



ARP/wARP

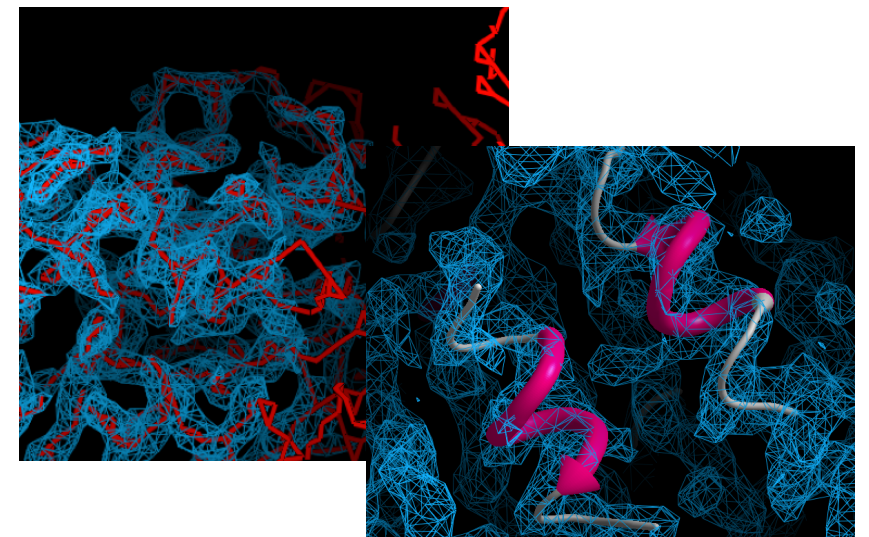
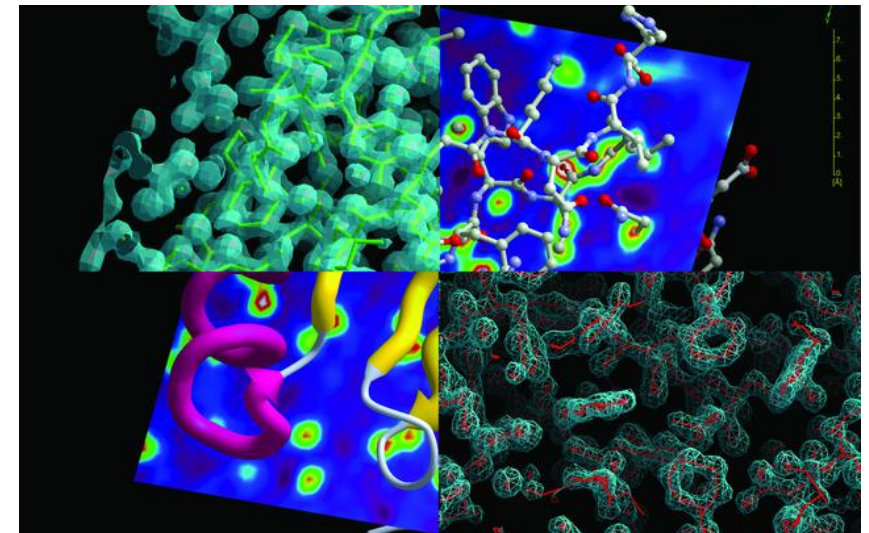
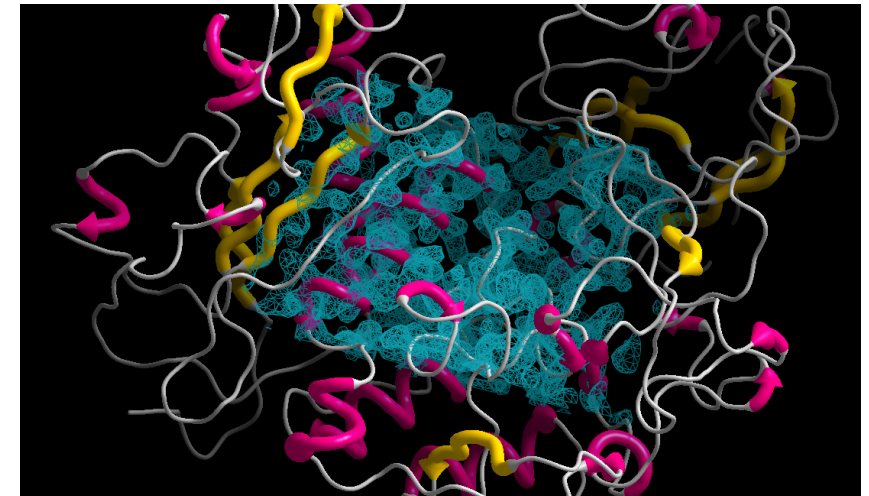
Hands-on Tutorial

Daria Beshnova and Joana Pereira

Lamzin Group, EMBL Hamburg

What will you learn?

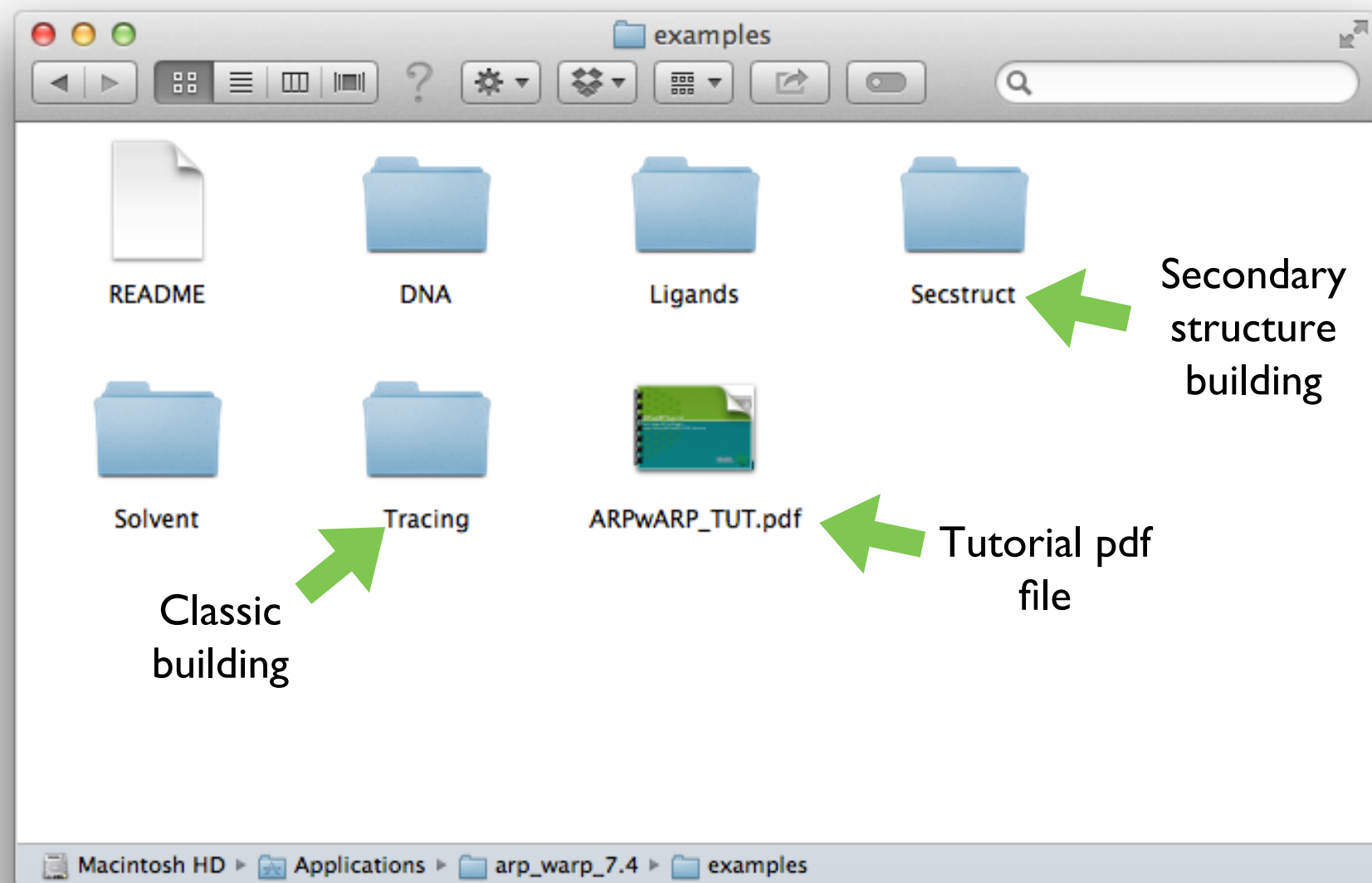
- 1 Automatically build a protein model from your electron density
- 2 Use several model-viewing options
- 3 Build helices and skeletons for a quick quality assessment of the initial map



What do you need?

Example data:

Applications/arp_warp_7.4/examples



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:

```
>Protein_A
GPGSGPGRGFGKRRHPKKLTPLAYKQFIPNVAEKT LGASG
RYEGKITRNSERFKELTPNYPNDIIFKDEENTGADRLMTQ
RCKDKLNALAI SVMNQWPGVKLRVTEGWDEDGHHSEESLH
YEGRAVDITTS DRDRSKYGMLARLAVEAGFDWVYYESKAH
IHCSVKAE
```

```
>Protein_B
GSTPITGPHIAYTEAVSDTQIMLKWTYIPSSNNNTPIQGF
YIYYRPTSDNDSDYKRDVVEGSKQWHMIGHLQPETSYDI
KMQCFNEGGESEFSNVMICETK
```

>Sequence

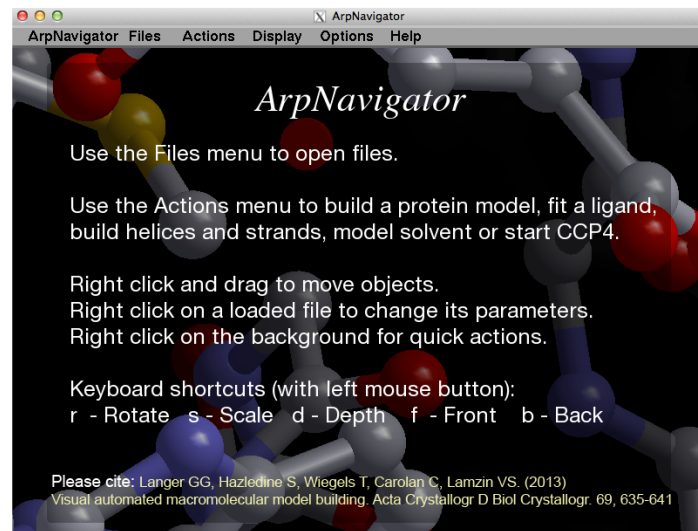
```
GPGSGPGRGFGKRRHPKKLTPLAYKQFIPNVAEKT LGASG
RYEGKITRNSERFKELTPNYPNDIIFKDEENTGADRLMTQ
RCKDKLNALAI SVMNQWPGVKLRVTEGWDEDGHHSEESLH
YEGRAVDITTS DRDRSKYGMLARLAVEAGFDWVYYESKAH
IHCSVKAEAAAAAAAAAAGSTPITGPHIAYTEAVSDTQI
MLKWTYIPSSNNNTPIQGFYIYYRPTSDNDSDYKRDVVE
GSKQWHMIGHLQPETSYDIKMQCFNEGGESEFSNVMICET
K
```

At least 10 alanines between both sequences!

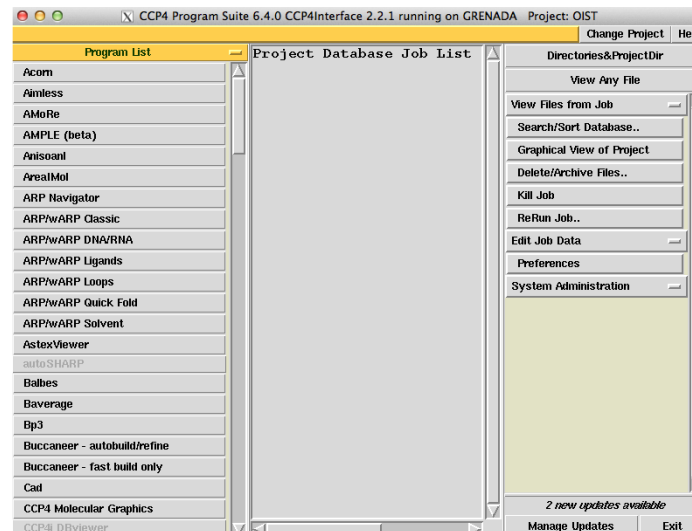


How to start it?

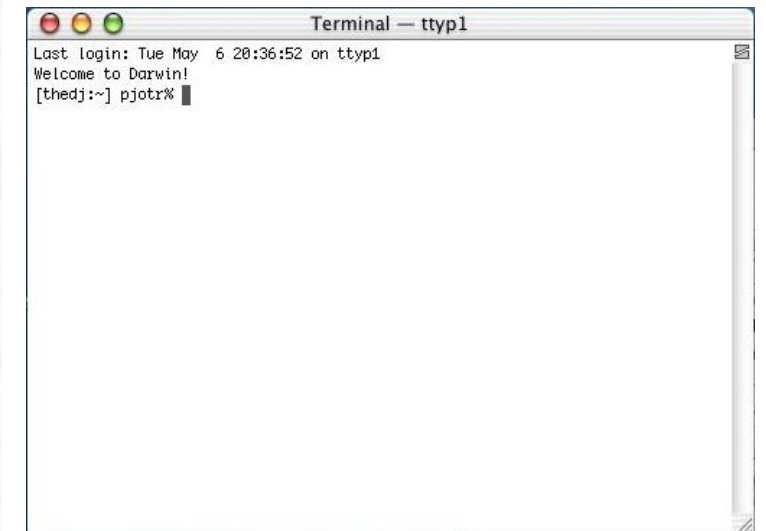
3 ways:



ArpNavigator



CCP4 Suite



Terminal

This tutorial!

Check the user
guide!

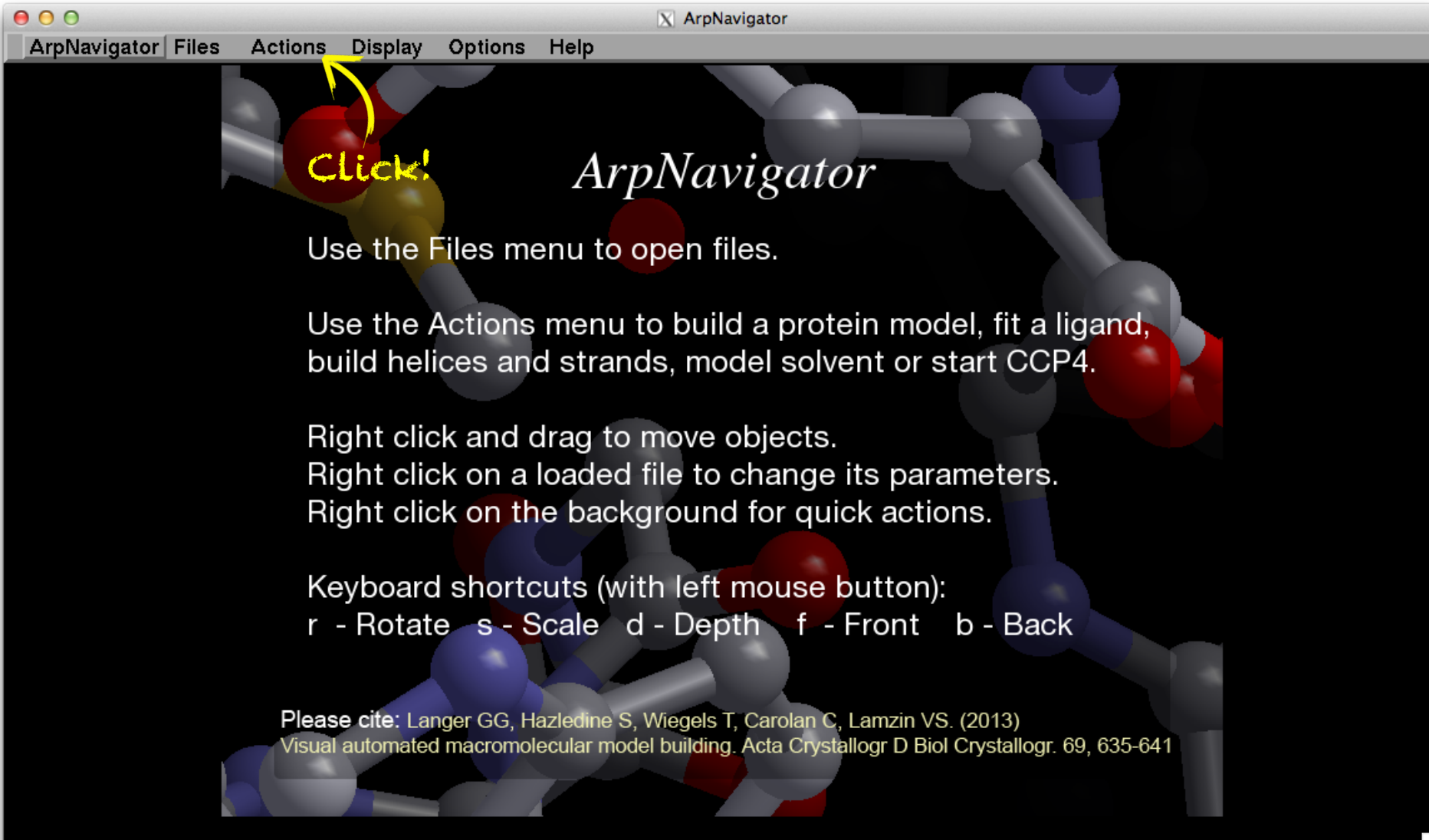
Classic Automated Model Building With ArpNavigator

A Click-on Tutorial

EMBL
Hamburg



Where to go...



The screenshot shows the ArpNavigator application window. The title bar reads 'ArpNavigator'. The menu bar includes 'ArpNavigator', 'Files', 'Actions', 'Display', 'Options', and 'Help'. The main window displays a 3D molecular model with atoms represented as spheres (red for oxygen, blue for nitrogen, grey for carbon) and bonds as sticks. A yellow arrow points to a red sphere with the text 'Click!' in yellow. The word 'ArpNavigator' is written in a large, stylized font in the center. Below the title bar, there is a list of instructions for using the software.

Click!

ArpNavigator

Use the Files menu to open files.

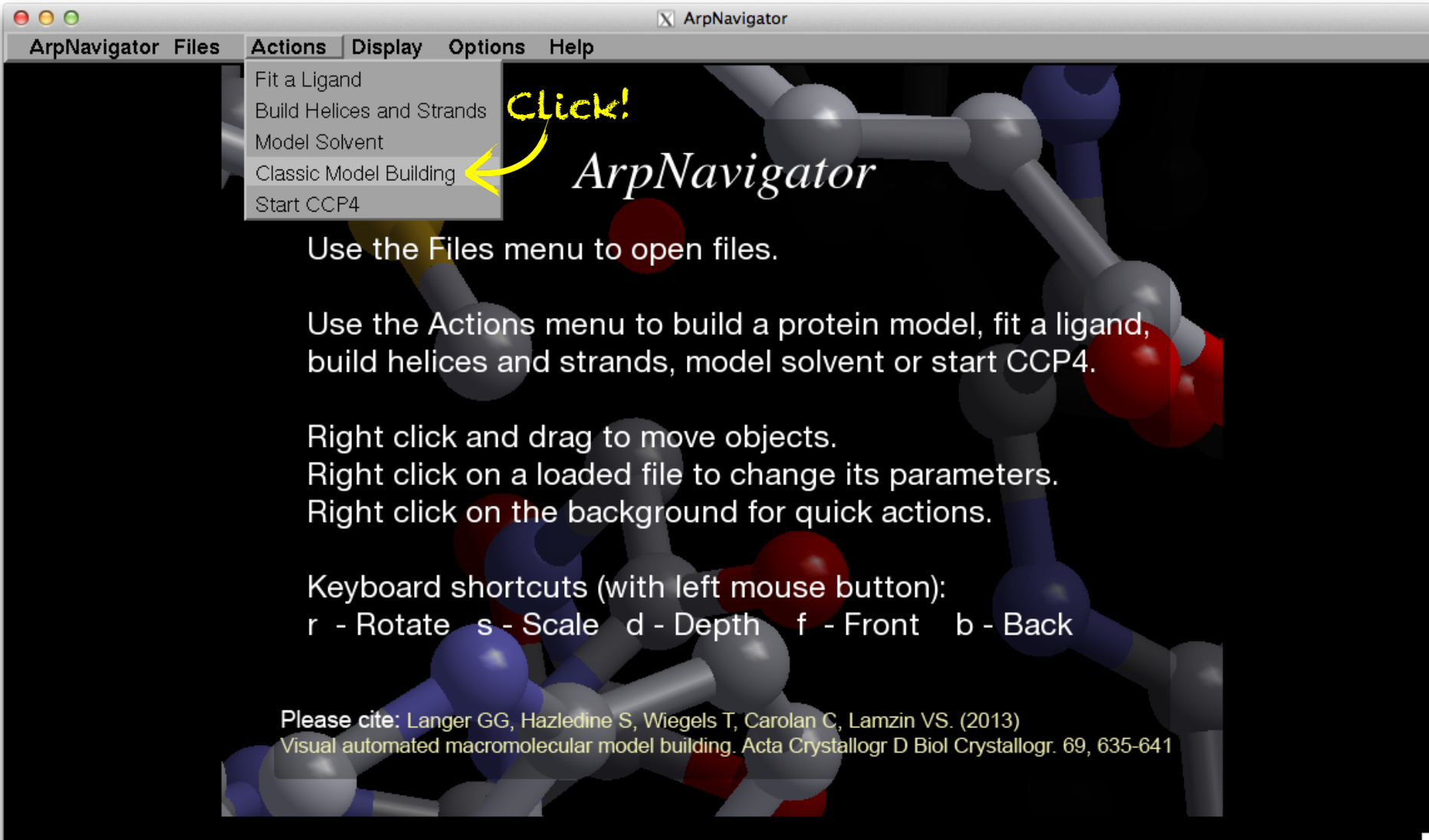
Use the Actions menu to build a protein model, fit a ligand, build helices and strands, model solvent or start CCP4.

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

ARP/wARP: Classic Model Building (arp_tracing)



The screenshot shows the ArpNavigator application window. The title bar reads 'ArpNavigator'. The menu bar includes 'ArpNavigator', 'Files', 'Actions', 'Display', 'Options', and 'Help'. The 'Actions' menu is open, showing options: 'Fit a Ligand', 'Build Helices and Strands', 'Model Solvent', 'Classic Model Building', and 'Start CCP4'. A yellow arrow points to 'Classic Model Building' with the text 'Click!' next to it. The background of the window displays a 3D molecular model with grey sticks for the protein backbone, blue spheres for nitrogen atoms, and red spheres for oxygen atoms. The word 'ArpNavigator' is written in a stylized font over the model.

Use the Files menu to open files.

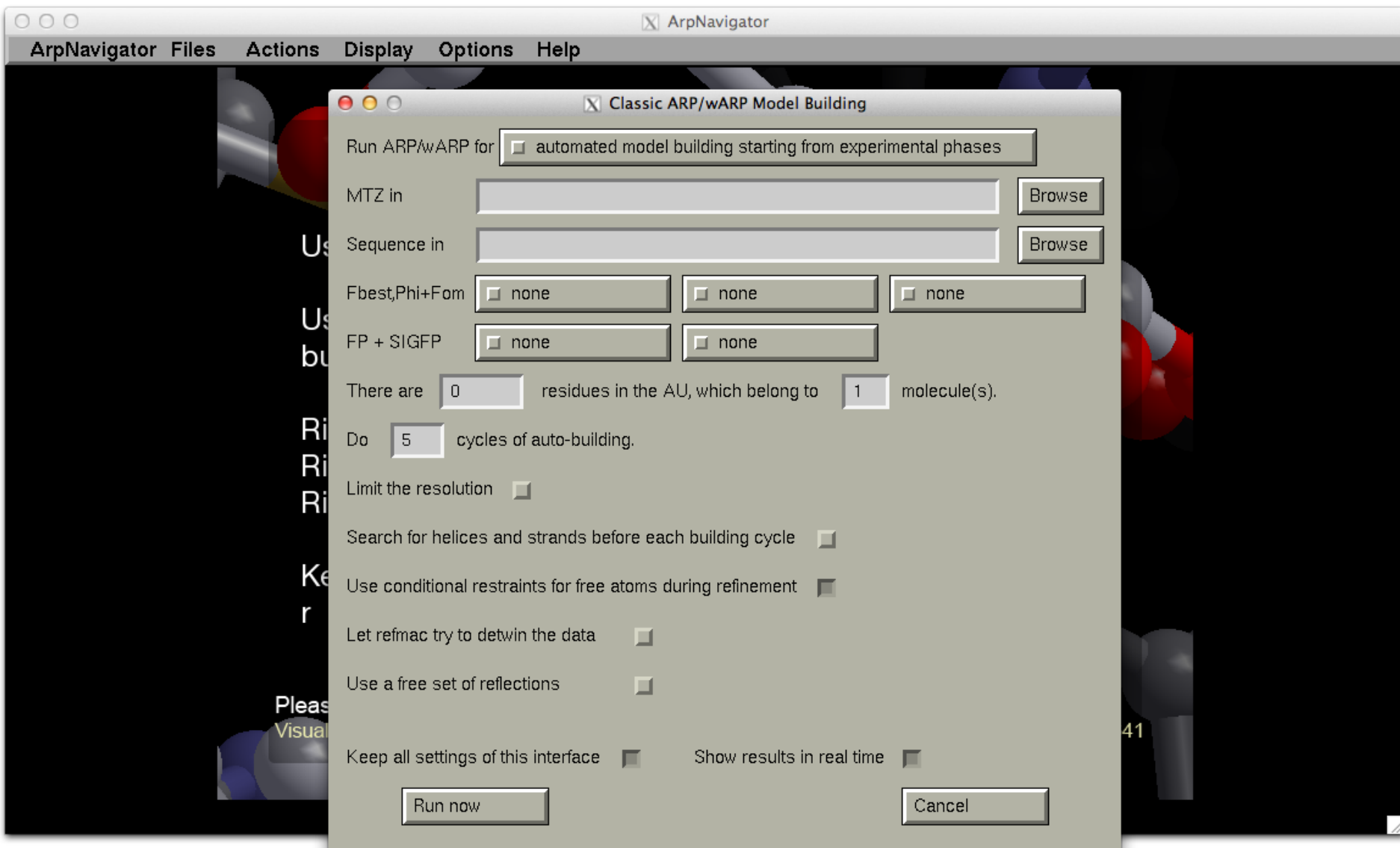
Use the Actions menu to build a protein model, fit a ligand, build helices and strands, model solvent or start CCP4.

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.

