Classic Automated Model Building and Secondary Structure Identification with ARP/wARP

Hands-on Tutorial

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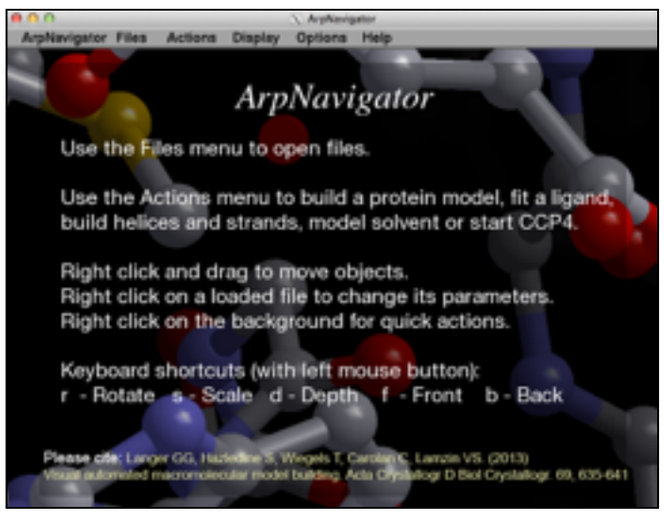
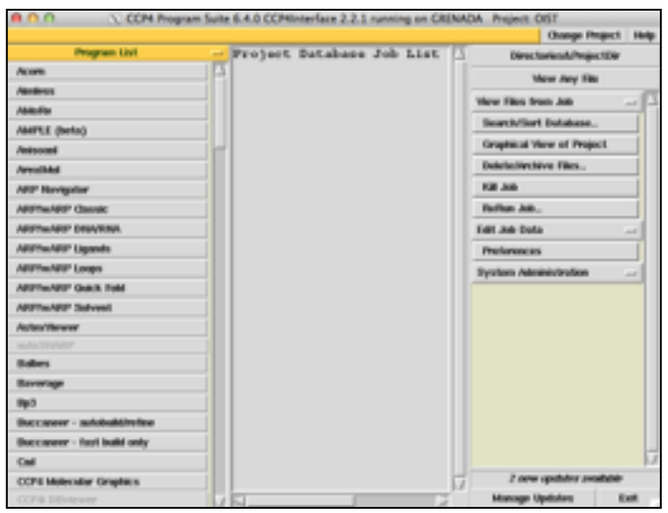
Lamzin Group, EMBL Hamburg

