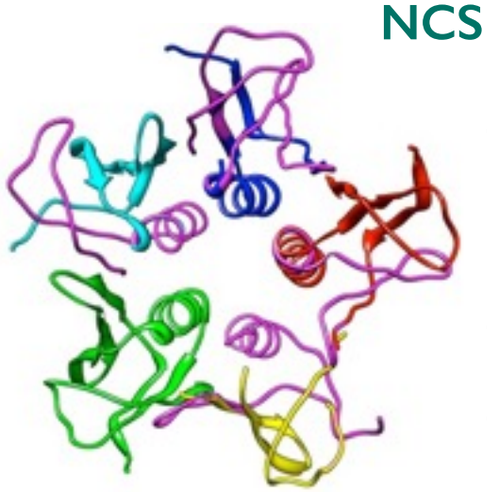
Resolution	Estimated fraction of automatically built protein structure
1.5 Å and higher	98% and higher
1.5-2.0 Å	91 - 98%
2.0-2.5 Å	81 - 91%
2.5-3.0 Å	67 - 81%
3.0-3.5 Å	51 - 67%

Protein model building at medium-to-low resolution in the best case generates incomplete and fragmented macromolecular models!

Methods to improve model building at lower resolution

There's a big effort now to improve automated model building at medium-to-low resolution:

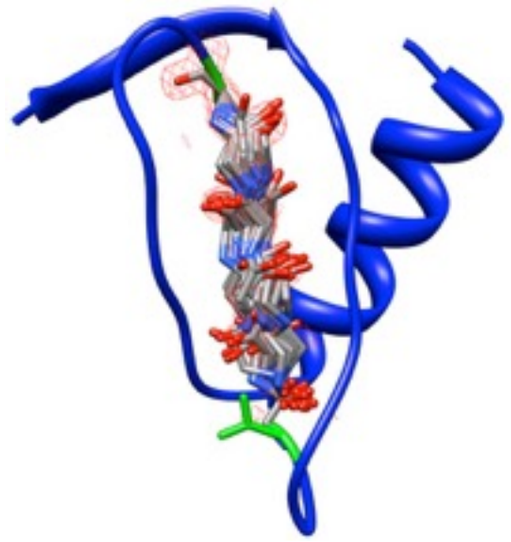
NCS detection and extension



- Detection of NCS related fragments and extension by "copy-paste"
- Improvements at 2.0-3.5 Å
- PNSextender
- +7% model completeness

Wiegels, T., & Lamzin, V. (2012)
Acta Crystallographica D

Sequence-independent loop fitting



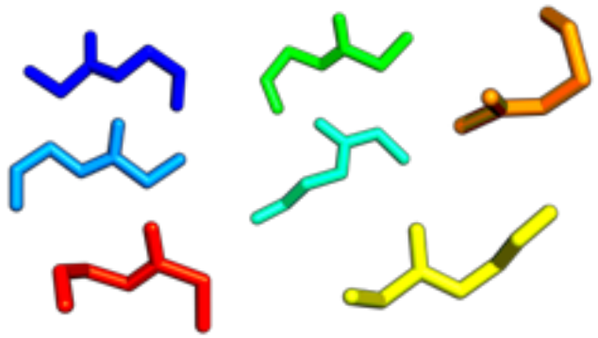
- Secondary structure prediction docking to find fragments that can be connected
- Search for links based on the gap size probability and a database of fragments
- Improvements at 3.0-3.8 Å
- +4% model completeness

Wiegels, T., Schwede, T., & Lamzin, V.
in preparation

Implemented already since version 7.4!

ValiFrag

- New conformational descriptors are being developed to evaluate main chain conformation during main chain tracing
- Expected improvements on built model quality and better fragment extension



Pereira, J., & Lamzin, V.
in preparation

Expected for version 8.0

NCS Detection and Extension

Non-Crystallographic Symmetry occurs if there are multiple subunits in the asymmetric unit of a crystal and some of them adopt almost the same tertiary structure:

We can use this information to extended fragmented models!

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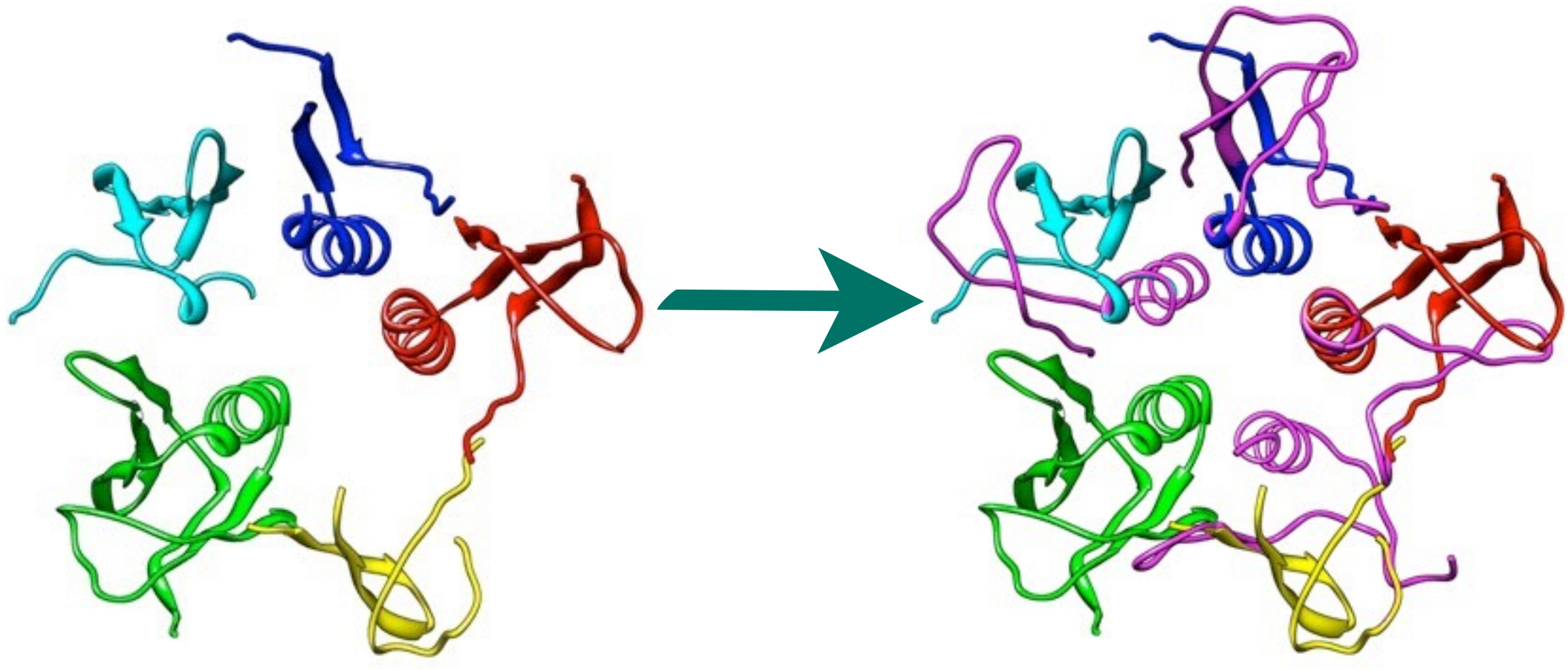

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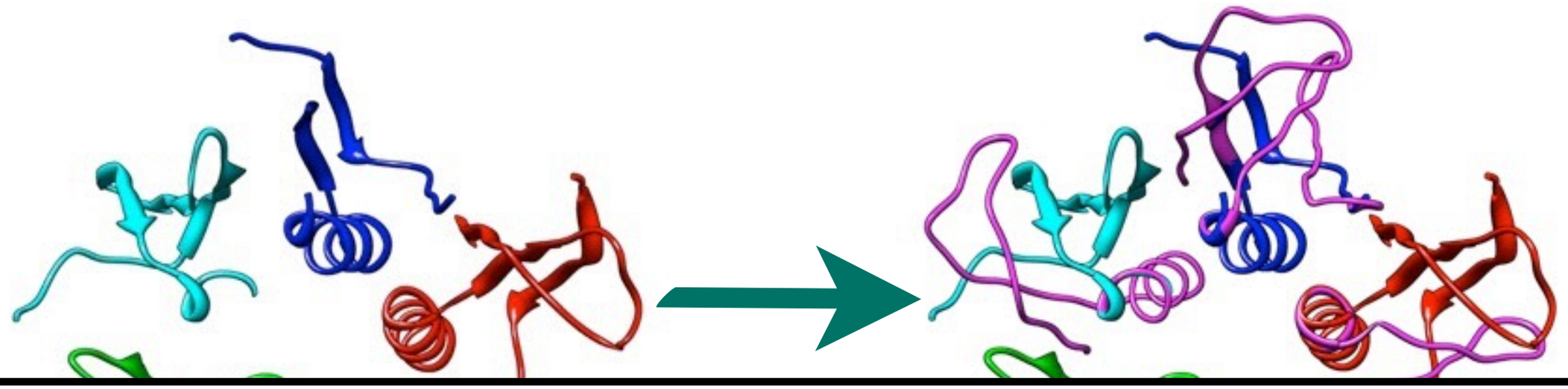

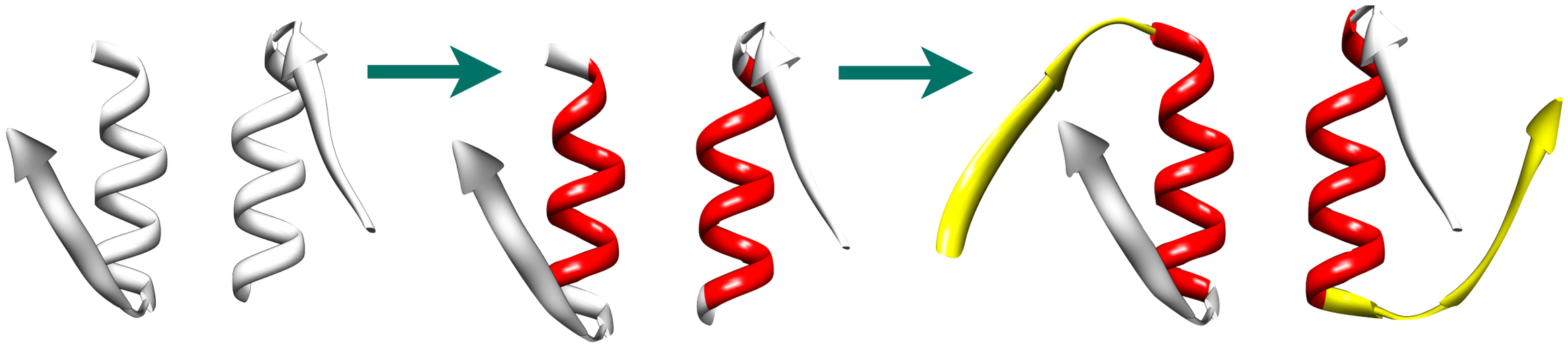

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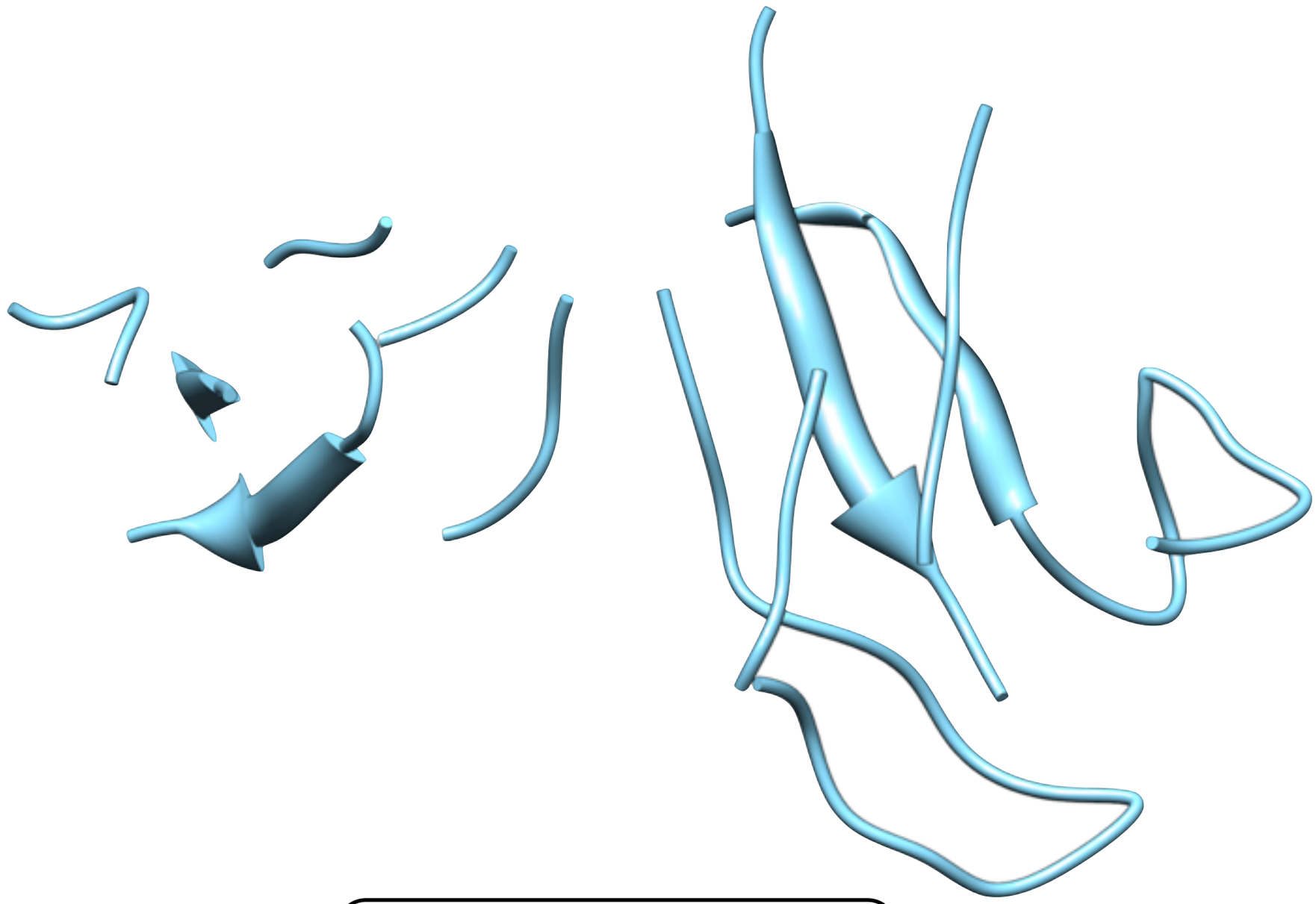


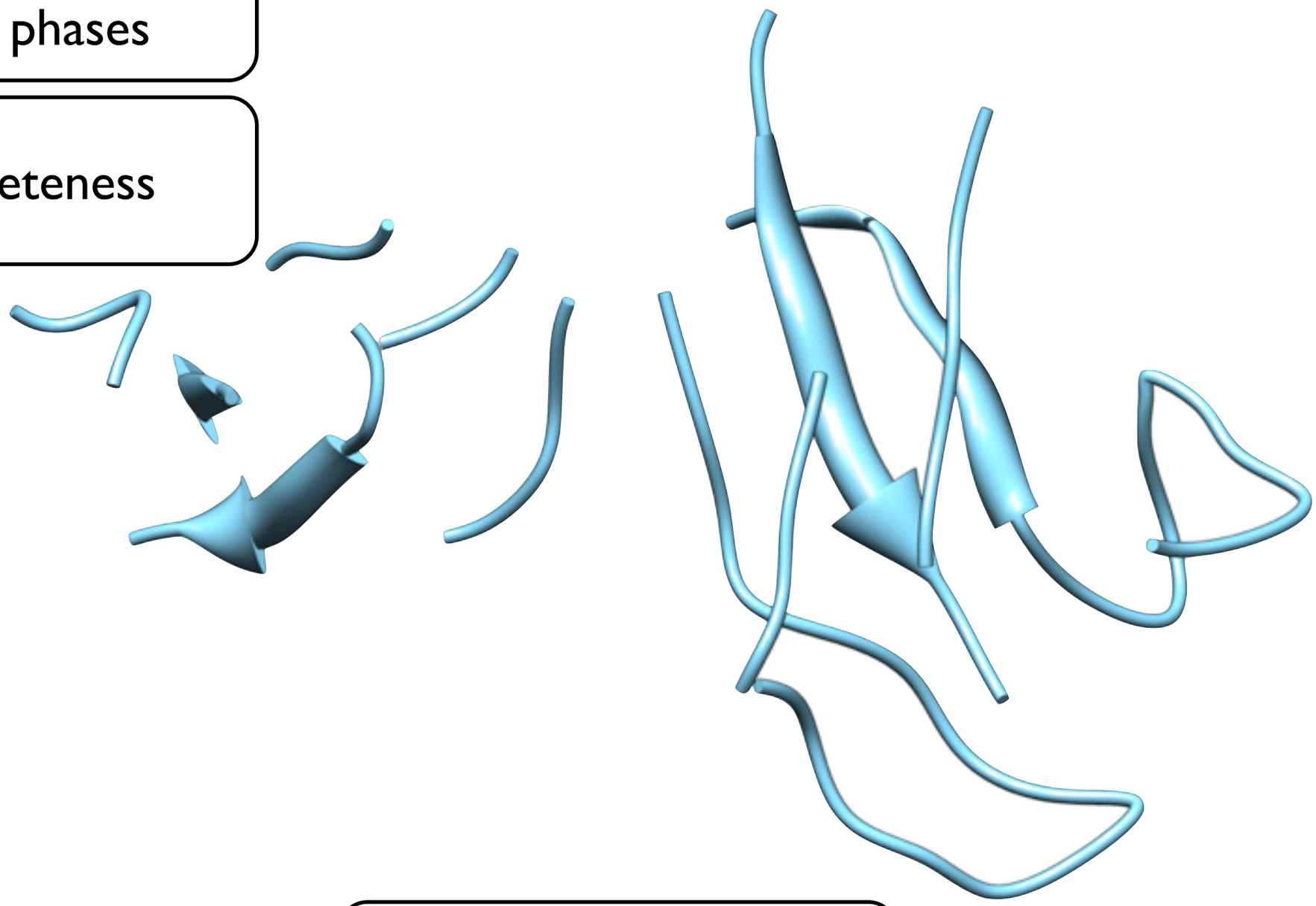
ARP/wARP

Data courtesy of Florian Sauer

NCS Detection and Extension

- 1.95 Å data
- poor initial phases

- 42% completeness



ARP/wARP

Data courtesy of Florian Sauer

NCS Detection and Extension

- 1.95 Å data
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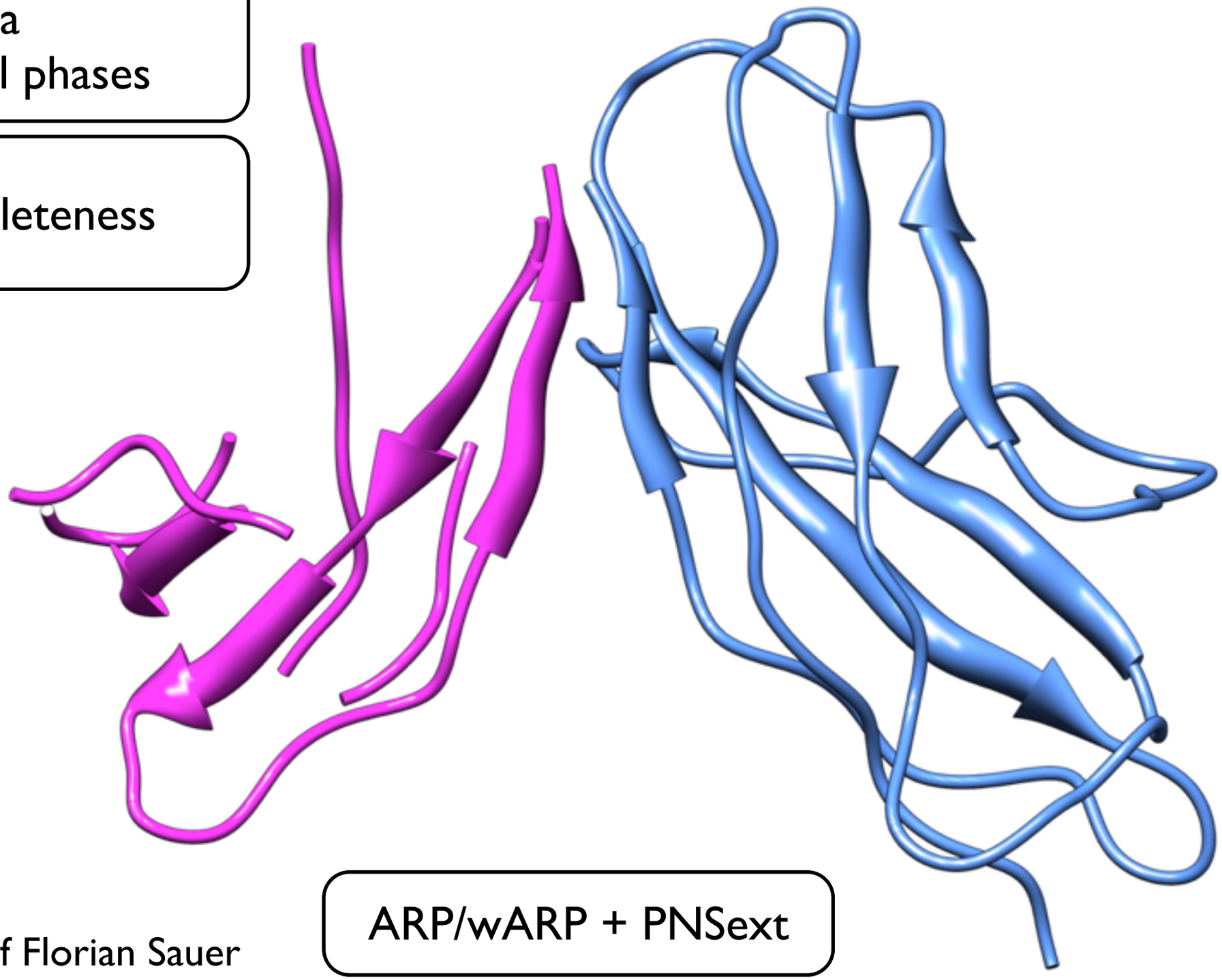
- 75% completeness