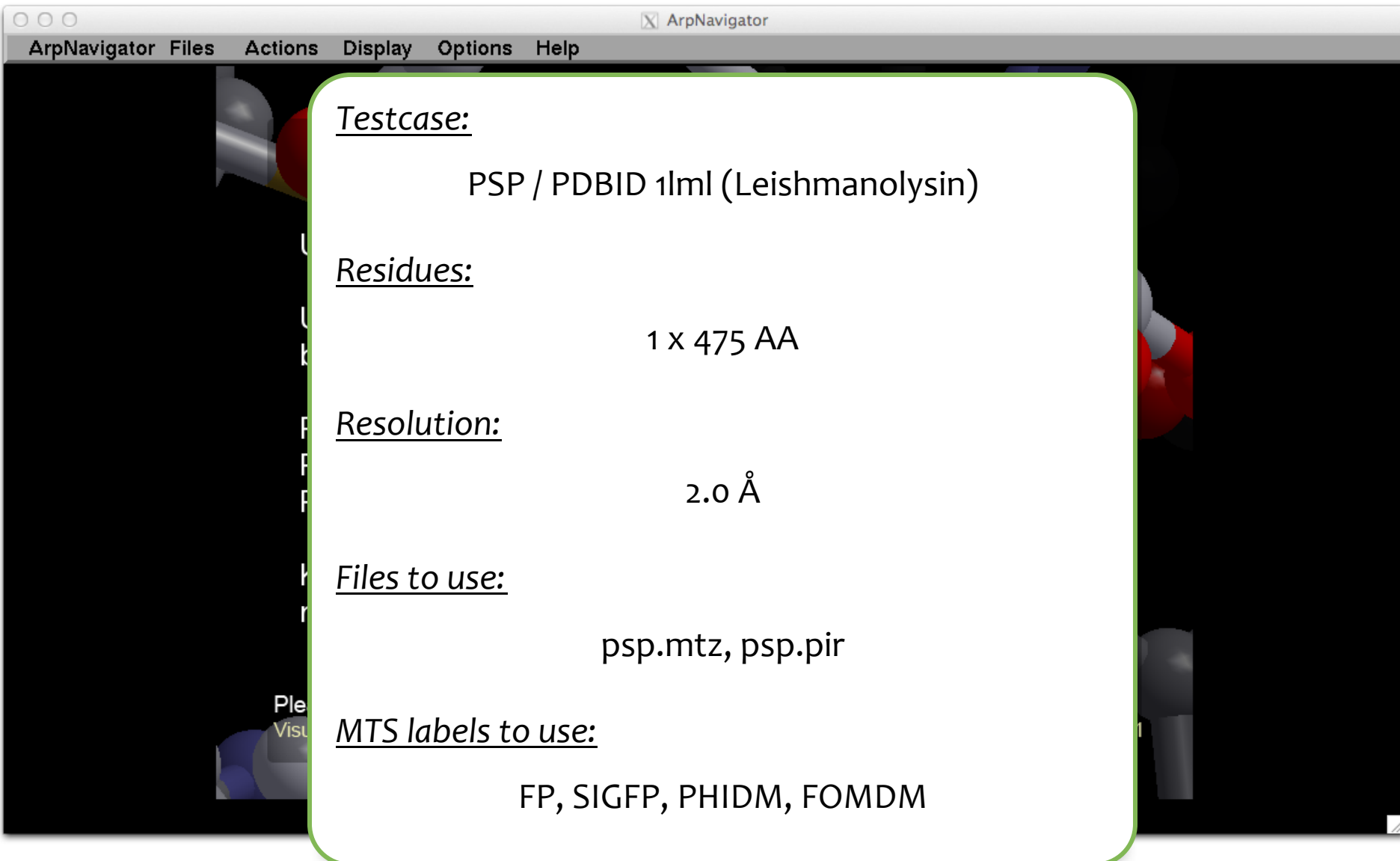
Keyboard shortcuts (with left mouse button):
r - Rotate s - Scale d - Depth f - Front b - Back

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

ARP/wARP: Classic Model Building (arp_tracing)



ARP/wARP: Classic Model Building (arp_tracing)



The screenshot shows the ArpNavigator application window. The title bar reads 'ArpNavigator'. The menu bar includes 'ArpNavigator', 'Files', 'Actions', 'Display', 'Options', and 'Help'. The main window displays a 3D molecular model with a central text box containing the following information:

Testcase:
PSP / PDBID 1lml (Leishmanolysin)

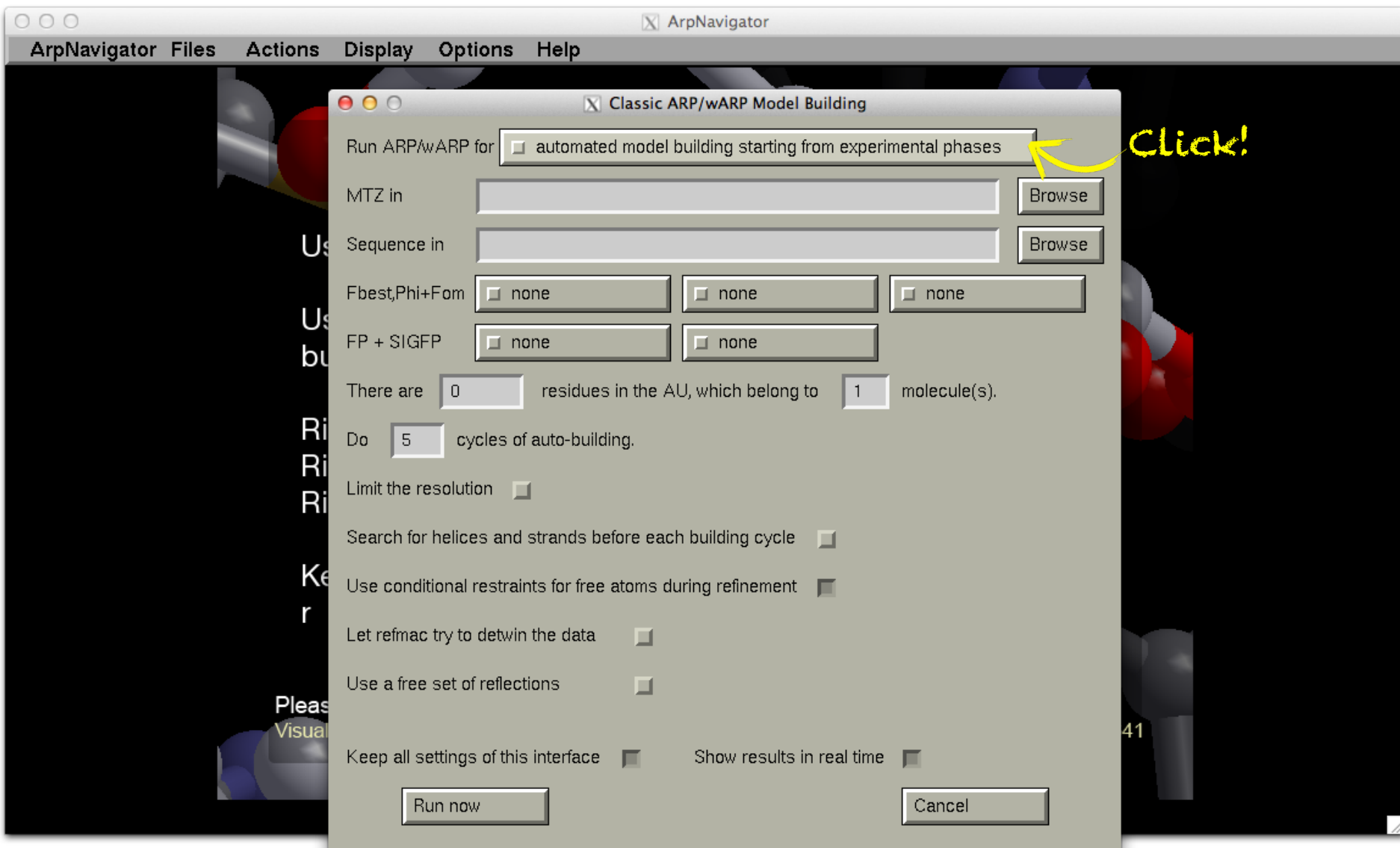
Residues:
1 x 475 AA

Resolution:
2.0 Å

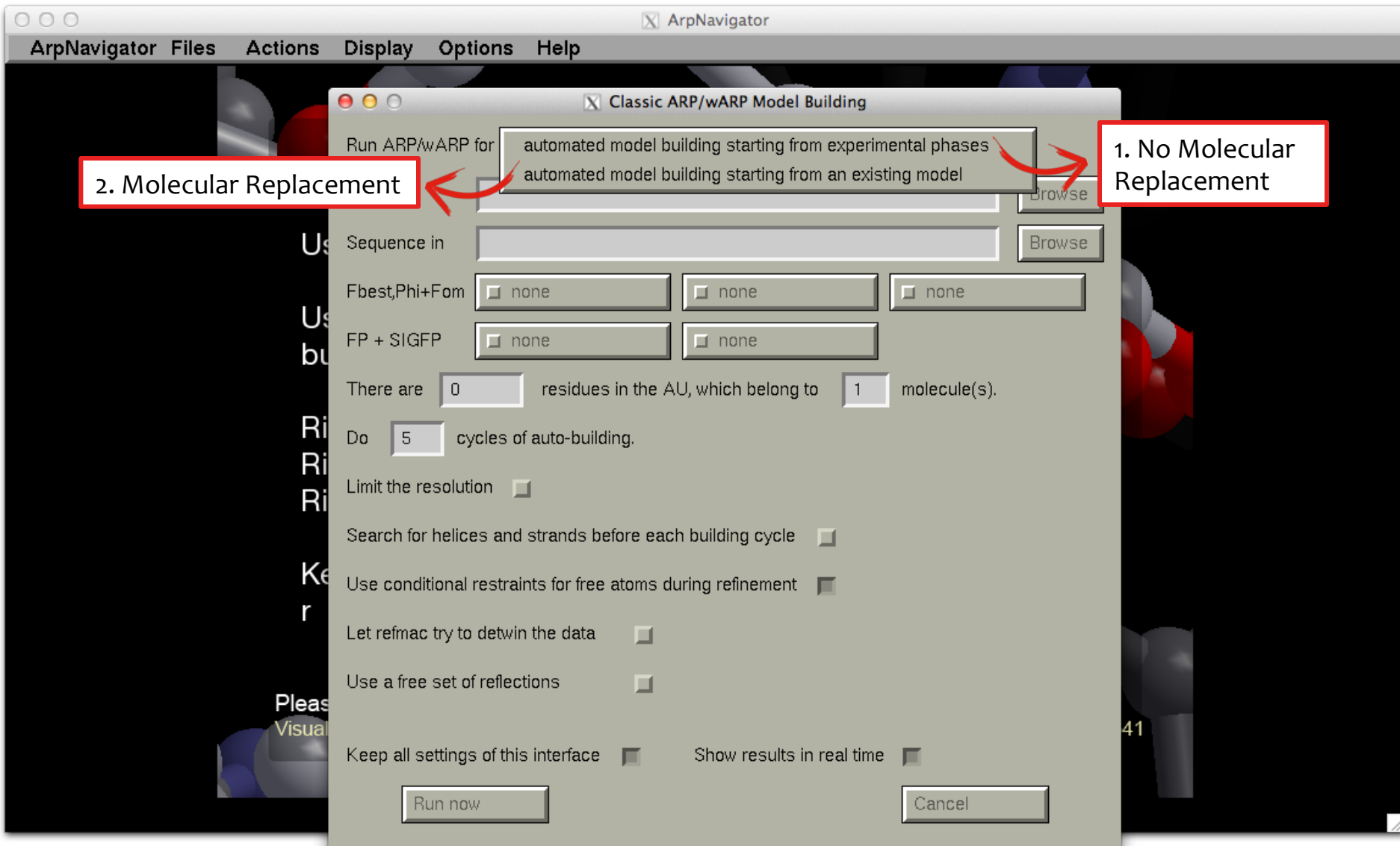
Files to use:
psp.mtz, psp.pir

MTS labels to use:
FP, SIGFP, PHIDM, FOMDM

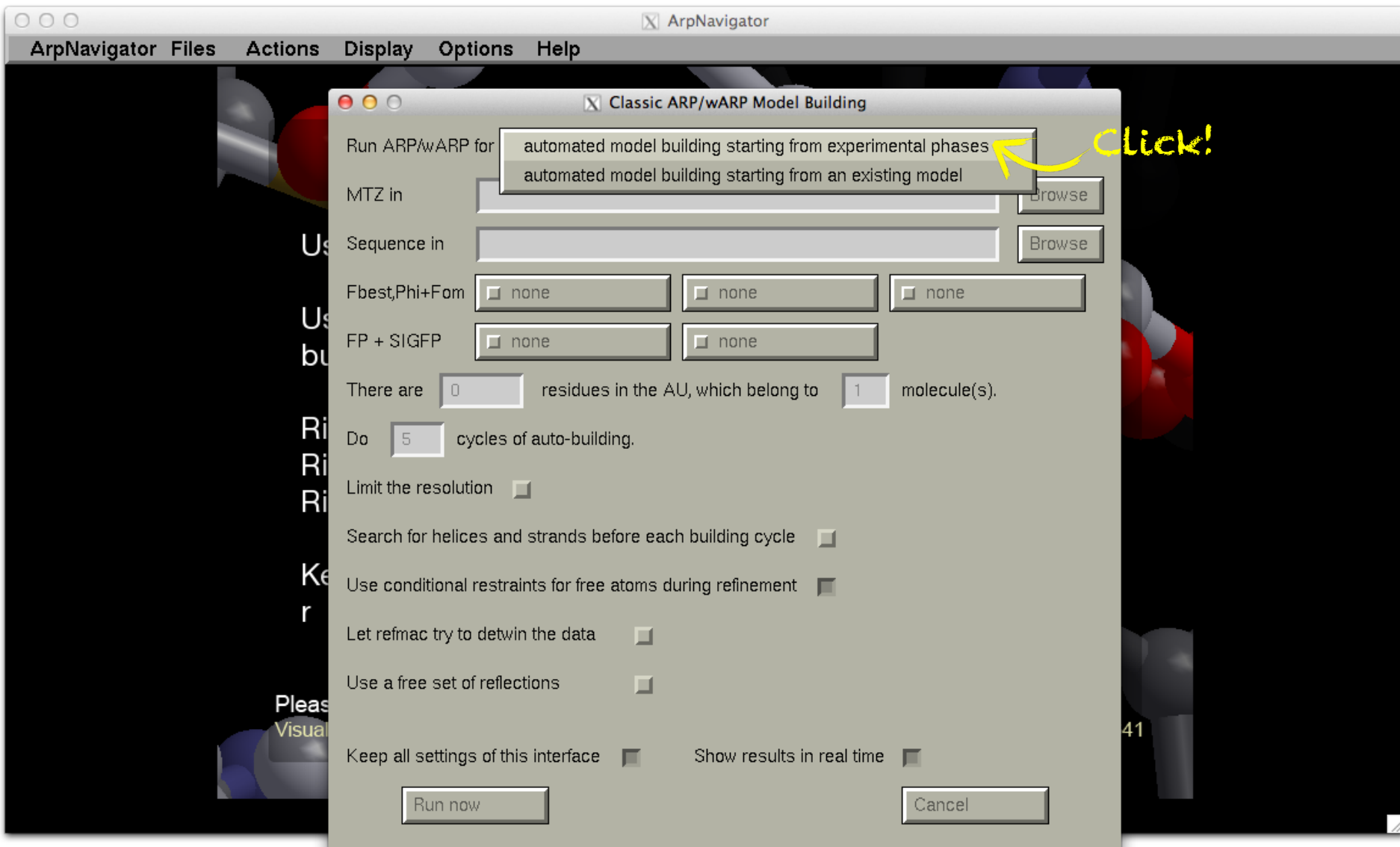
ARP/wARP: Classic Model Building (arp_tracing)



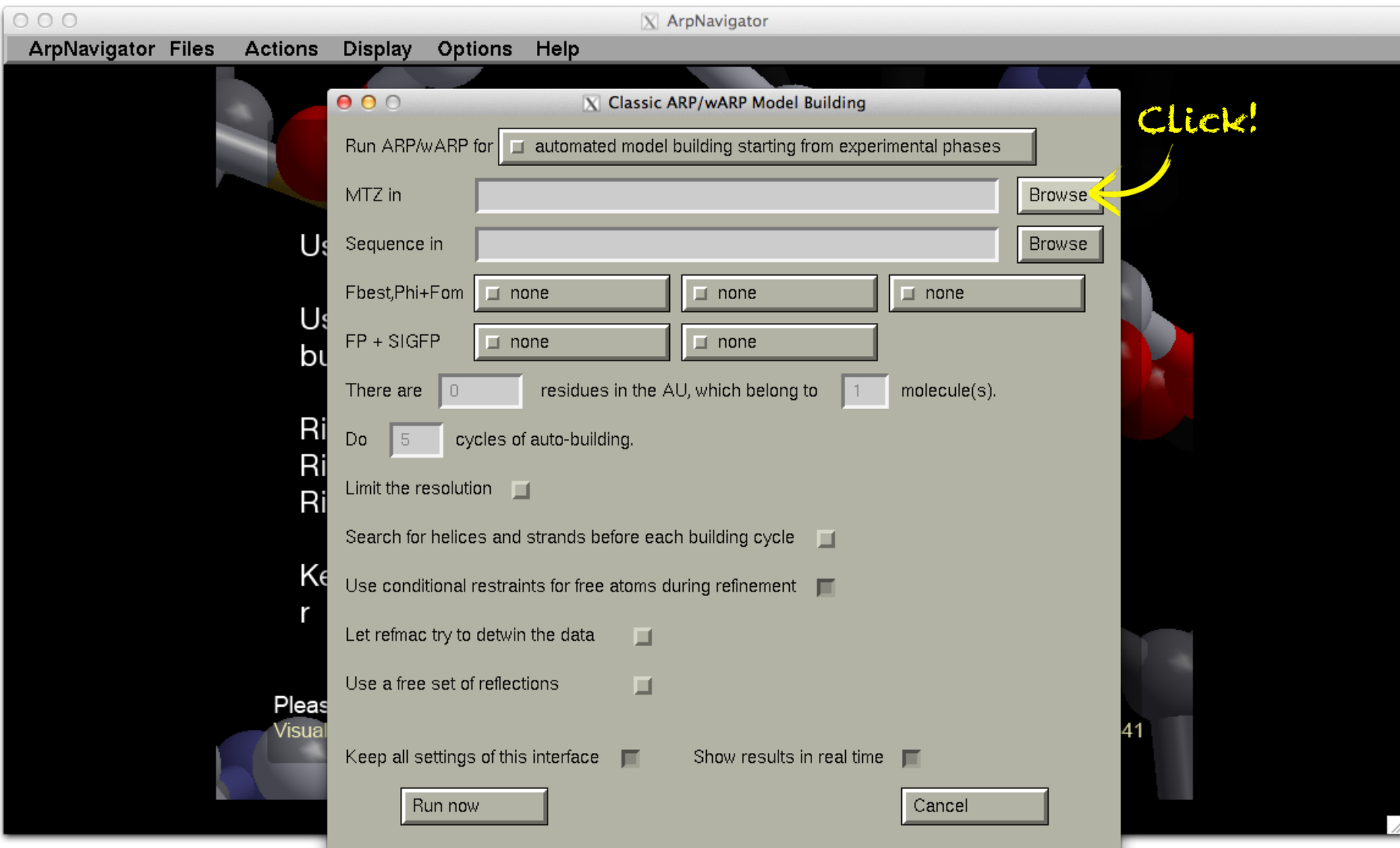
ARP/wARP: Classic Model Building (arp_tracing)



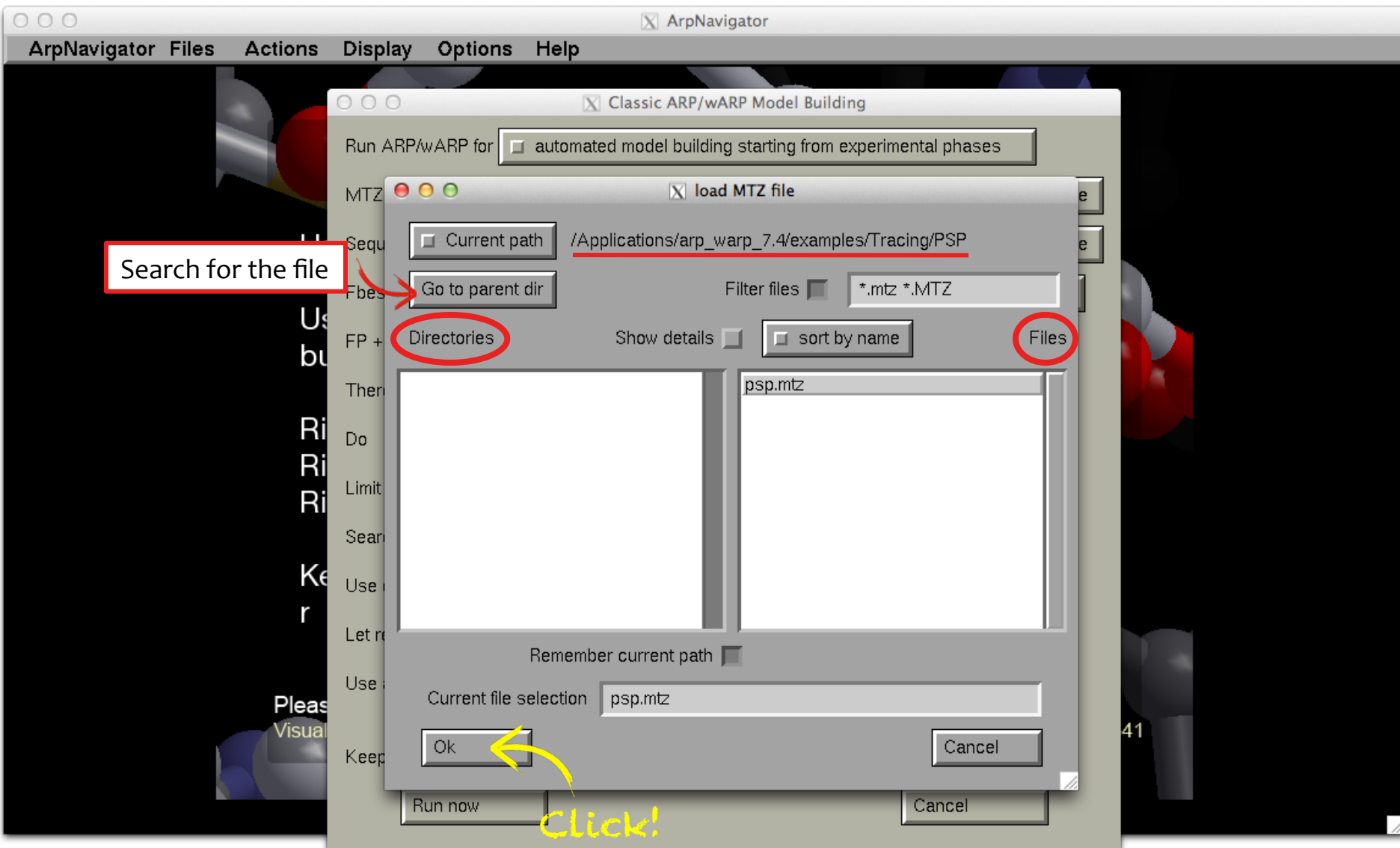
1. From Experimental Phases



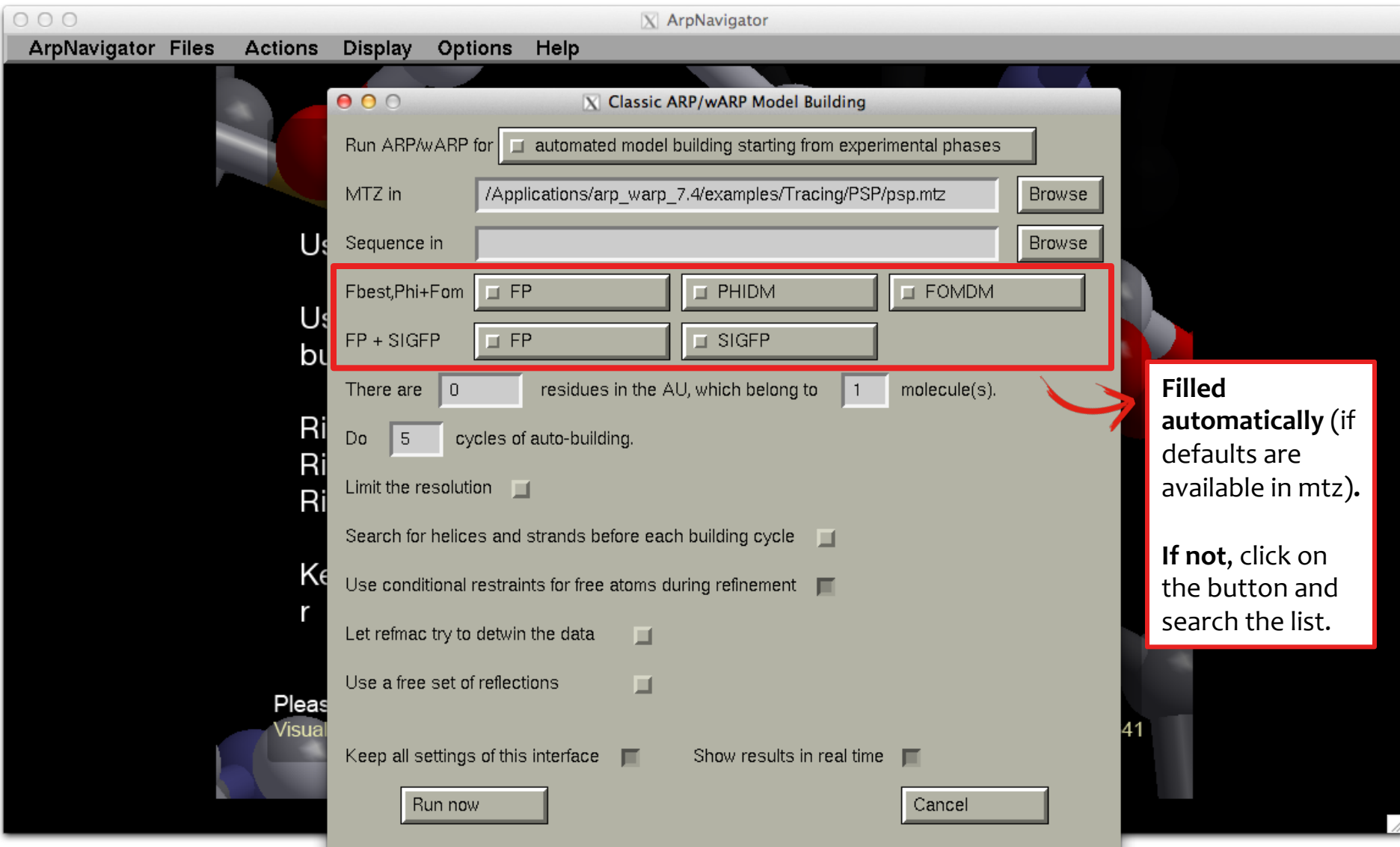
1.1. Input Files: MTZ File



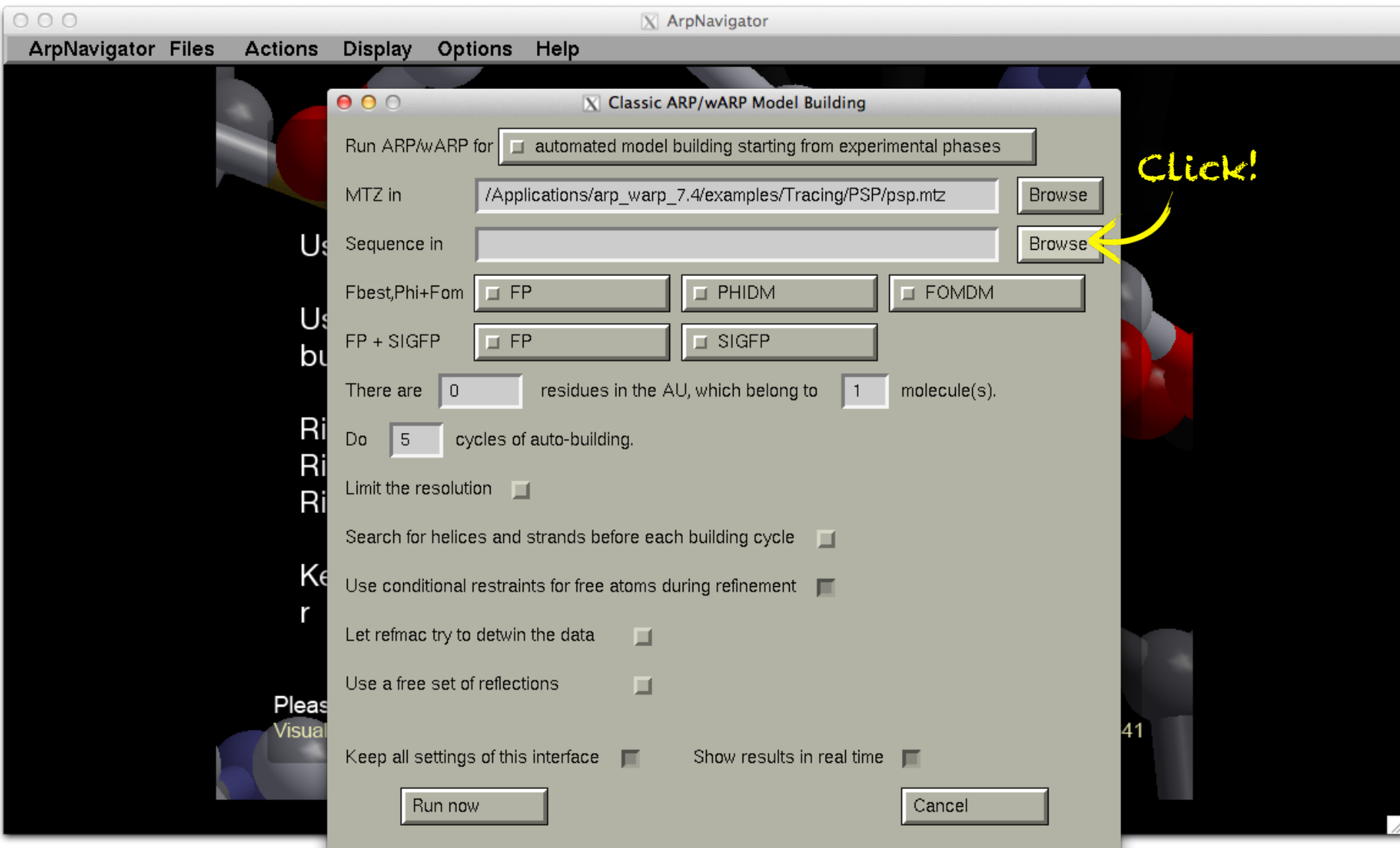
1.1. Input Files: MTZ File



1.1. Input Files: MTZ File



1.1. Input Files: Sequence



1.1. Input Files: Sequence

ArpNavigator Files Actions Display Options Help

Classic ARP/wARP Model Building

Run ARP/wARP for ☐ automated model building starting from experimental phases

MTZ ☐ load sequence file

☐ Current path /Applications/arp_warp_7.4/examples/Tracing/PSP

Filter files ☐ *.pir *.seq *.fasta

☐ Directories Show details ☐ sort by name ☐ Files

psp.fasta
psp.pir

Remember current path ☐

Current file selection psp.pir

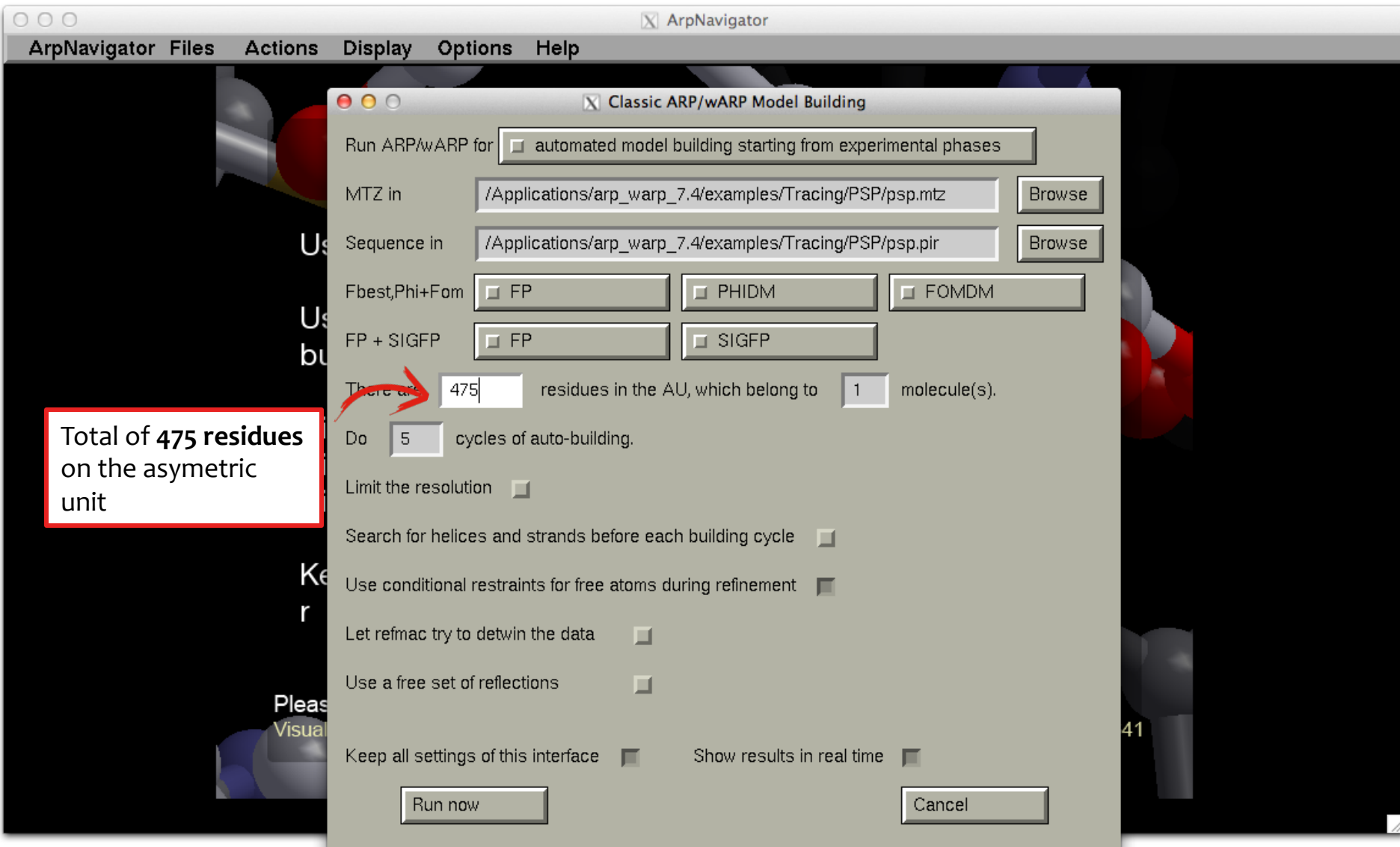
Search for the file

Click!