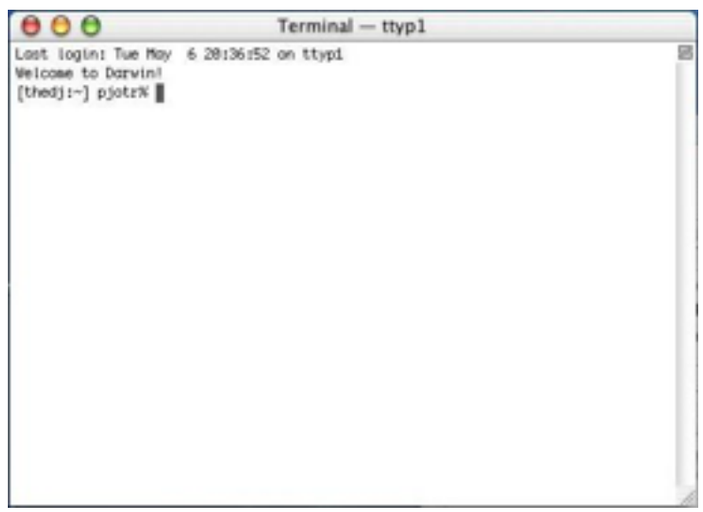
EMBL 40 YEARS | 1974–2014

How to 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

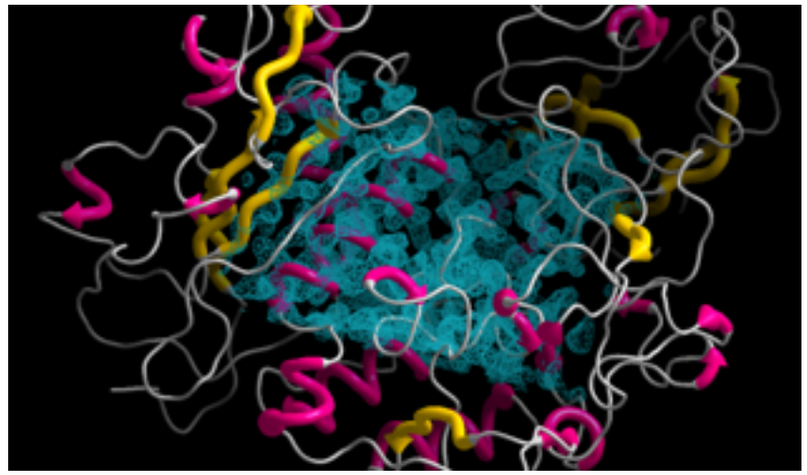
Good for Windows users

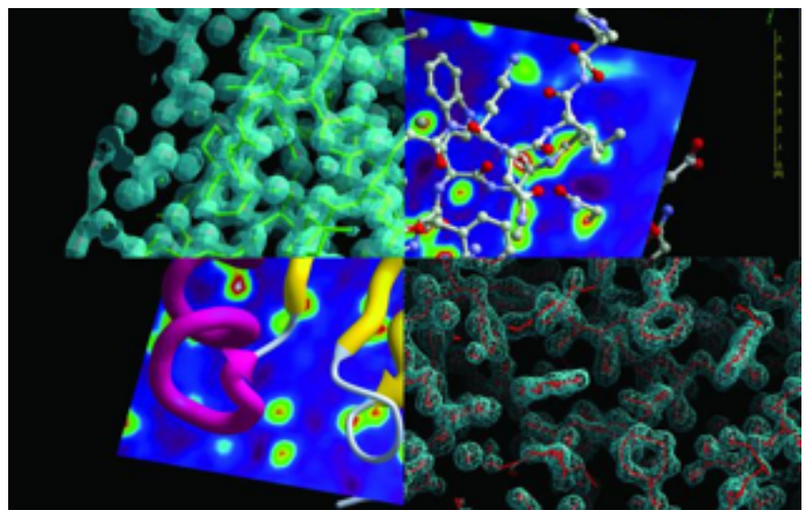
Only for protein automated model building

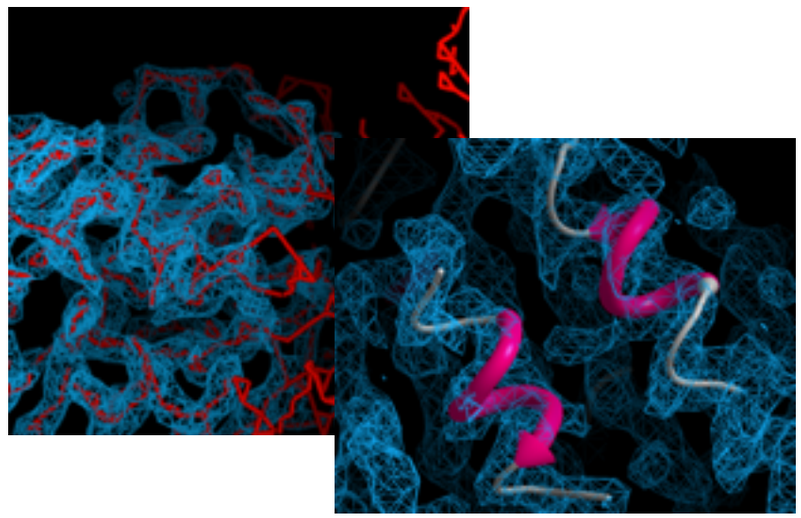
Jobs don't run your computer but on our cluster in Hamburg

What will you learn?

1. Open ArpNavigator from CCP4
2. Use ArpNavigator to build protein models
3. Use ArpNavigator to build secondary structure elements and skeletons to evaluate map quality
4. Run ARP/wARP for protein model building from CCP4 gui