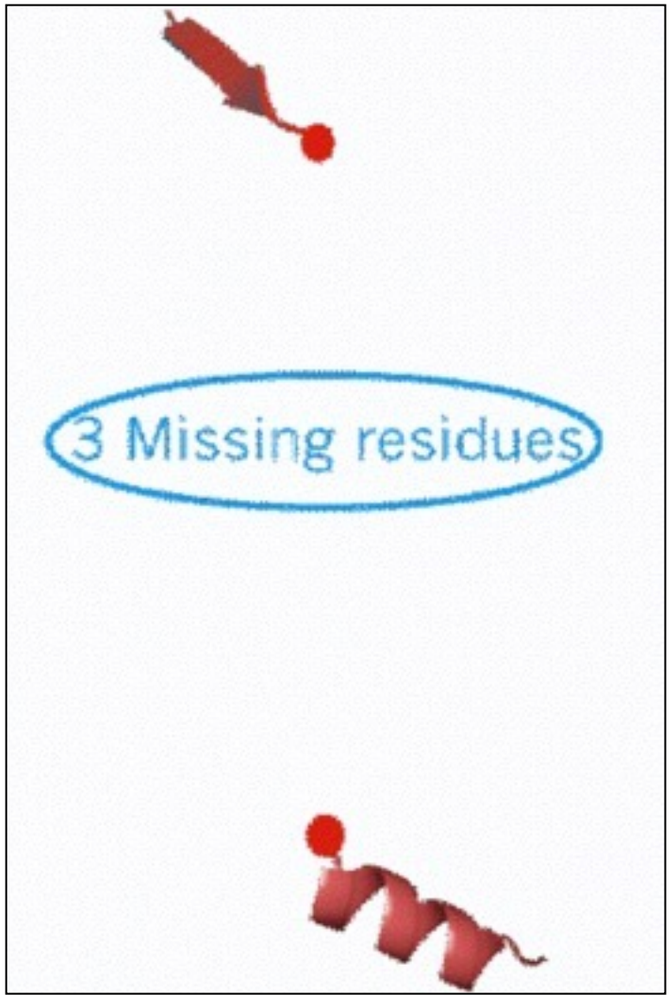
ARP/wARP + PNSext

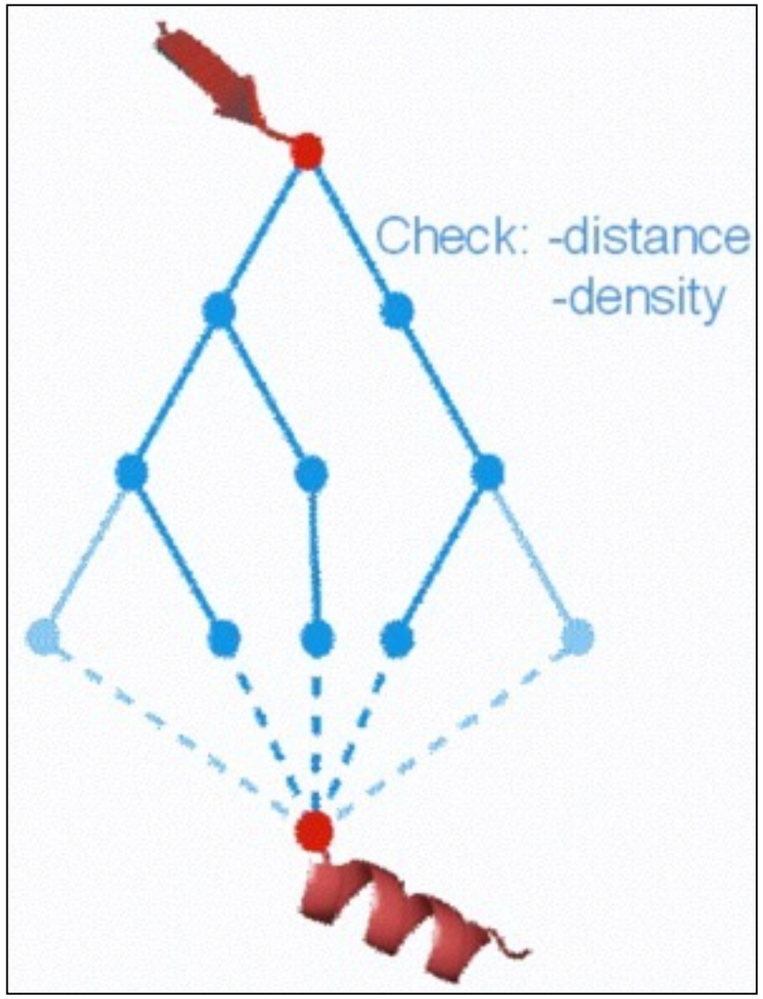
Data courtesy of Florian Sauer

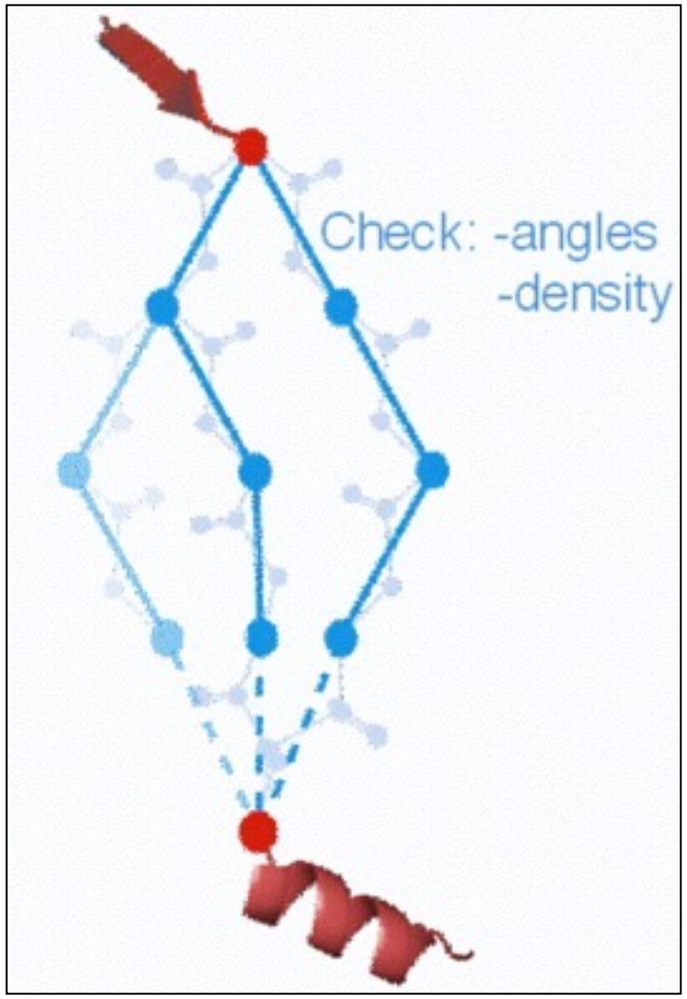
Modelling Loops With *a priori* Knowledge

Chain fragments are built and **docked to sequence**

- using **knowledge of angles** between anchors
- **check with density** to see if modeled loops are valid







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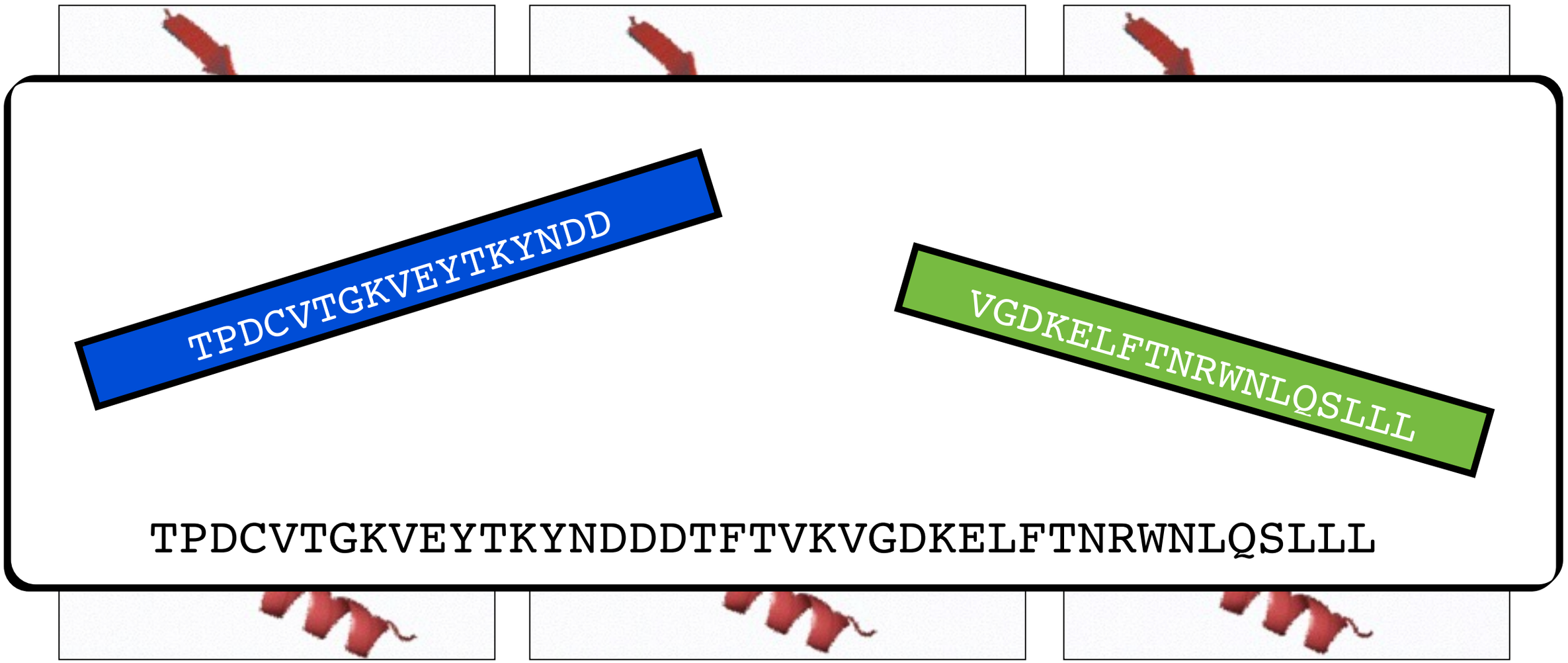

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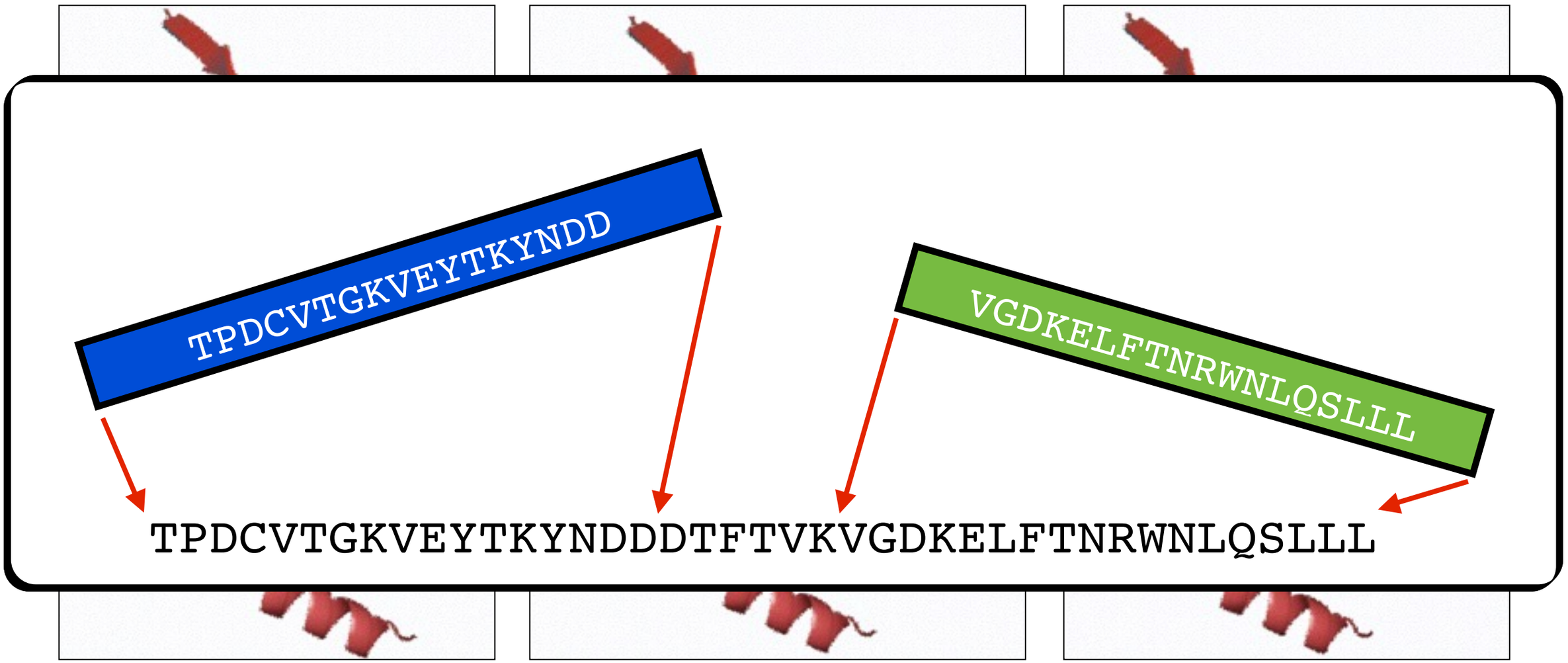

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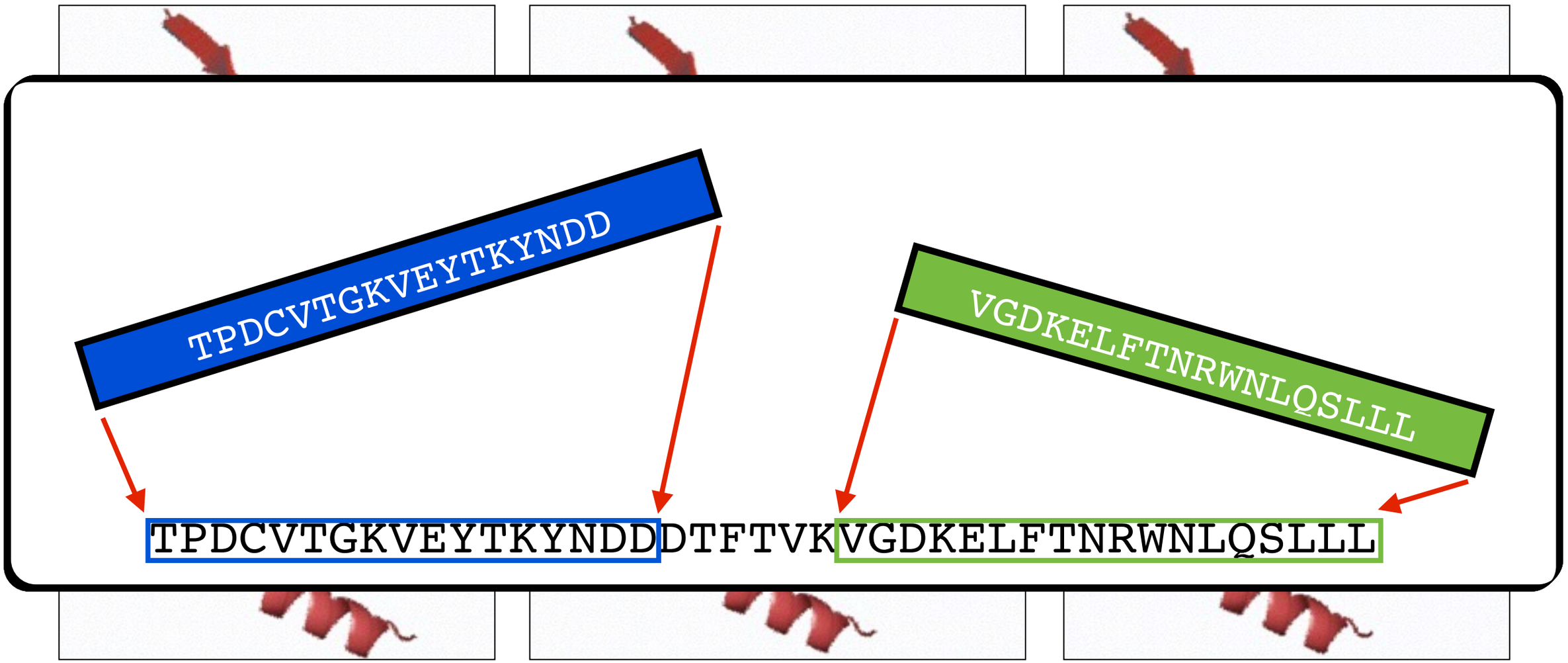

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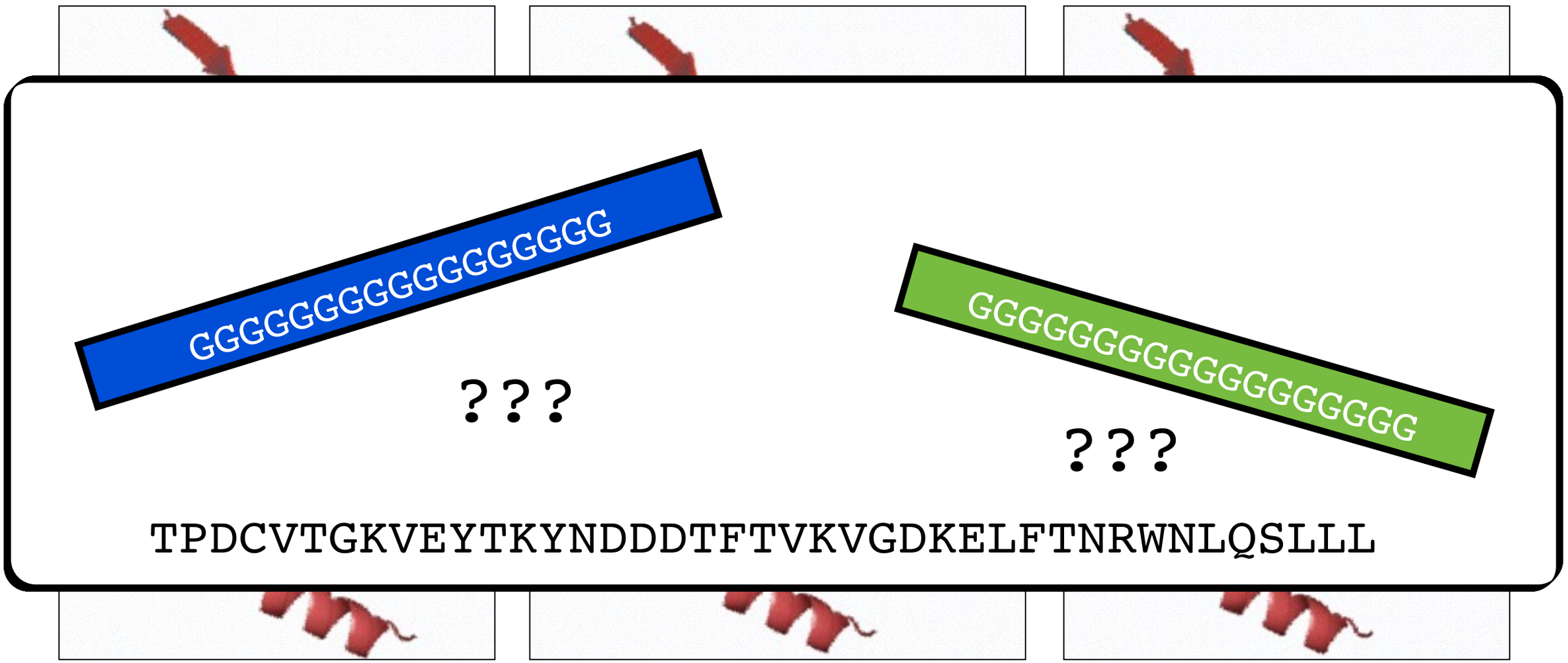