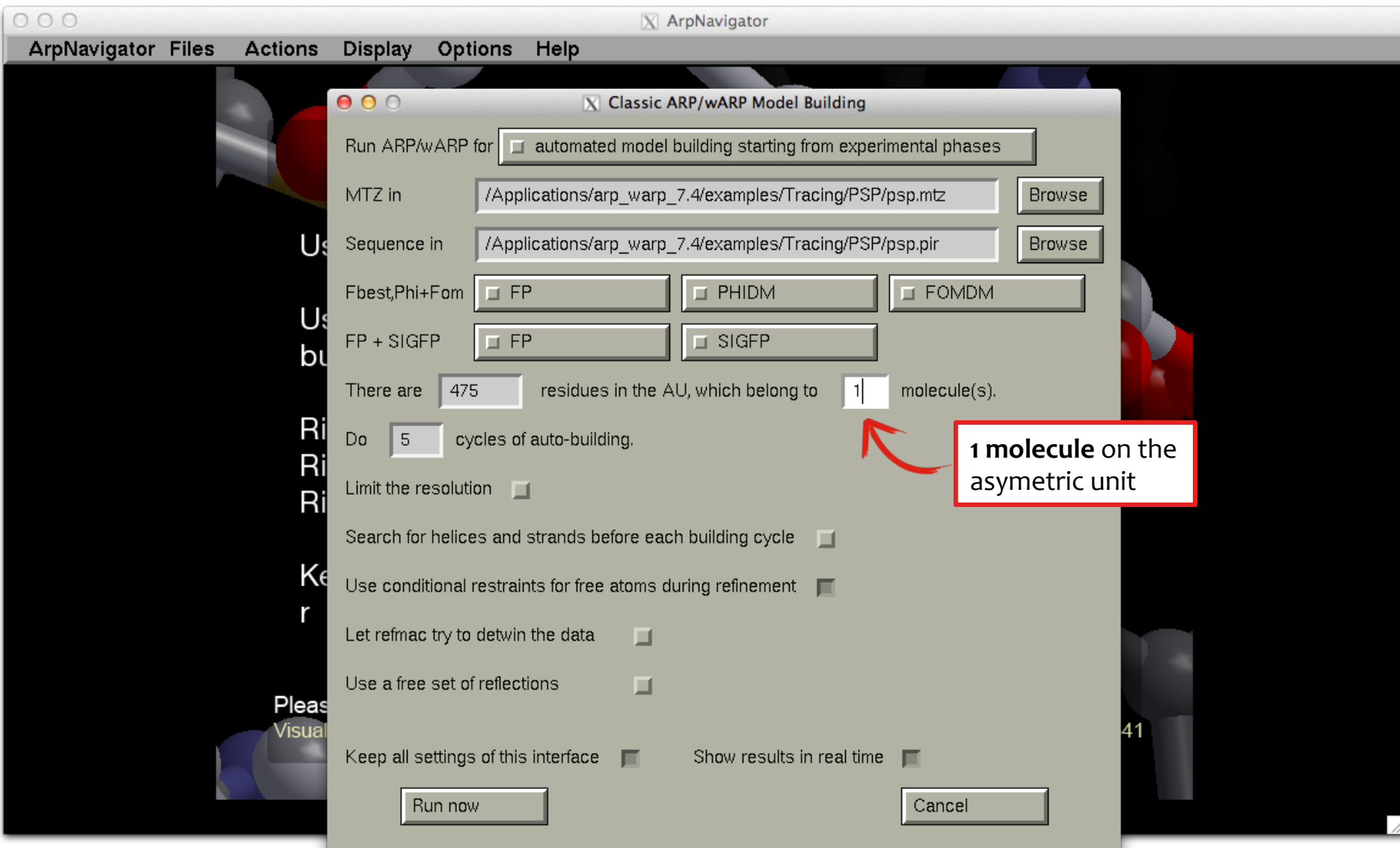
Required format (.pir):

- The first line starts with '>'
- The second line should be blank
- 1 letter code
- In the case of heteromers, separate different sequences with around 10 alanines

1.2. Required Parameters



1.2. Required Parameters



1.2. Required Parameters

Define the number of cycles of building

ArpNavigator

Files Actions Display Options Help

Classic ARP/wARP Model Building

Run ARP/wARP for ☐ automated model building starting from experimental phases

MTZ in

Sequence in

Fbest,Phi+Fom ☐ FP ☐ PHIDM ☐ FOMDM

FP + SIGFP ☐ FP ☐ SIGFP

There are residues in the AU, which belong to molecule(s).

Do cycles of auto-building.

Limit the resolution ☐

Search for helices and strands before each building cycle ☐

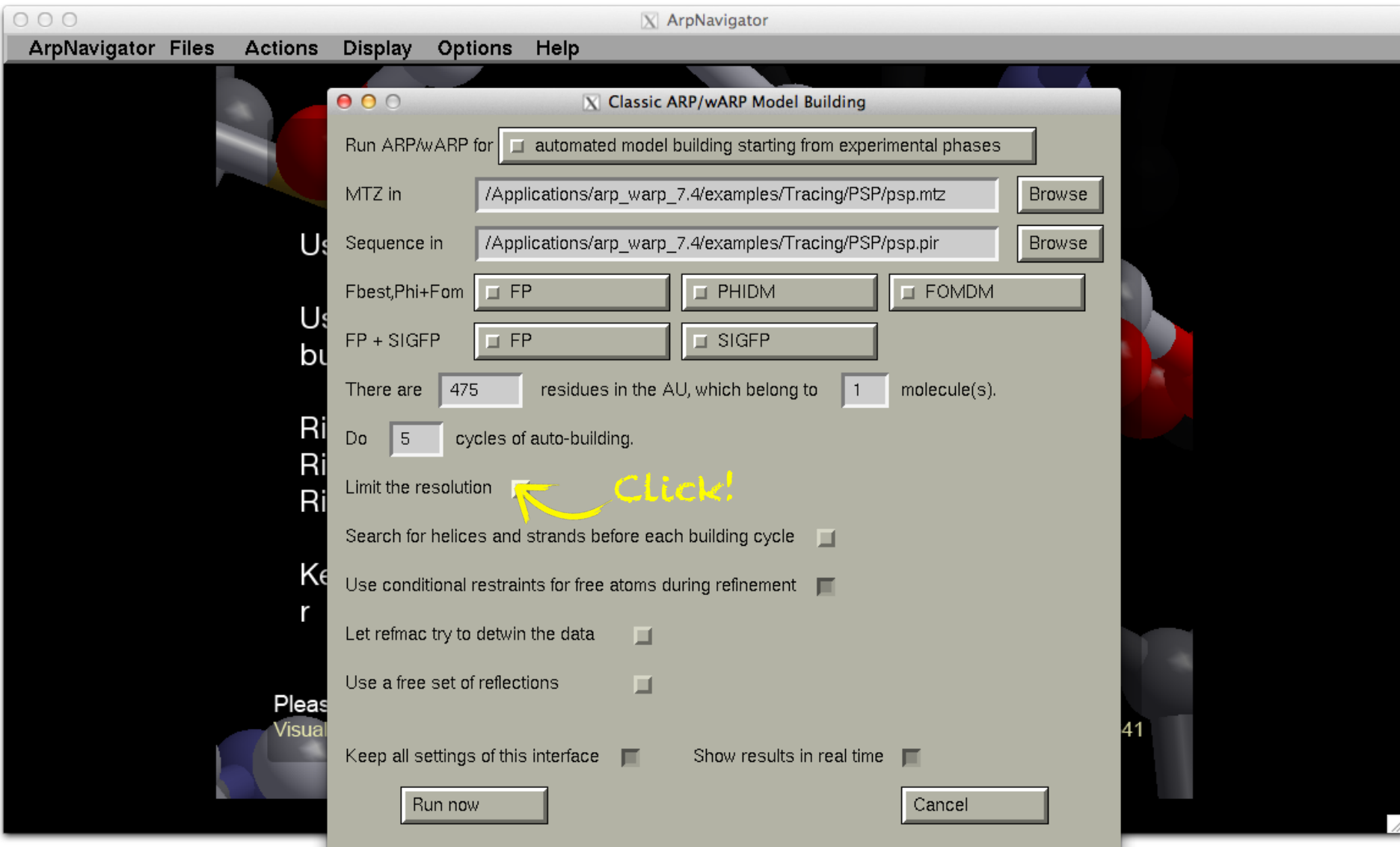
Use conditional restraints for free atoms during refinement ☐

Let refmac try to detwin the data ☐

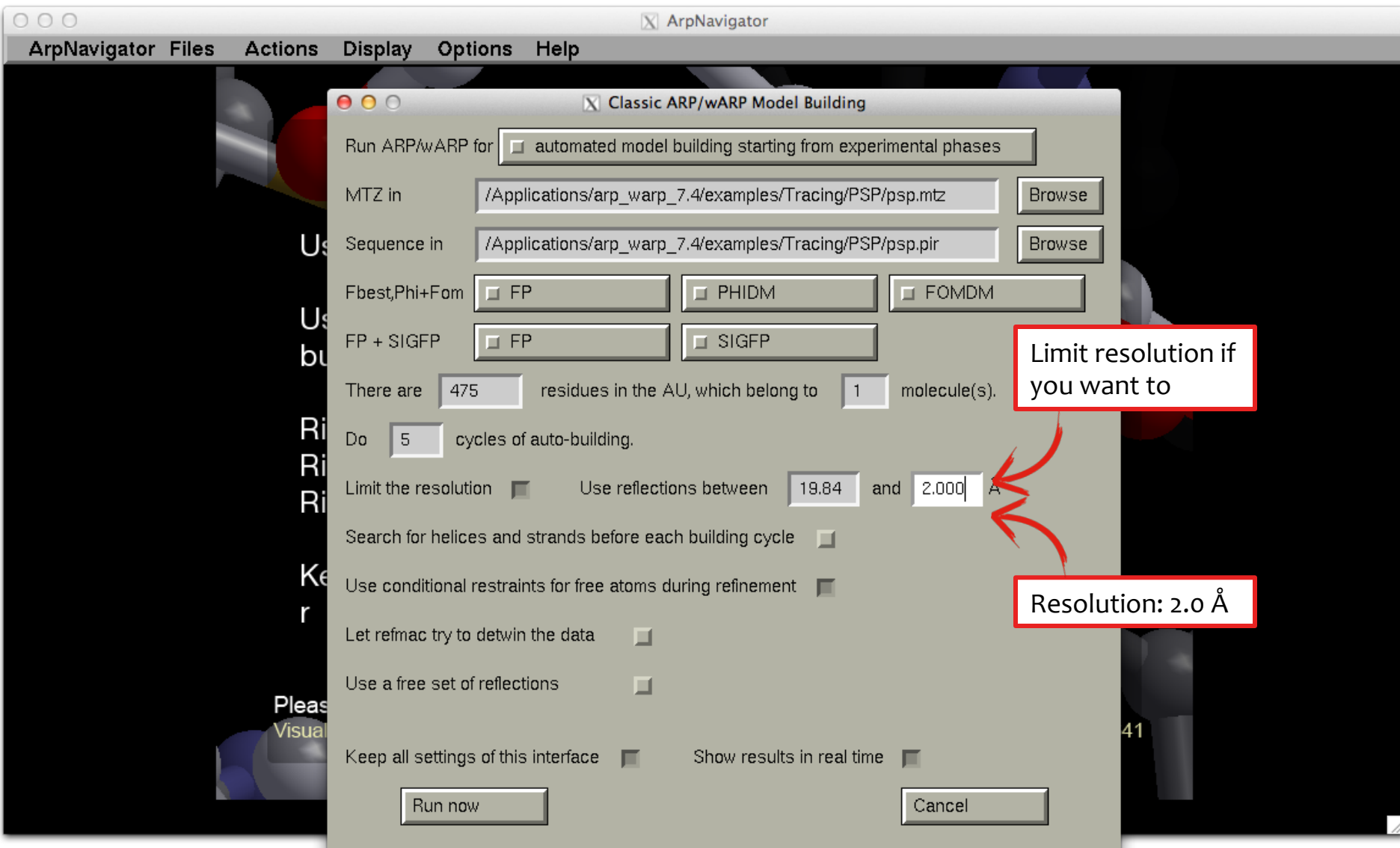
Use a free set of reflections ☐

Keep all settings of this interface ☐ Show results in real time ☐

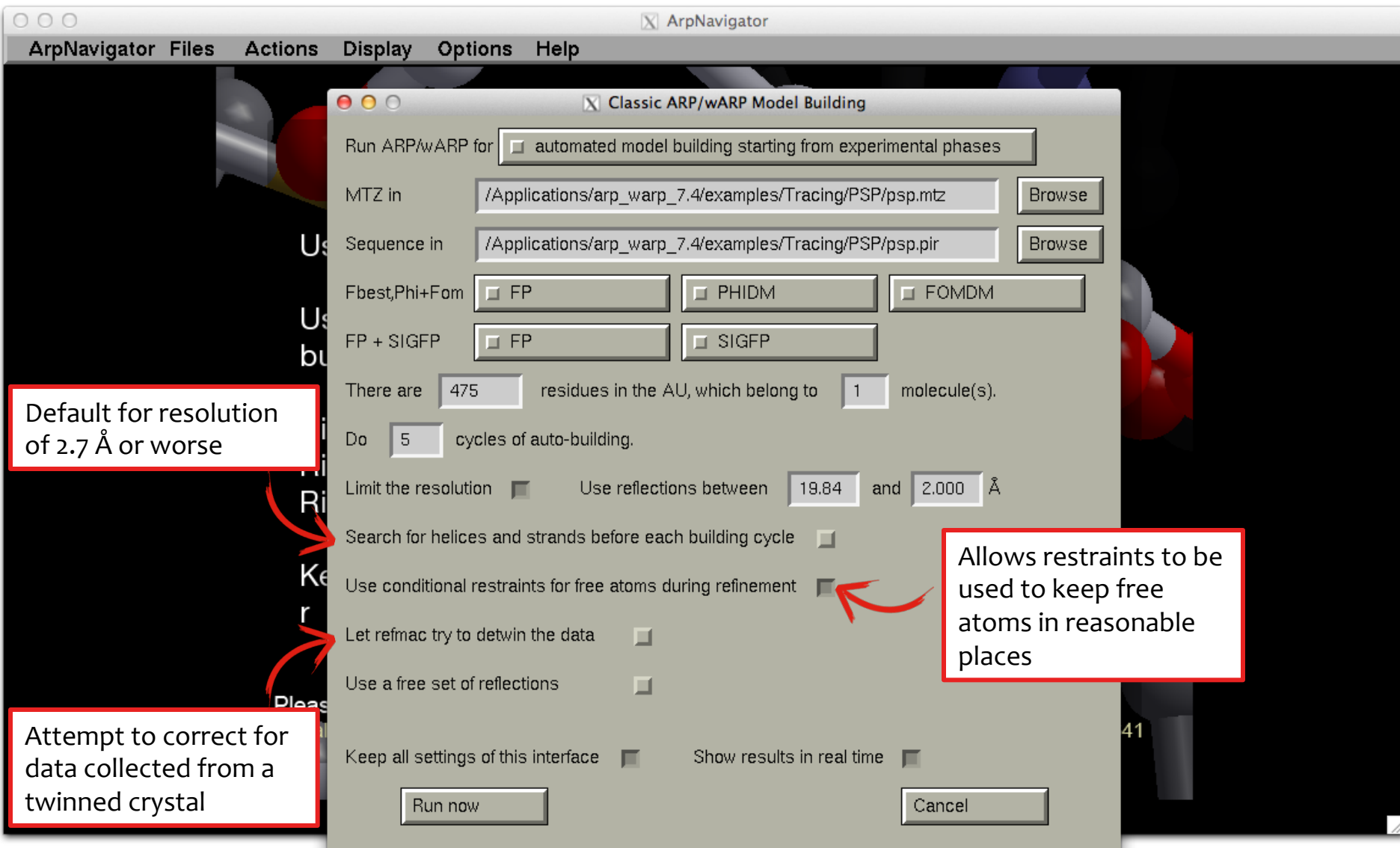
1.3. Resolution



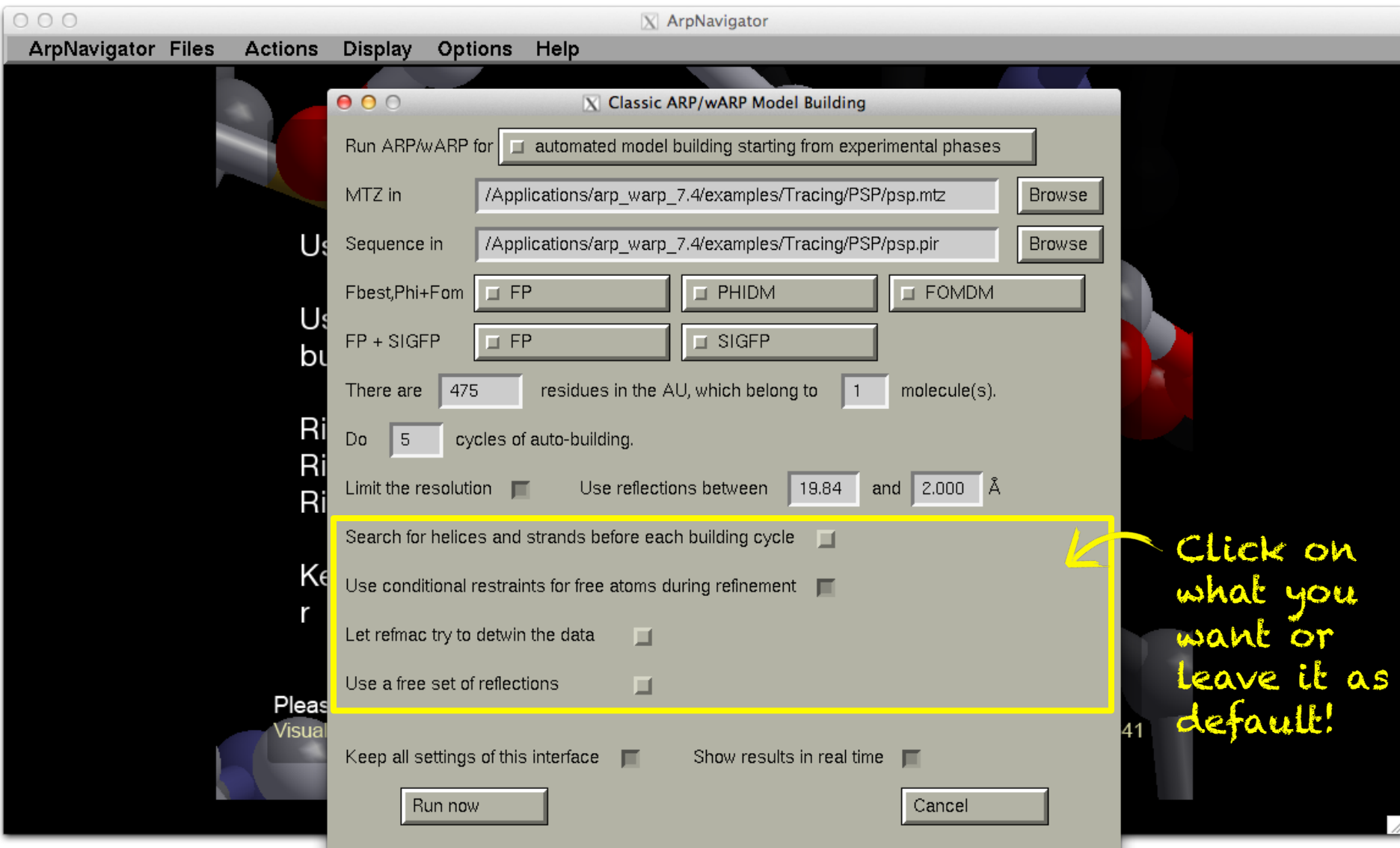
1.3. Resolution



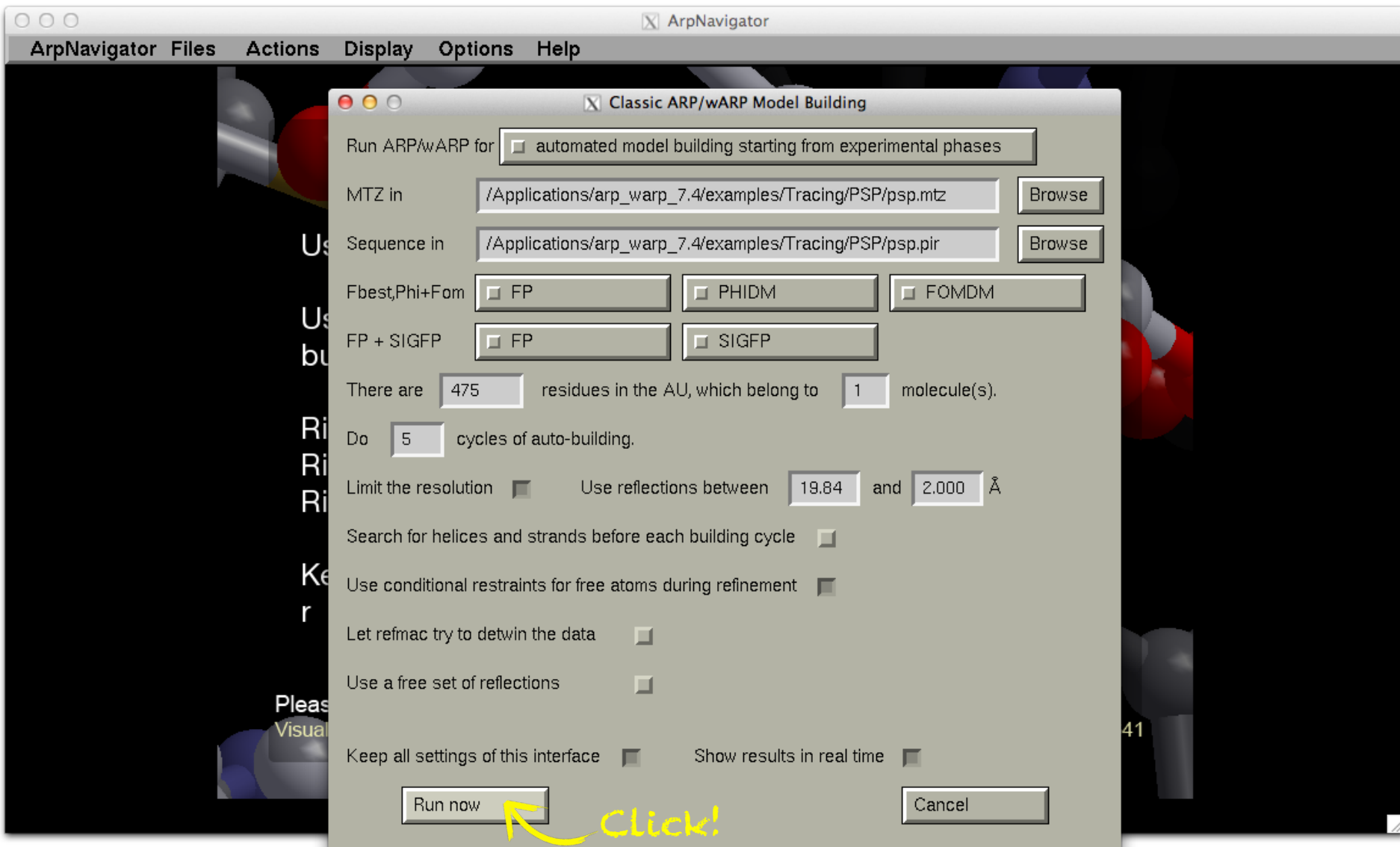
1.4. Flow Parameters



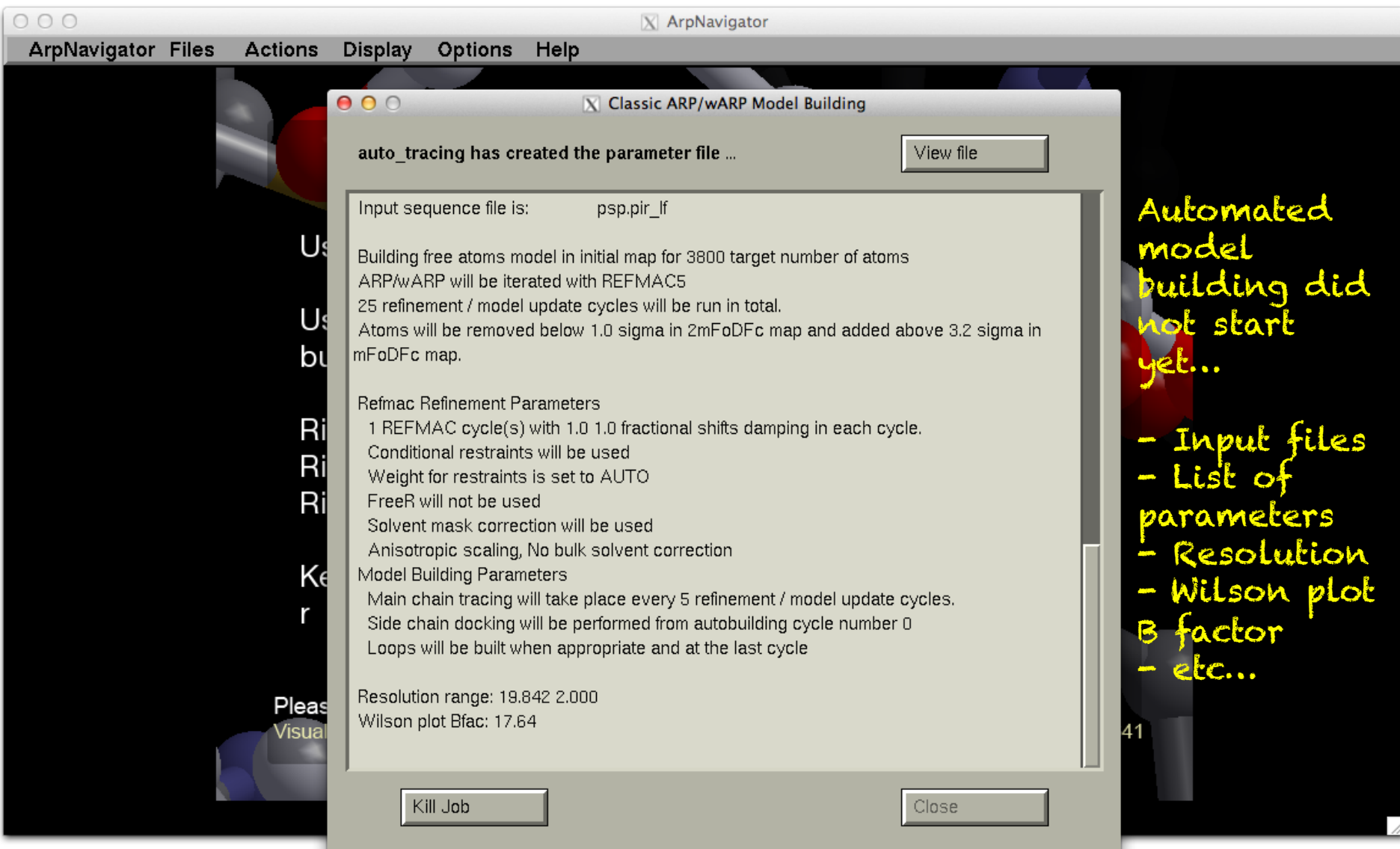
1.4. Flow Parameters



1.5. Run The Job



1.5. Run The Job – Log File



Automated
model
building did
not start
yet...

- Input files
- List of parameters
- Resolution
- Wilson plot
- B factor
- etc...

1.5. Run The Job – Log File

Automated
model building
started!