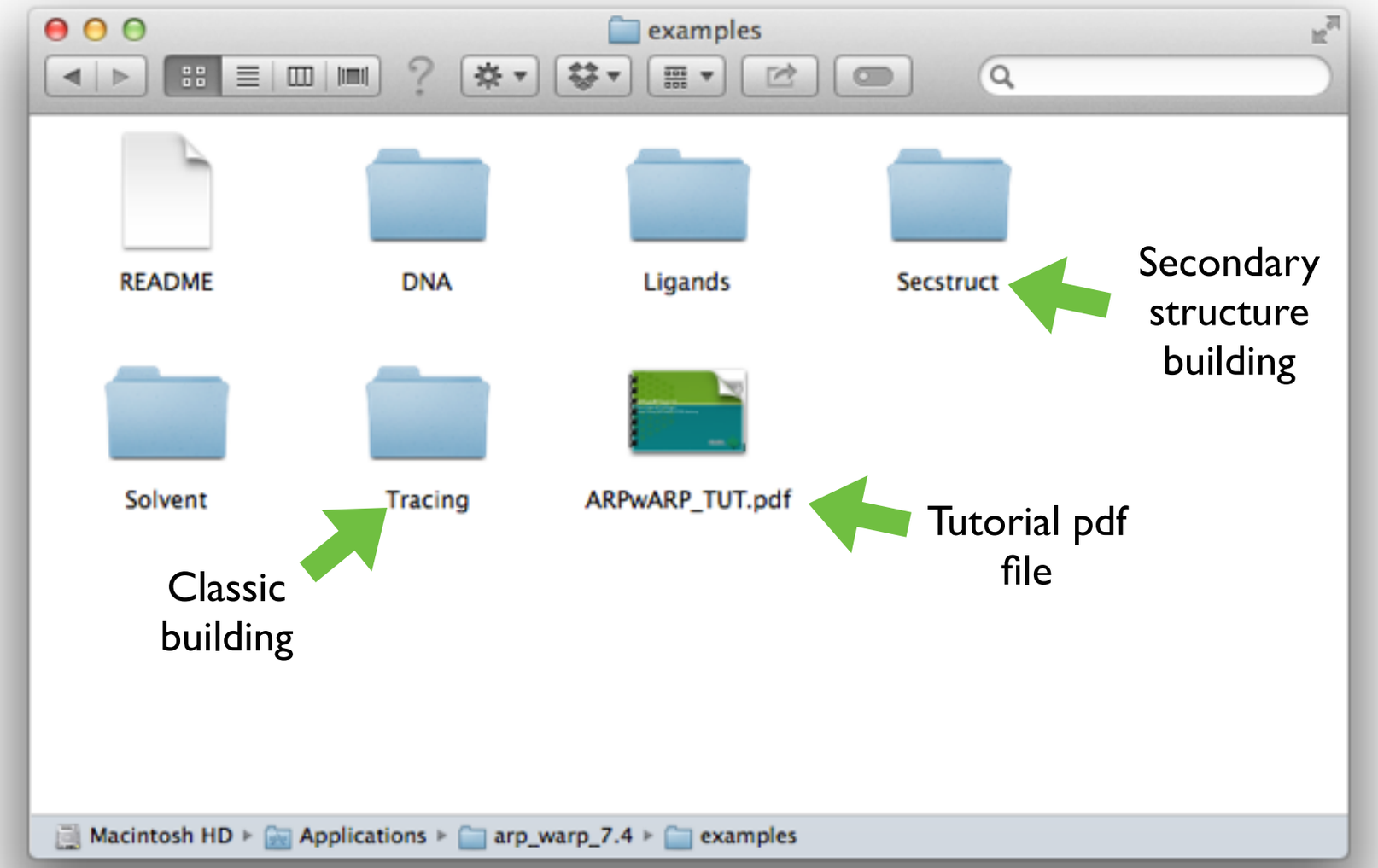




What do you need?

Example data:

/arp_warp_7.4/examples



Or try your own data ;)

What do you need?

- MTZ file (e.g, PSP.mtz)
- Sequence file (e.g, PSP.fasta or PSP.pir)

Fasta format

>Protein_name
PROTEINSEQUENCE

Pir format

>Protein_type;protein_IDcode
Description of the protein
PROTEINSEQUENCE

- Number of residues on the asymmetric unit (e.g., 475)
- Number of molecules on the asymmetric unit (e.g., 1)

(the number of NCS related molecules)

For everything

Only for protein chain tracing

One thing to have into account…

The sequence file when you have a hetero-multimer:

Both ways are valid!

```
>Protein_A
GPGSGPGRGFGKRRHPKKLTPLAYKQFIPNVAEKTLGASG
RYEGKITRNSERFKELTPNYNPDIIFKDEENTGADRLMTQ
RCKDKLNALAISVMNQWPGVKLRVTEGWDEDGHHSEESLH
YEGRAVDITTSDRDRSKYGMLARLAVEAGFDWVYYESKAH
IHCSVKAE

>Protein_B
GSTPITGPHIAYTEAVSDTQIMLKWTYIPSSNNNTPIQGF
YIYYRPTDSDNDSDYKRDVVEGSKQWHMIGHLQPETSYDI
KMQCFNEGGESEFSNVMICETK
```

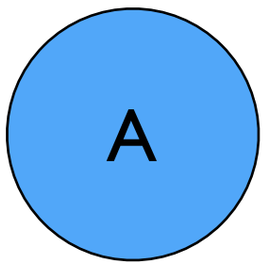
```
>Sequence

GPGSGPGRGFGKRRHPKKLTPLAYKQFIPNVAEKTLGASG
RYEGKITRNSERFKELTPNYNPDIIFKDEENTGADRLMTQ
RCKDKLNALAISVMNQWPGVKLRVTEGWDEDGHHSEESLH
YEGRAVDITTSDRDRSKYGMLARLAVEAGFDWVYYESKAH
IHCSVKAEAAAAAAAAAAGSTPITGPHIAYTEAVSDTQI
MLKWTYIPSSNNNTPIQGFYIYYRPTDSDNDSDYKRDVVE
GSKQWHMIGHLQPETSYDIKMQCFNEGGESEFSNVMICET
K
```

At least 10 alanines between both sequences!