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When **no sequence** has been **docked** - **no loop building!**

- Search for **missing fragments** in a **structural database**

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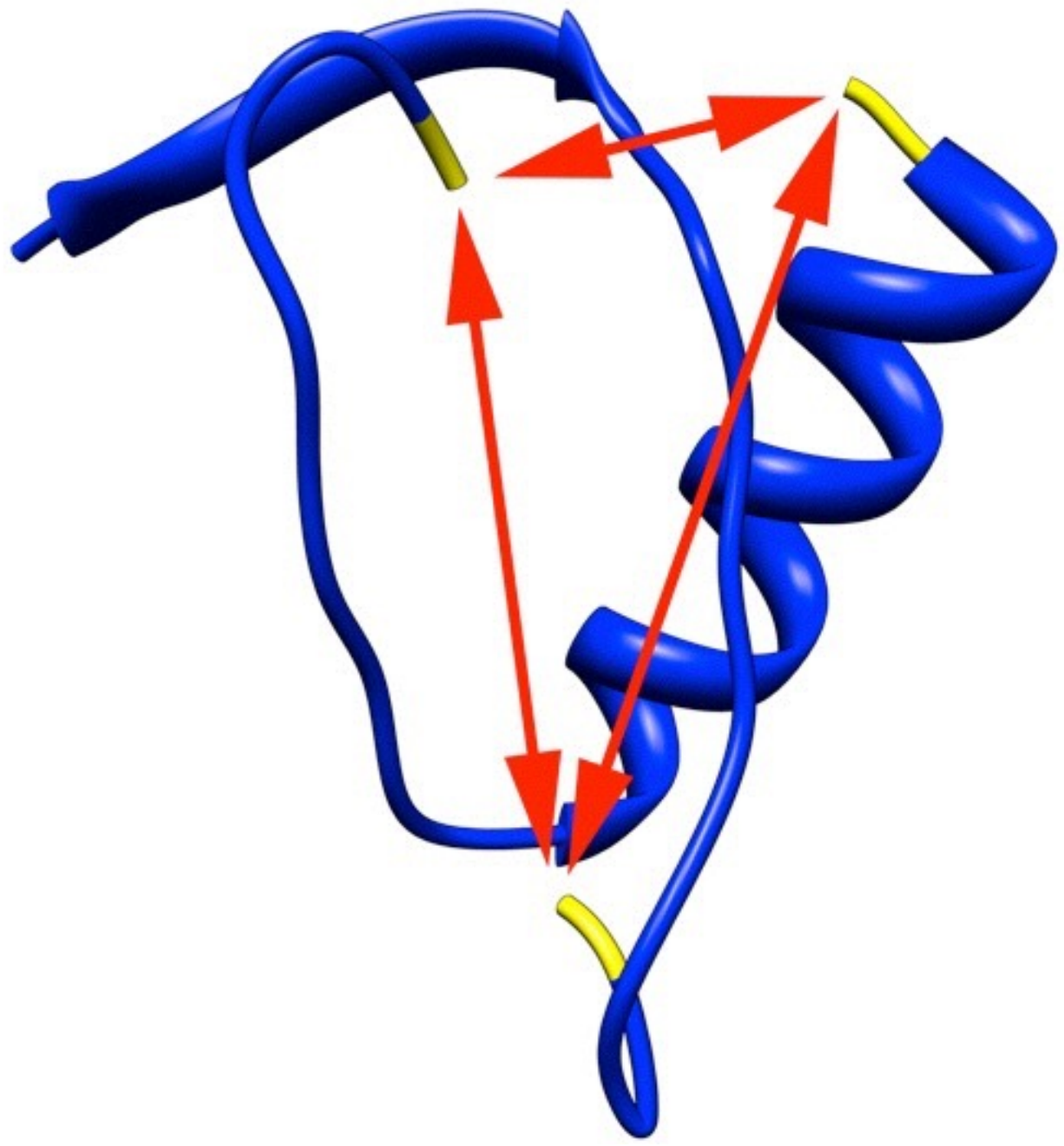

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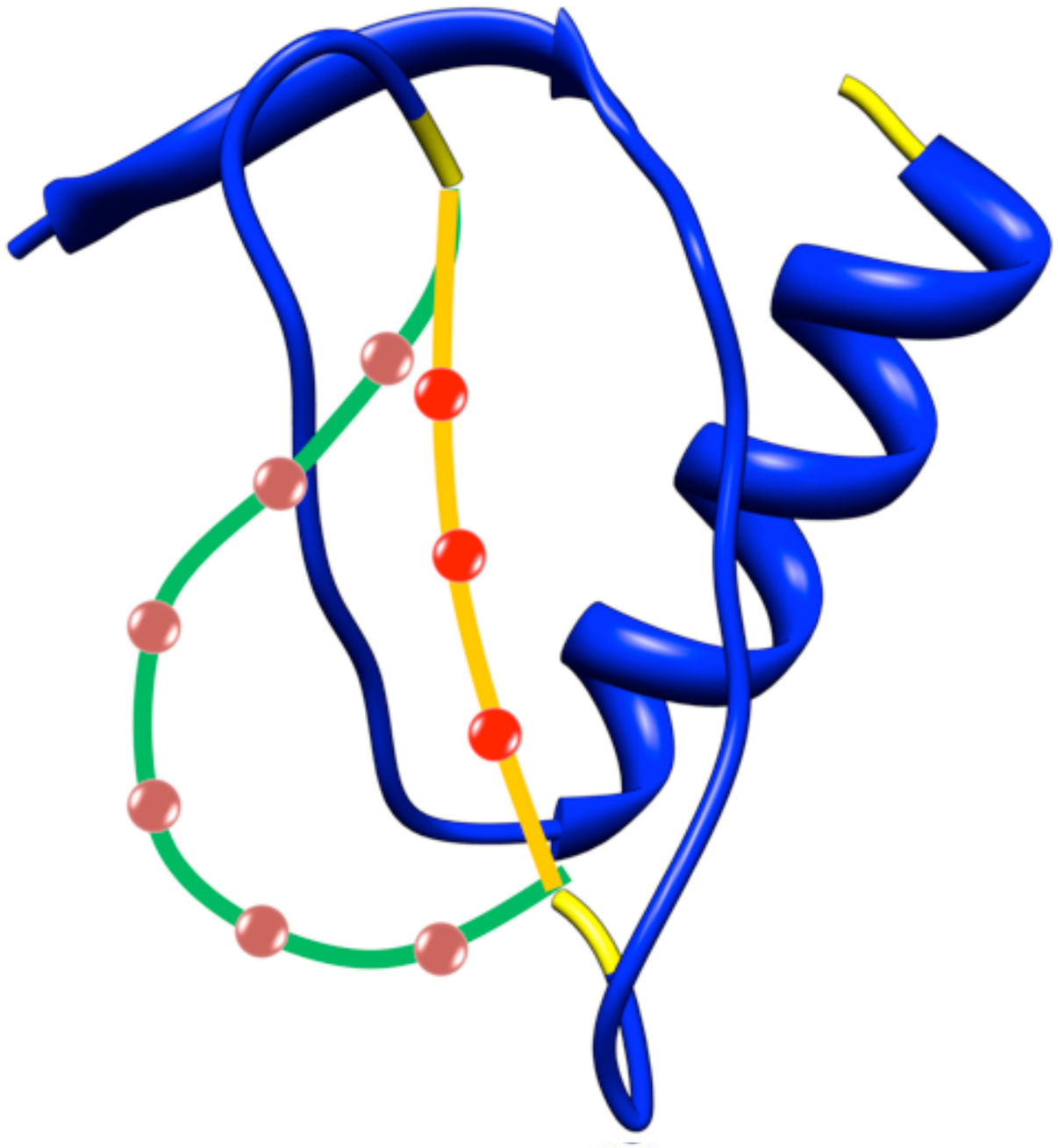

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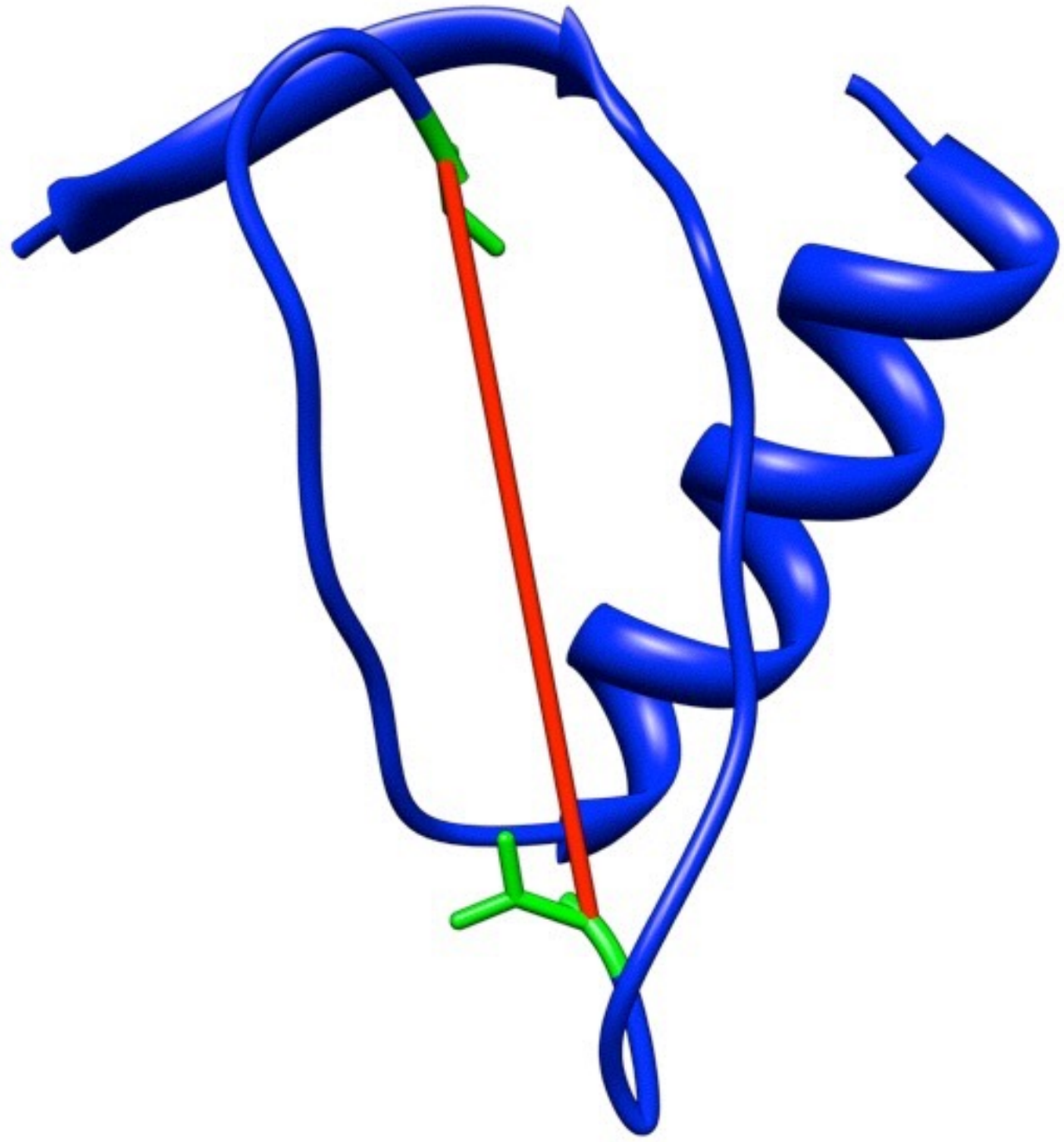

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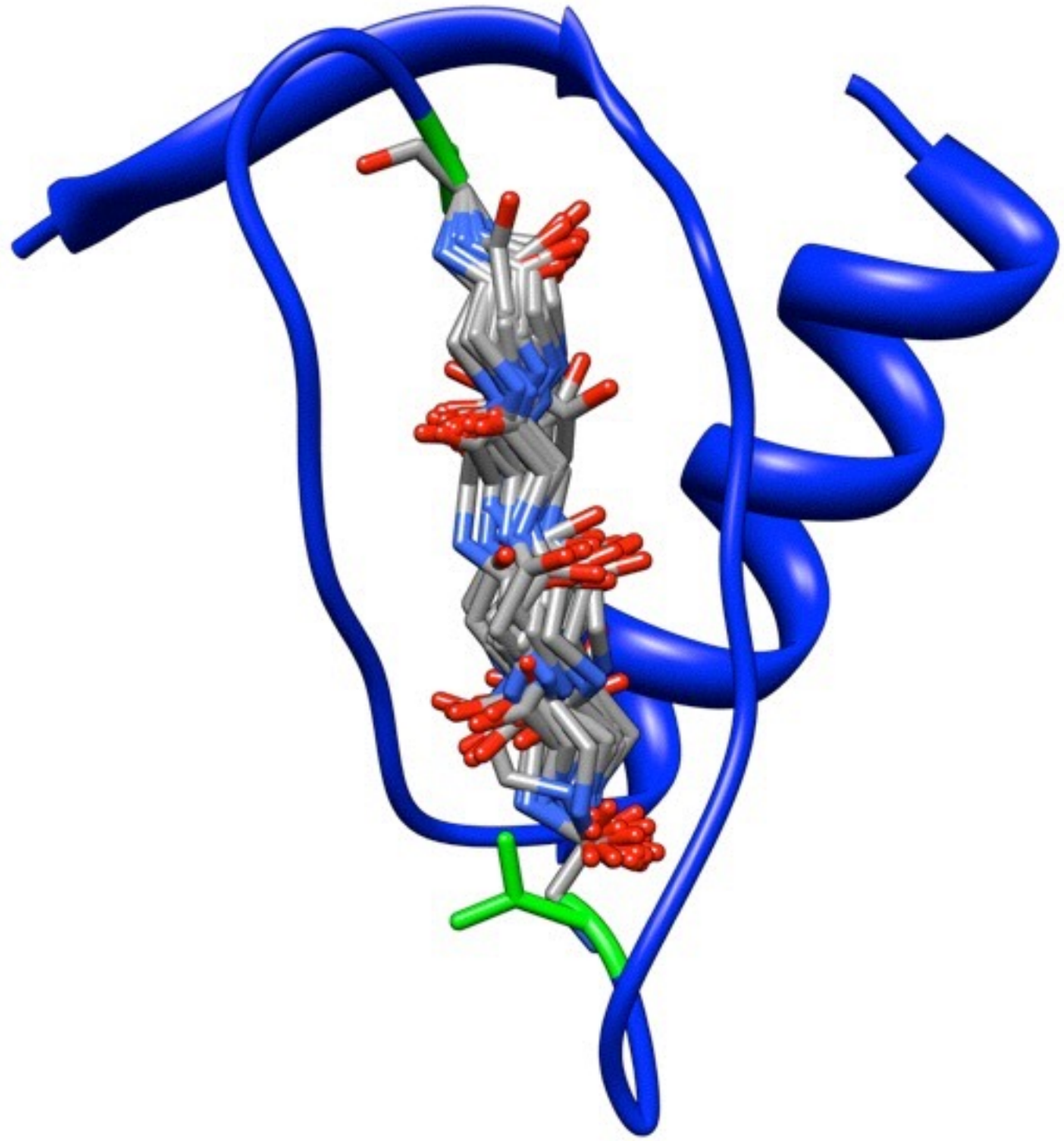

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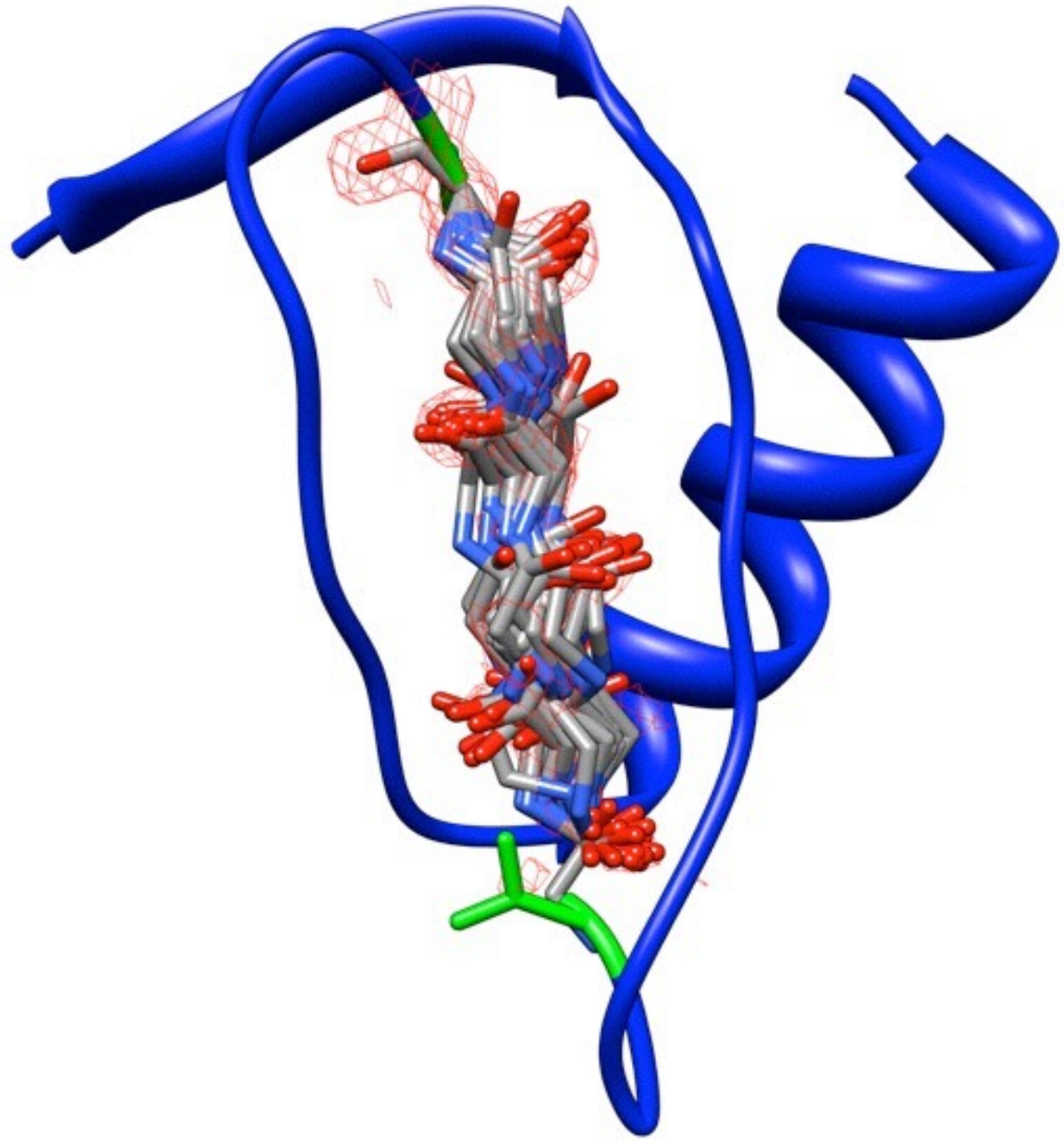