- Model evolution
- Model completeness
- Fragments
- Residues docked into sequence
- Loop building
- R-factor
- Sequence coverage

ArpNavigator Files Actions Display Options Help

Classic ARP/wARP Model Building

auto_tracing has created the parameter file ... [View file](#)

Building Cycle 0 Atomic shape factors 1.99 1.74

Round 1: 350 peptides, 45 chains. Longest chain 34 peptides. Score 0.591
Round 2: 382 peptides, 34 chains. Longest chain 36 peptides. Score 0.726
Round 3: 382 peptides, 27 chains. Longest chain 50 peptides. Score 0.769
Round 4: 403 peptides, 22 chains. Longest chain 56 peptides. Score 0.819
Round 5: 416 peptides, 22 chains. Longest chain 48 peptides. Score 0.831
Taking the results from Round 5

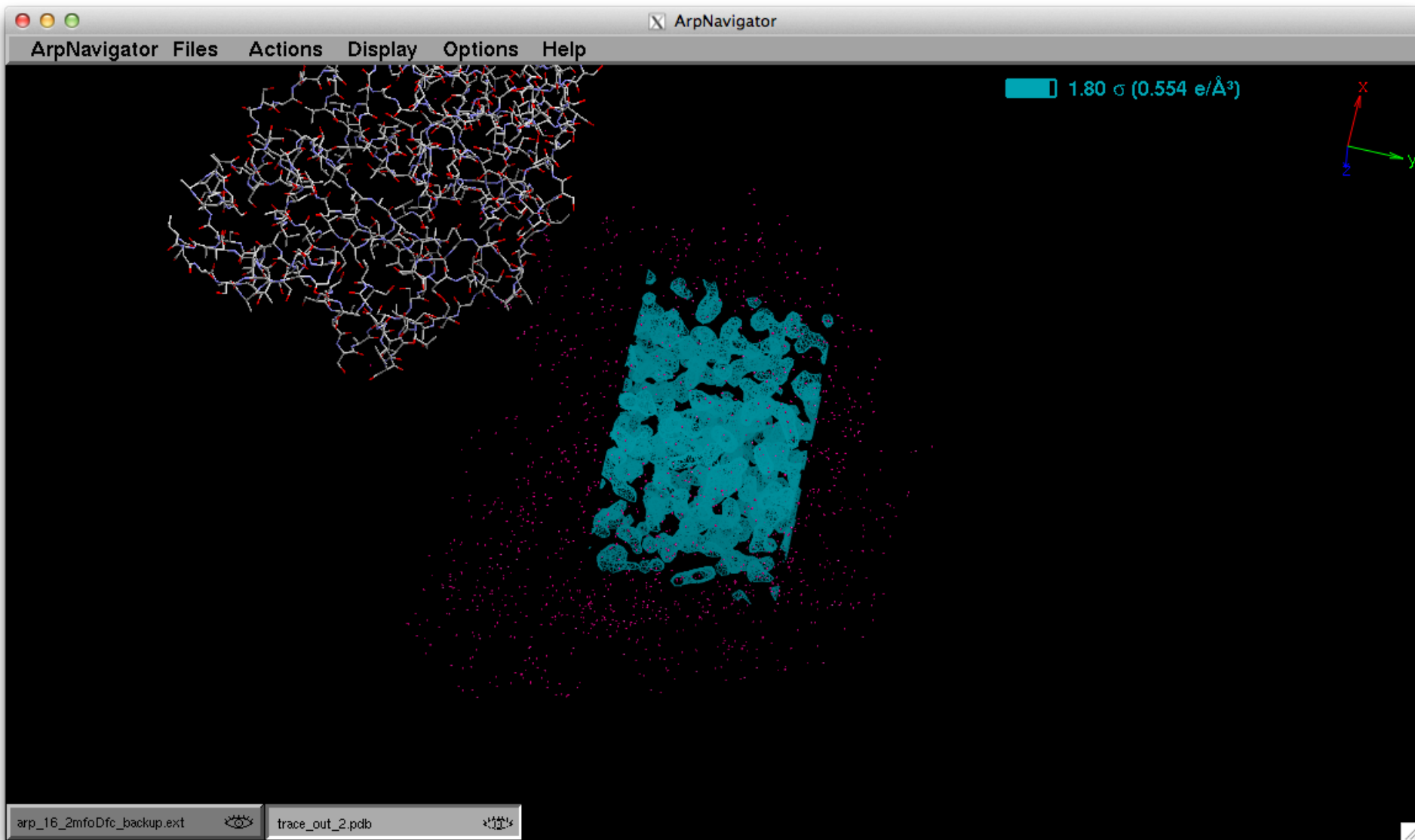
Chains 22, Residues 394, Estimated correctness of the model 97.7 %
2 chains (74 residues) have been docked in sequence

42571 reflections (99.67 % complete) and 4857 restraints for refining 3894 atoms.
3000 conditional restraints added.
Observations/parameters ratio is 2.73

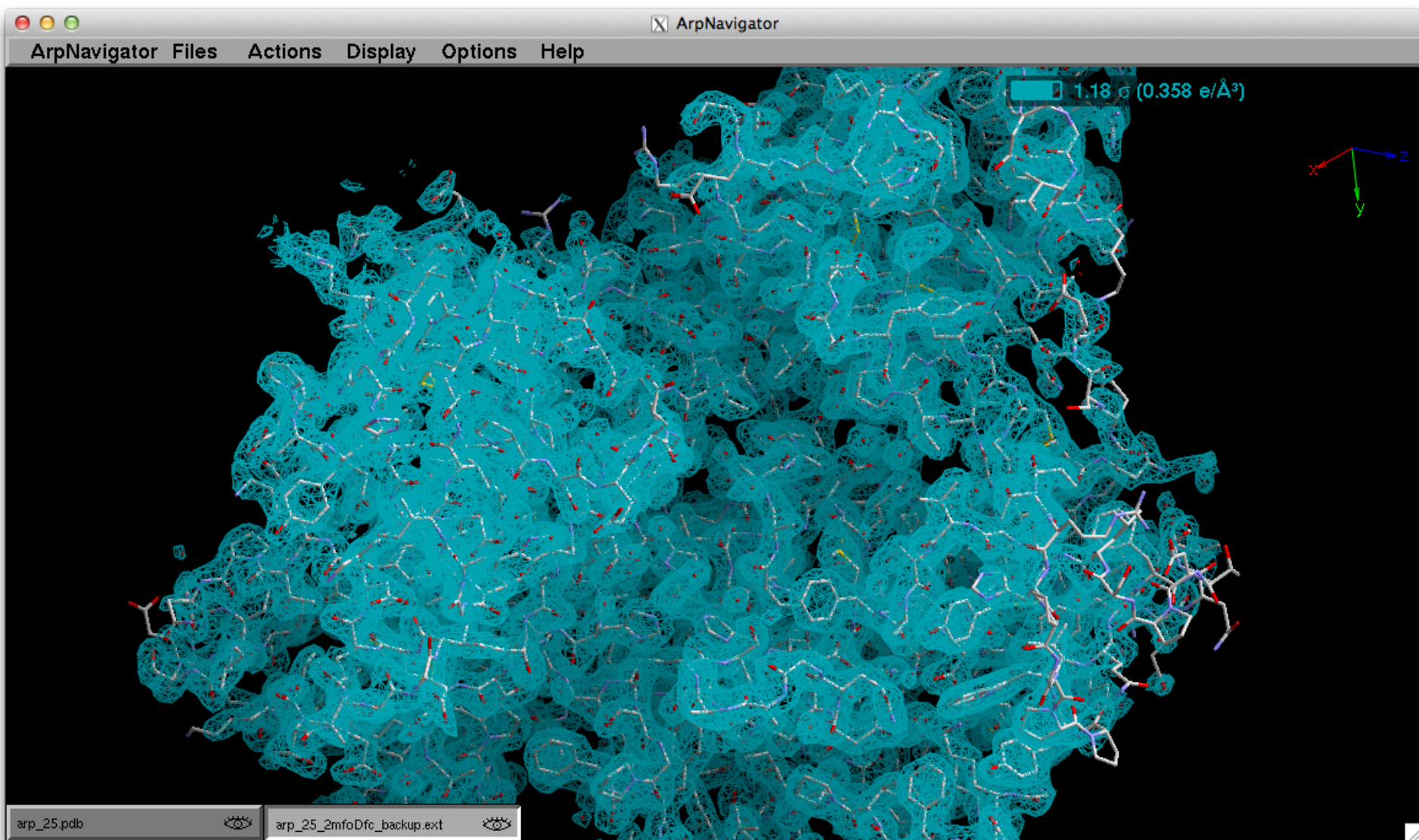
Cycle 1: After refinac, R = 0.3466 (Rfree = 0.000) for 3894 atoms.
Found 133 (133 requested) and removed 66 (66 requested) atoms.
Cycle 2: After refinac, R = 0.2938 (Rfree = 0.000) for 3959 atoms.
Found 135 (135 requested) and removed 67 (67 requested) atoms.
Cycle 3: After refinac, R = 0.2625 (Rfree = 0.000) for 4021 atoms.
Found 137 (137 requested) and removed 59 (68 requested) atoms.
Cycle 4: After refinac, R = 0.2410 (Rfree = 0.000) for 4096 atoms.
Found 111 (140 requested) and removed 52 (70 requested) atoms.

[Kill Job](#) [Close](#) **Click!**

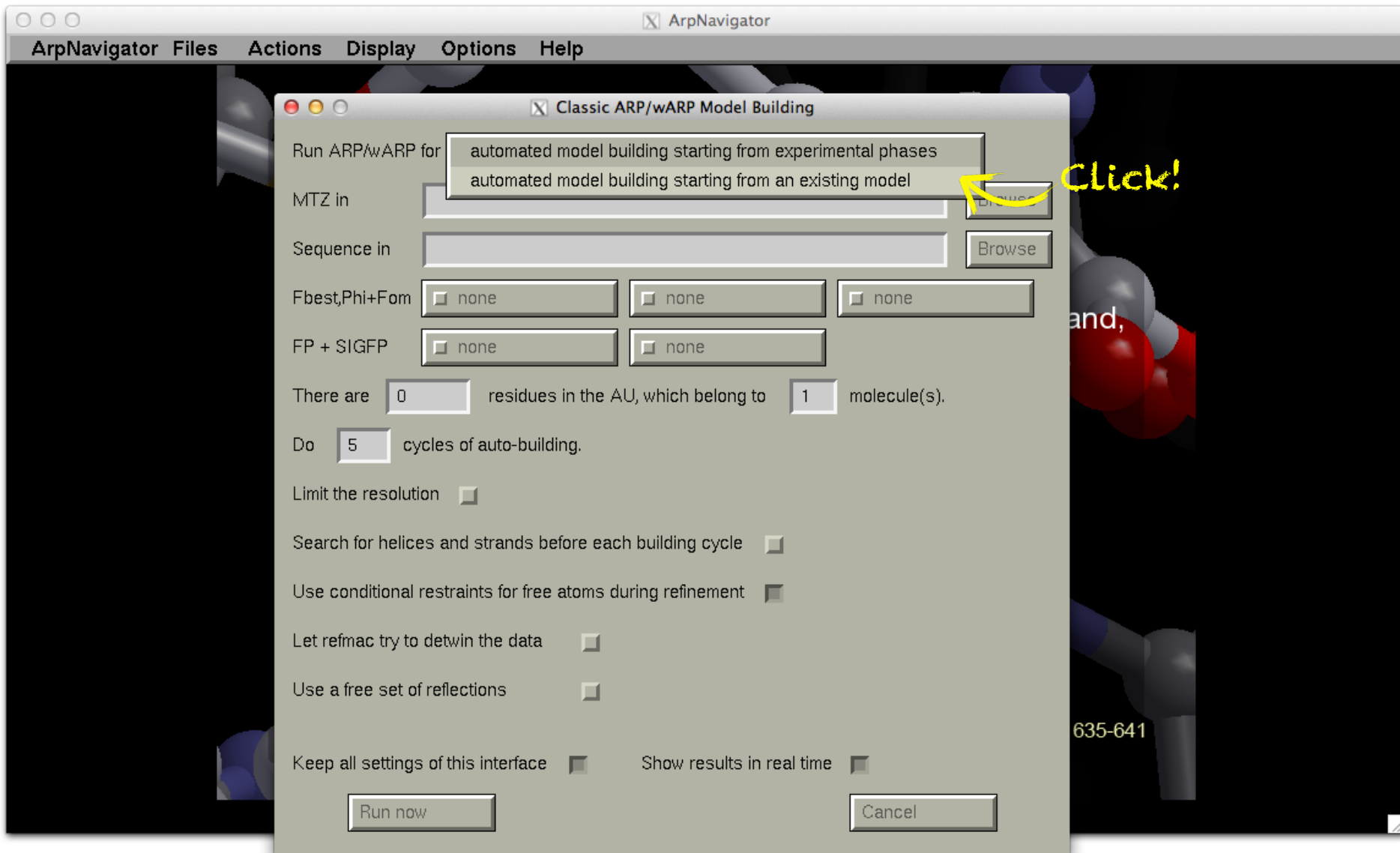
1.5. Run The Job – Live Model Building



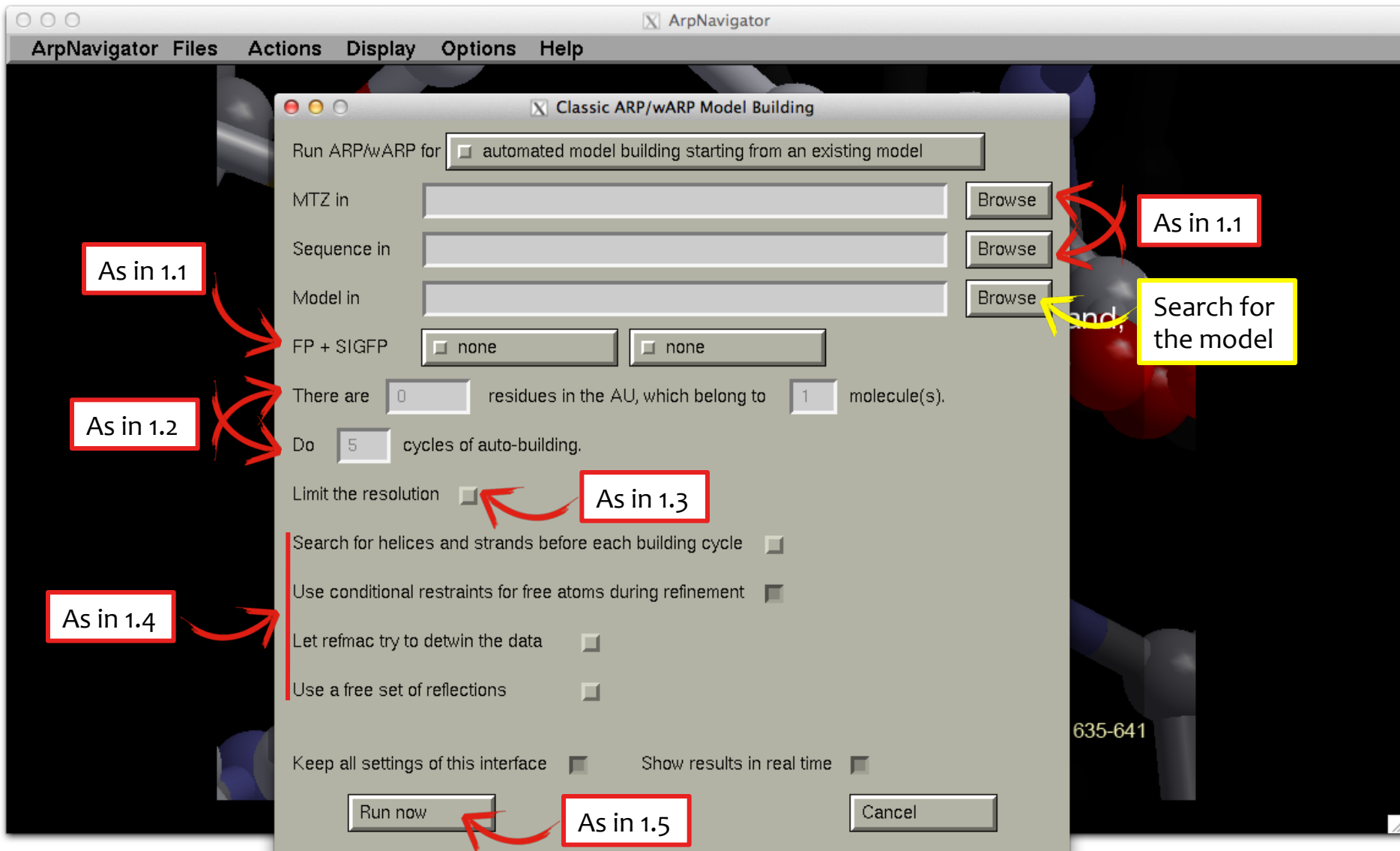
1.5. Run The Job – Live Model Building



2. Molecular Replacement



2. Molecular Replacement



For any questions...

The Developers

Contact us anytime!

Victor Lamzin Philipp Heuser

Ioan Vancea Joana Pereira

Daria Beshnova

Or just visit our website!

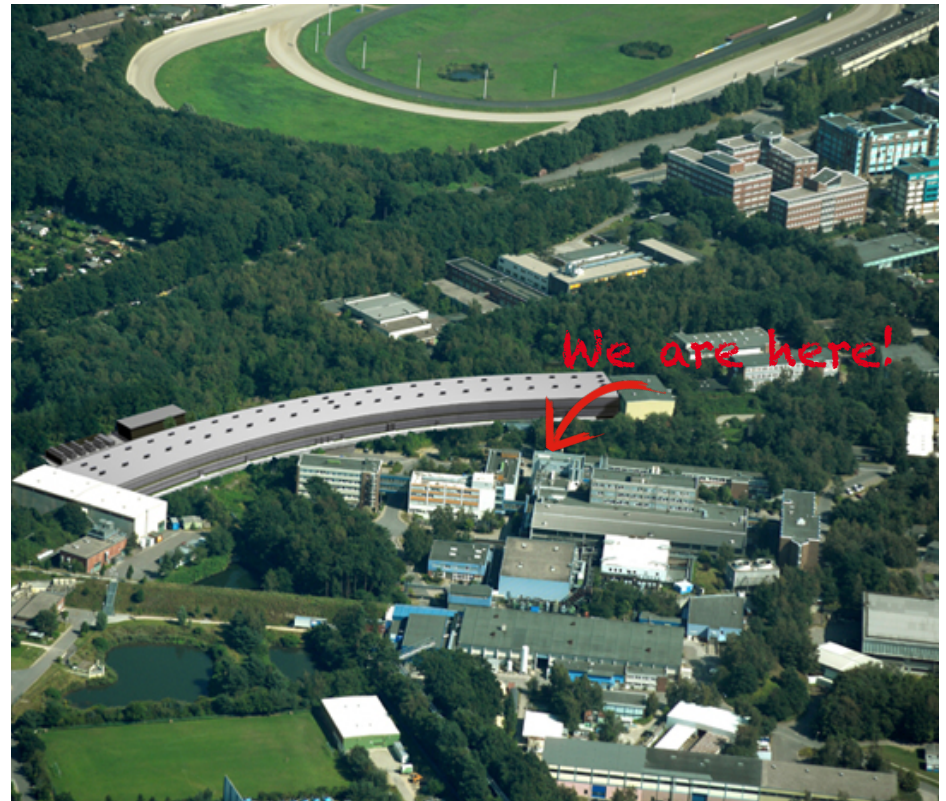
<http://www.embl-hamburg.de/ARP/>



User guide

Frequently asked questions

Tutorials



EMBL @ Desy Hamburg

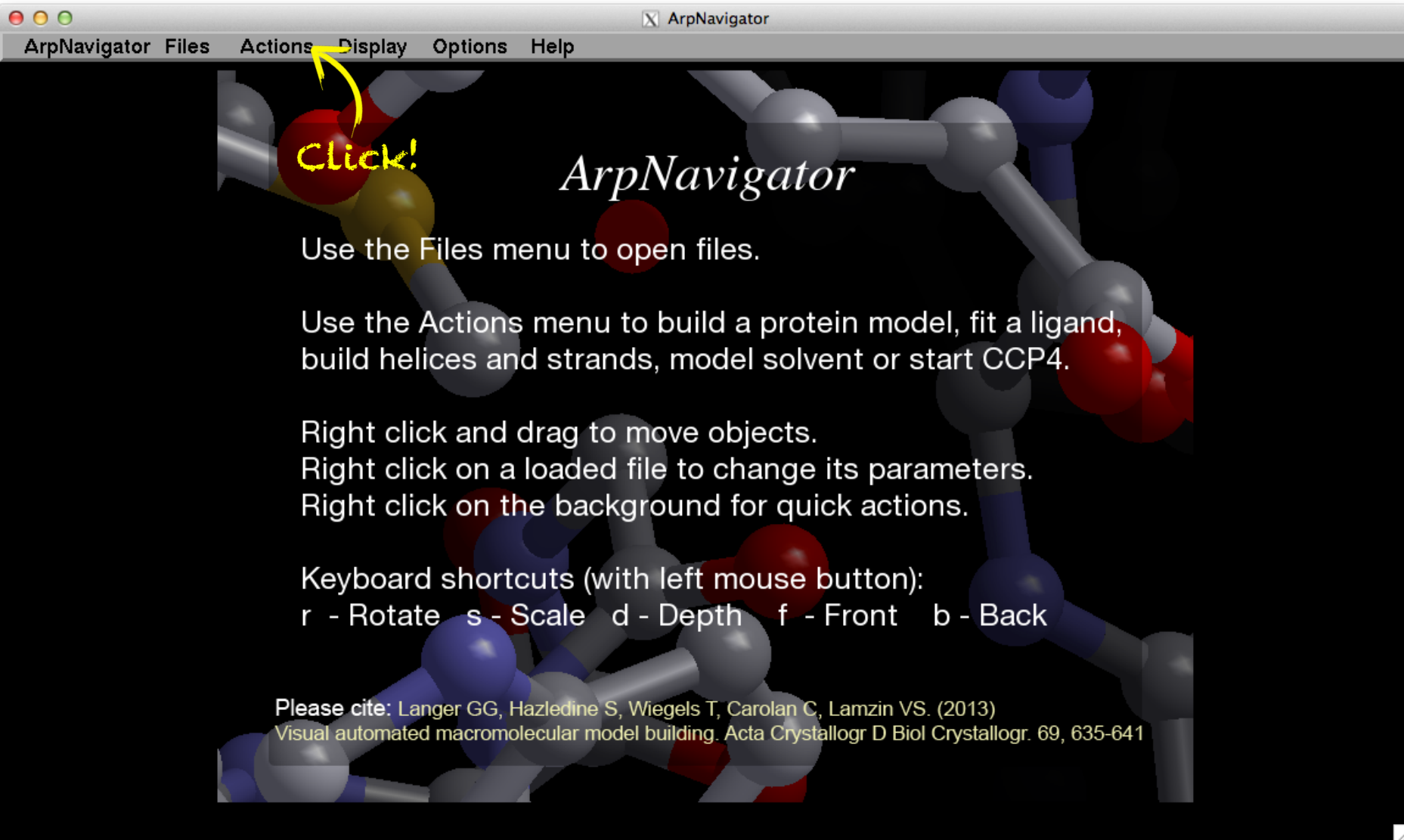
Automated Building of Secondary Structure Elements With ArpNavigator

A Click-on Tutorial

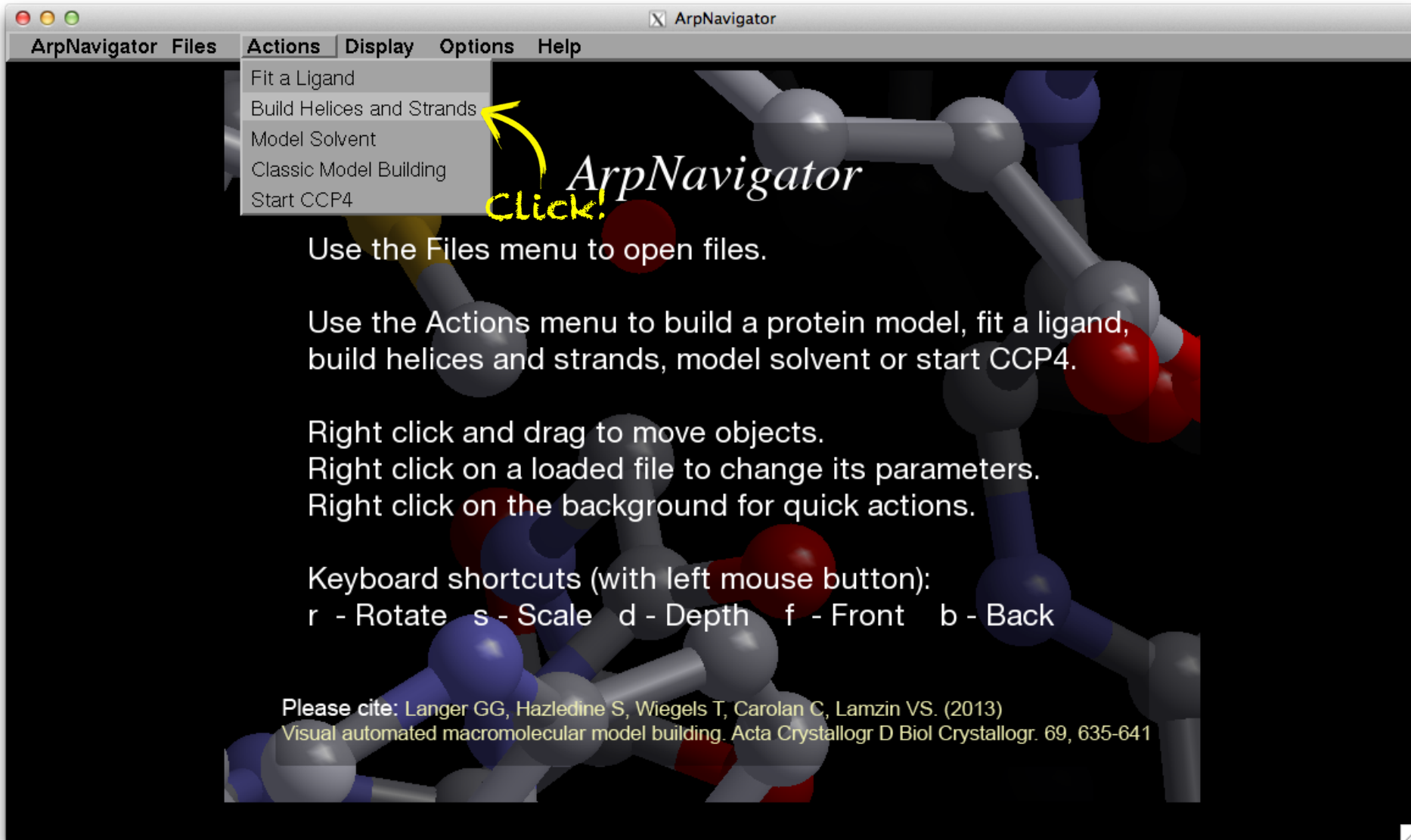
EMBL
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Where to go...



ARP/wARP: Secondary Structure (albe)



The screenshot shows the ArpNavigator application window. The title bar reads 'ArpNavigator'. The menu bar includes 'ArpNavigator', 'Files', 'Actions', 'Display', 'Options', and 'Help'. The 'Actions' menu is open, showing options: 'Fit a Ligand', 'Build Helices and Strands', 'Model Solvent', 'Classic Model Building', and 'Start CCP4'. A yellow arrow points to 'Build Helices and Strands' with the text 'Click!' next to it. The background displays a 3D molecular model of a protein structure with grey sticks, blue spheres, and red spheres.

ArpNavigator

Click!

Use the Files menu to open files.

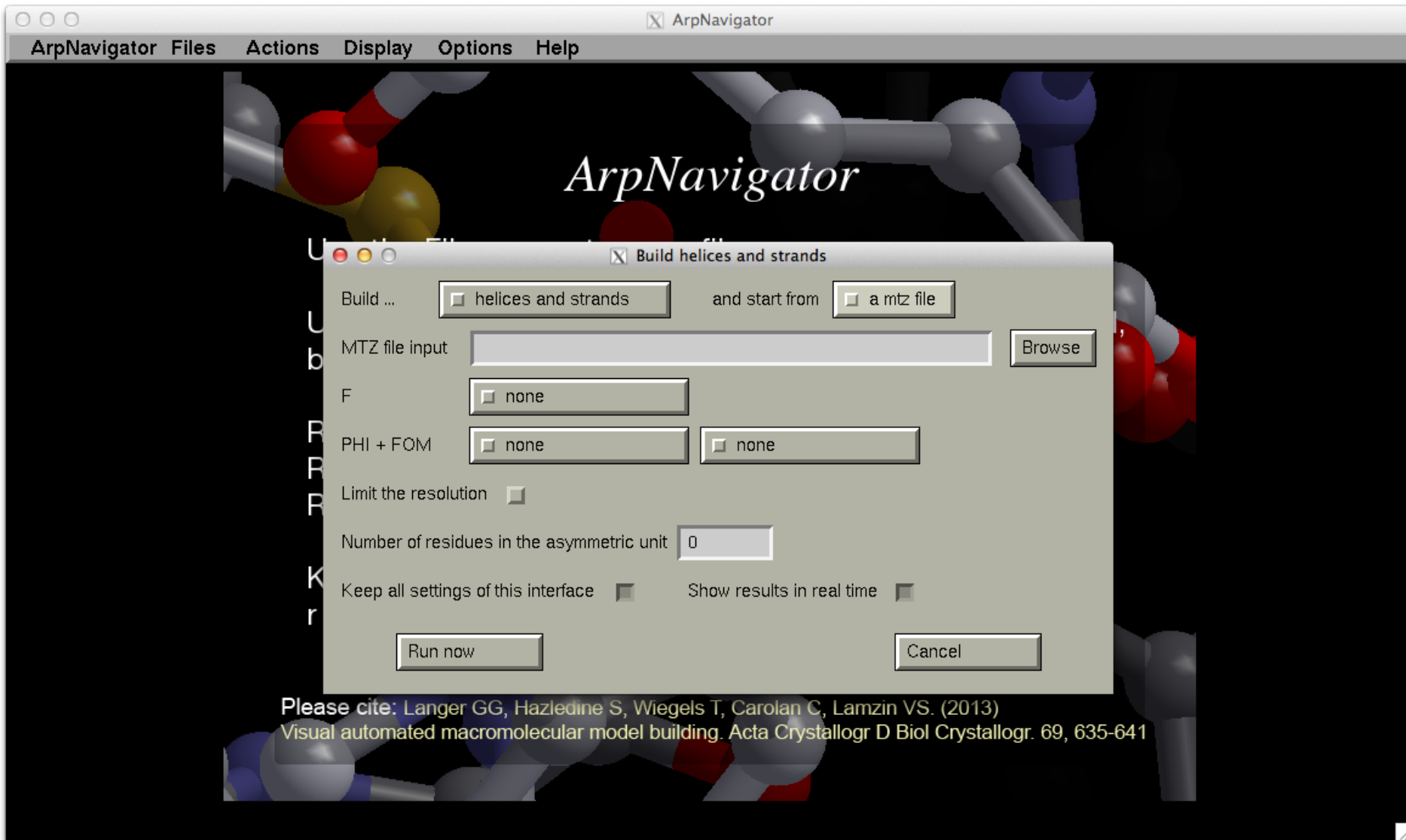
Use the Actions menu to build a protein model, fit a ligand, build helices and strands, model solvent or start CCP4.