Dealing with residue and molecule number

Monomers:



residues A: X

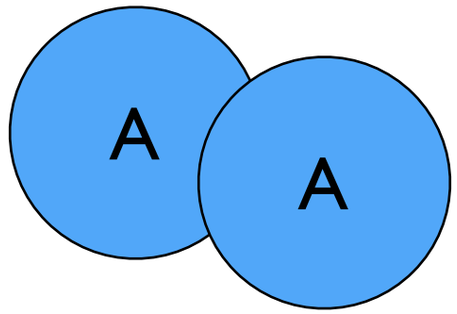
expected residues: X

mol. ass. unit: 1

Sequence file:

```
>Protein_A
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG
```

Homo-multimers:



residues A: X

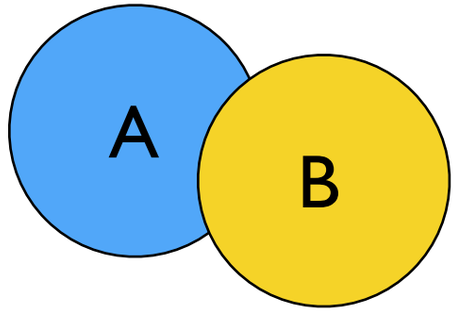
 # expected residues: 2X

 # mol. ass. unit: 2

Sequence file:

```
>Protein_A
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG
```

Hetero-multimers:



residues A: X

residues B: W

 # expected residues: X+W

 # mol. ass. unit: 1

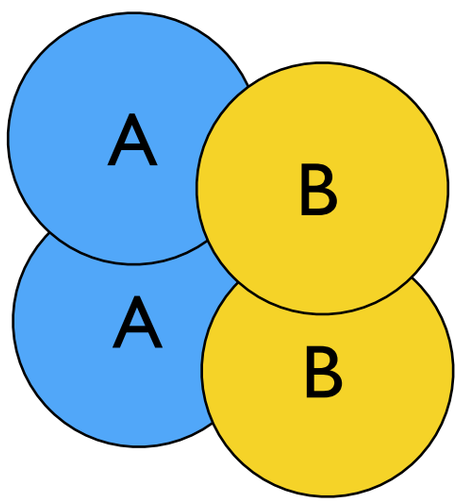
Sequence file:

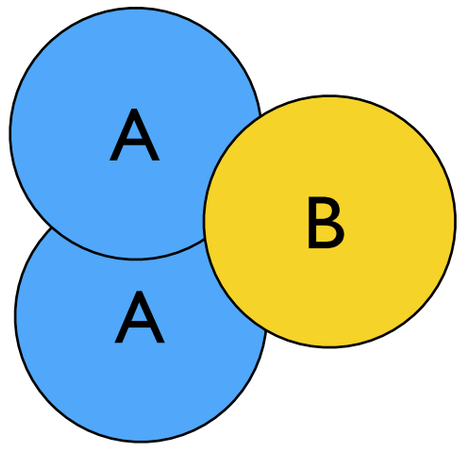
```
>Protein_A
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG

>Protein_B
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG
```

Dealing with residue and molecule number

Hetero-multimers:





residues A: X

residues B: W

 # expected residues: 2(X+W)

 # mol. ass. unit: 2

Sequence file:

```
>Protein_A
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG

>Protein_B
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG
```