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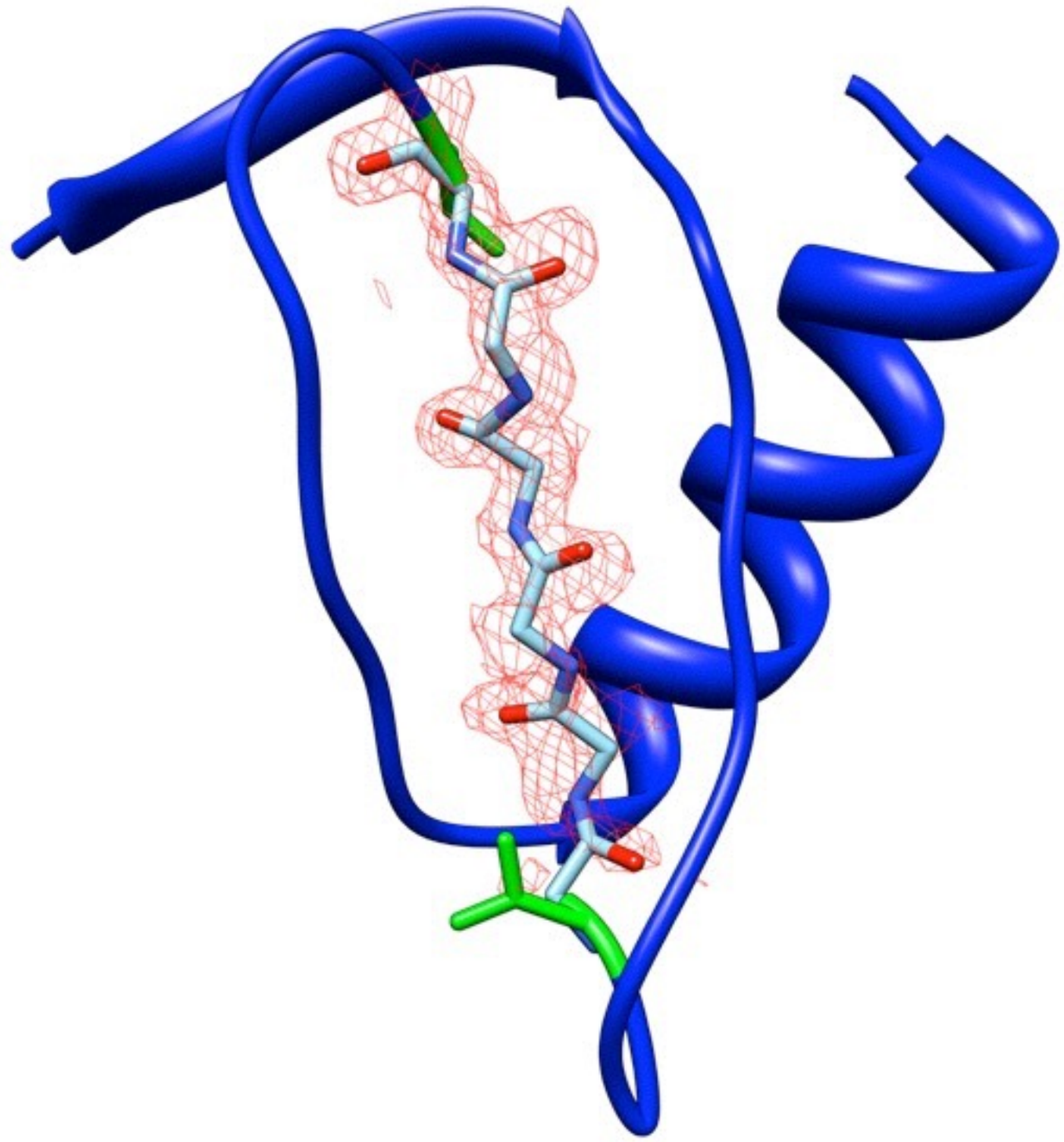

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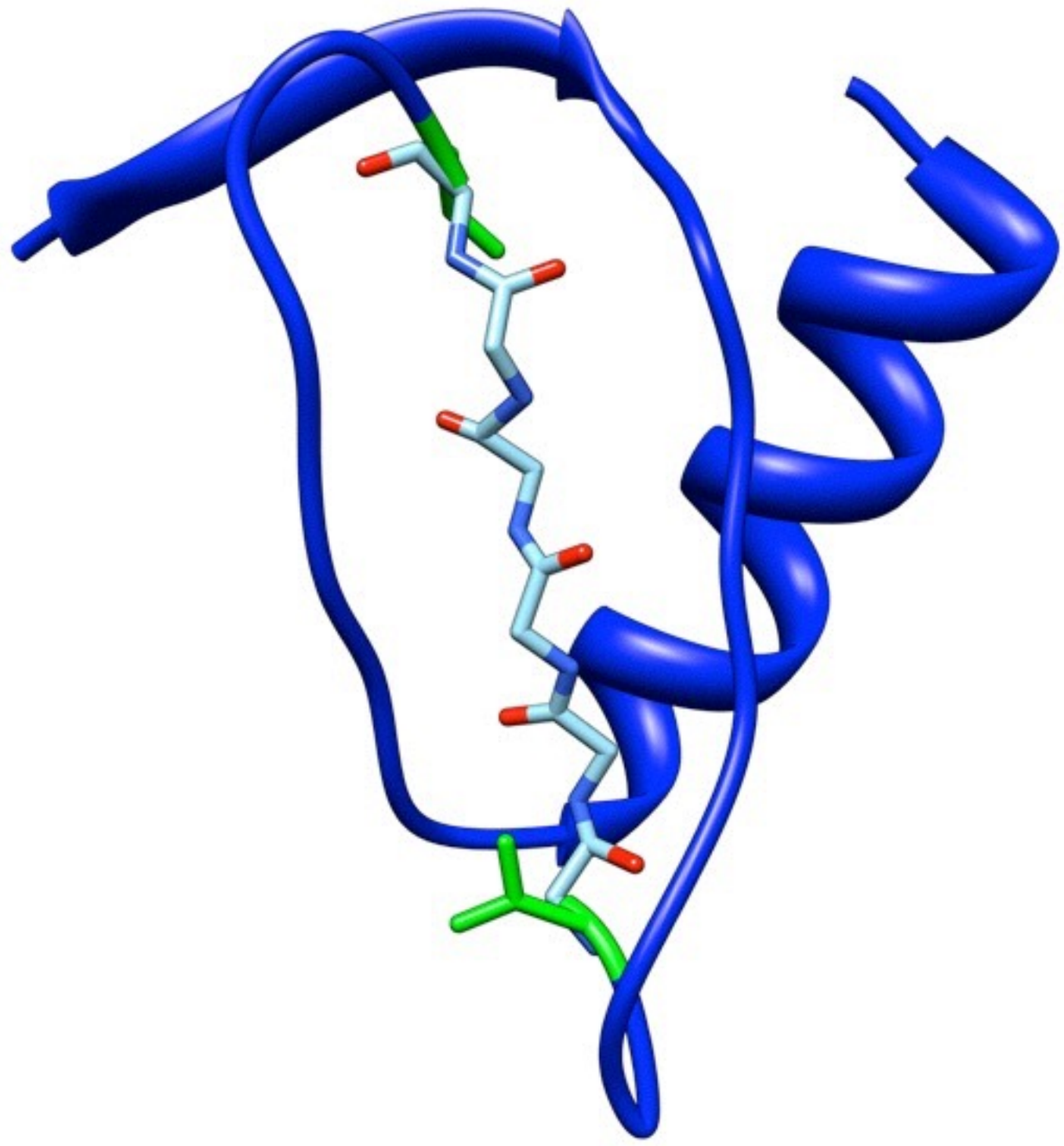

Modelling Loops With *a priori* Knowledge

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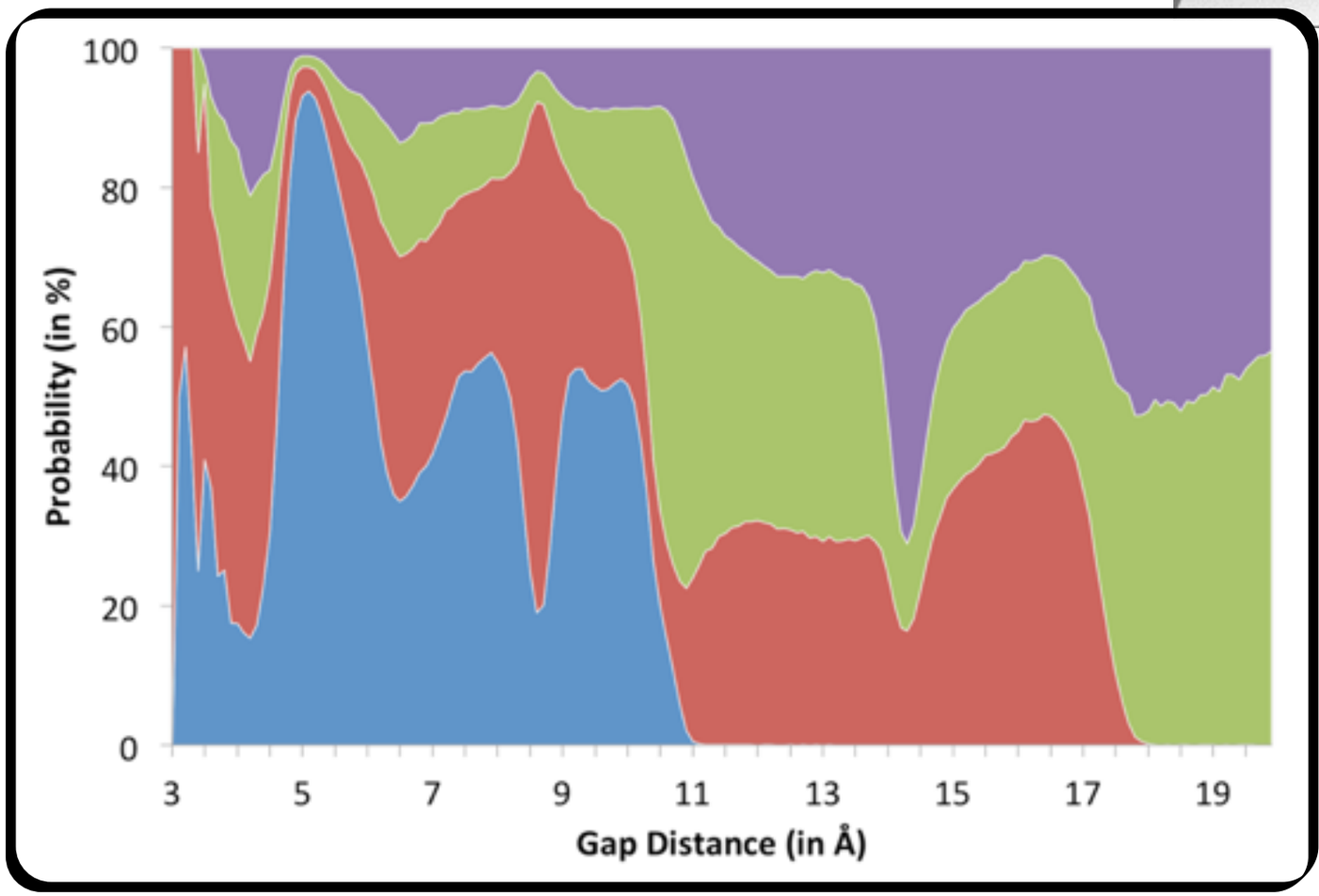
Docking results

Modelling Loops With *a priori* Knowledge

Docking results

Distance statistics



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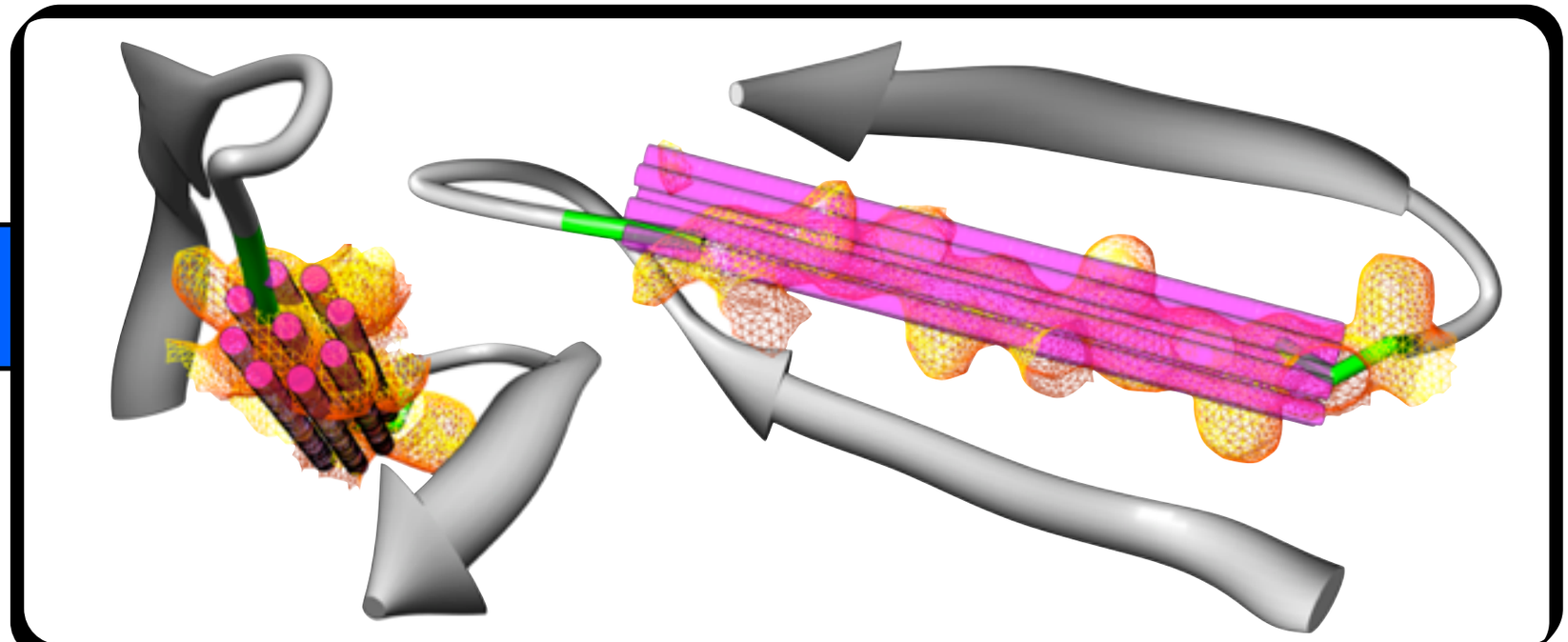

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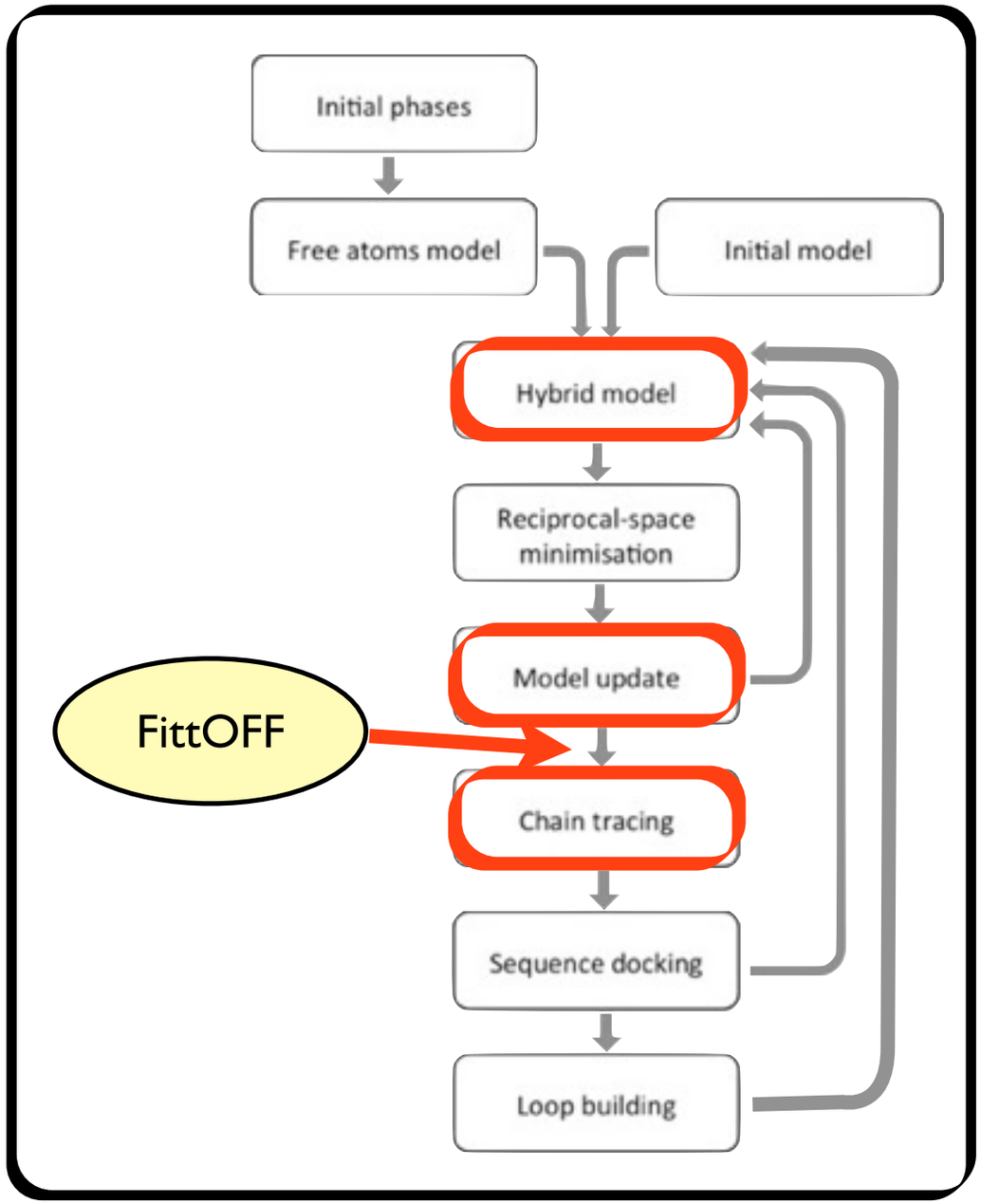

FRAGRA

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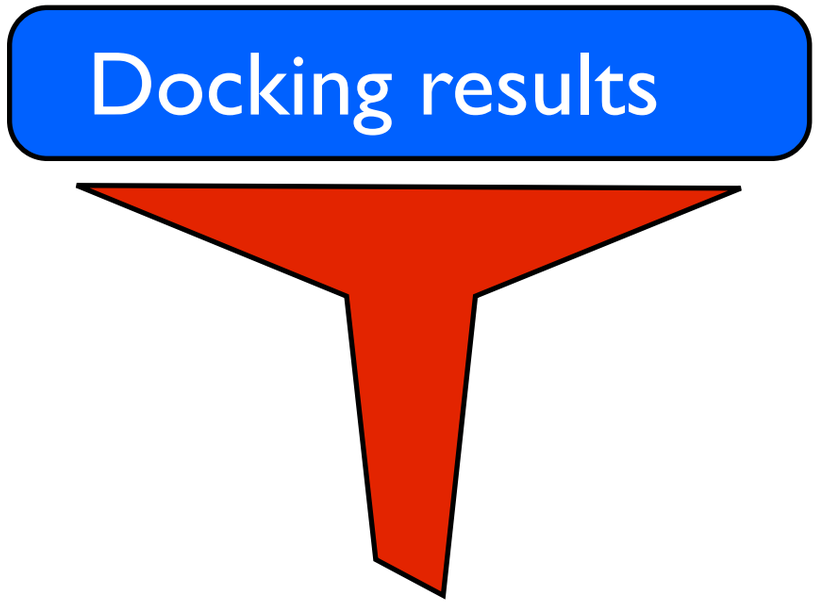
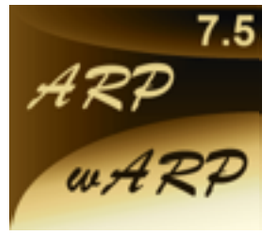


10 protein test structures with resolution 3.0 to 3.8 Å, up to 300 residues

	Model Completeness	Residues / Fragment	Sequence Coverage
Top Results	+ 12%	+ 98%	+ 59%
Average	+ 4%	+ 25%	+ 7%

Secondary structure modelling



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Good to evaluate map quality!

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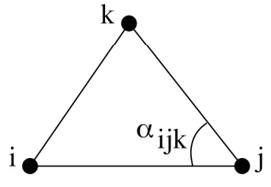
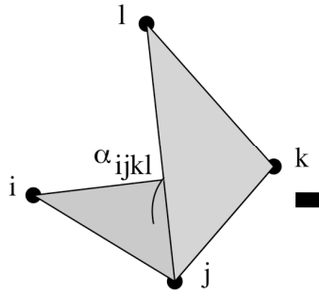
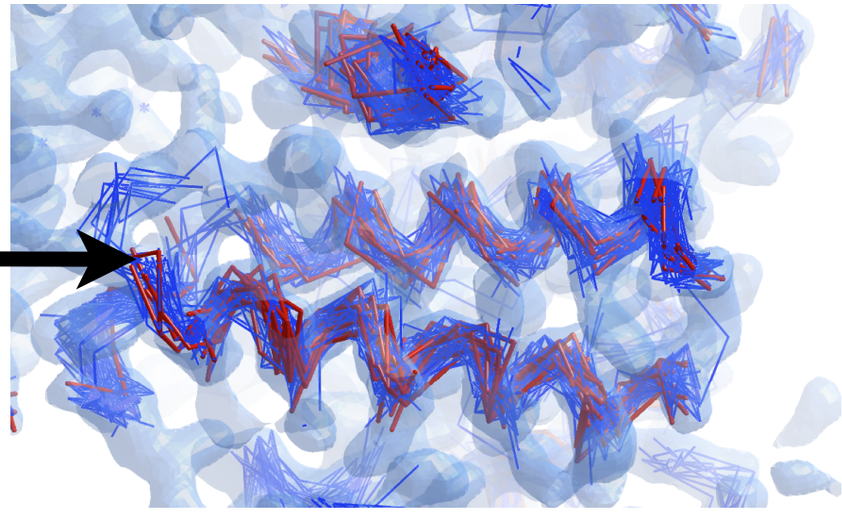
  (3 to 5 Cα candidates) are built.