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.

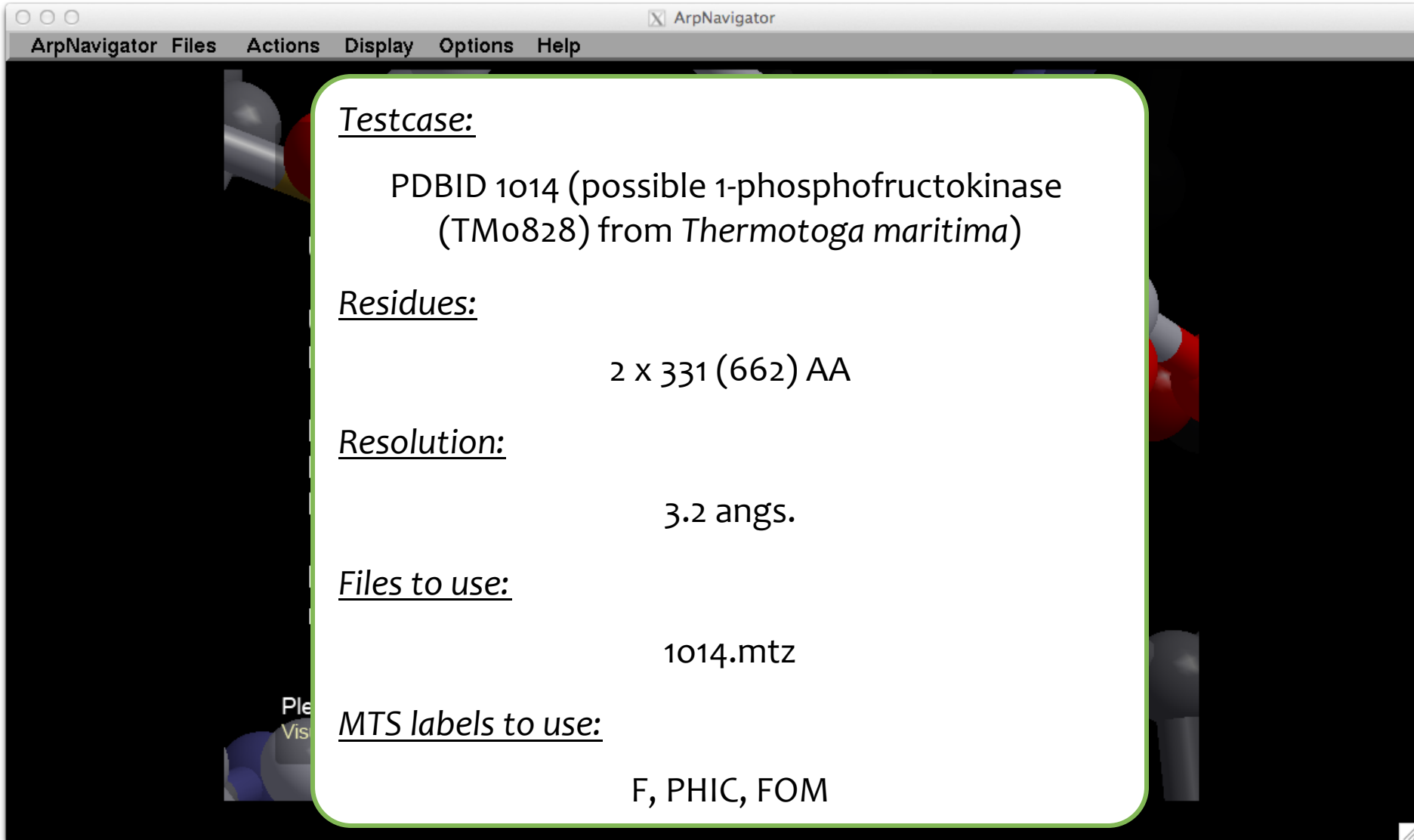
Keyboard shortcuts (with left mouse button):
r - Rotate s - Scale d - Depth f - Front b - Back

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

ARP/wARP: Secondary Structure (albe)



ARP/wARP: Secondary Structure (albe)



ArpNavigator Files Actions Display Options Help

Testcase:

PDBID 1014 (possible 1-phosphofructokinase (TMO828) from *Thermotoga maritima*)

Residues:

2 x 331 (662) AA

Resolution:

3.2 ang.

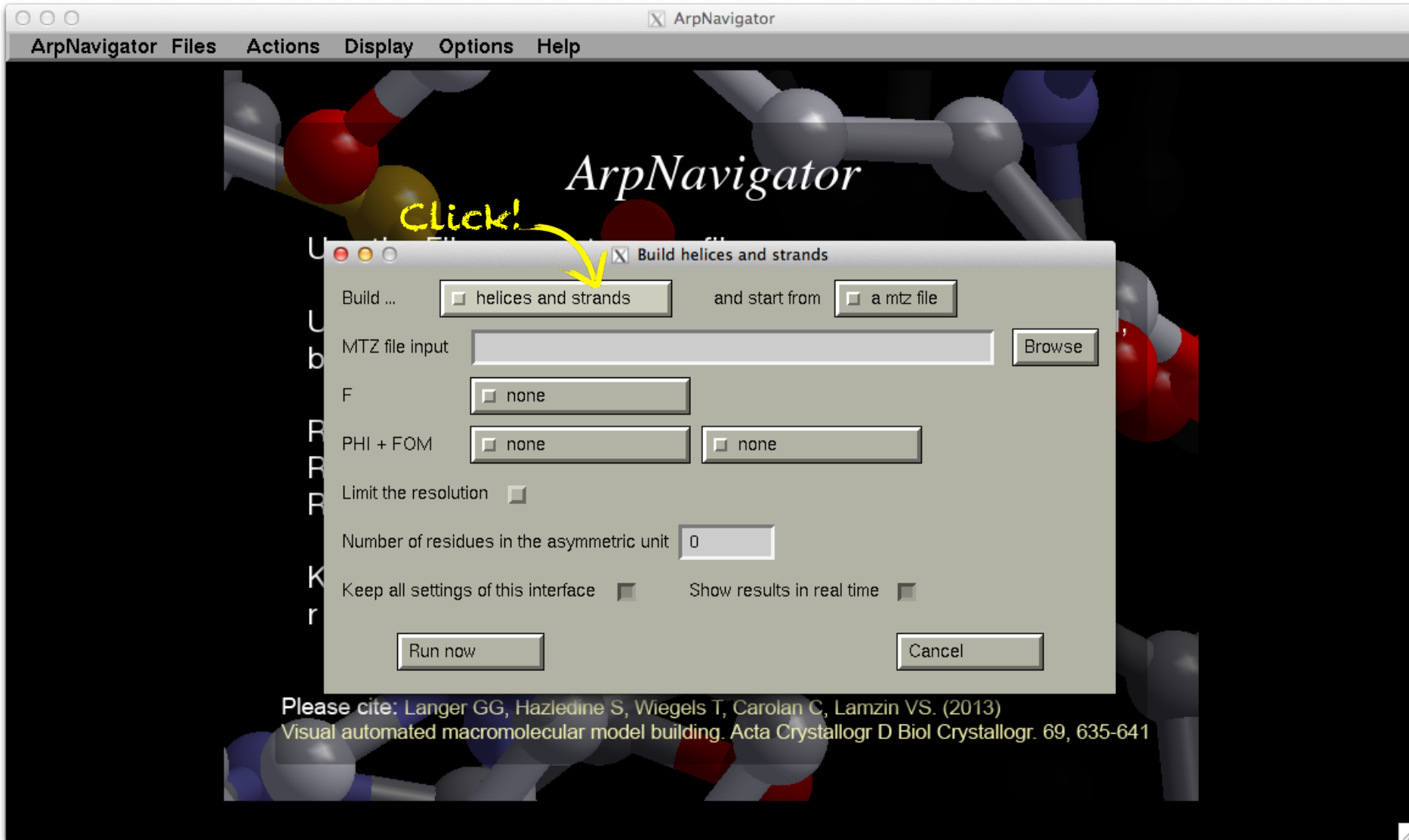
Files to use:

1014.mtz

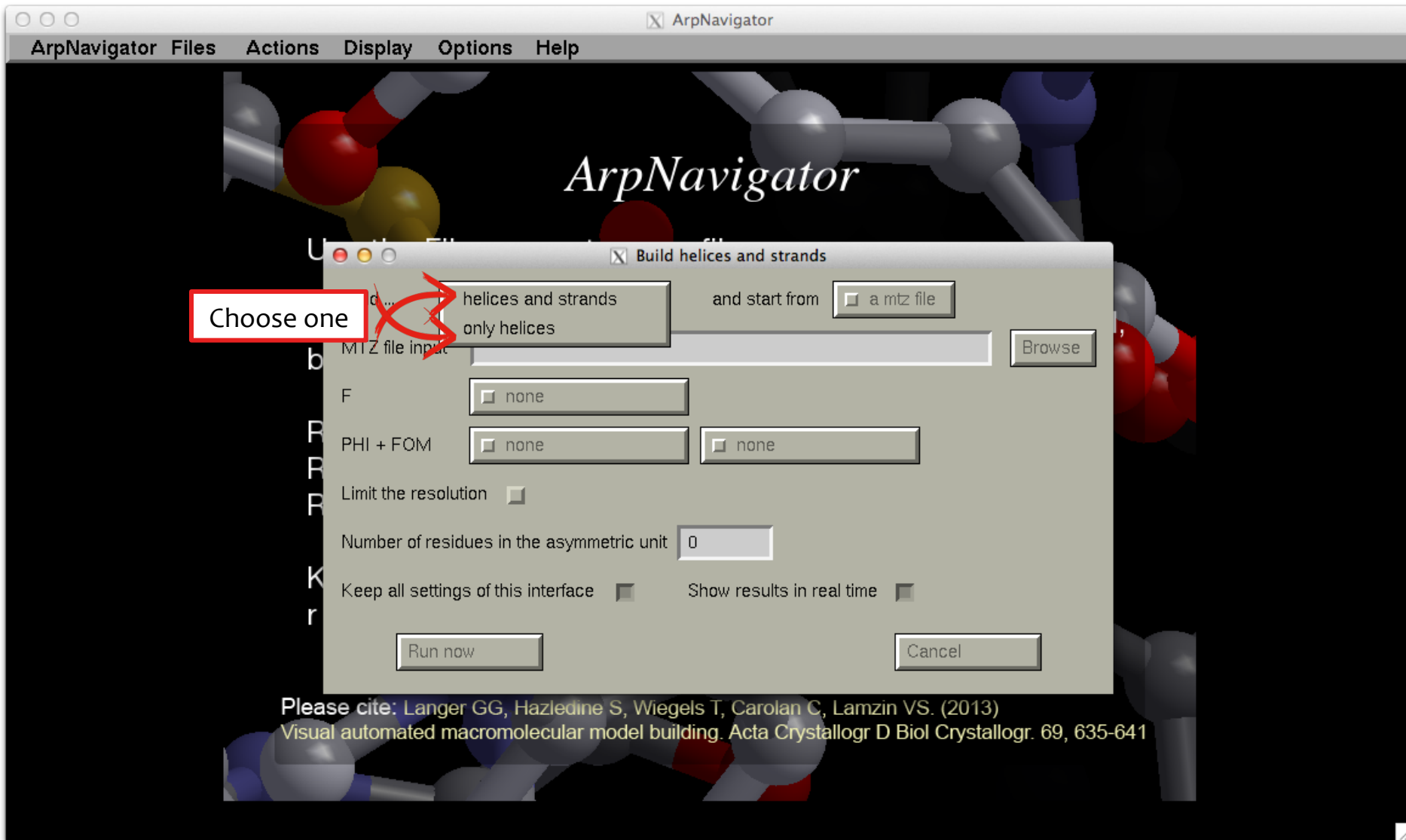
MTS labels to use:

F, PHIC, FOM

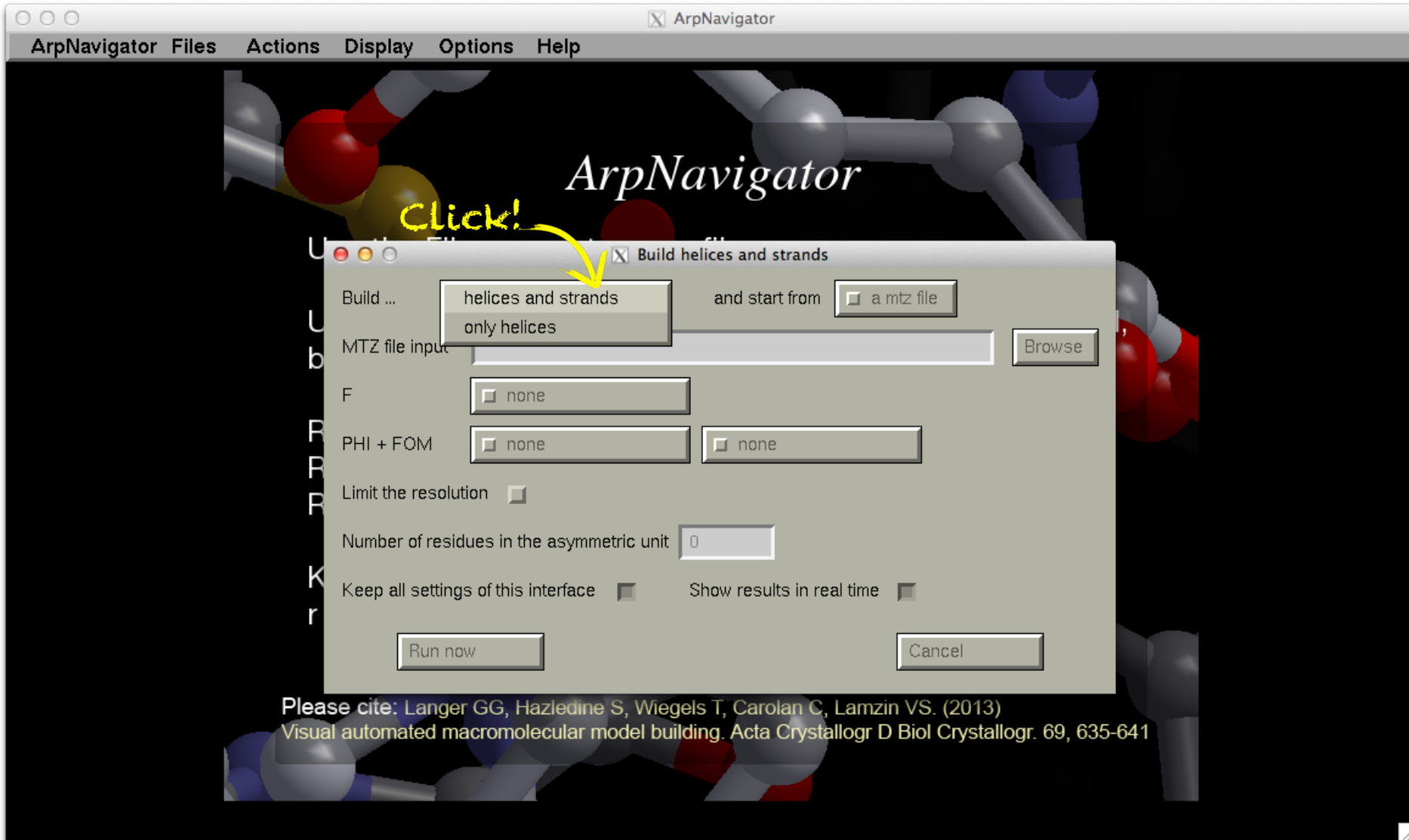
ARP/wARP: Secondary Structure (albe)



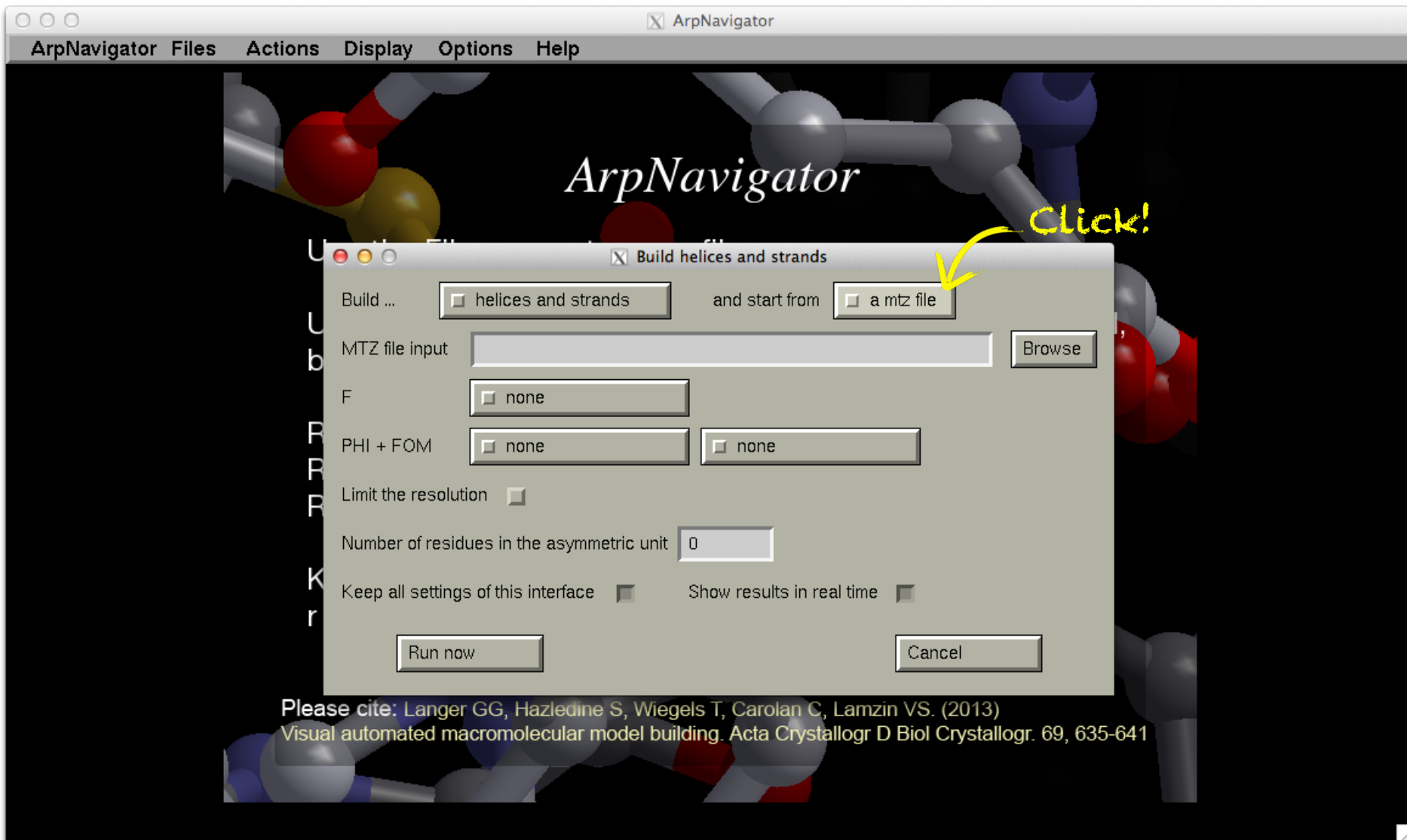
ARP/wARP: Secondary Structure (albe)