residues A: X

residues B: W

 # expected residues: 2X+W

 # mol. ass. unit: 1

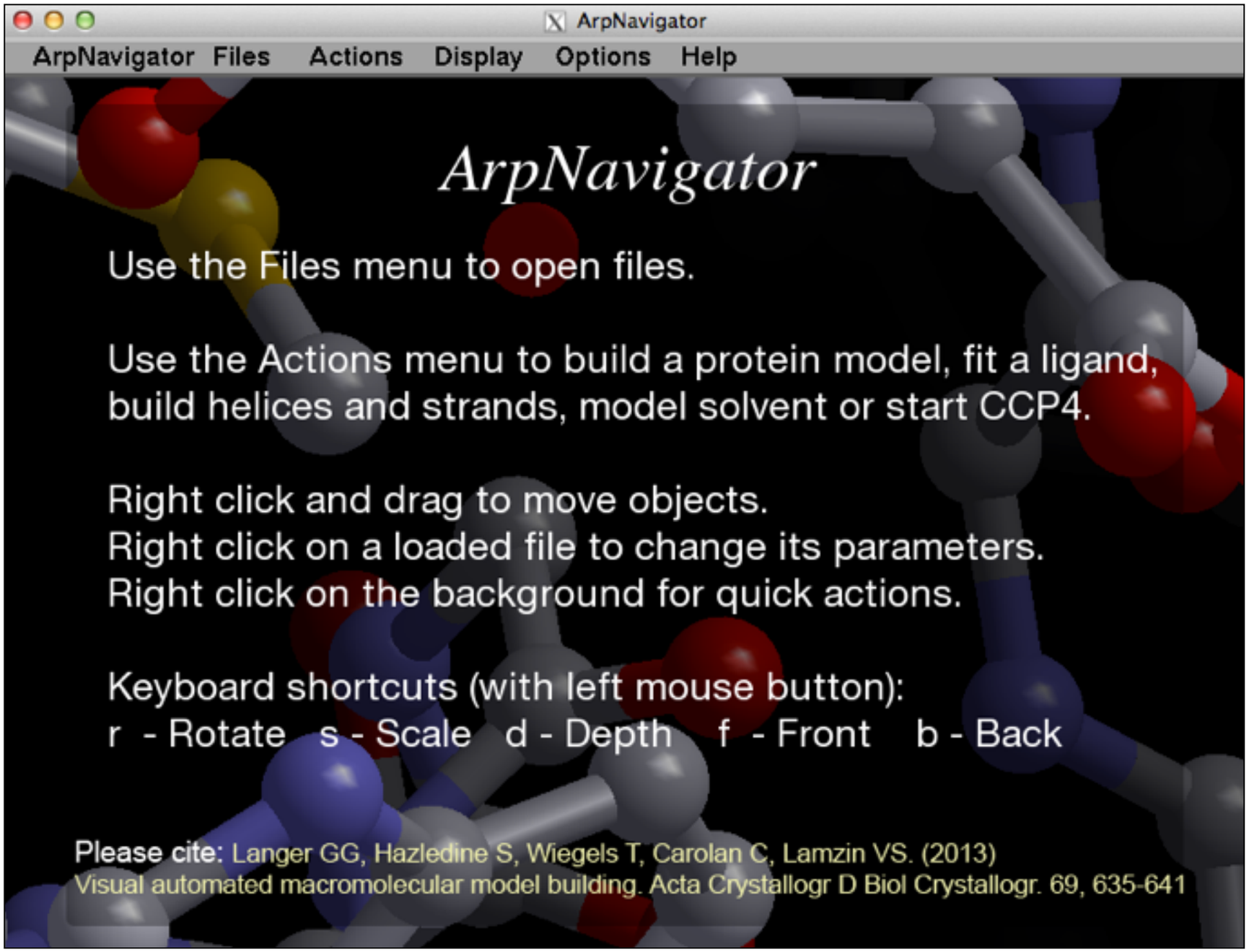
Sequence file:

```
>Protein_A
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG

>Protein_B
GPGSGPGRGFGKRRHPKKLTPLAYKQ
FIPNVAEKTLGASG
```