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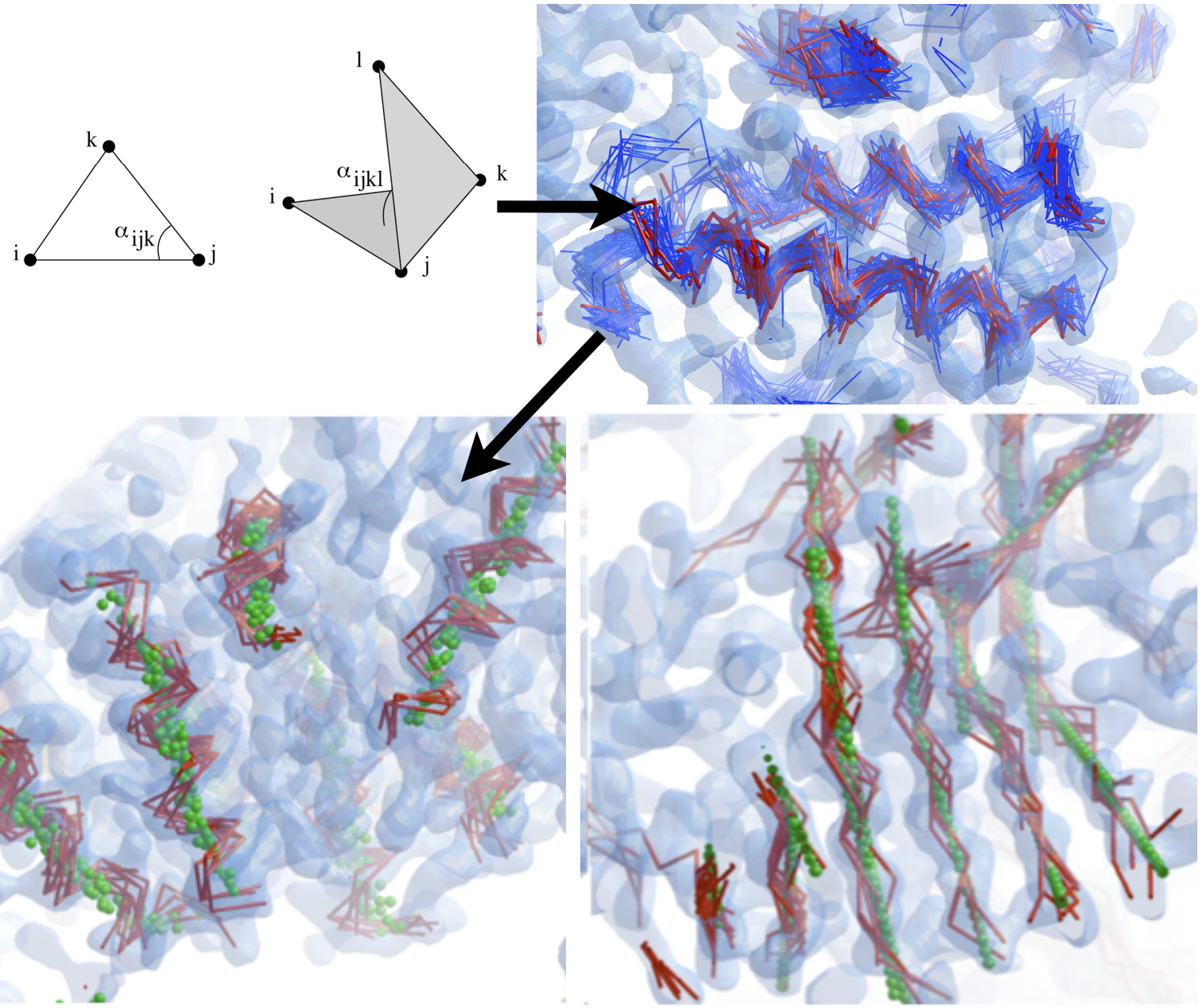
At low resolution, one can try to find **secondary structure elements** on the map:

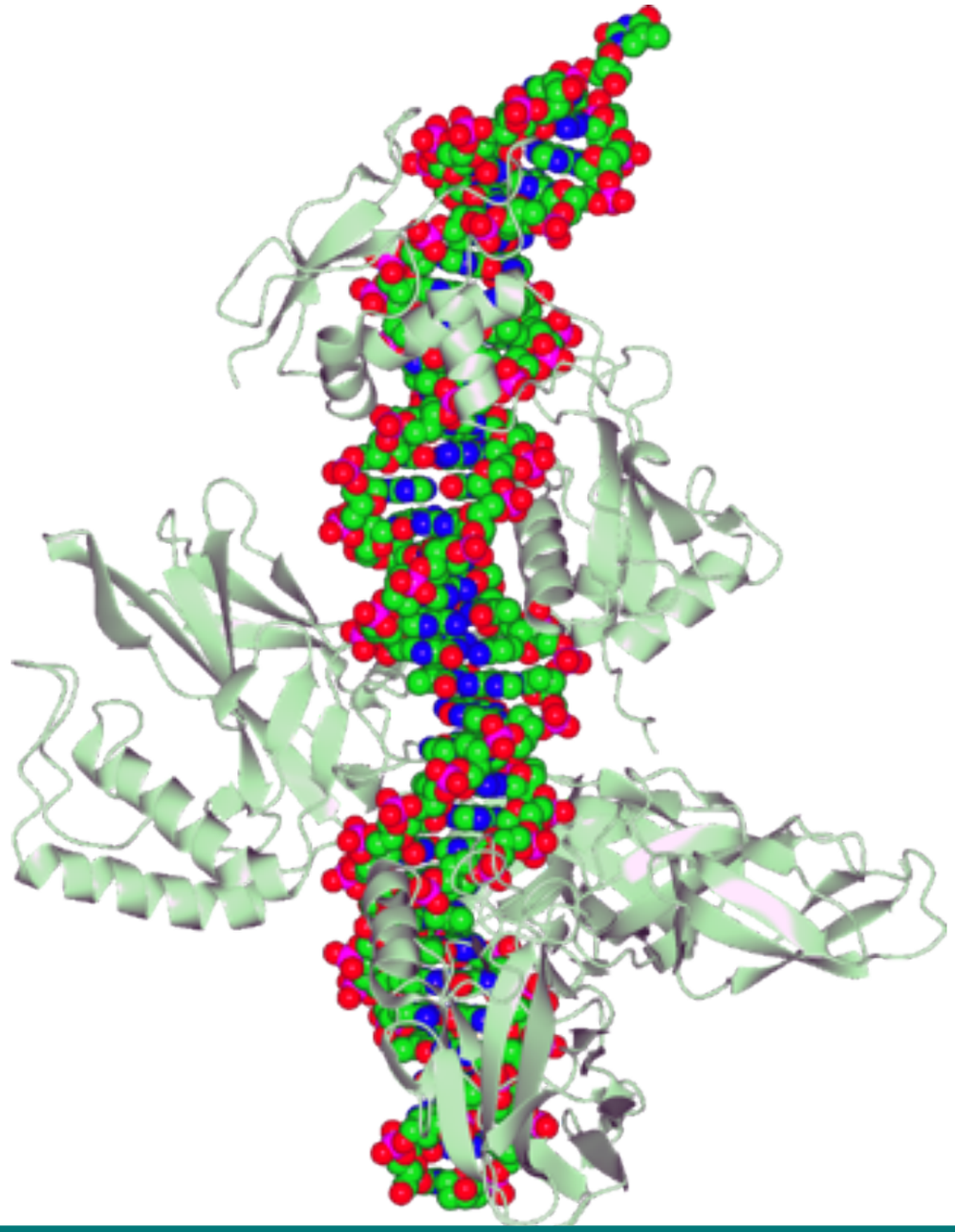
- **Short helix/strand fragments** (3 to 5 Cα candidates) are built.
- Longer traces are formed and the **best are kept** (in red)
- Traces are **clustered**
- Assemblies are **averaged**

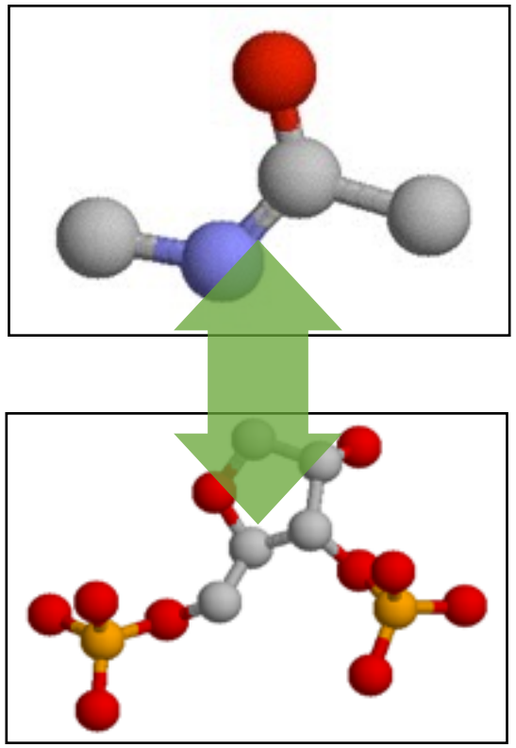
Good to evaluate map quality!

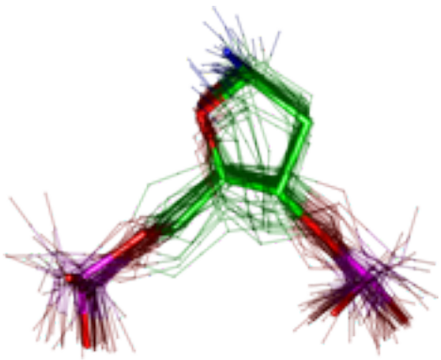


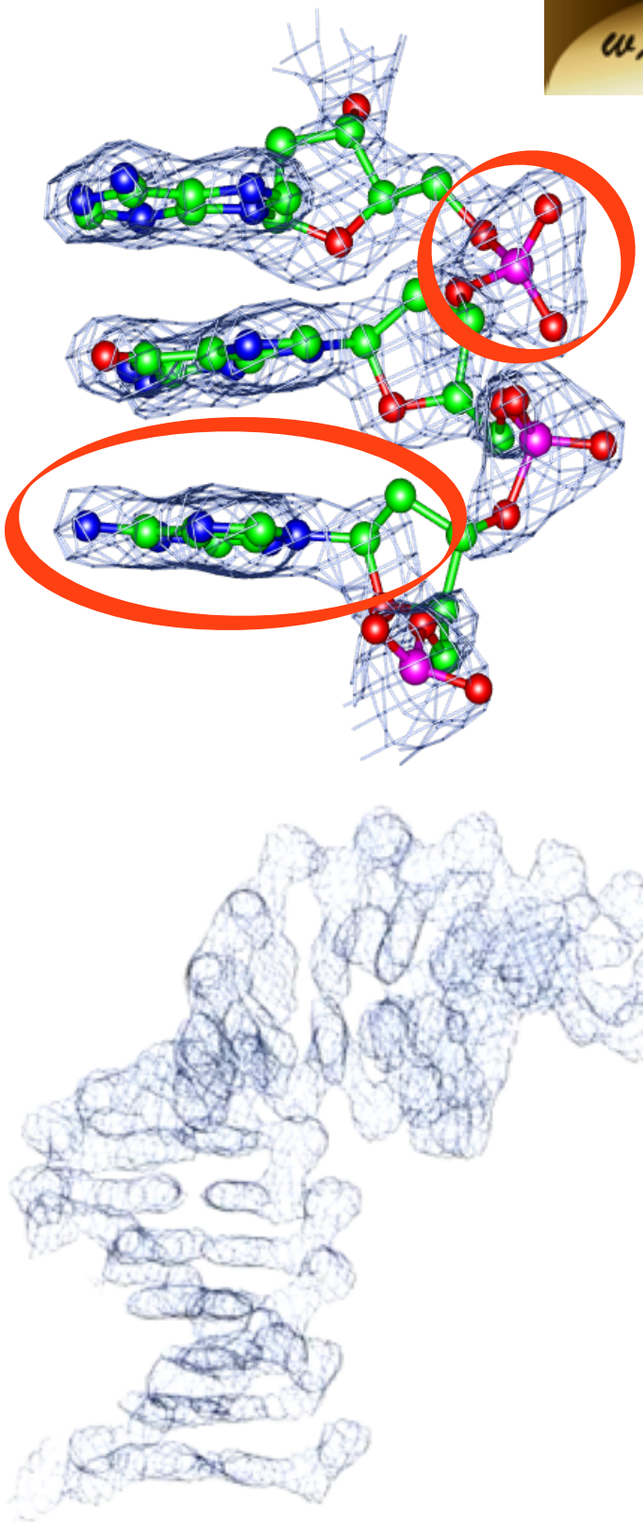
Tracing RNA/DNA Chains

ARP/wARP is just not about building protein models, it can also build **nucleic acids**:









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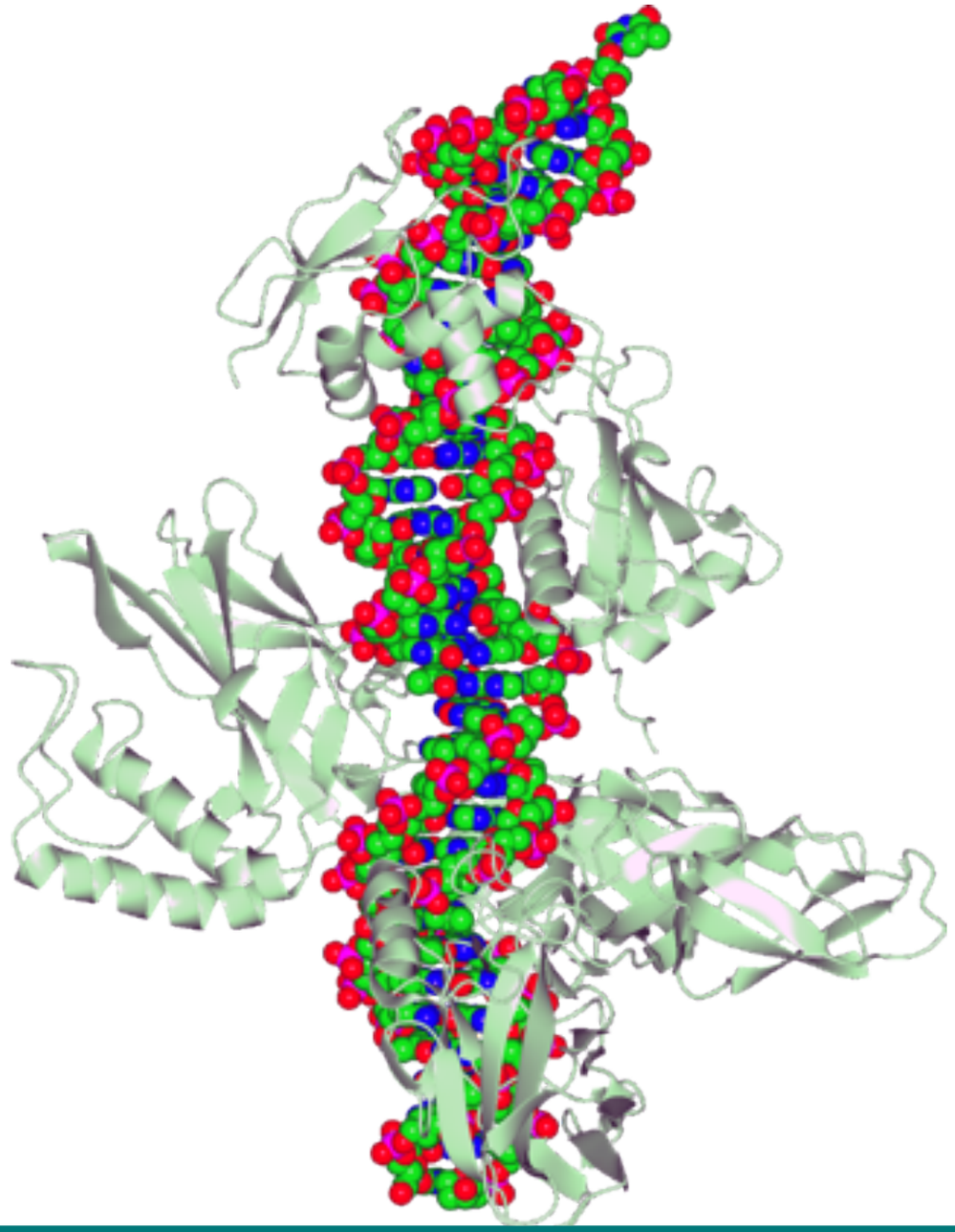
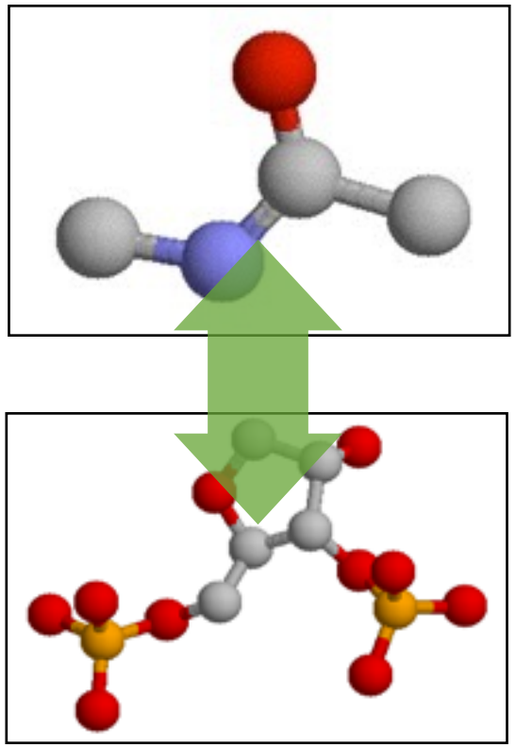
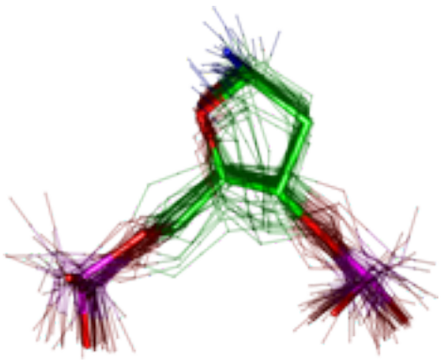
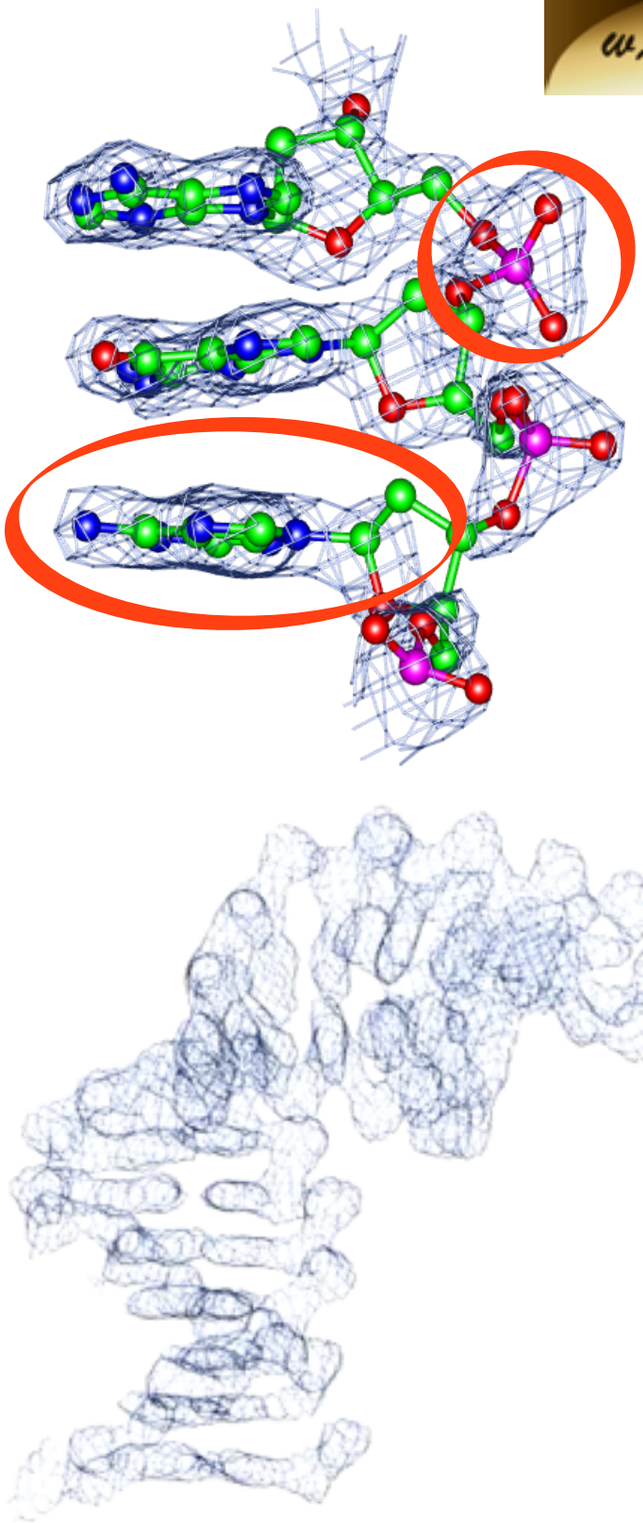