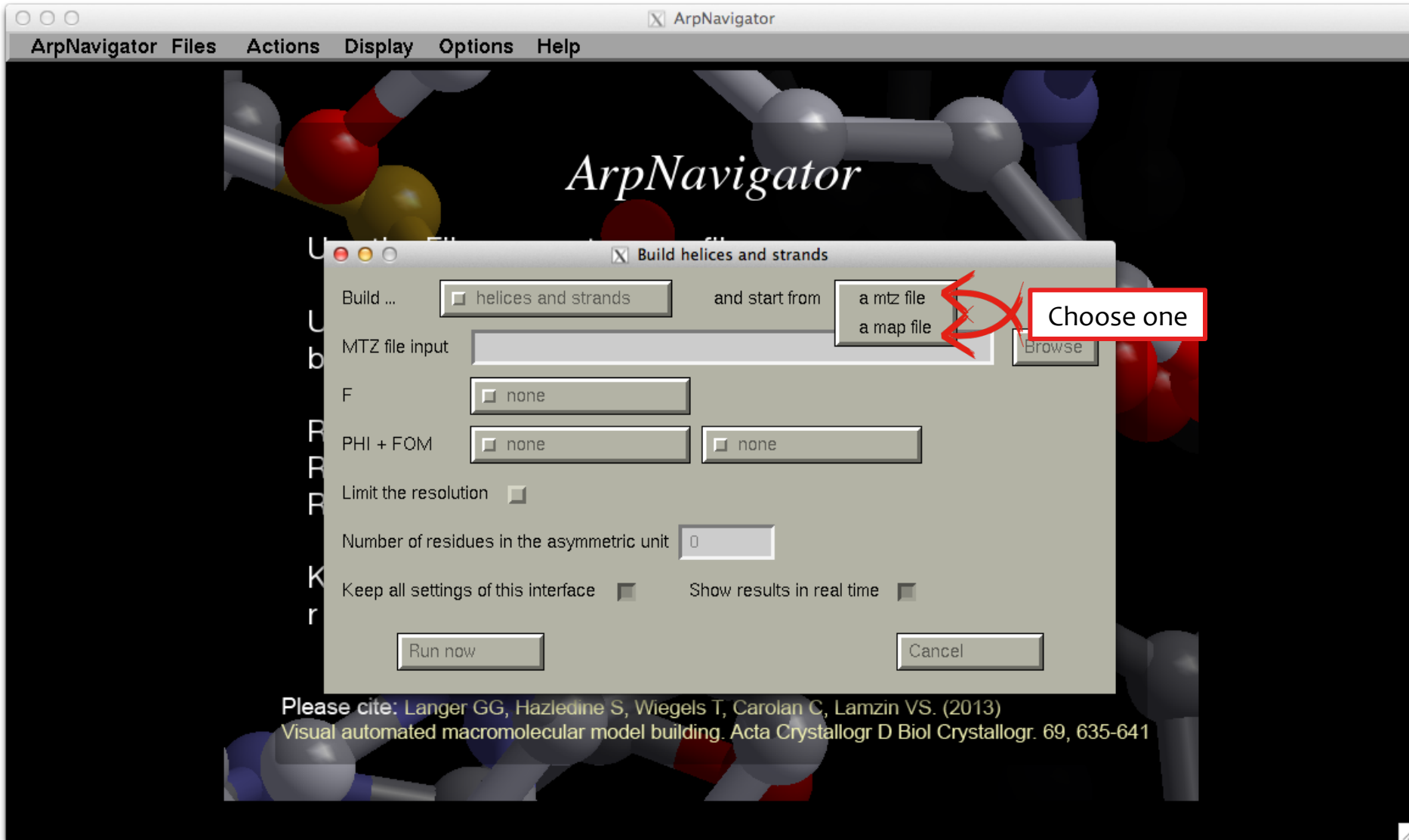
1. Building of Helices and Strands



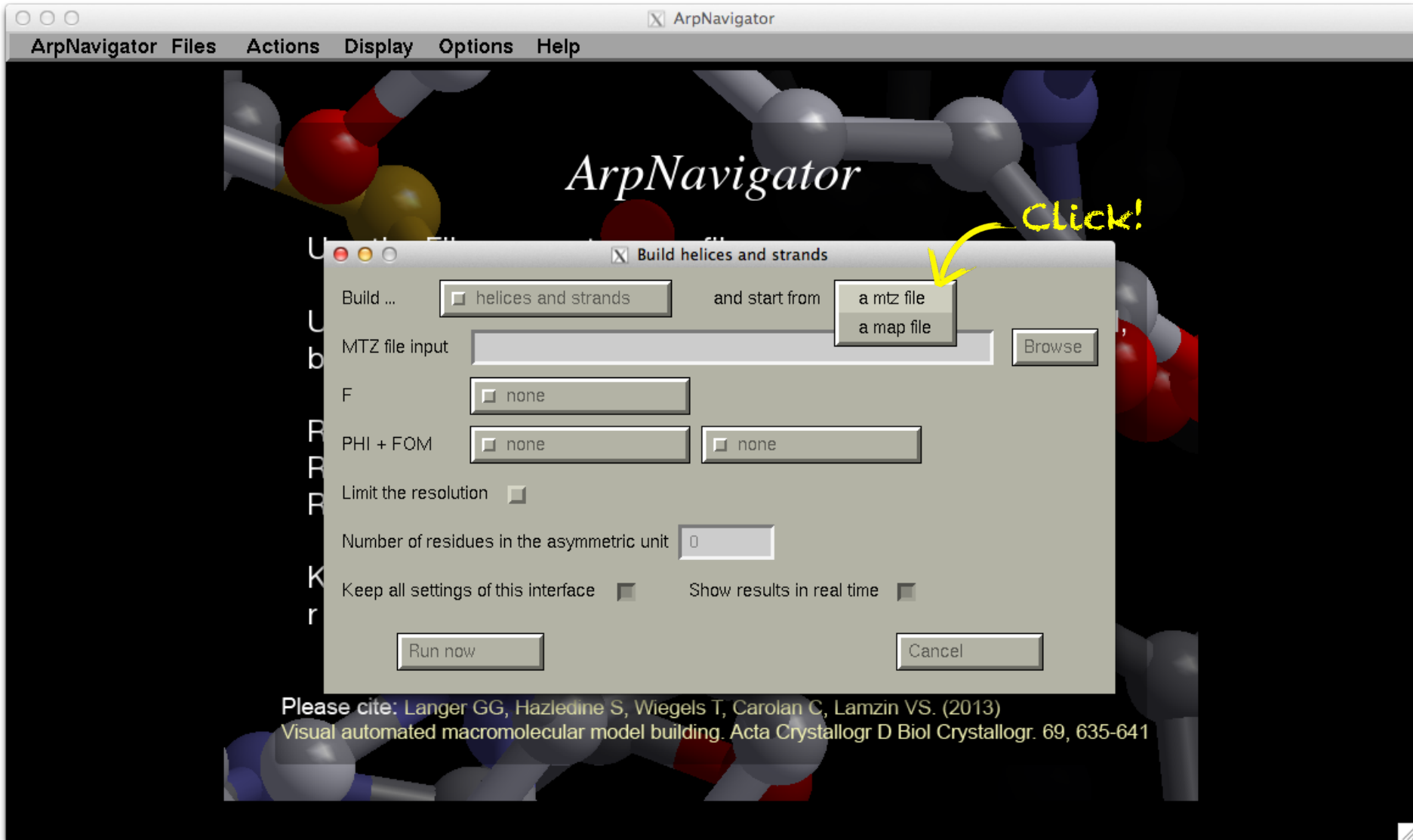
1. Building of Helixes and Strands



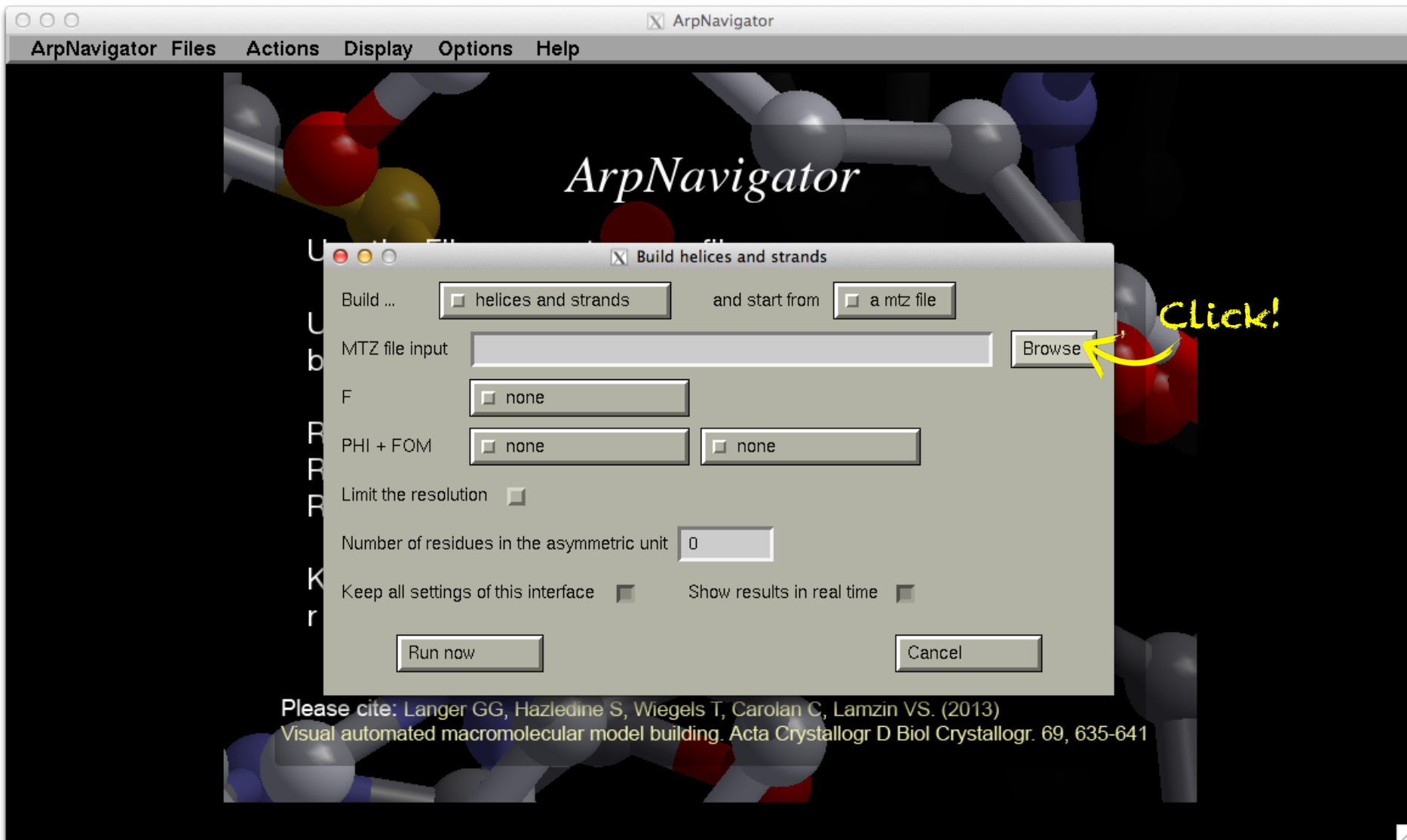
1. Building of Helixes and Strands



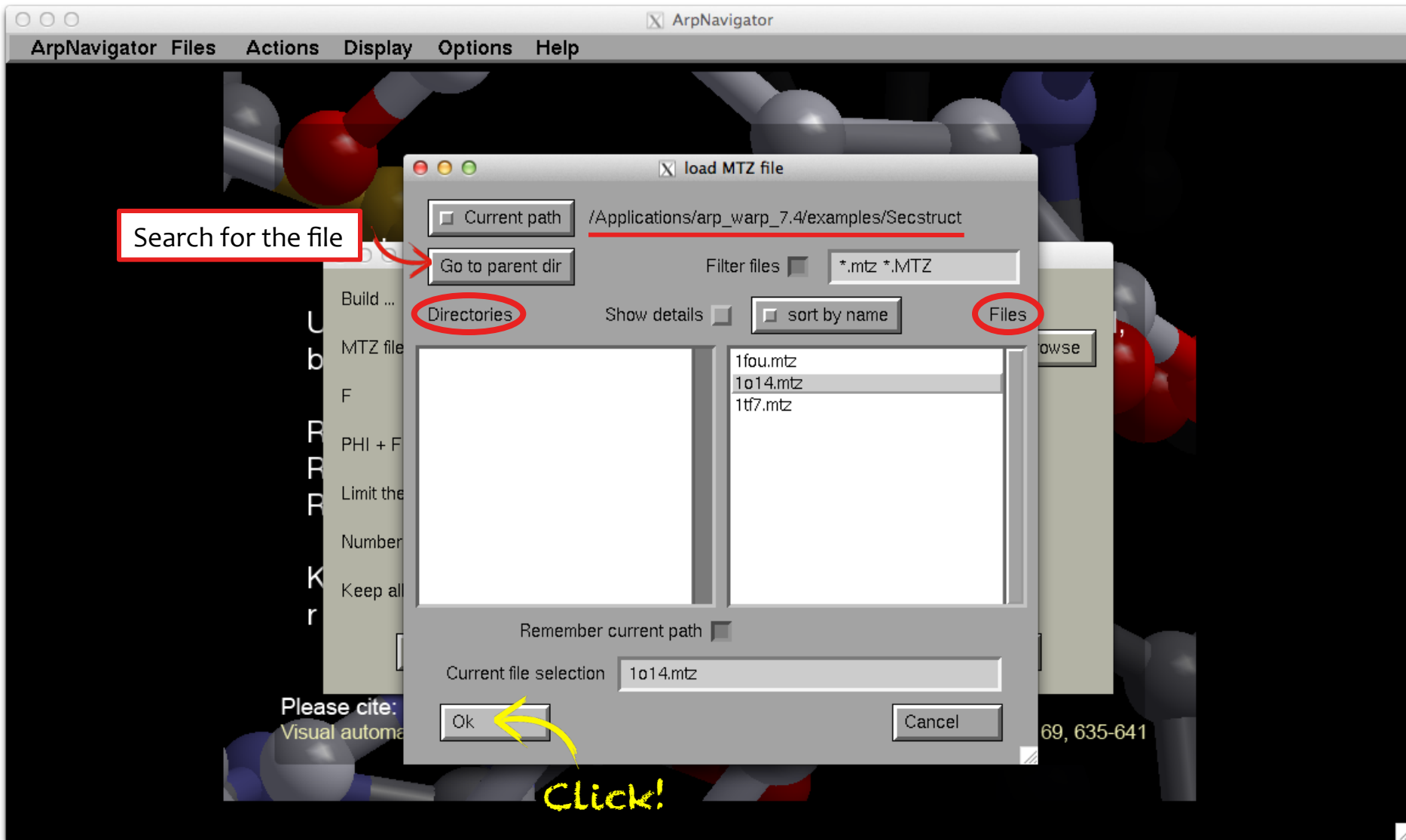
1.1. Start From MTZ File



1.1.1. Input Files: MTZ File



1.1.1. Input Files: MTZ File



1.1.1. Input Files: MTZ File

ArpNavigator Files Actions Display Options Help

ArpNavigator

Build ... ☒ helices and strands and start from ☒ a mtz file

MTZ file input /Applications/arp_warp_7.4/examples/Secstruct/1o14.mtz Browse

F ☒ F

PHI + FOM ☒ PHIC ☒ FOM

Limit the resolution ☐

Number of residues in the asymmetric unit 0

Keep all settings of this interface ☒ Show results in real time ☐

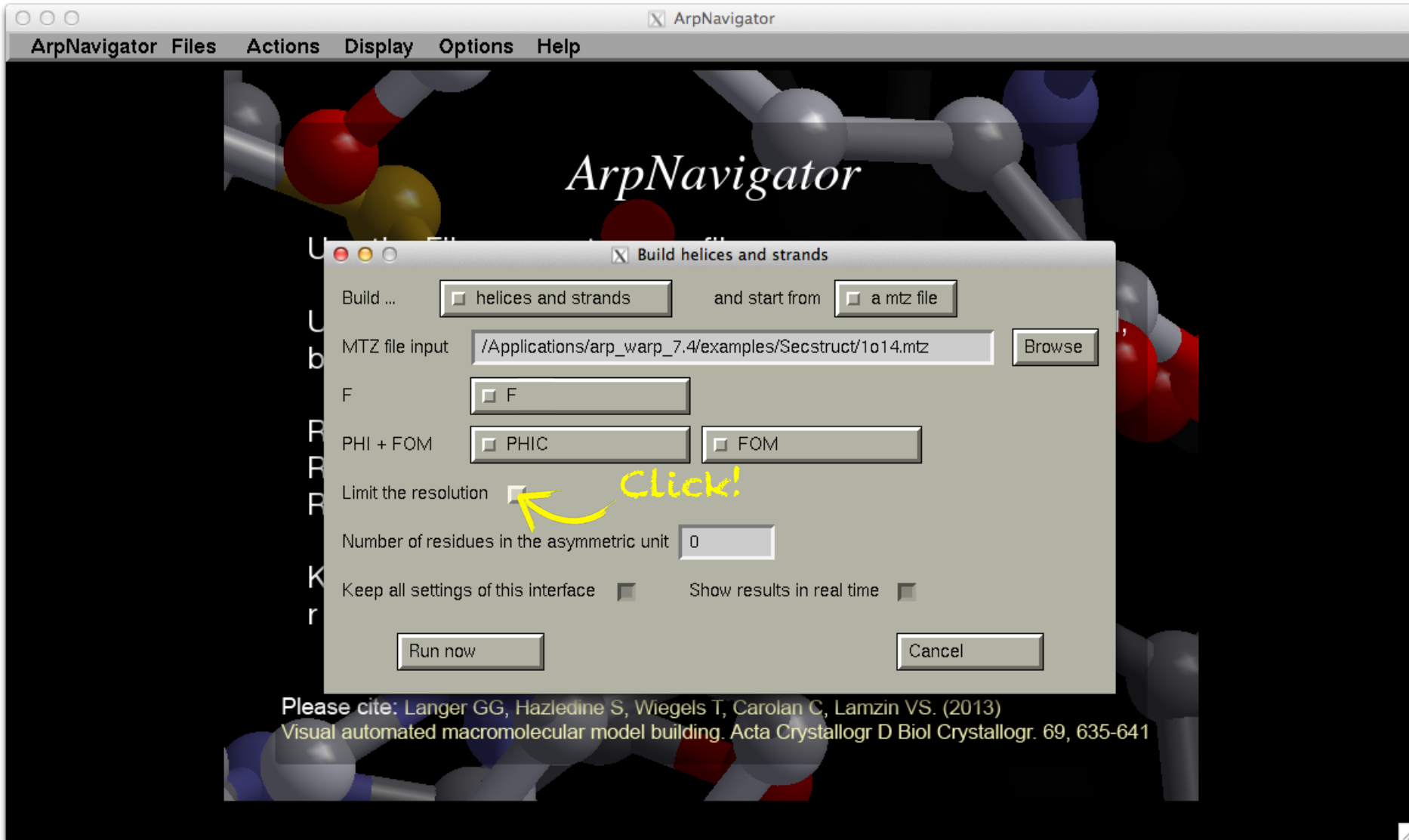
Run now Cancel

Filled automatically (if defaults are available in mtz).

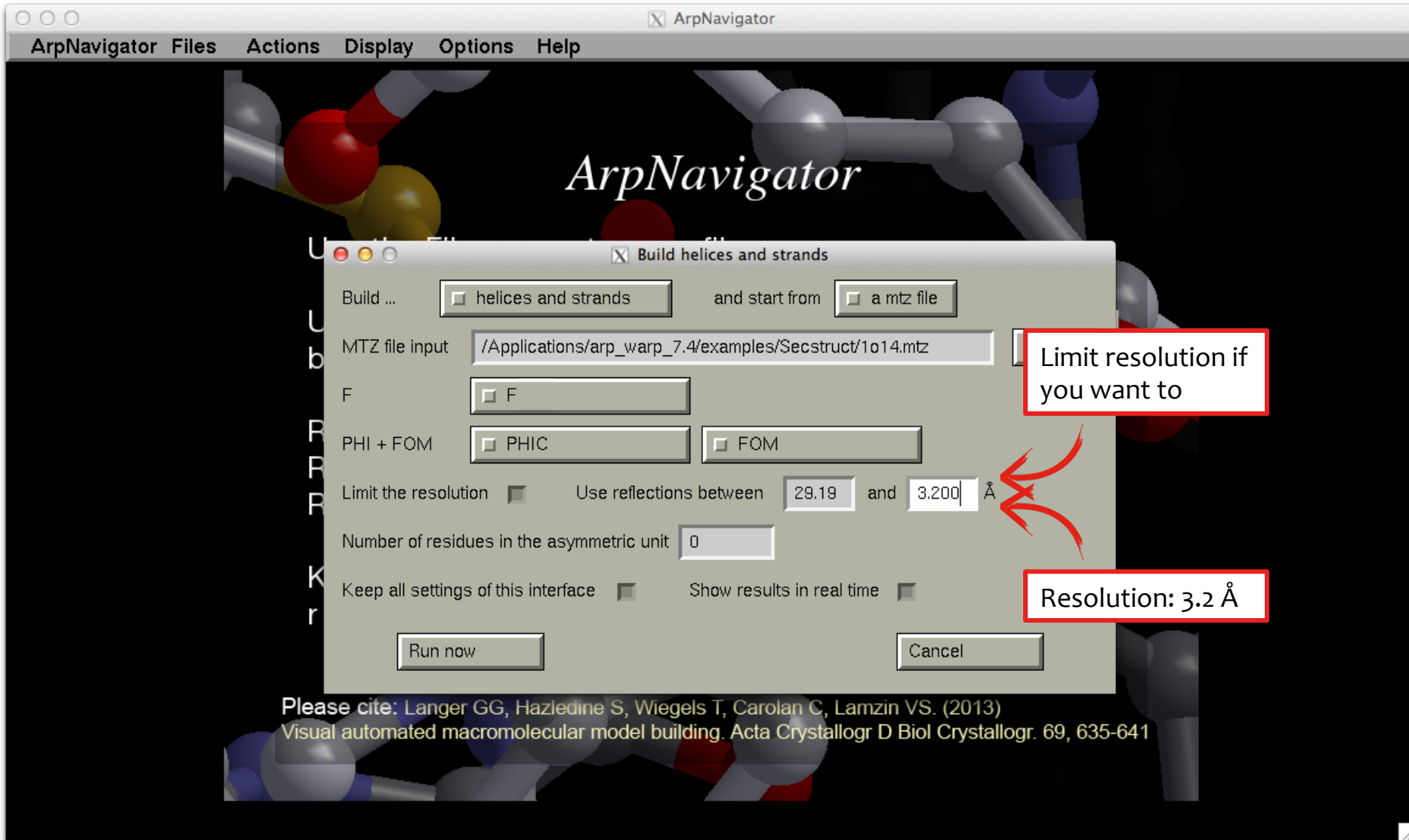
If not, click on the button and search the list.

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

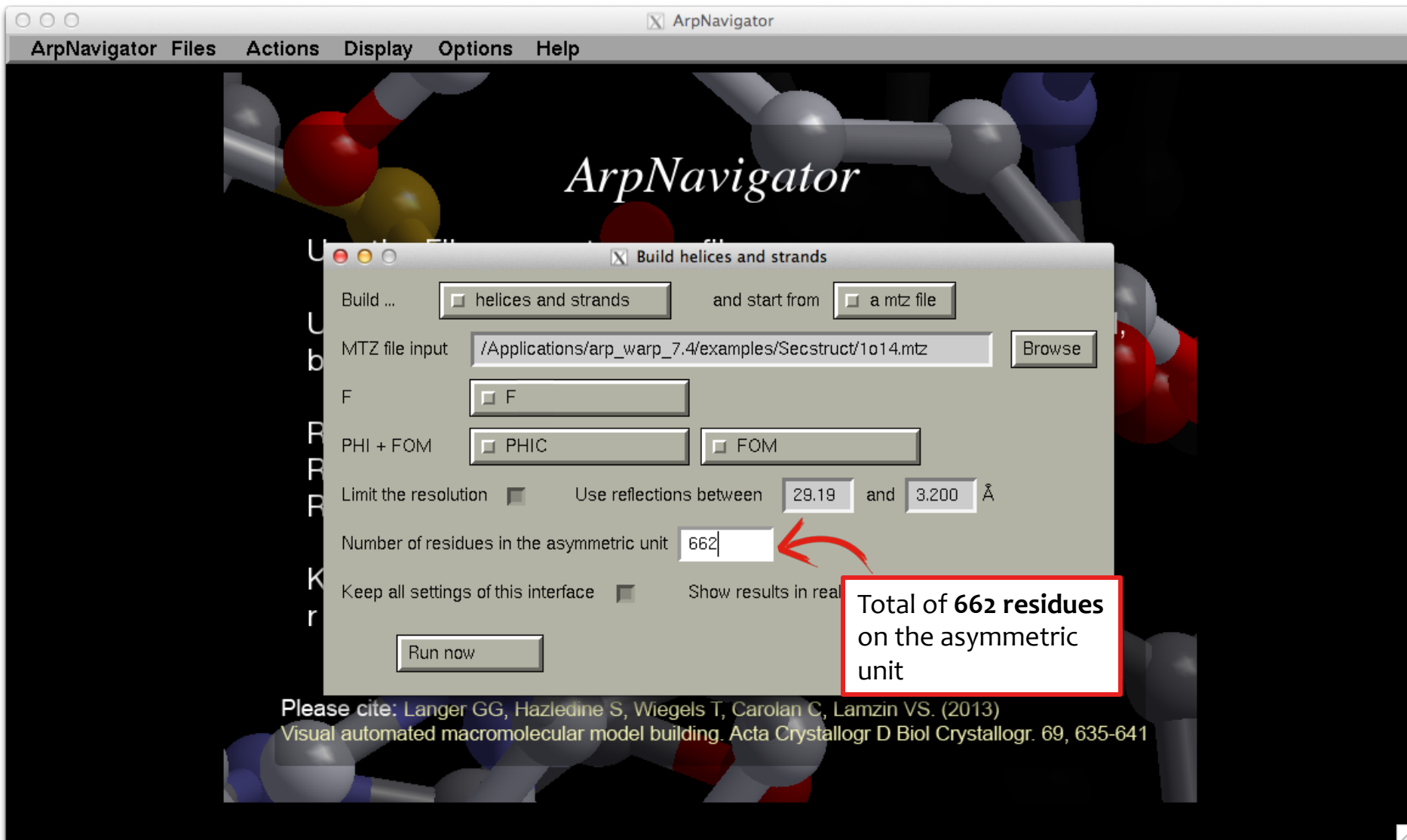
1.1.2. Resolution



1.1.2. Resolution



1.1.3. Required Parameters



ArpNavigator

Build helices and strands

Build ... ☐ helices and strands and start from ☐ a mtz file

MTZ file input /Applications/arp_warp_7.4/examples/Secstruct/1o14.mtz Browse

F ☐ F

PHI + FOM ☐ PHIC ☐ FOM

Limit the resolution ☐ Use reflections between 29.19 and 3.200 Å

Number of residues in the asymmetric unit 662

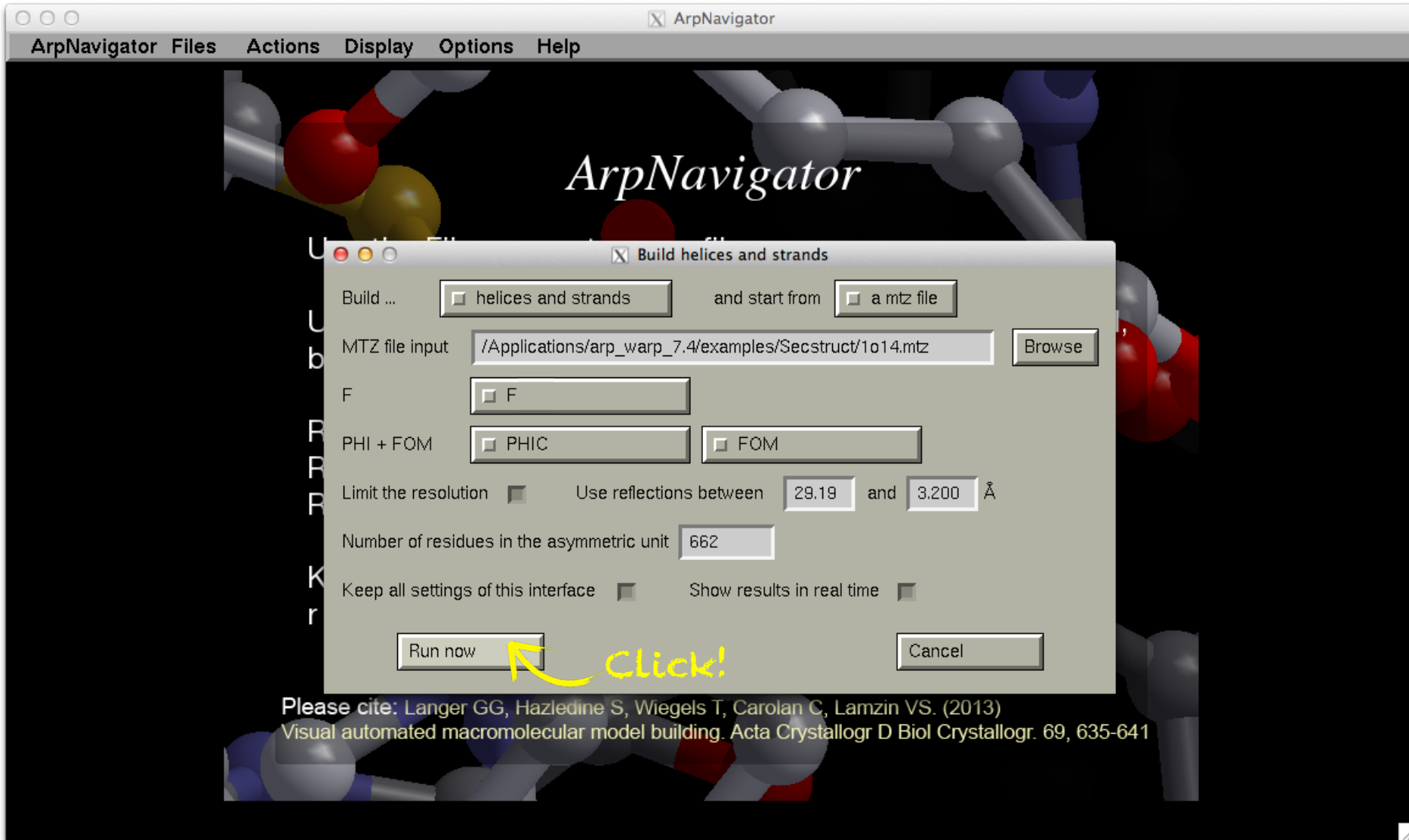
Keep all settings of this interface ☐ Show results in real

Run now

Total of 662 residues on the asymmetric unit

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

1.1.4. Run The Job



1.1.4. Run The Job – Log File

The screenshot shows the ArpNavigator software interface. The main window displays a 3D molecular model of a protein structure. A dialog box titled "Build helices and strands" is open in the center, displaying the following text:

auto_albe has created the parameter file ... [View file](#)

19 helical and 22 stranded fragments

242 helical CAs, 162 stranded CAs and 363 candidate peptide connections

The longest chain comprises 16 peptides

Residues 402 Chain fragments 41 Connectivity index 0.7729 Tracing score 0.5443

Normal termination of warp_albe

Buttons: [Kill Job](#) [Close](#)

Handwritten notes on the right side of the dialog box:

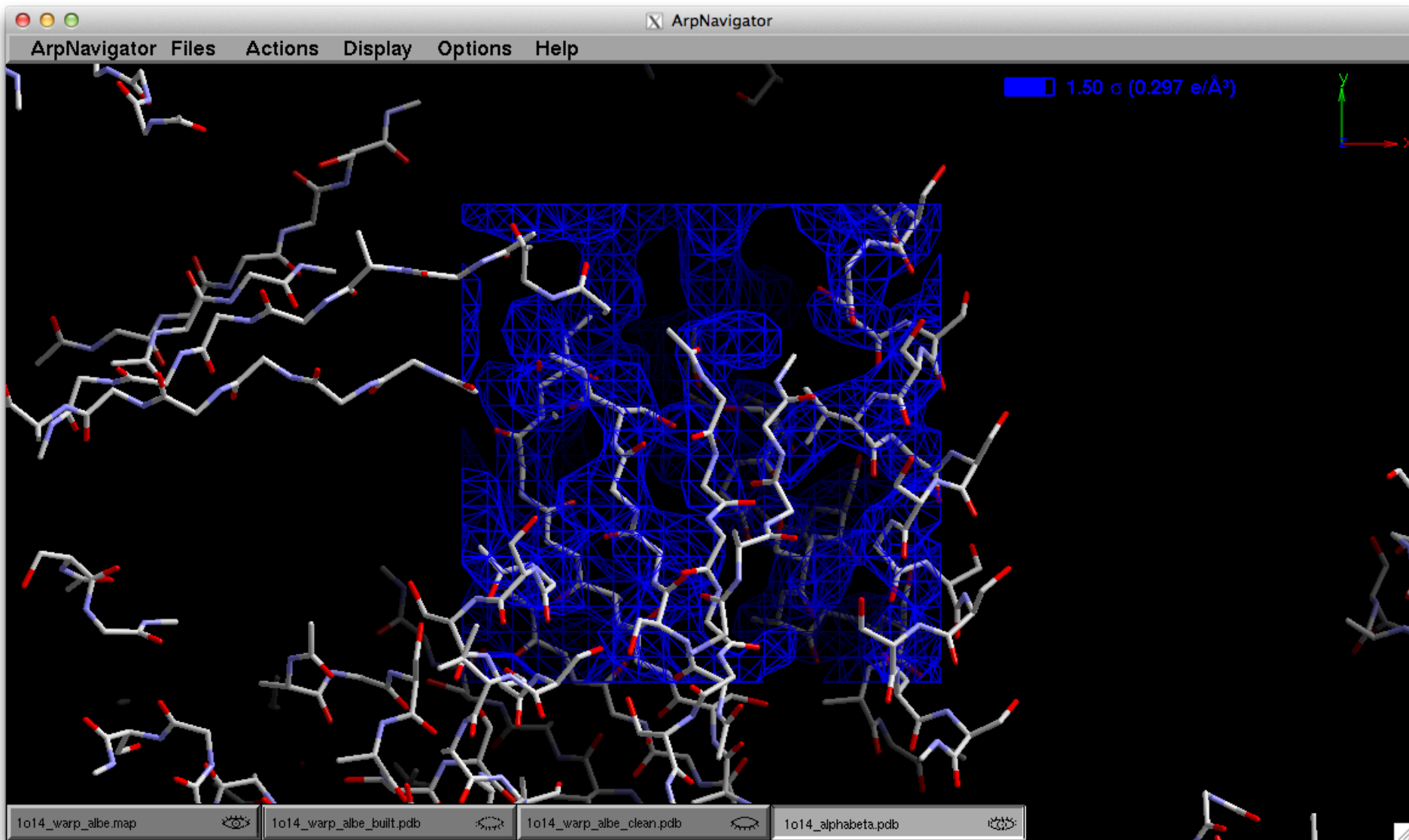
- Fragments found
- Sec structure found
- Etc.

A yellow arrow points to the "Close" button with the handwritten text "Click!".

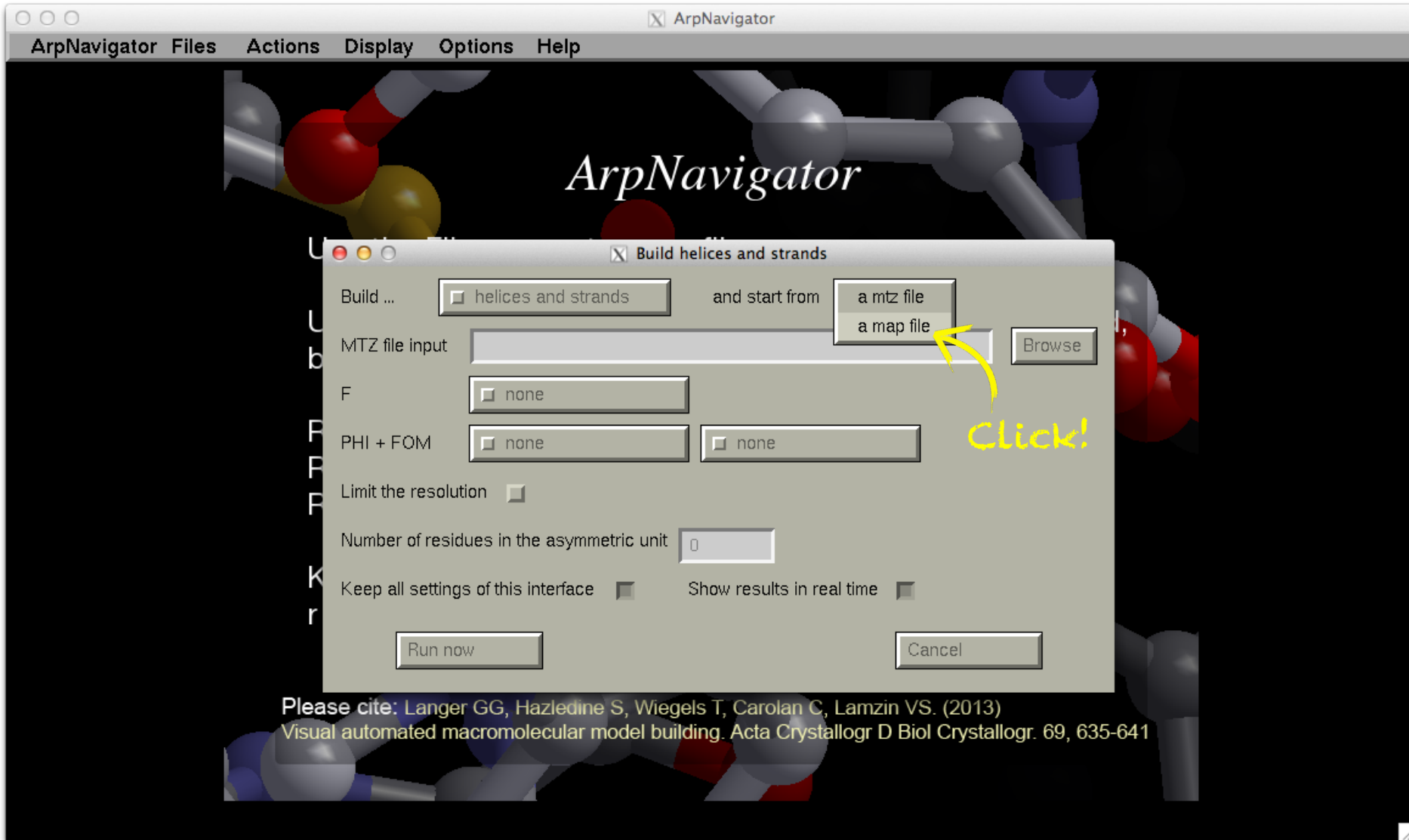
The bottom of the ArpNavigator window shows a taskbar with the following files:

- 1o14_warp_albe.map
- 1o14_warp_albe_built.pdb
- 1o14_warp_albe_clean.pdb
- 1o14_alphabeta.pdb

1.1.4. Run The Job – Live Model Building



1.2. Start From MAP File



1.2.1. Input Files: MAP File

ArpNavigator Files Actions Display Options Help

ArpNavigator

Build ... ☐ helices and strands and start from ☐ a map file

MAP file input Browse

Number of residues in the asymmetric unit As in 1.1.3.