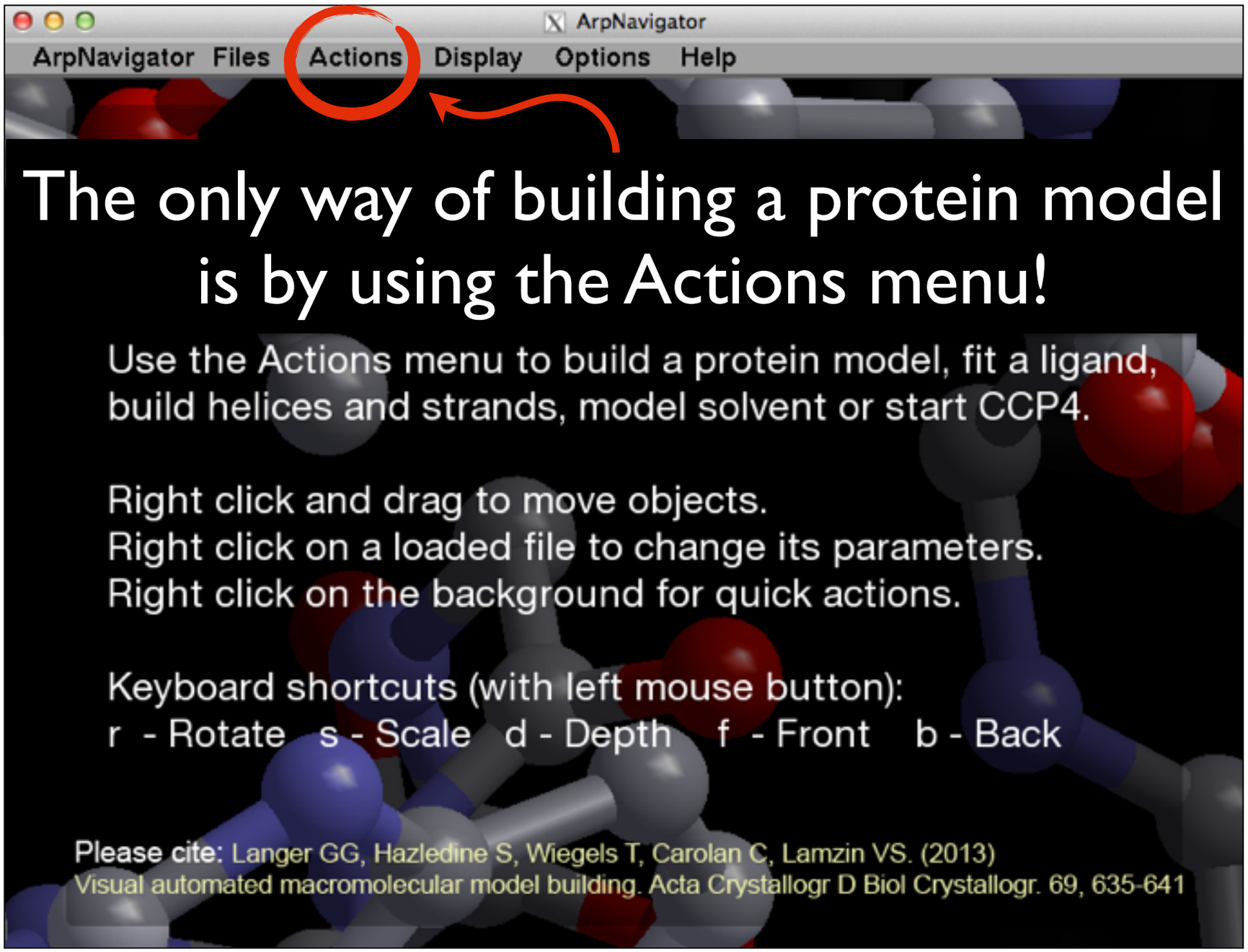
Putting the hands on the work

This is the main window of ArpNavigator:



Putting the hands on the work

This is the main window of ArpNavigator:



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

ArpNavigator

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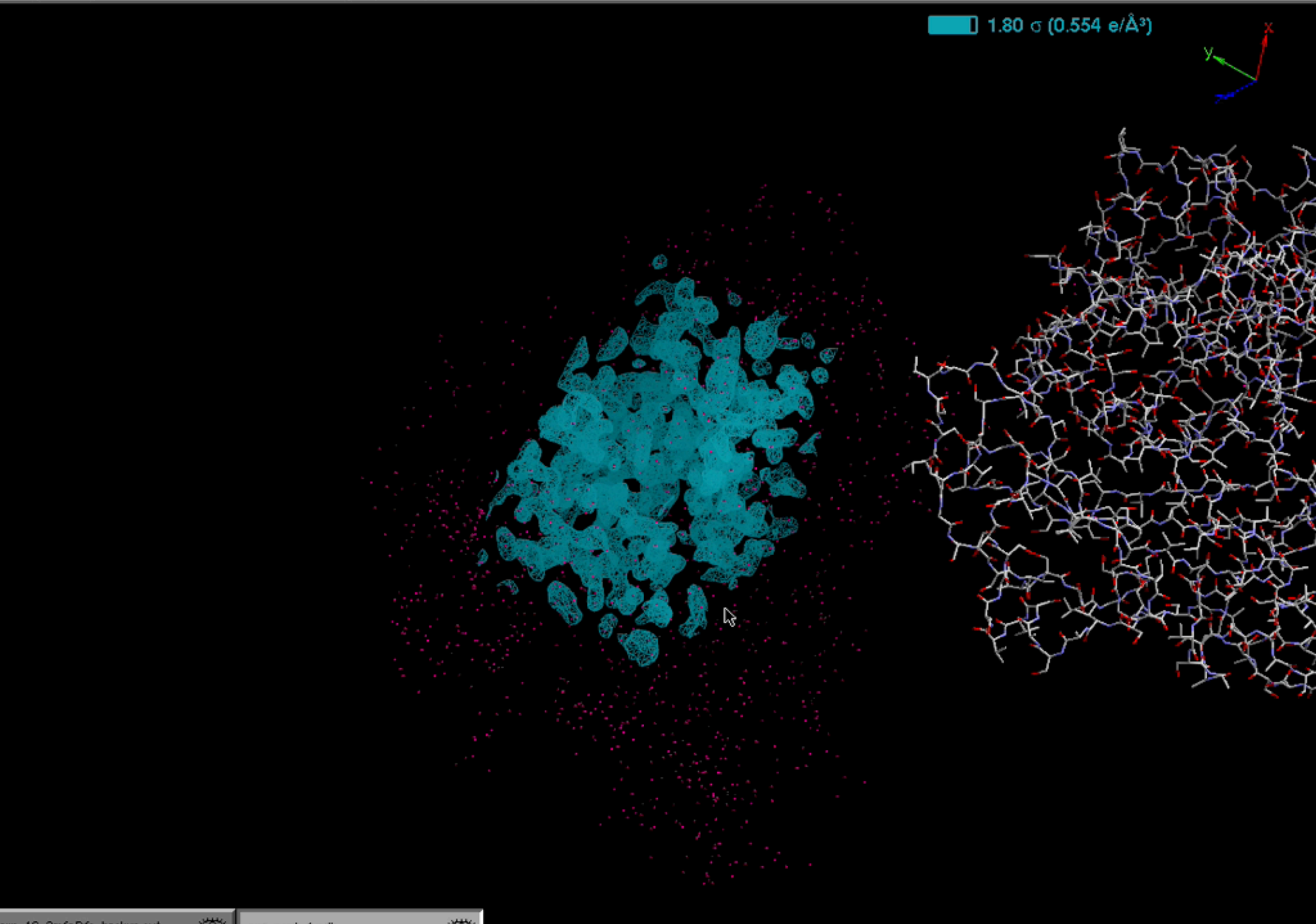
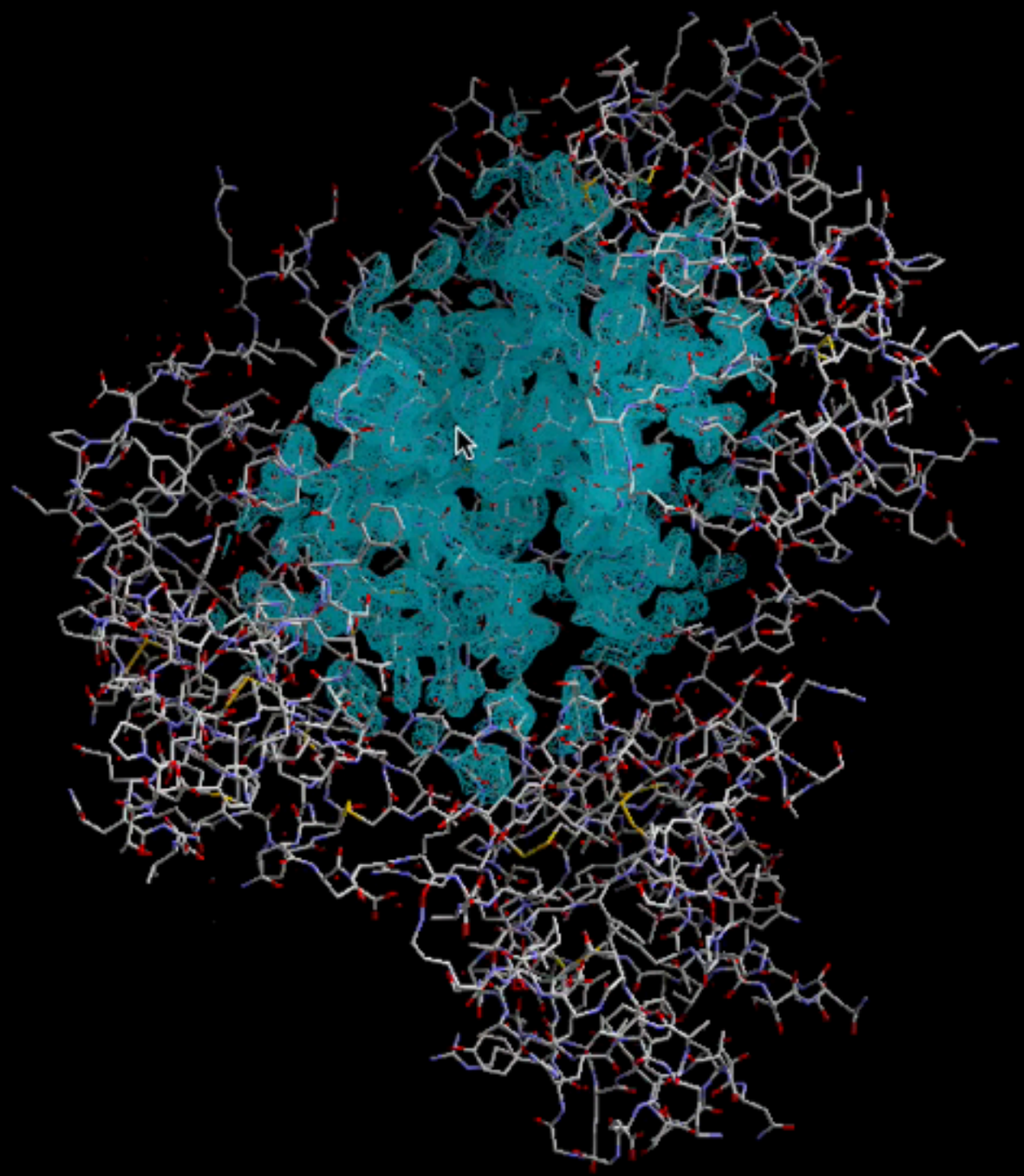