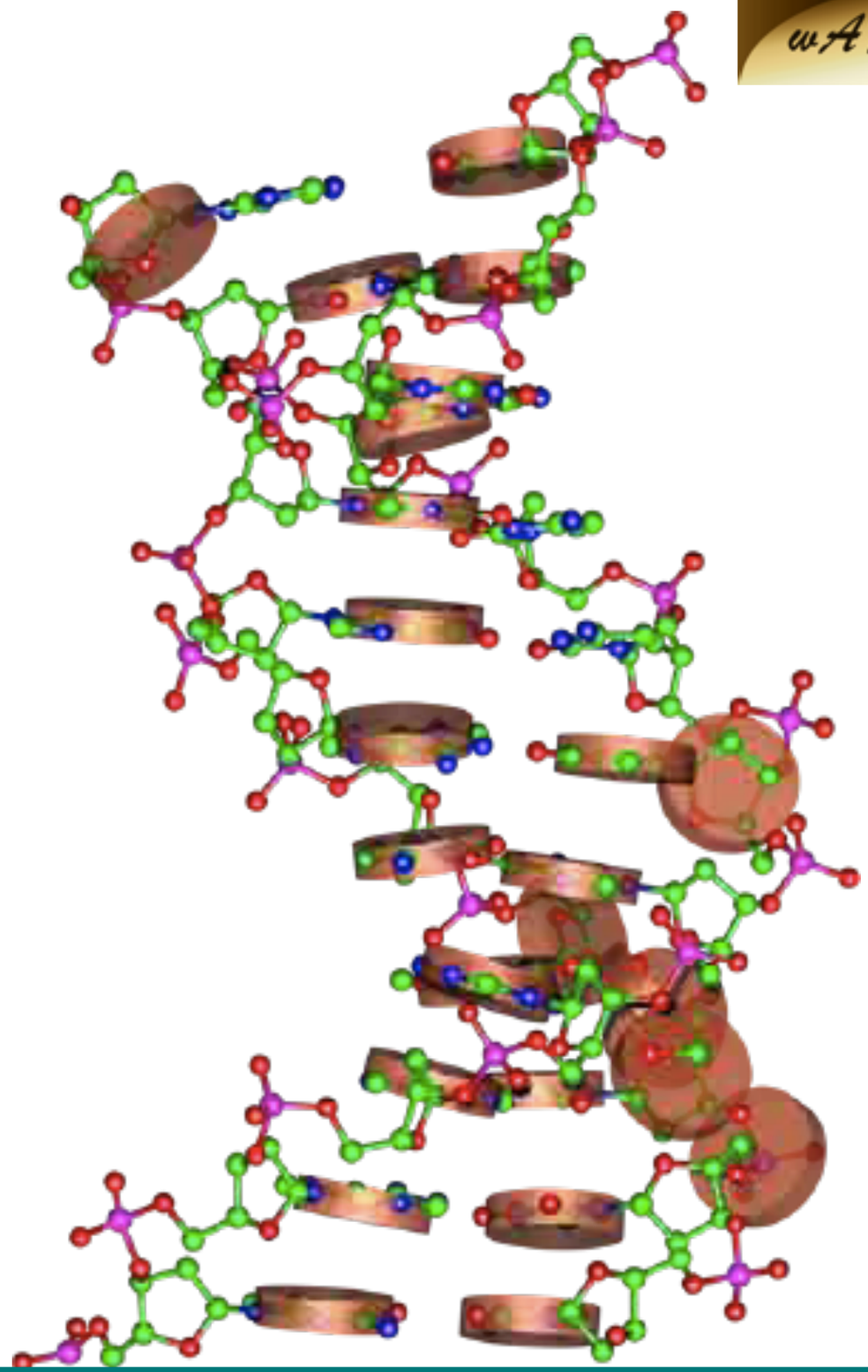




Tracing RNA/DNA Chains

- Detection of
  - **phosphate backbone** and
  - **nucleobase planes**
- using pattern recognition algorithms

1p7h (2.5 Å)	
Completeness	0,88
Noise level	0,69
Positional r.m.s.d.:	0.5 Å
Angular Difference	5°

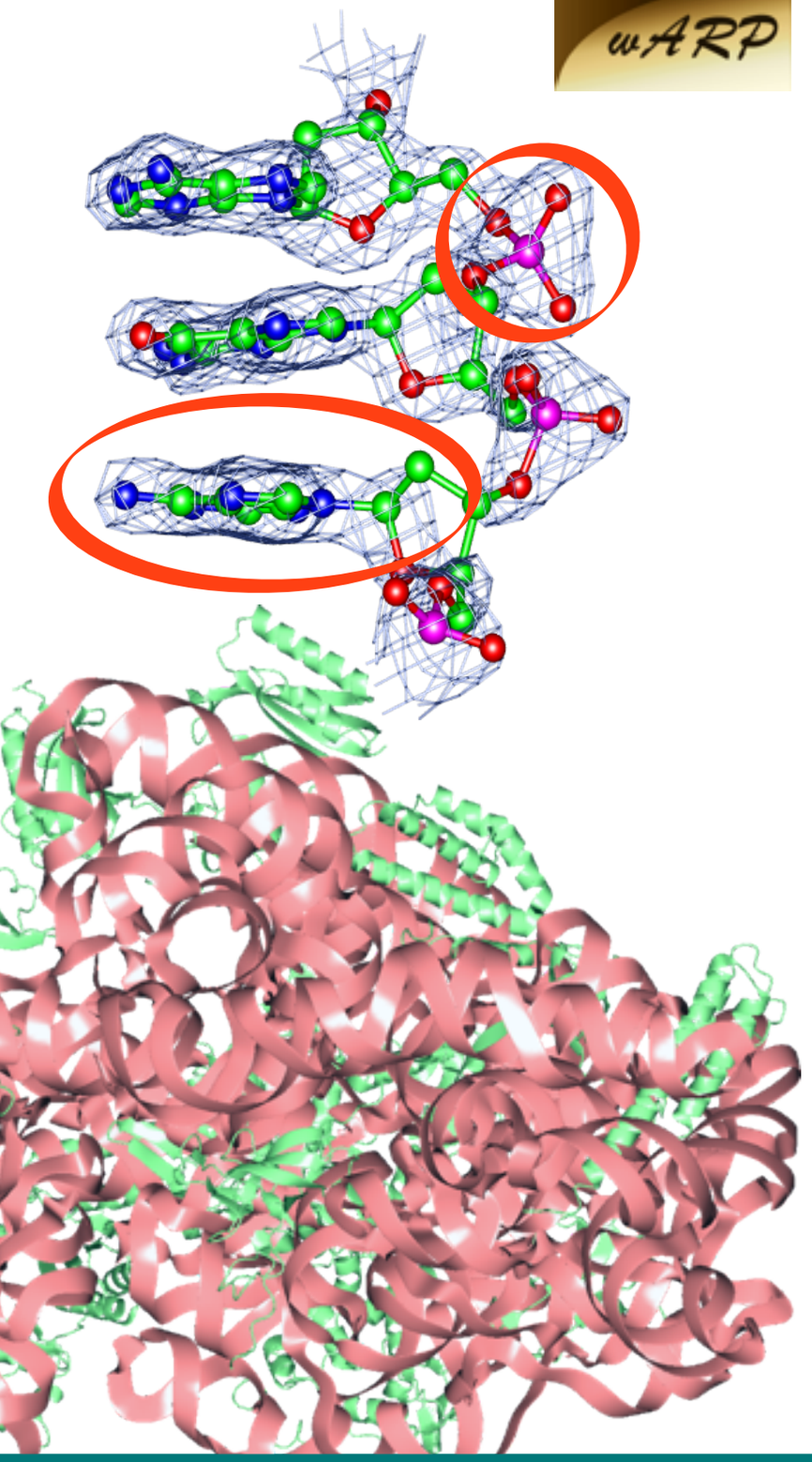


Tracing RNA/DNA Chains

- The **30S ribosomal subunit**
  - Resolution: 3.05 Å
  - Experimental phases (MCC 0.73)

- Automatic model building with ARP/wARP
  - modelled 1,302 out of 1,513 nucleotides **(86%)**
  - backbone r.m.s.d. to reference: **0.7 Å**
  - Located 1,121 nucleobases with **0.6 Å** accuracy in location and 12° in orientation

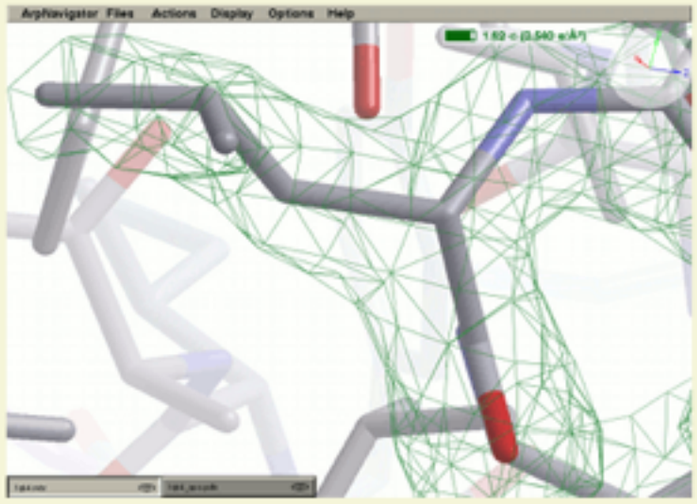
- Backbone fragmented in 75 chains
- Built in **around 6h**
- (*cf.* several **months** of manual work)



Where can I find it?

http://www.embl-hamburg.de/ARP/

ARP/wARP Copyright 2013
by European Molecular Biology Laboratory



Click on the images above to zoom.

ARP/wARP: Crystallographic Macromolecular Model Building Version 7.4

Builds proteins, RNA/DNA, secondary structure, side chains, loops, solvent and ligands.

Download available for Mac and Linux.

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Model building also available over the web.

Web Service

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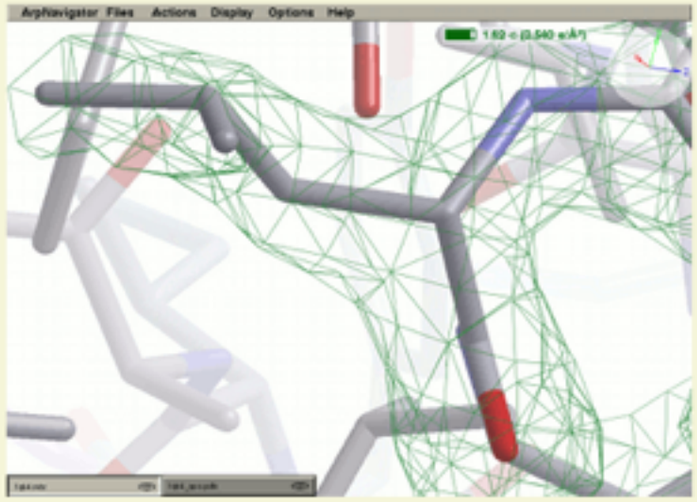

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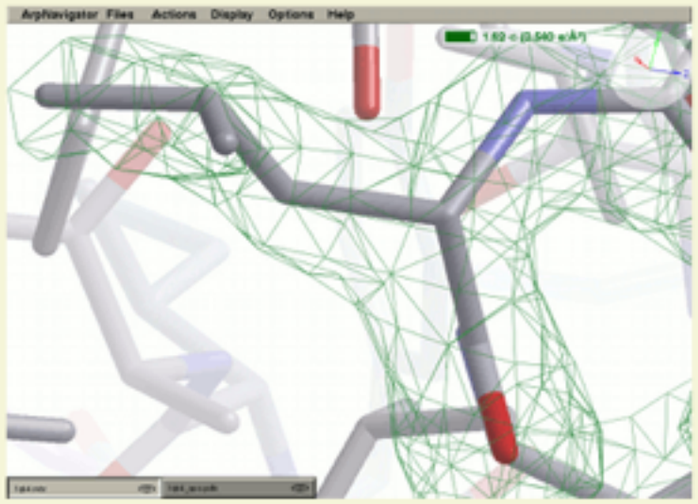

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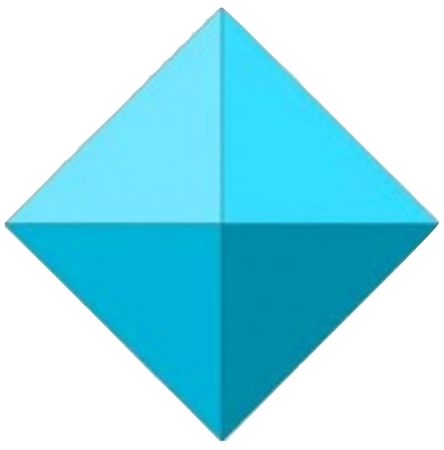
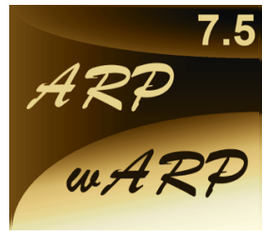
Only for Mac or Linux!!

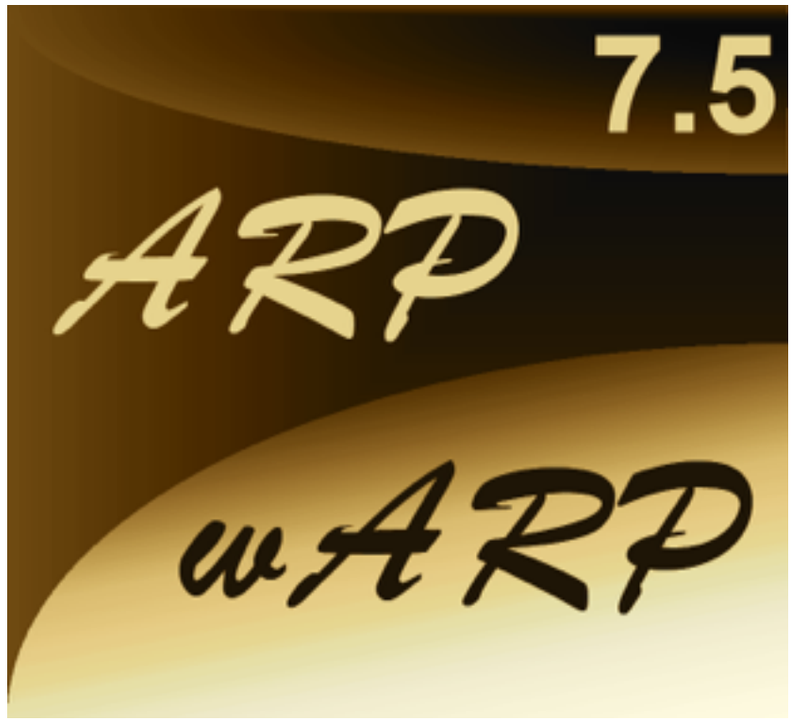
Good for Windows users!!

Collaboration with CCP4

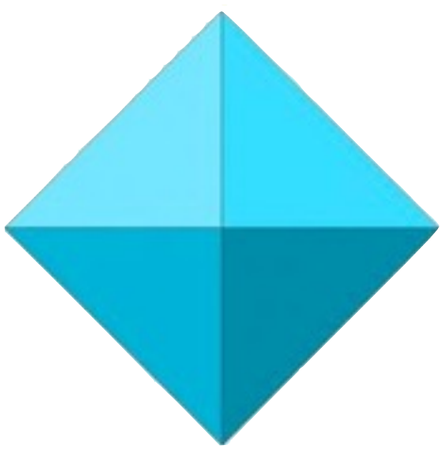


CCP4





Collaboration with CCP4



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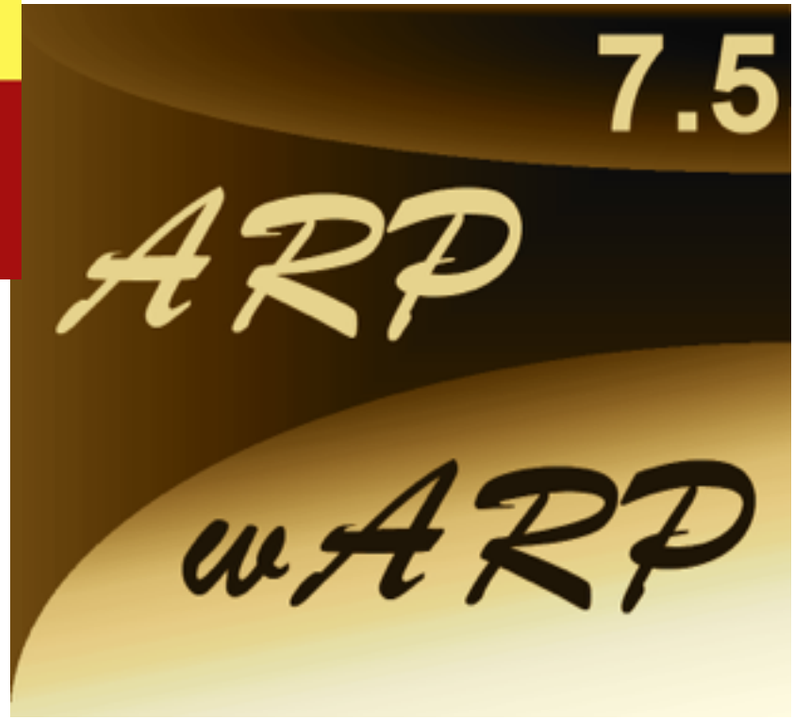

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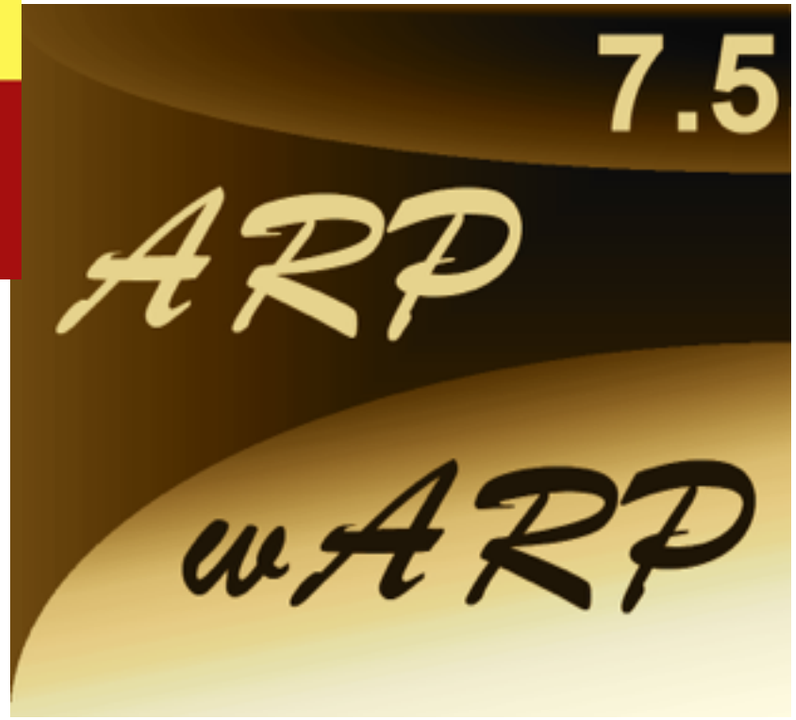
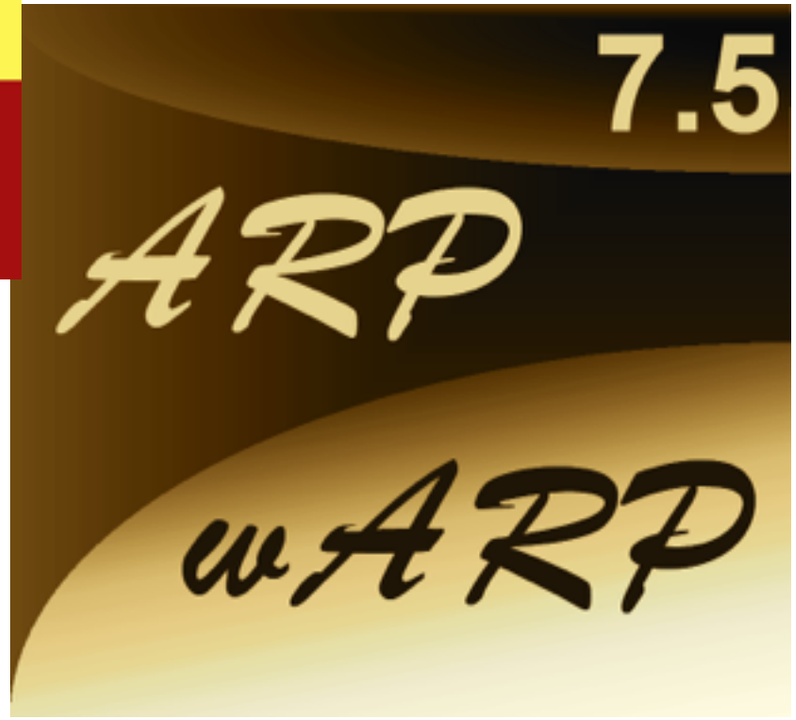


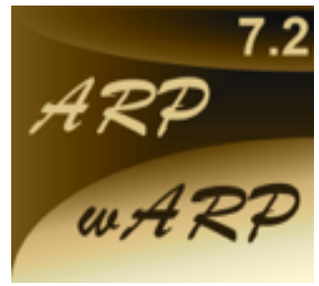
- Joint release
  - CCP4 6.5 and ARP/wARP 7.5

Collaboration with CCP4



- Joint release
  - CCP4 6.5 and ARP/wARP 7.5
  - one installer, no worries!