Keep all settings of this interface ☐ Show results in real time ☐

Run now As in 1.1.4. Cancel

Search for map file

Does not need:

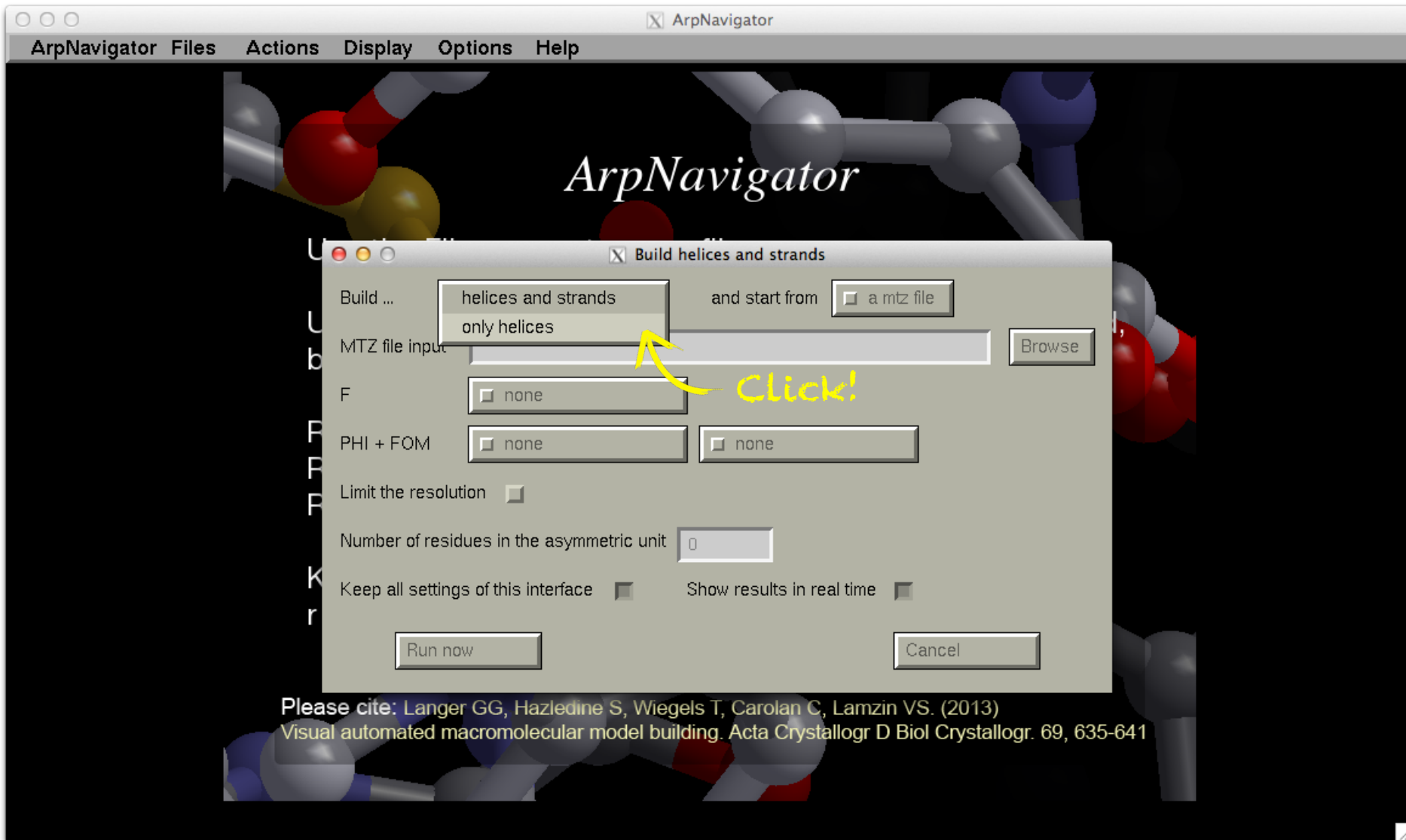
- MTS labels

Does not allow:

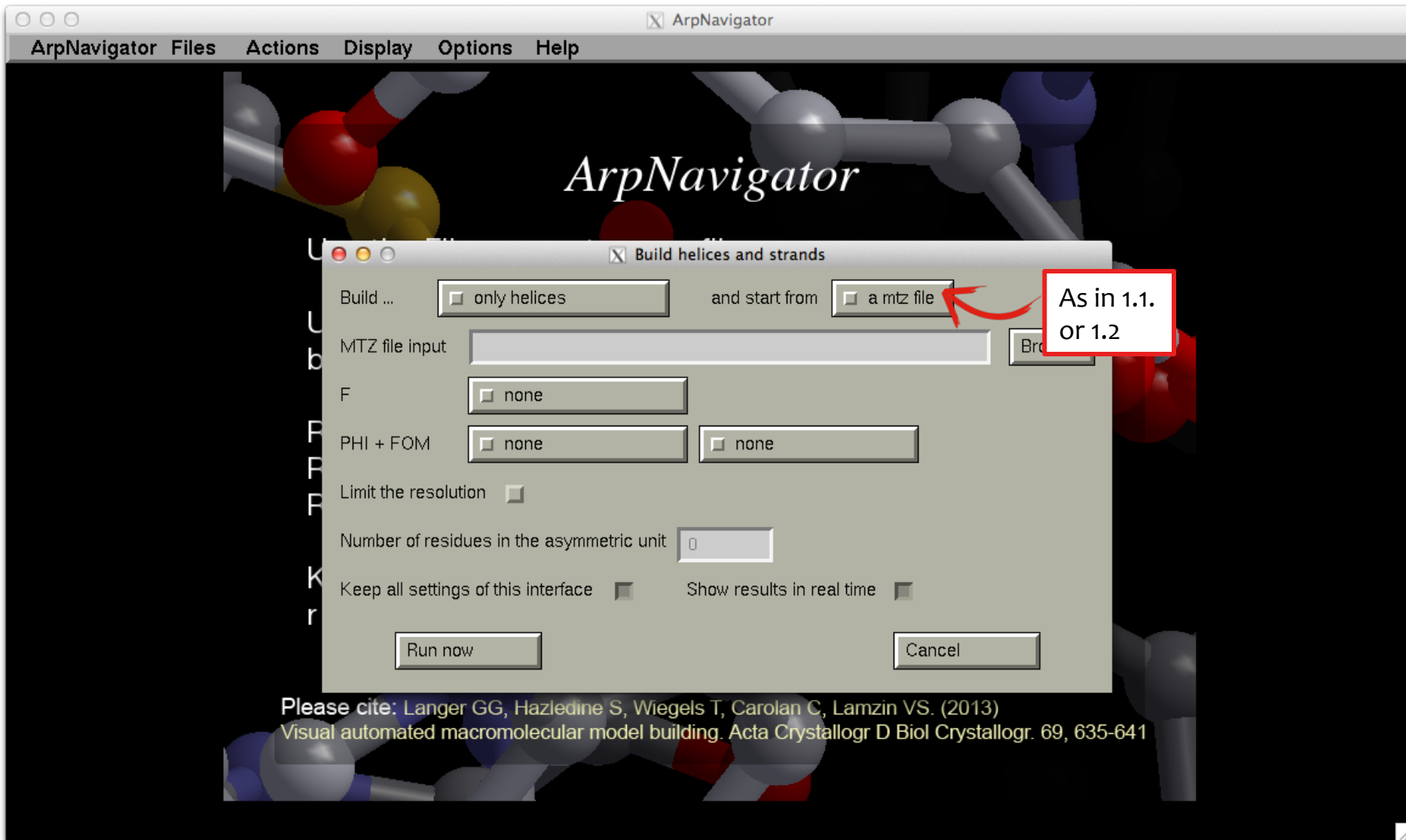
- Resolution restriction

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

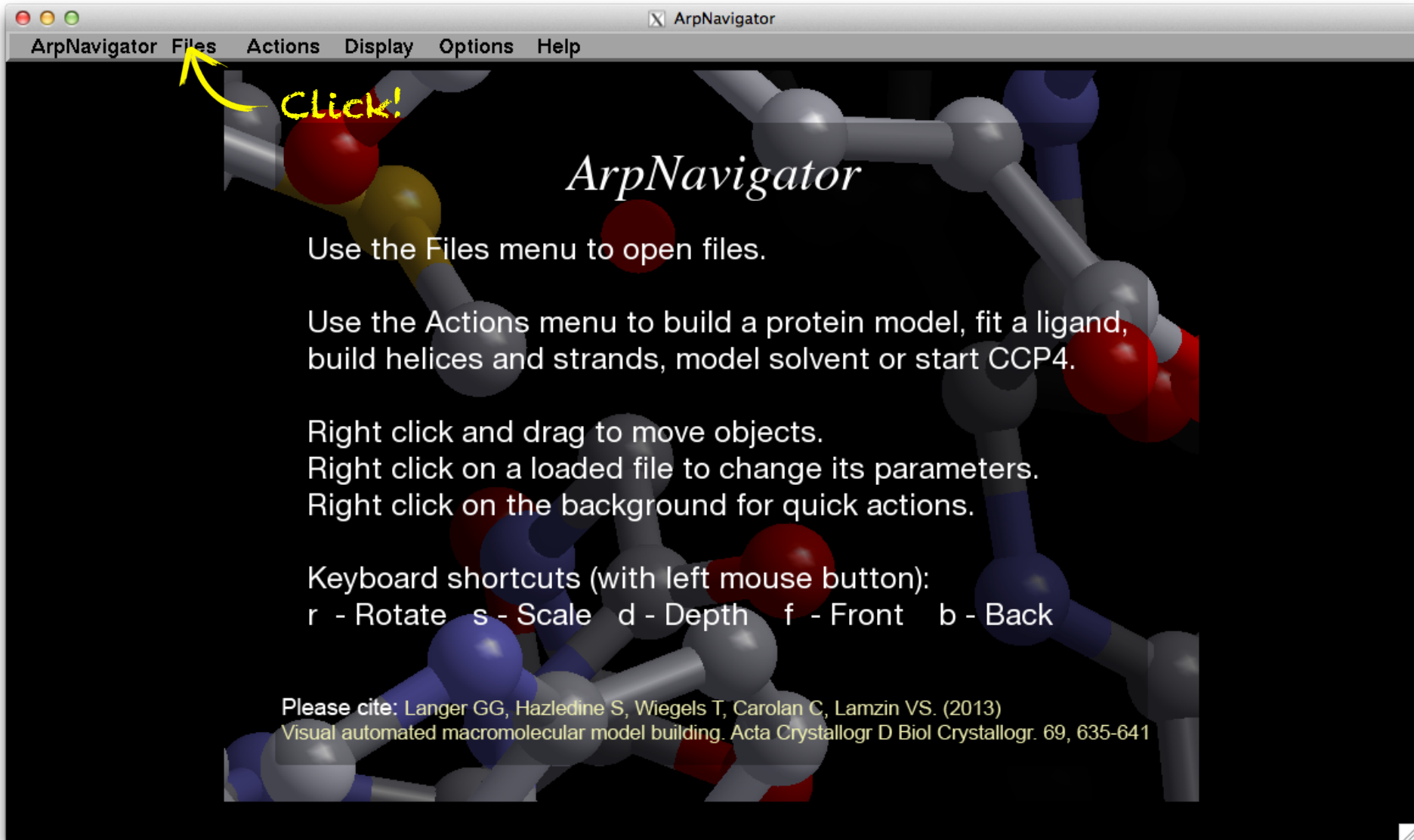
2. Building of Helixes Only



2. Building of Helixes Only



Build Secondary Structure and Skeletons Quickly



The image shows a screenshot of the ArpNavigator software window. The title bar reads 'ArpNavigator'. The menu bar includes 'ArpNavigator', 'Files', 'Actions', 'Display', 'Options', and 'Help'. A yellow arrow points to the 'Files' menu with the text 'Click!' in yellow. The main area displays a 3D molecular model with atoms represented by spheres (red for oxygen, blue for nitrogen, grey for carbon) and bonds as sticks. The word 'ArpNavigator' is written in a large, white, serif font in the center. Below it, several instructions are listed in white text. At the bottom, a citation is provided.

ArpNavigator

Use the Files menu to open files.

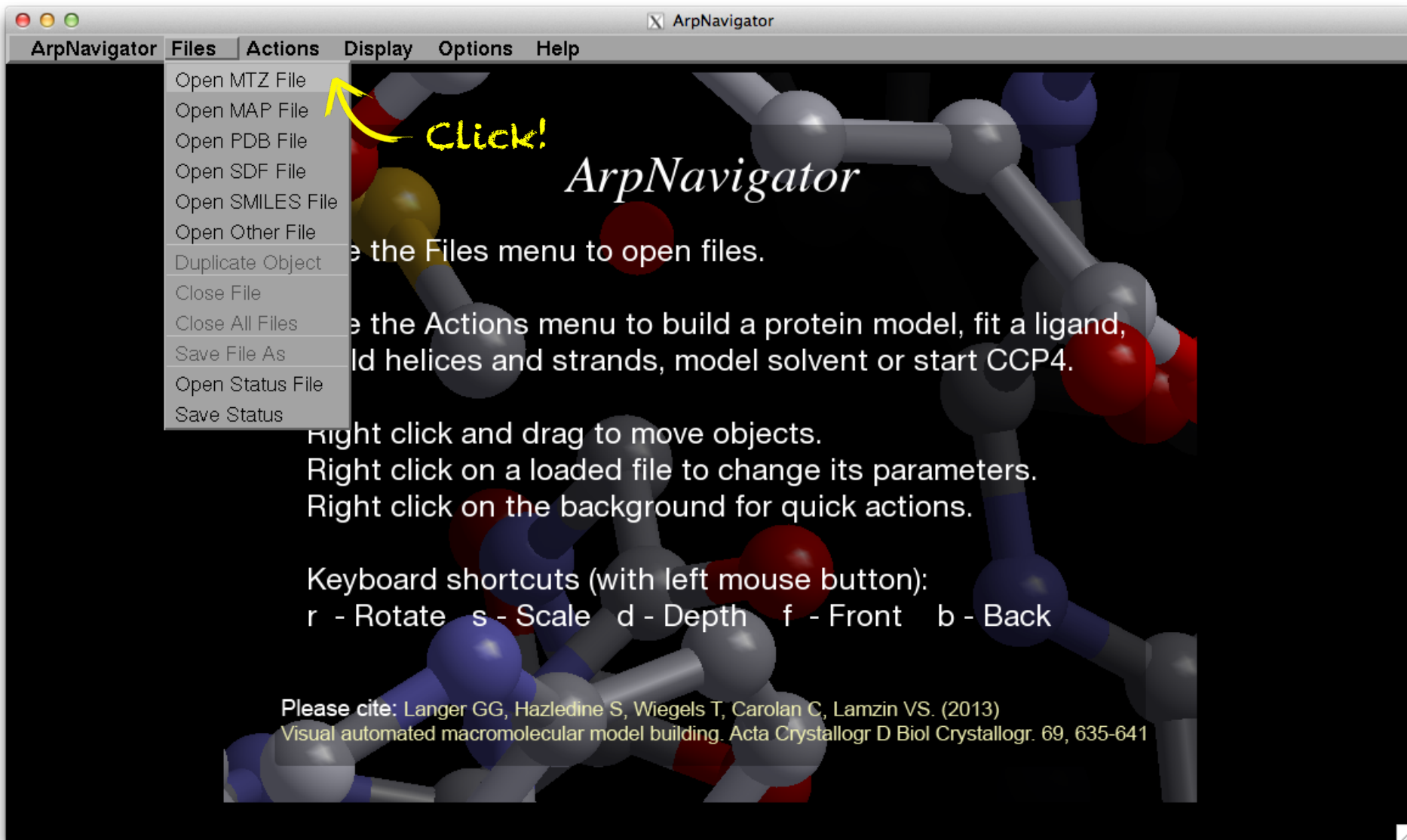
Use the Actions menu to build a protein model, fit a ligand, build helices and strands, model solvent or start CCP4.

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

1. Load MTZ File



ArpNavigator

Files Actions Display Options Help

- Open MTZ File
- Open MAP File
- Open PDB File
- Open SDF File
- Open SMILES File
- Open Other File
- Duplicate Object
- Close File
- Close All Files
- Save File As
- Open Status File
- Save Status

Click!

ArpNavigator

Use the Files menu to open files.

Use the Actions menu to build a protein model, fit a ligand, add 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.

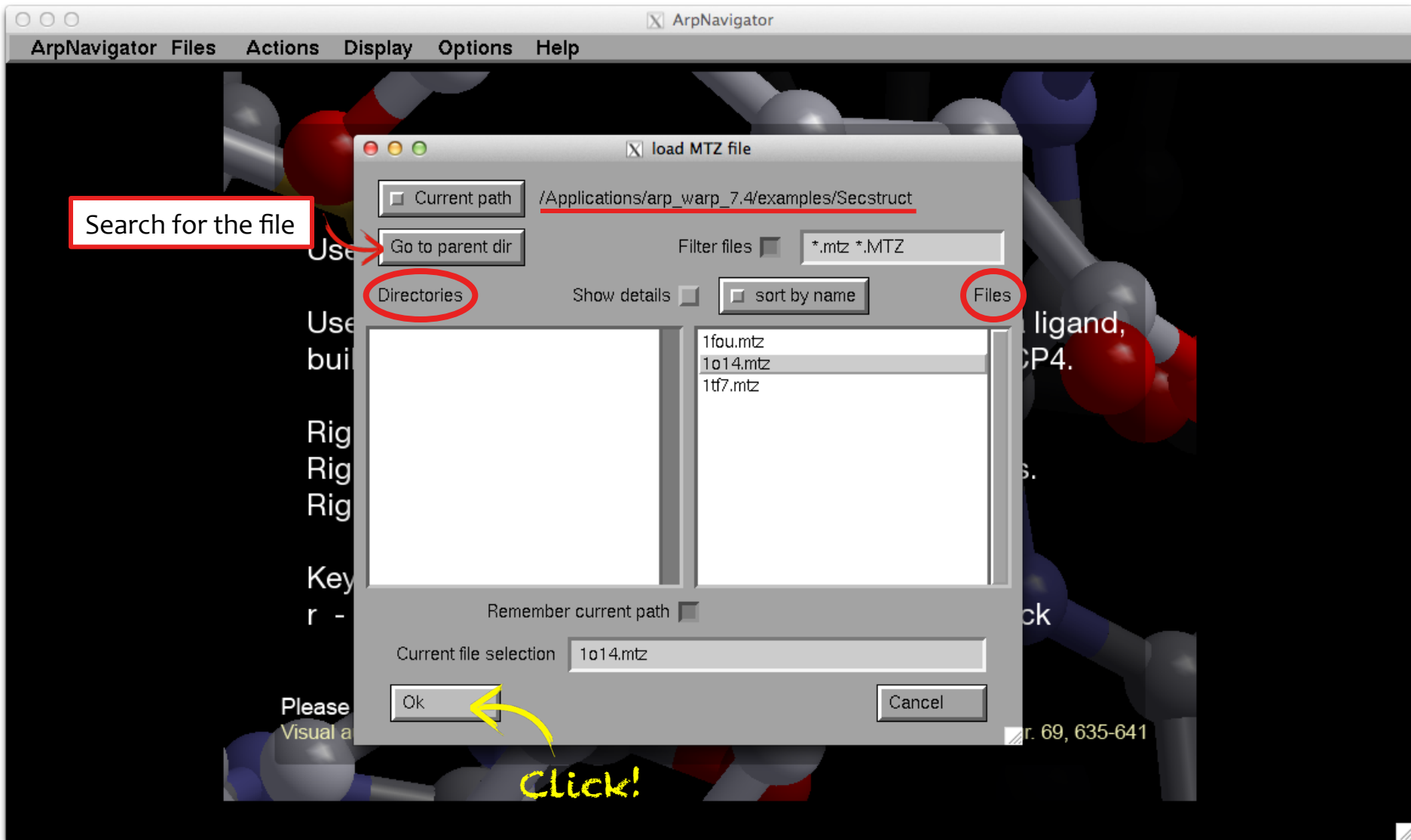
Right click on the background for quick actions.

Keyboard shortcuts (with left mouse button):

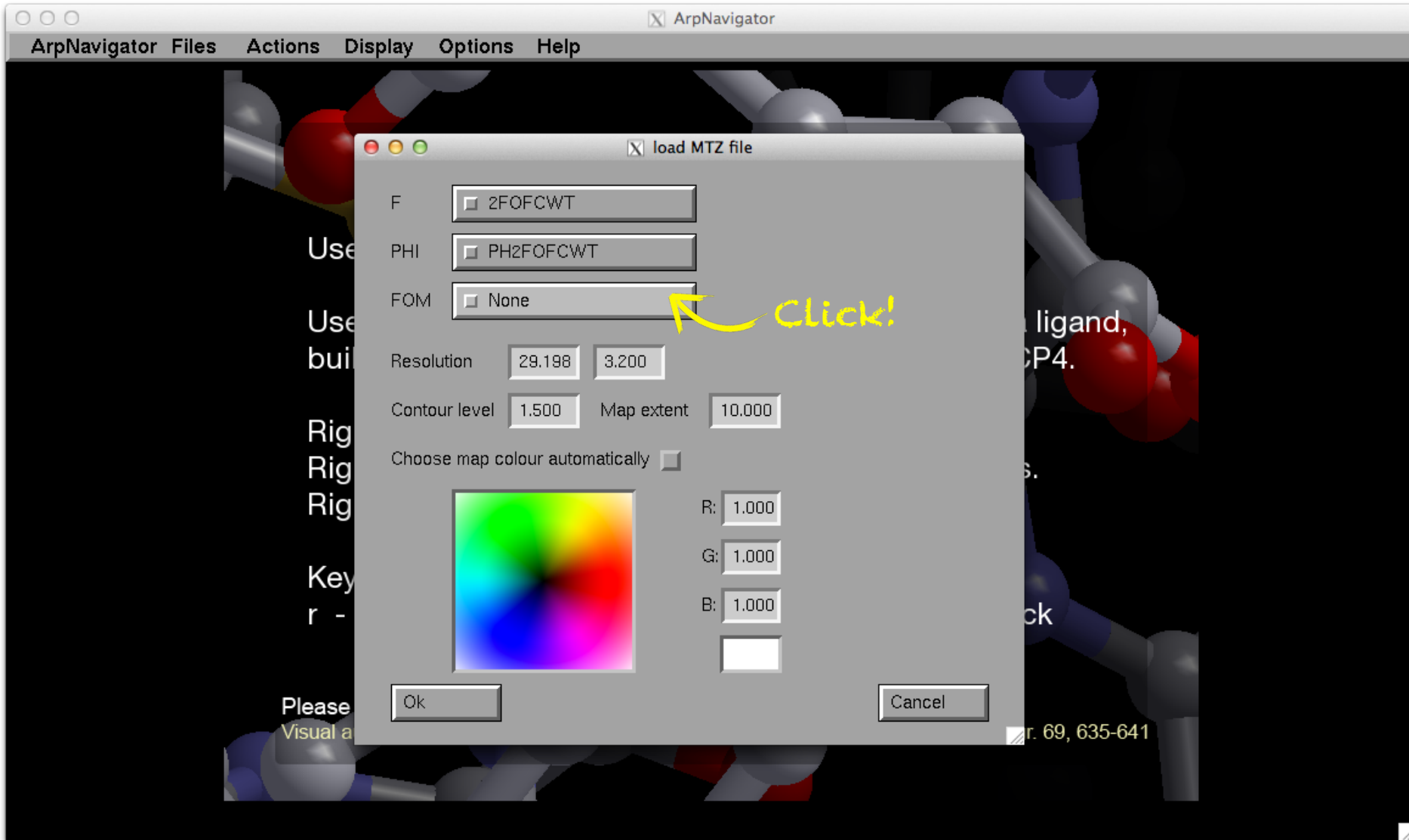
r - Rotate s - Scale d - Depth f - Front b - Back