arp_16_2mfoDfc_backup.ext

arp_pept_4.pdb

ArpNavigator

ArpNavigator Files Actions Display Options Help

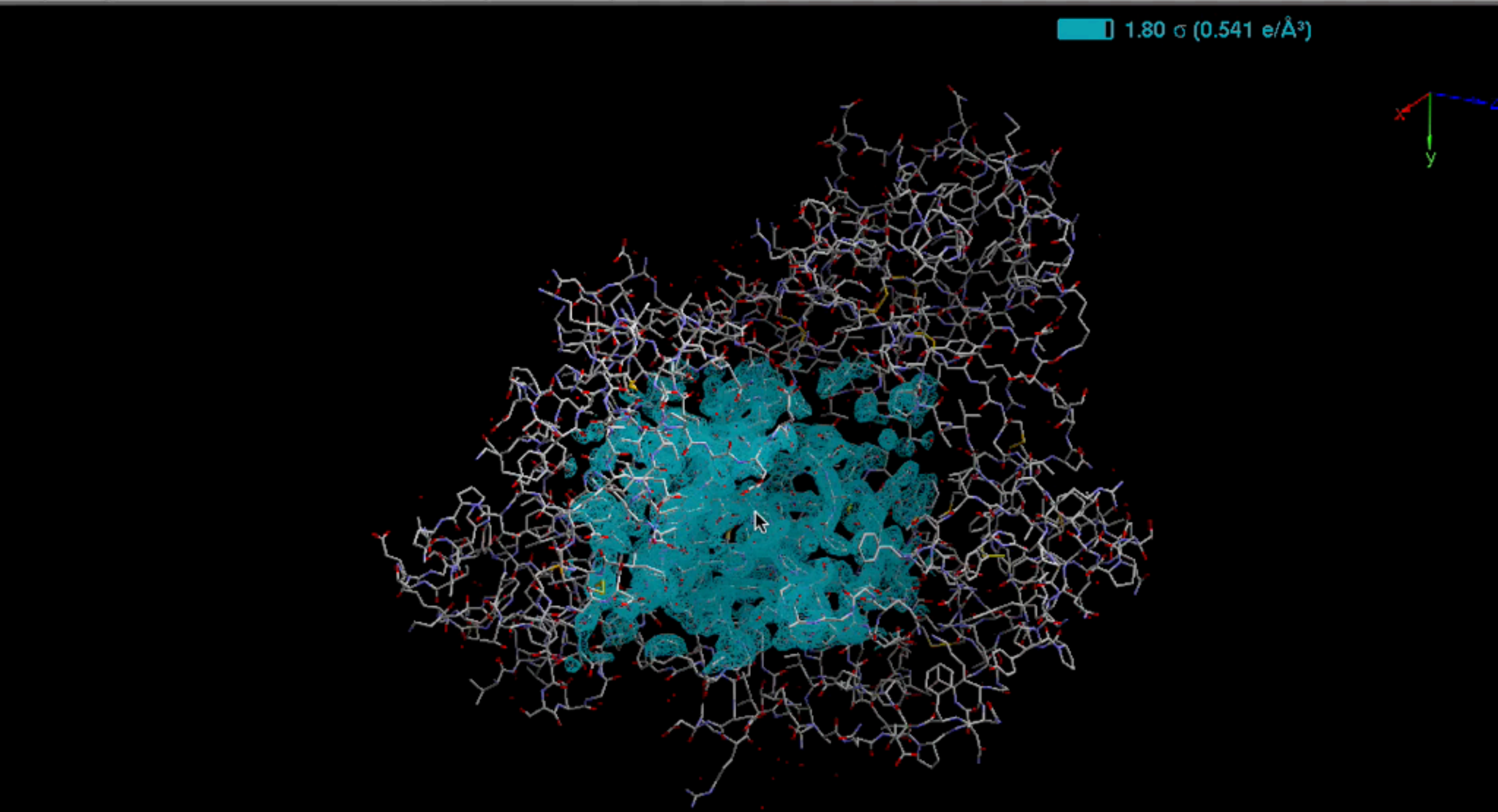


arp_25.pdb

arp_25_2mfoDfc_backup.ext

ArpNavigator

ArpNavigator Files Actions Display Options Help



arp_25.pdb

arp_25_2mfoDfc_backup.ext

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

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