What can I find in ARP/wARP right now?



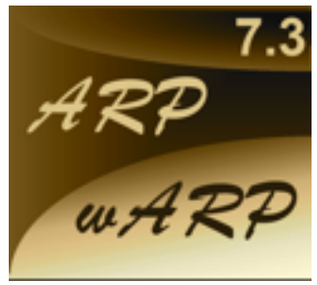
Changes in Version 7.5

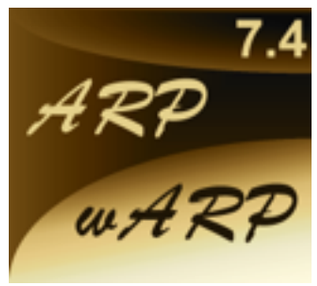
- Increased performance of protein model building through:
  - improved polypeptide recognition,
  - NCS-restraints,
  - atom update,
  - SAD-refinement option,
  - estimation of solvent content
  - and model accuracy

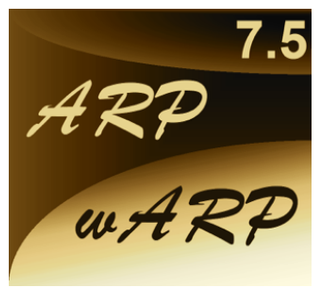
- Improved stability of beta-strand, DNA/RNA and solvent building

- "Fit Ligand" incorporates 84 most common ligands now
  - and uses cif files defining bond, torsion and plane restraints

- Incremental improvements in auto-depth view and menus of ArpNavigator







ArpNavigator

Last year, we made the cover of Acta Crystallographica D because we launched **ArpNavigator**:

- The primary intuitive interface for interacting with the automated model building processes
- Real time visualisation of model building
- Can be used by both experienced and novice users
- It controls the setup of computational tasks and displays the intermediate steps
- Allows model visualisation, map quality check and figure production

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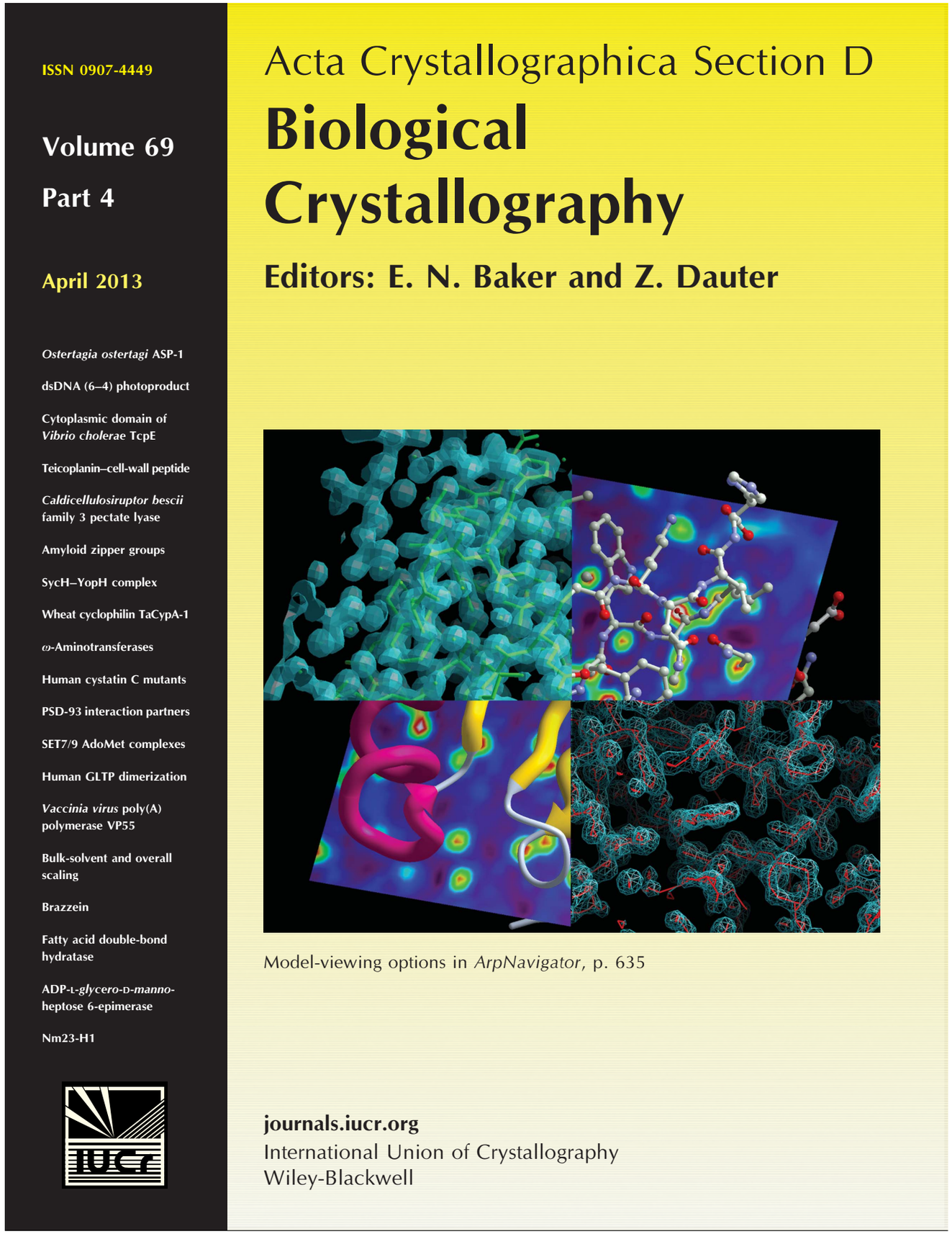
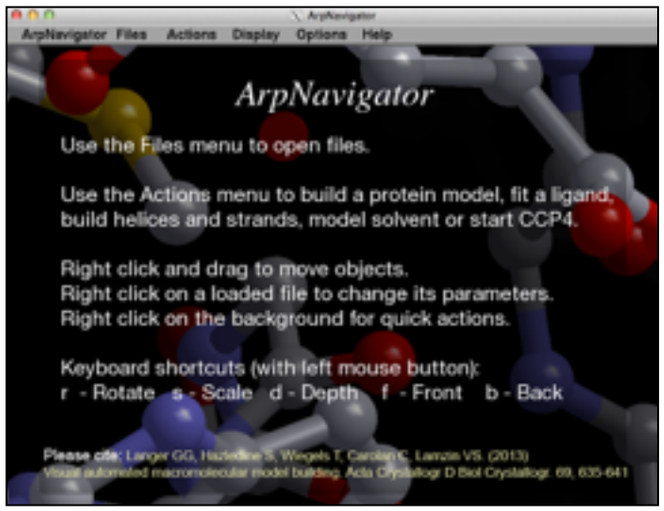
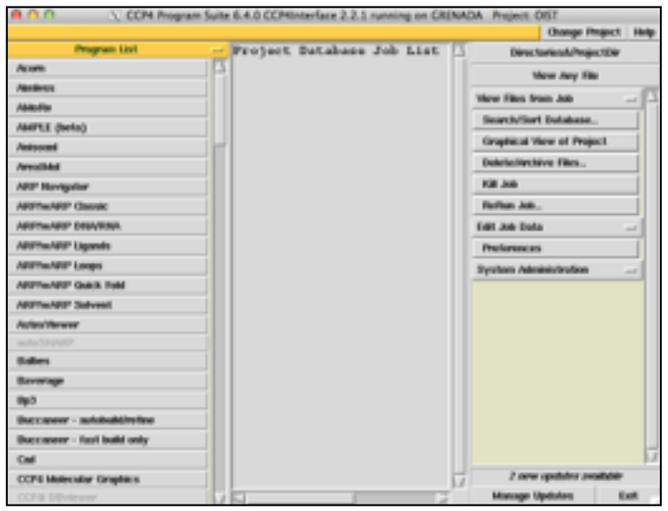
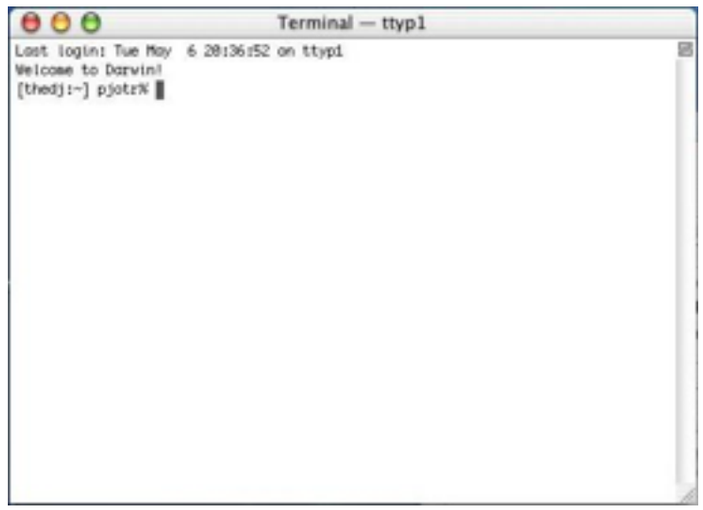


How do I use ARP/wARP?

There are 4 main ways to use ARP/wARP:







ArpNavigator

Intuitive interaction with automated model building

Real time visualisation of model building

Automated setup of computational tasks

Displays the intermediate steps

CCP4 Suite

Model building job saved in your project directory

Extra options for automated model building

Job submission to Hamburg cluster

Possibility to share data with developers

Terminal

Good for expert users

Complete control on the parameters to use

Check user guide for the commands

Web Service

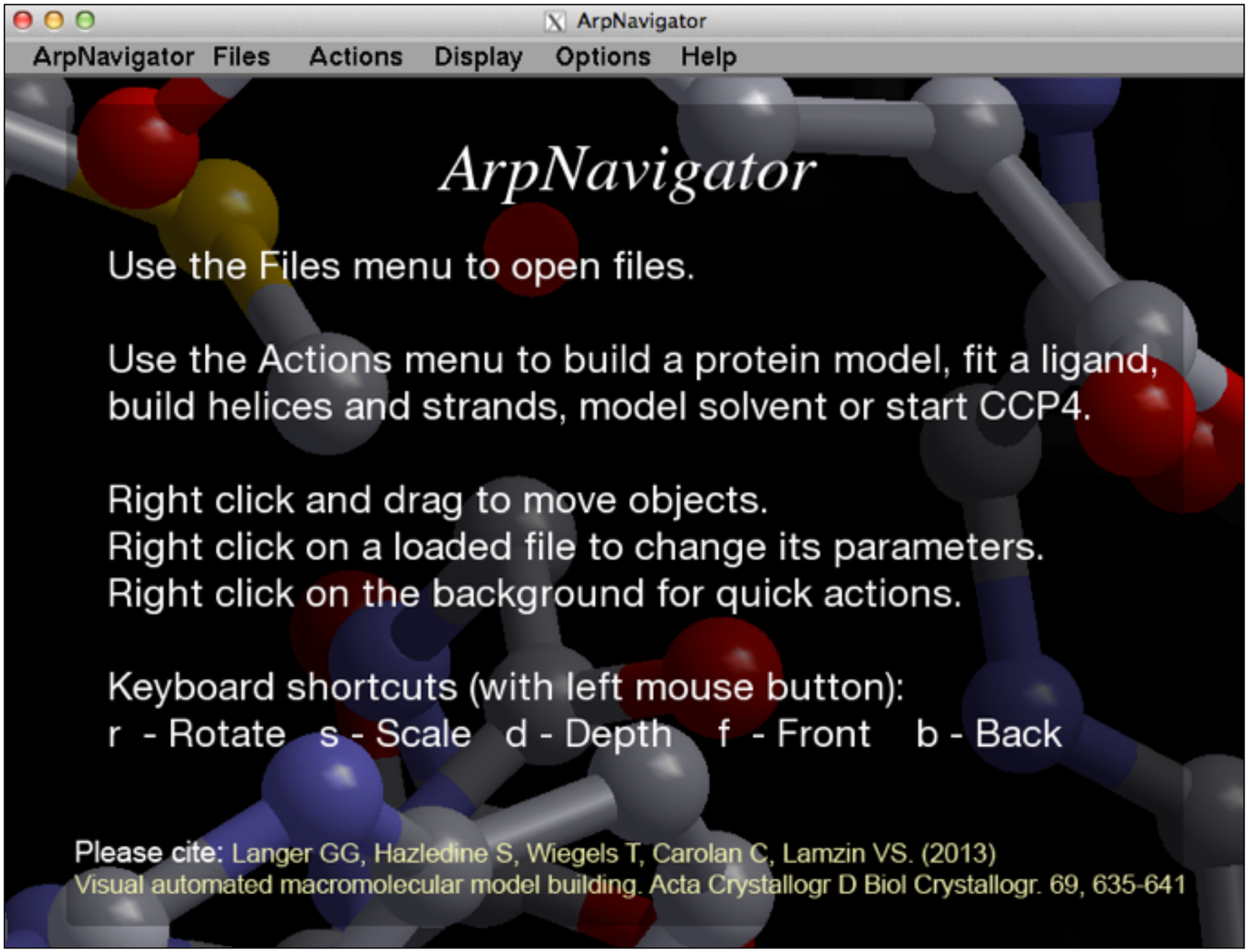
Good for Windows users

Only for protein automated model building

Jobs don't run your computer but on our cluster in Hamburg

Putting the hands on the work

This is the main window of ArpNavigator:



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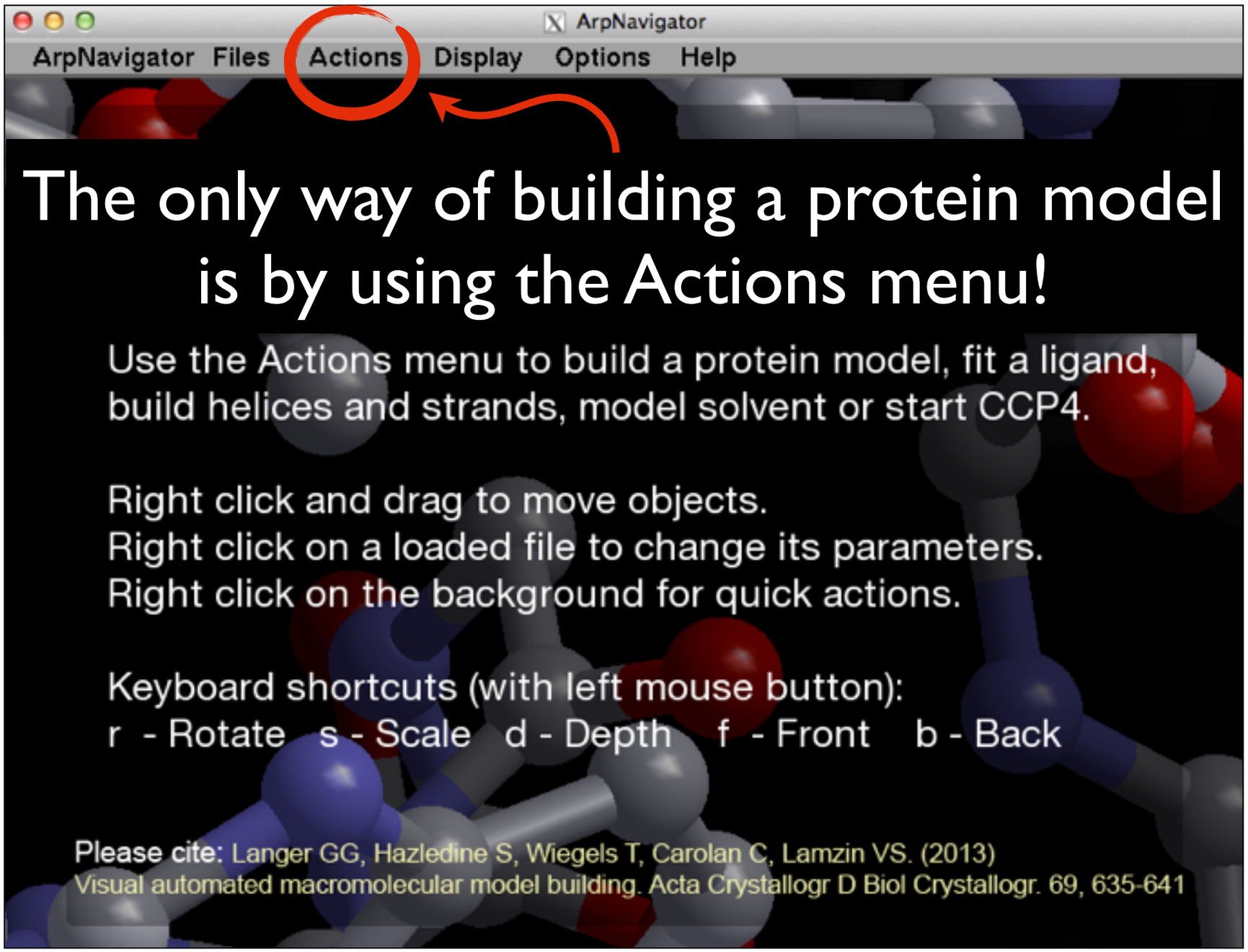

ArpNavigator

ArpNavigator Files Actions Display Options Help

ArpNavigator

Use the Files menu to open files.

Use the Actions menu to build a protein model, fit a ligand, build helices and strands, model solvent or start CCP4.

Right click and drag to move objects.
Right click on a loaded file to change its parameters.
Right click on the background for quick actions.

Keyboard shortcuts (with left mouse button):
r - Rotate s - Scale d - Depth f - Front b - Back

Please cite: Langer GG, Hazledine S, Wiegels T, Carolan C, Lamzin VS. (2013) Visual automated macromolecular model building. Acta Crystallogr D Biol Crystallogr. 69, 635-641

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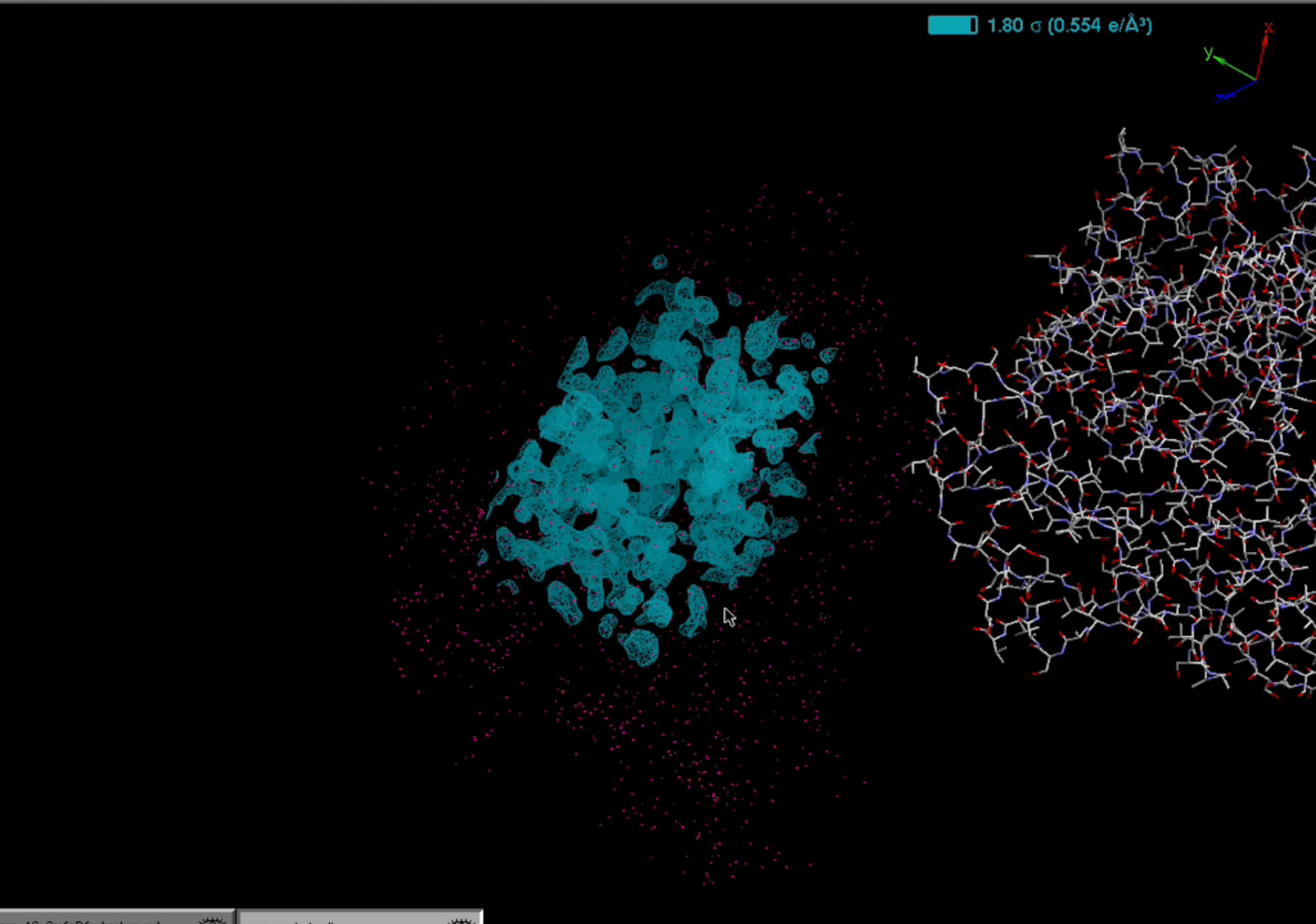

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arp_pept_4.pdb

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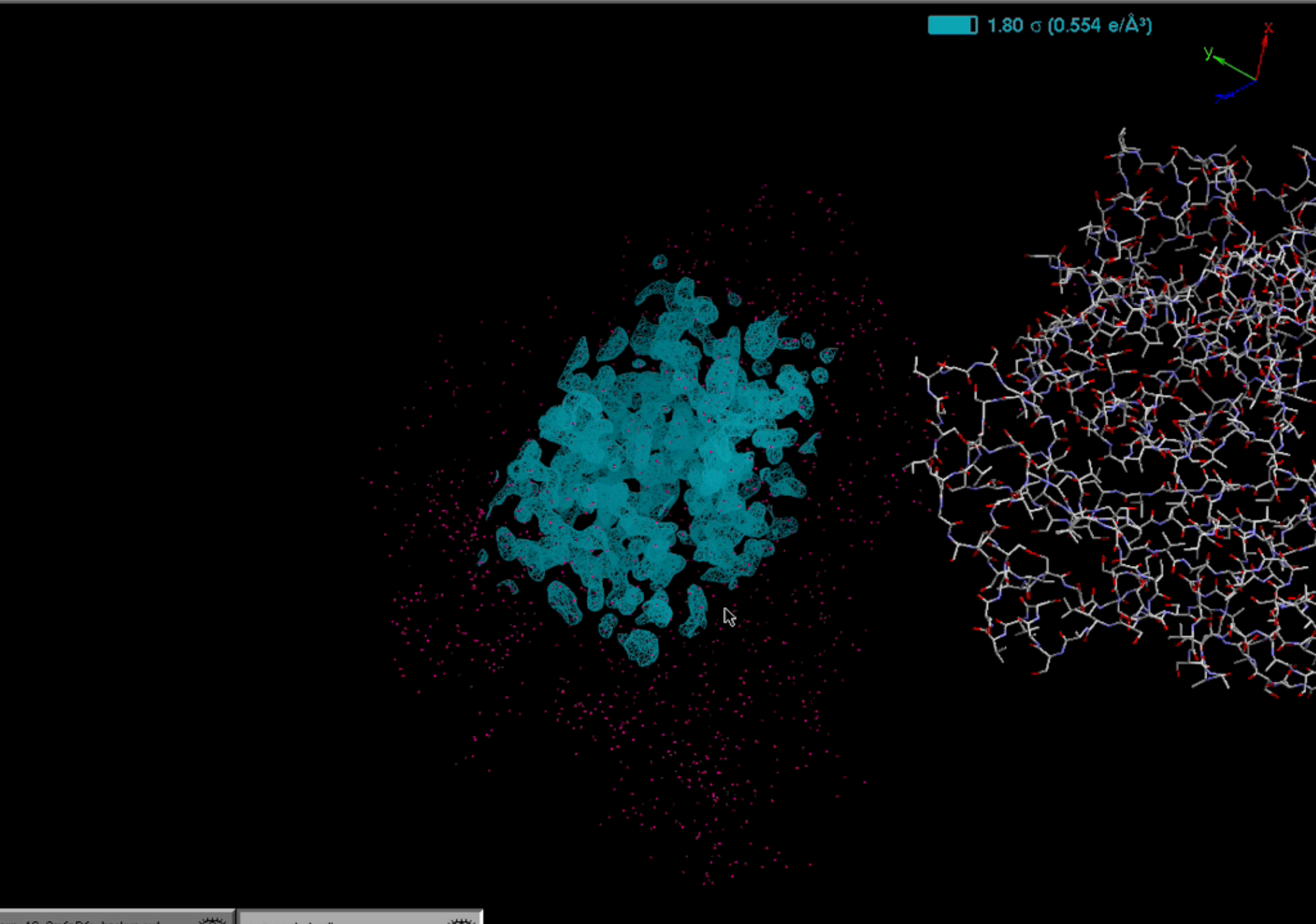

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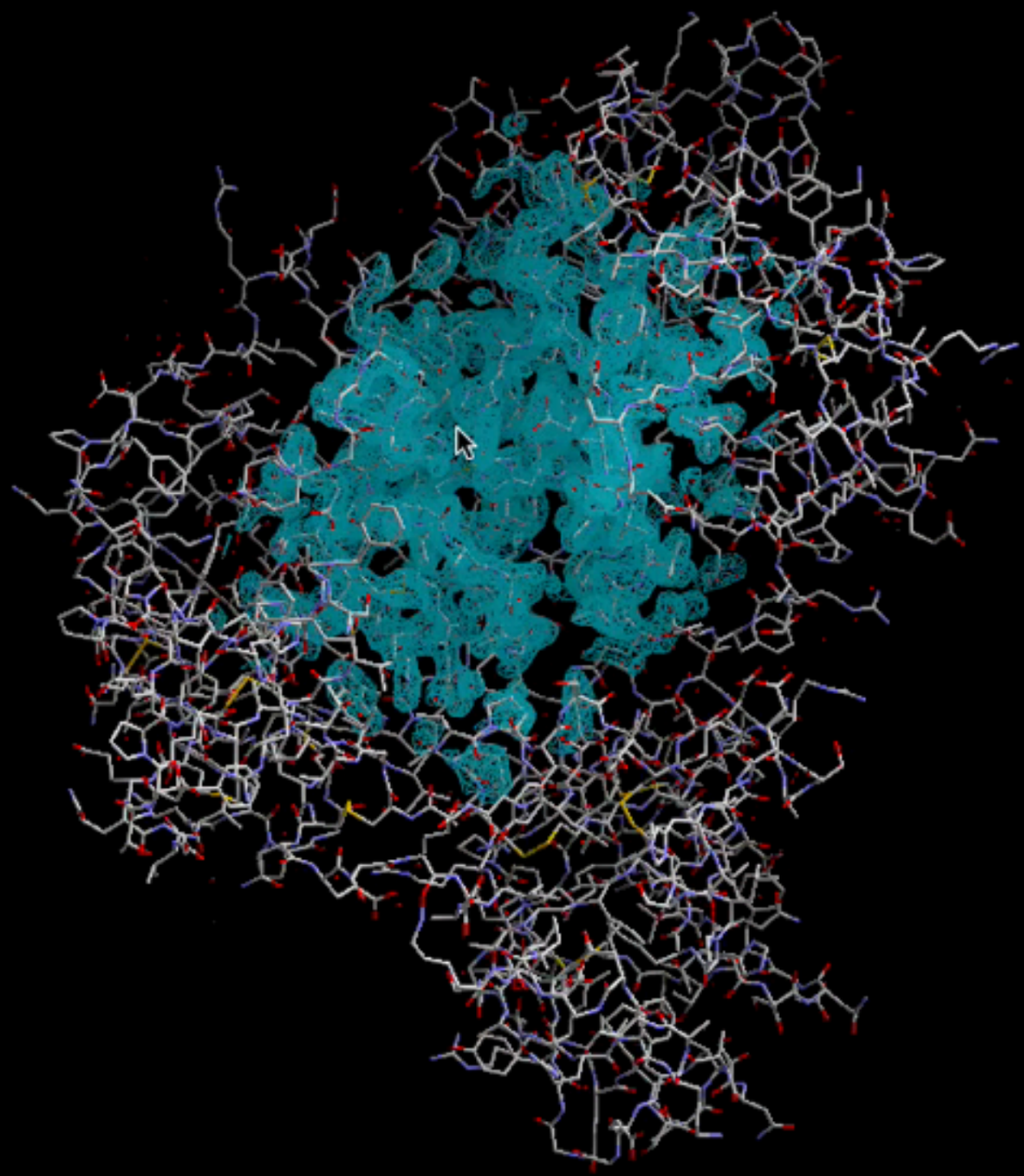

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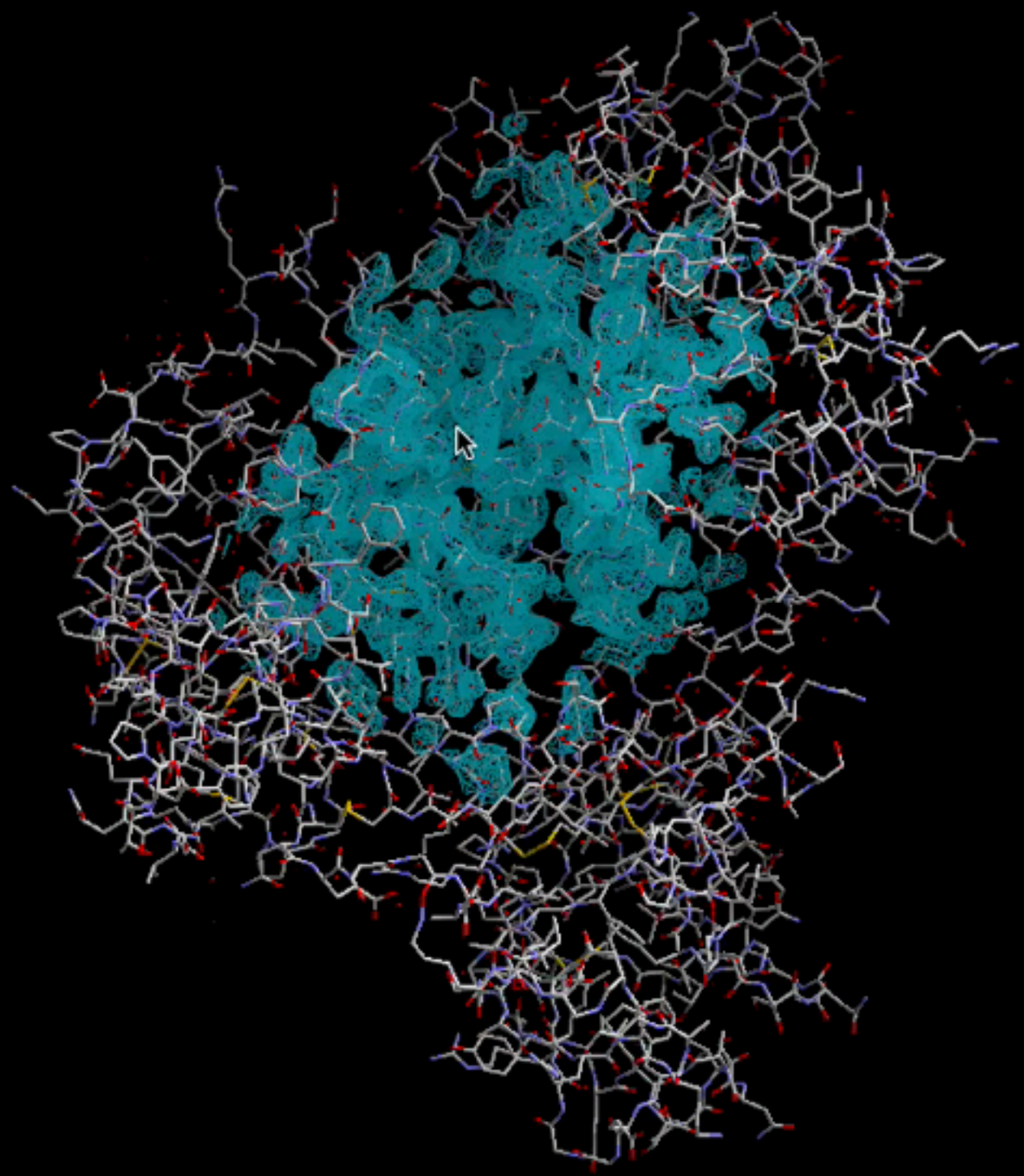

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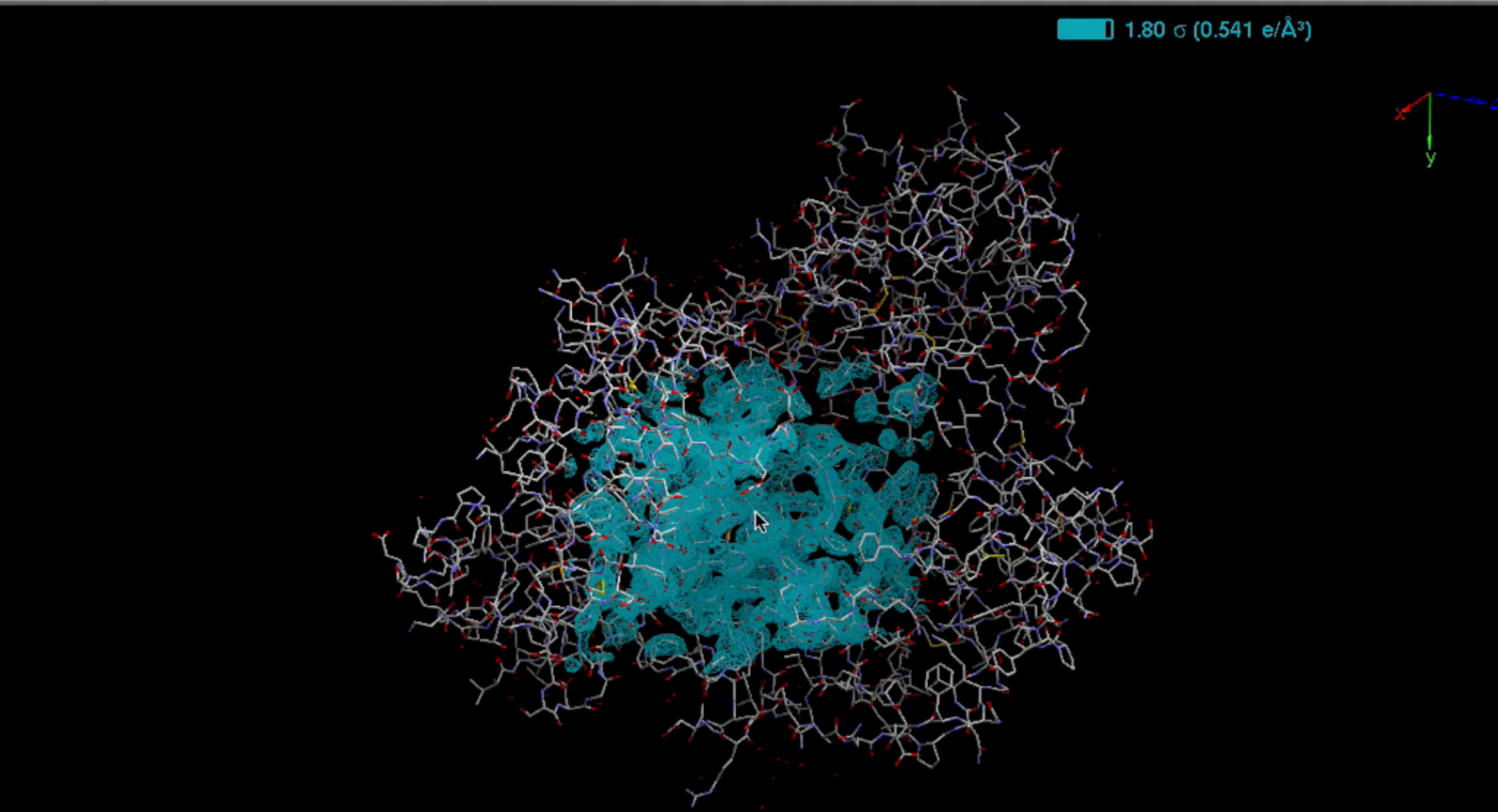

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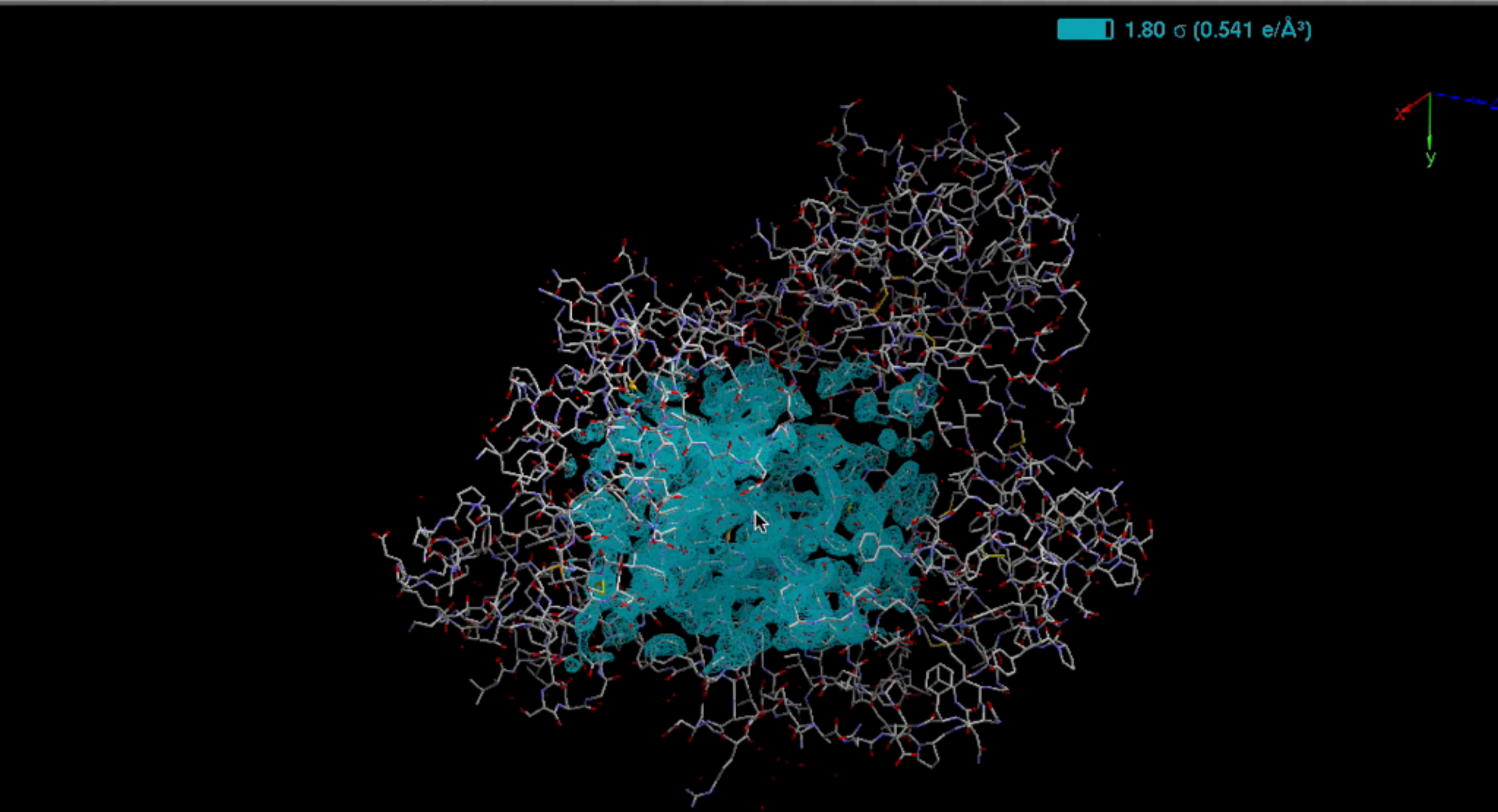

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The people - The power!

Collaborators

EMBL Hamburg: Gleb Bourenkov, Santosh Panjikar

MRC Laboratory, Cambridge : Garib Murshudov's group

Rutherford Appleton Laboratory: CCP4 team

Previous Members

Ciaran Carolan, Tim Wiegels

Funding