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

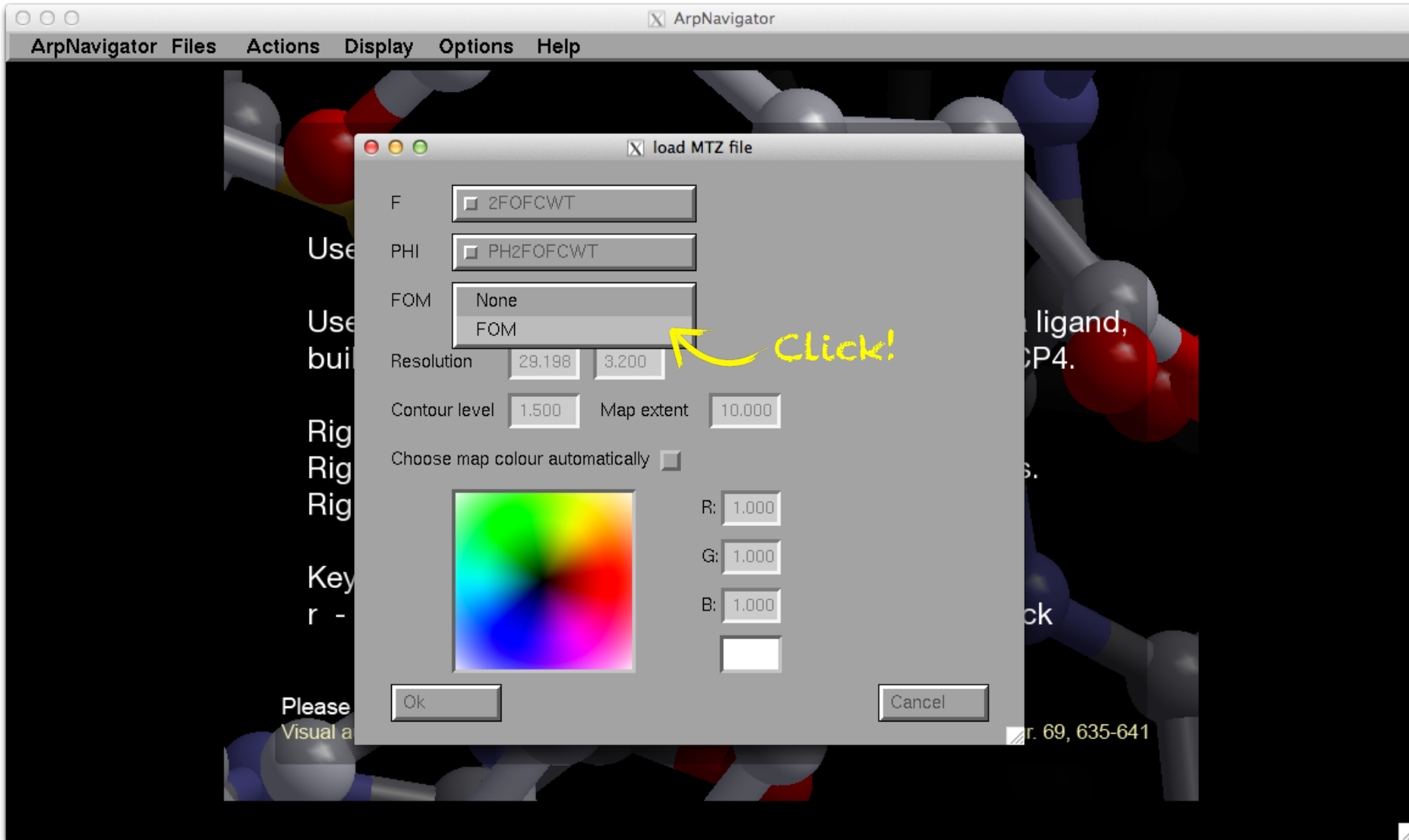
1. Load MTZ File



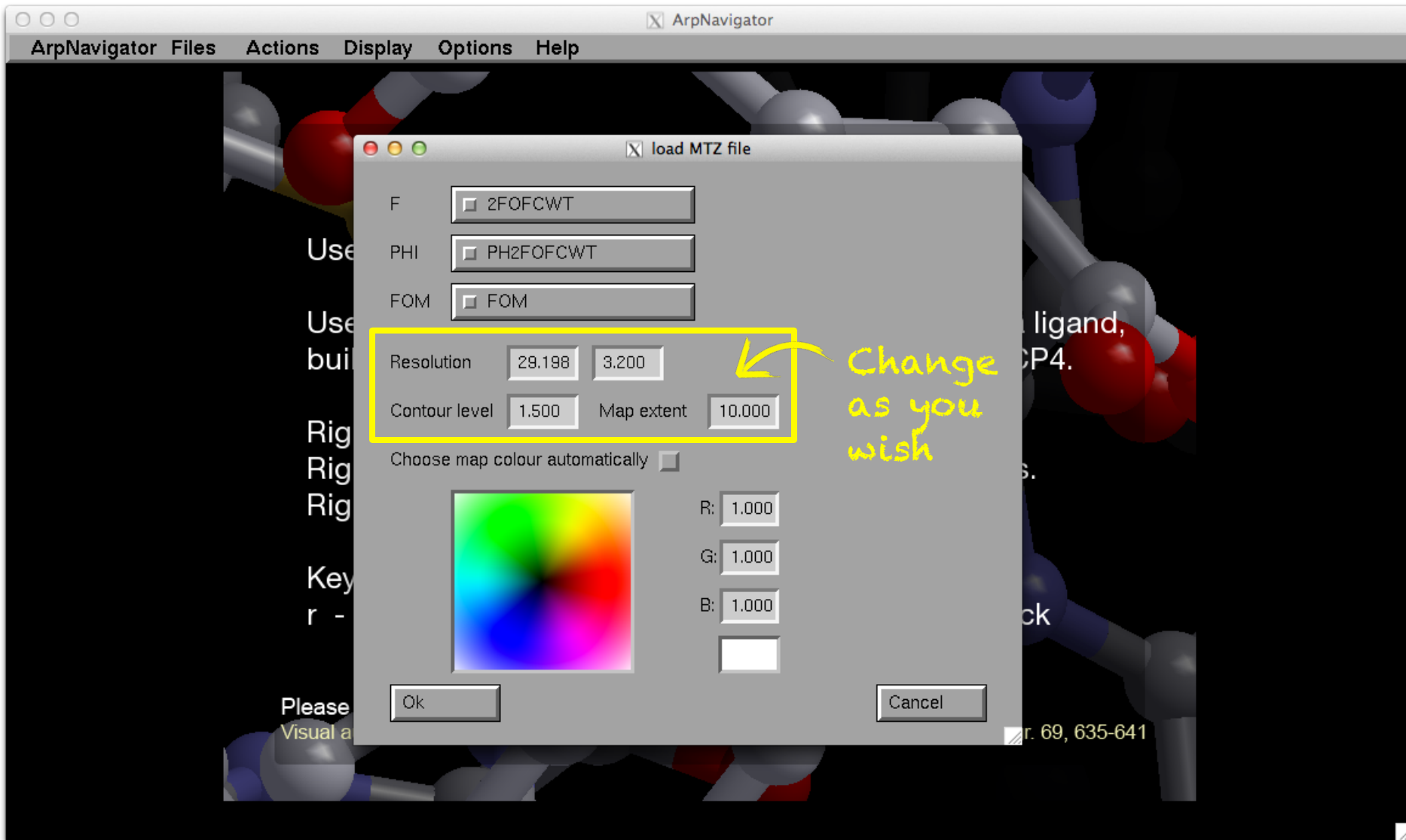
1. Load MTZ File



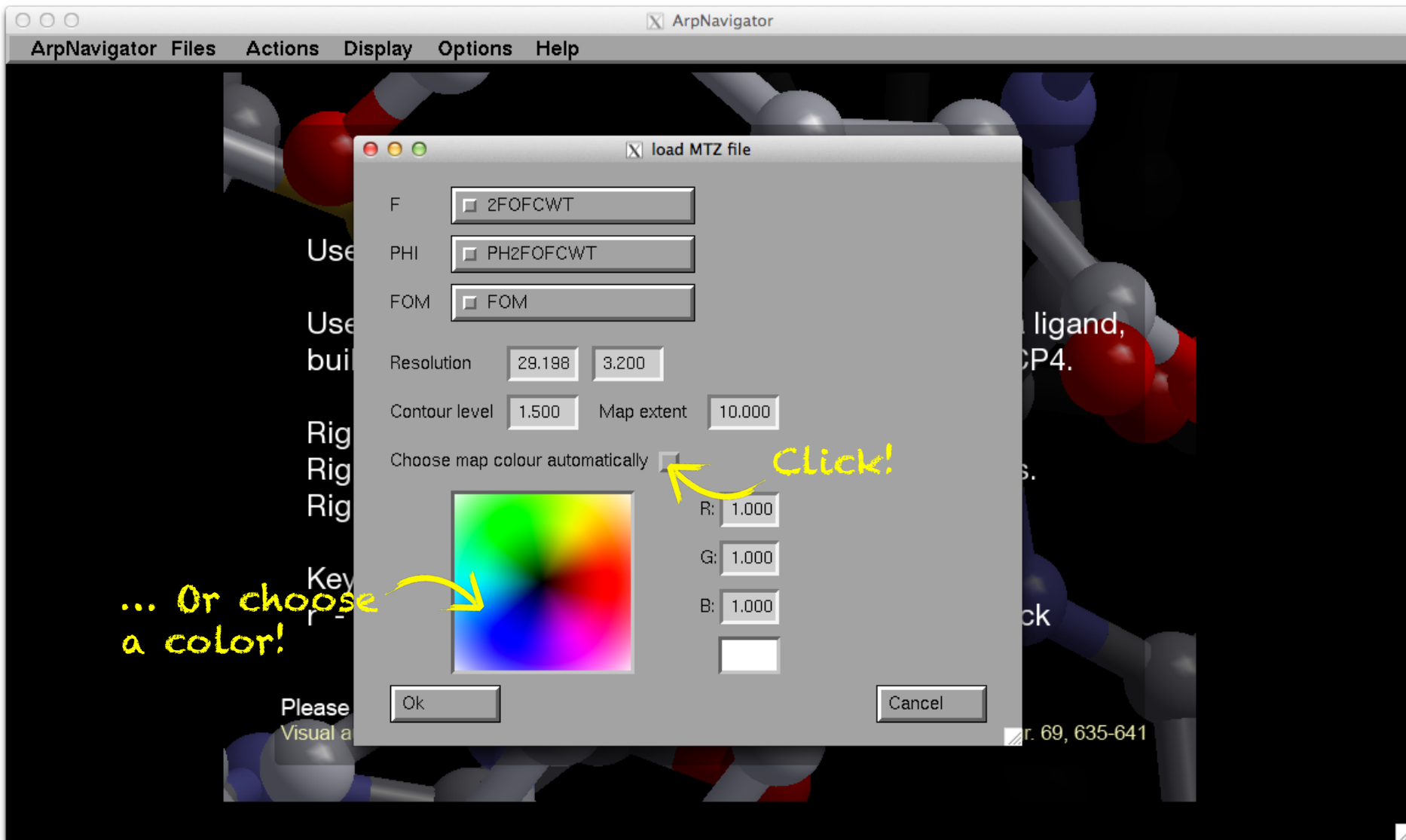
1. Load MTZ File



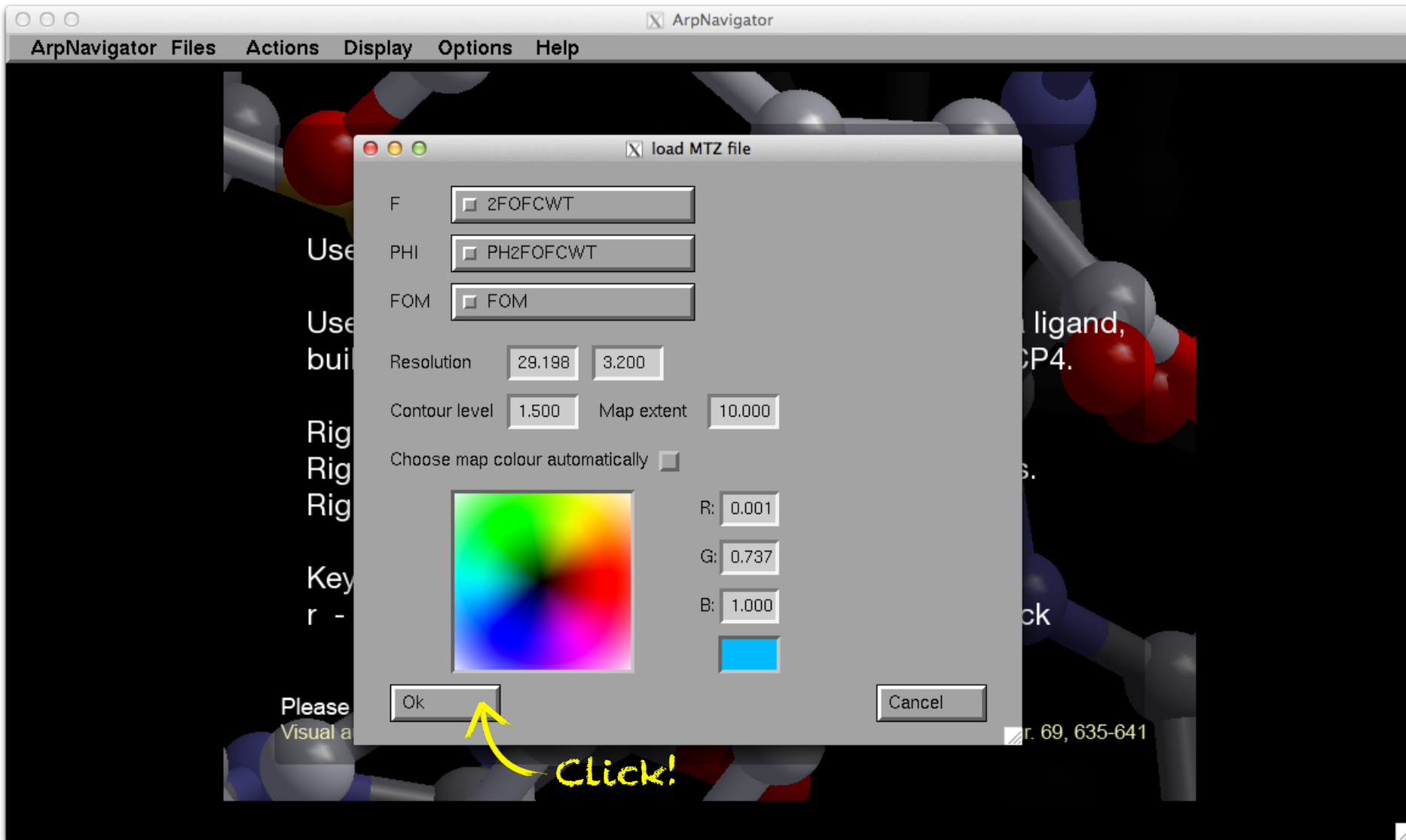
1. Load MTZ File



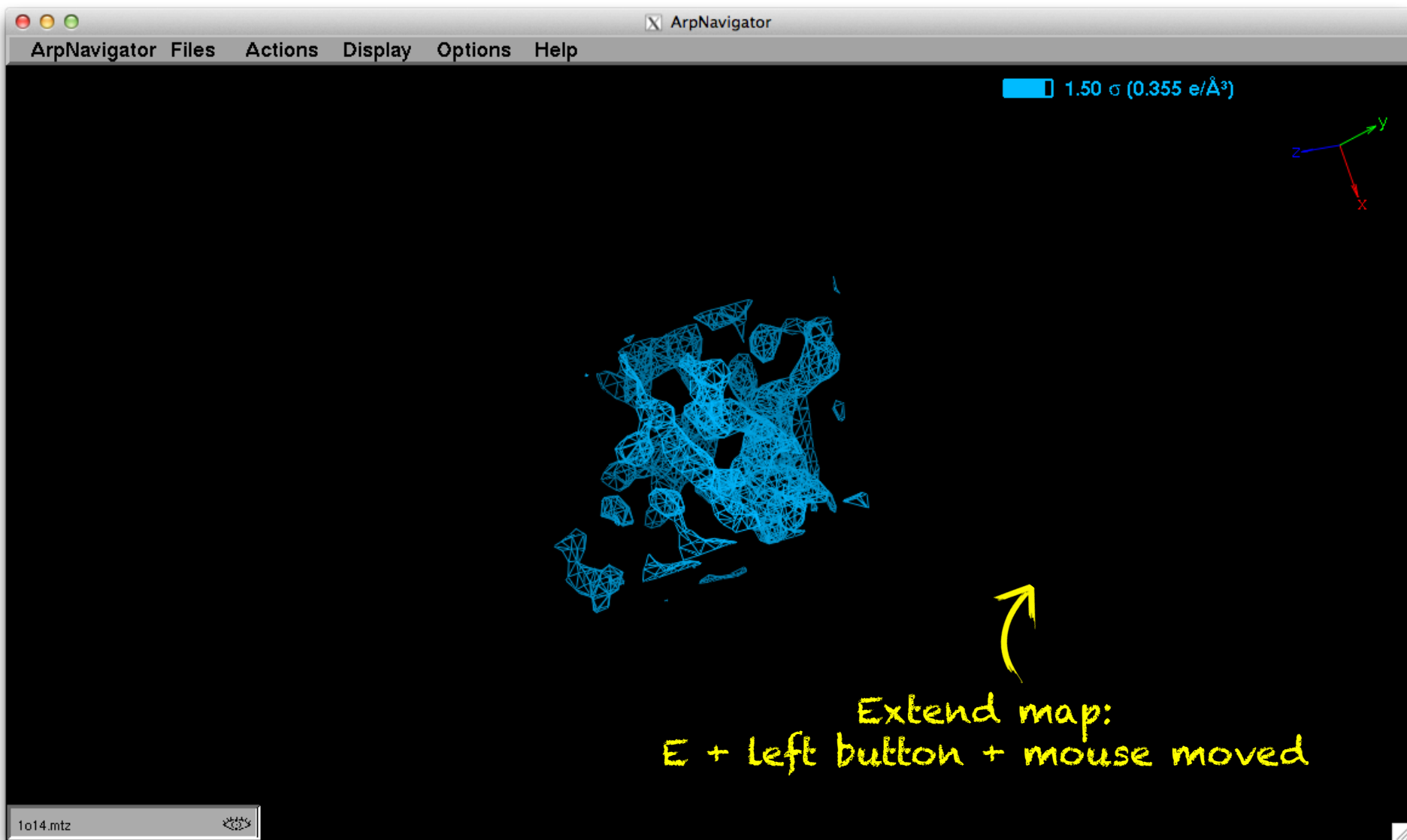
1. Loading MTZ File



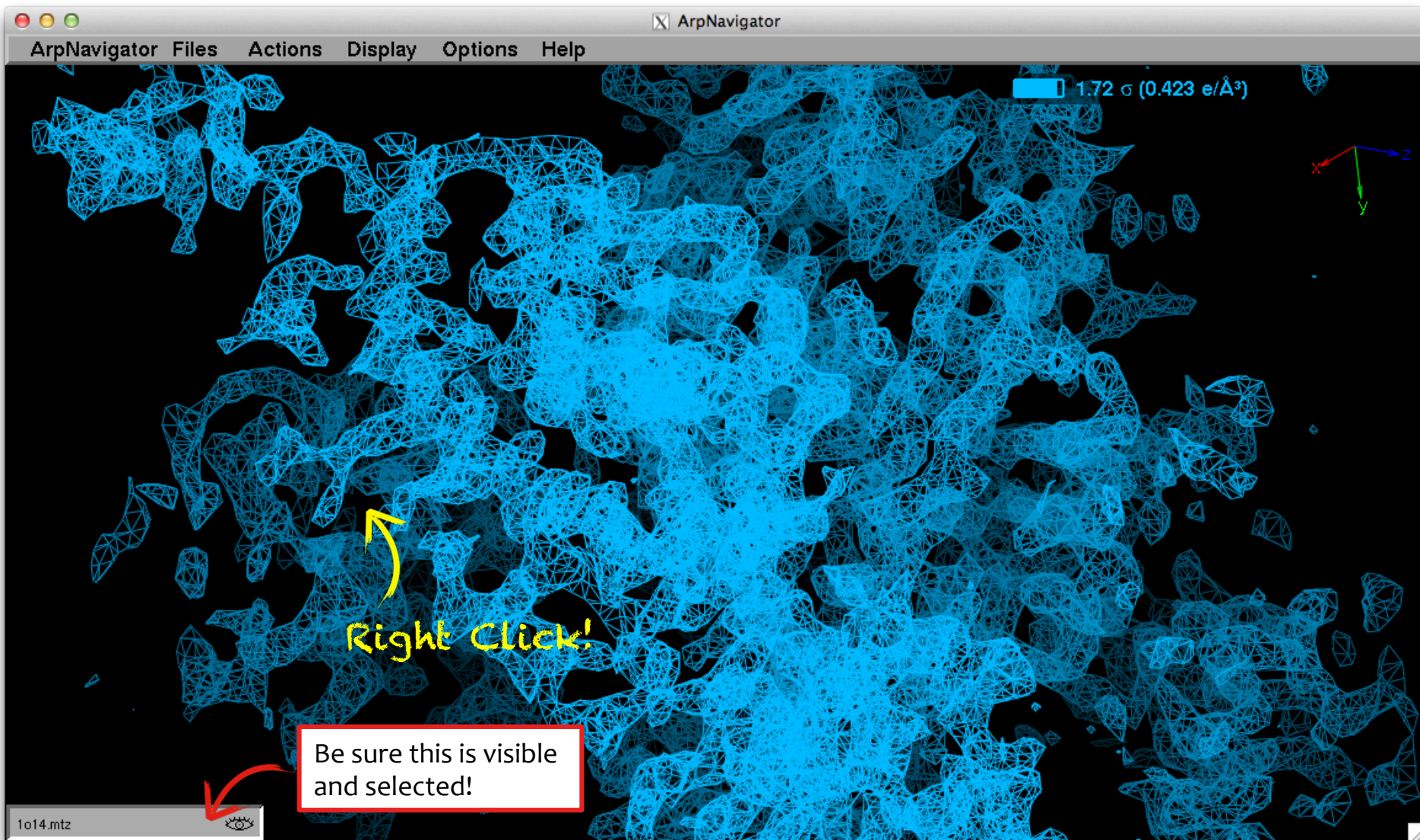
1. Load MTZ File



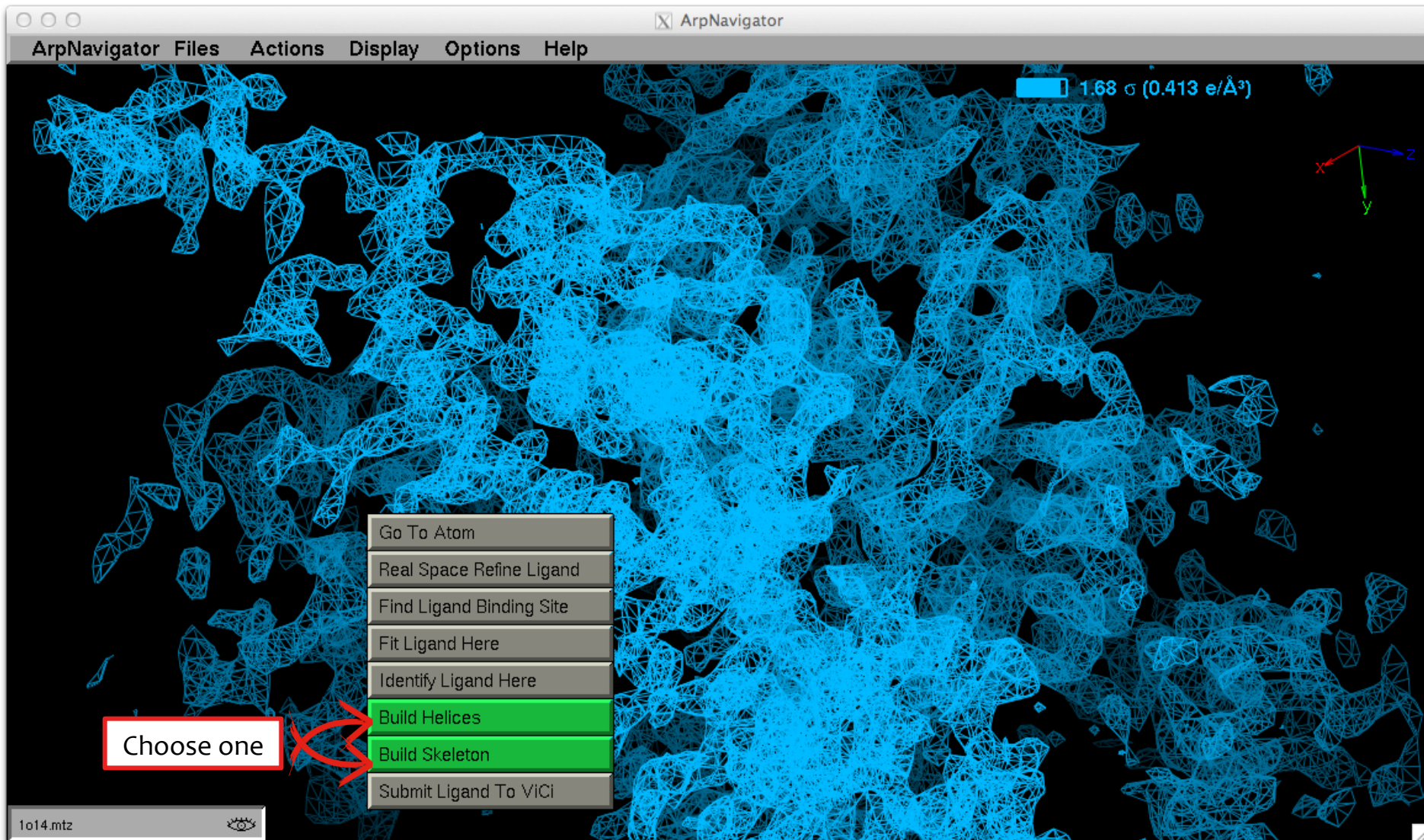
1. Load MTZ File



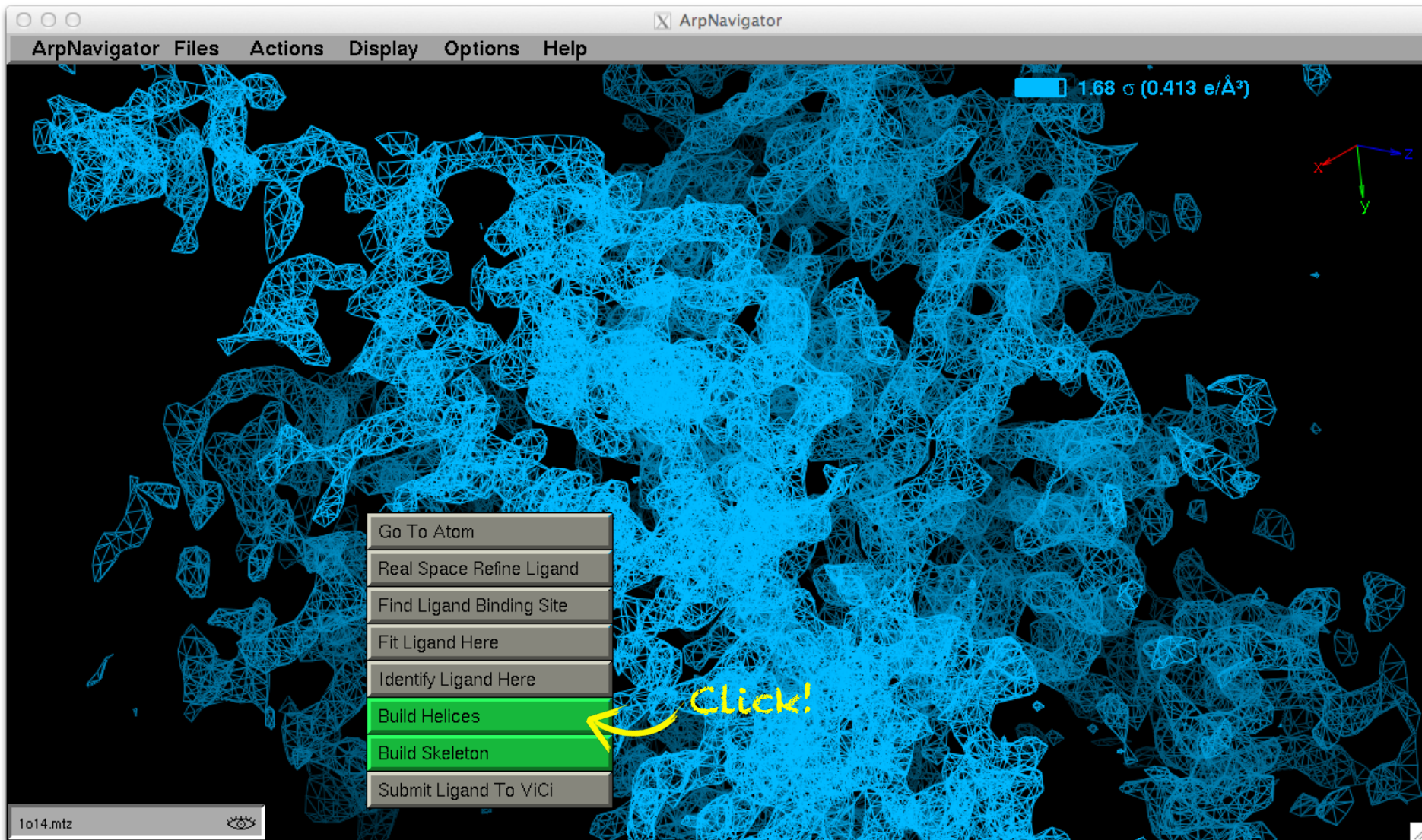
2. Build Helices (Only) or Skeletons



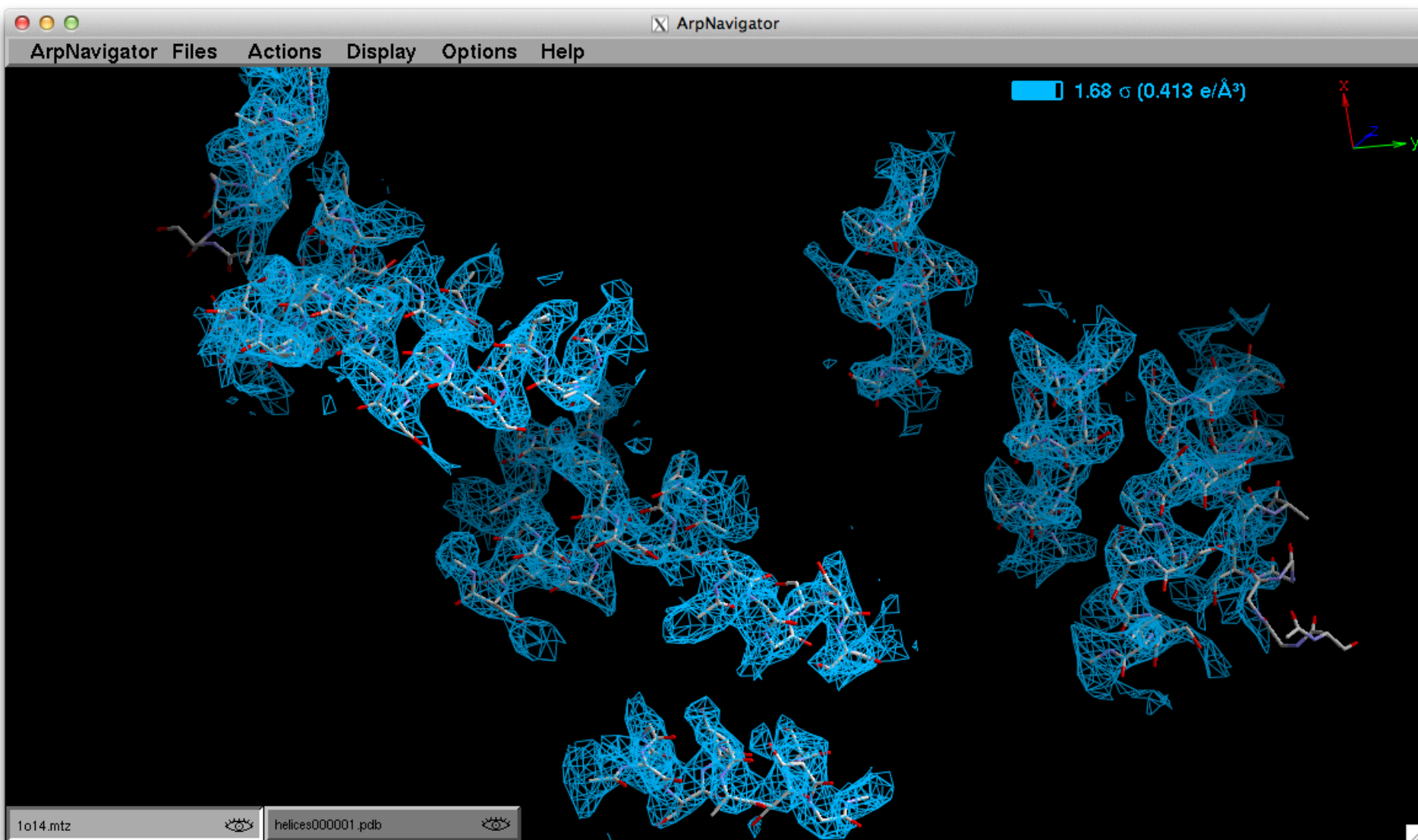
2. Build Helices (Only) or Skeletons



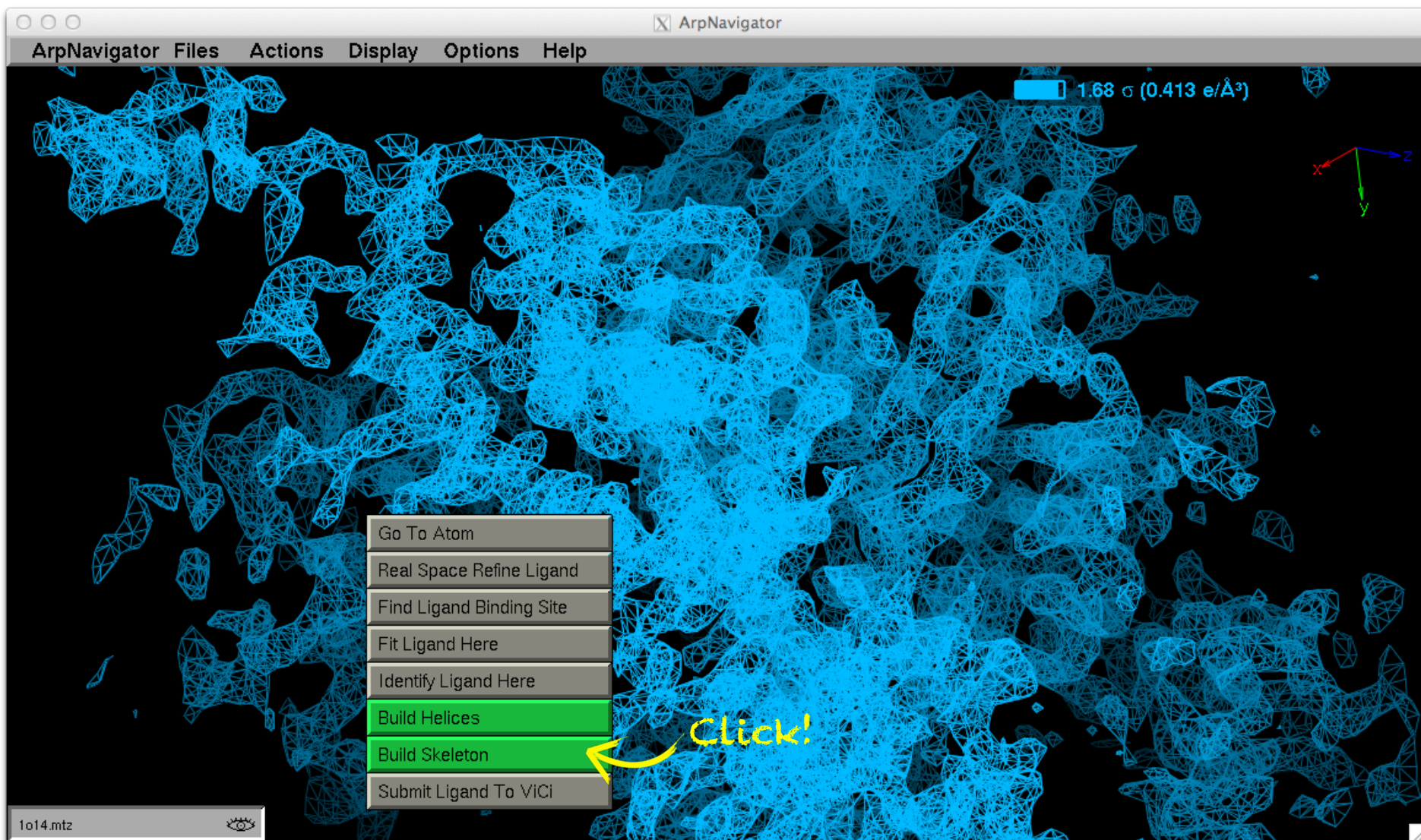
2.1. Build Helices (Only)



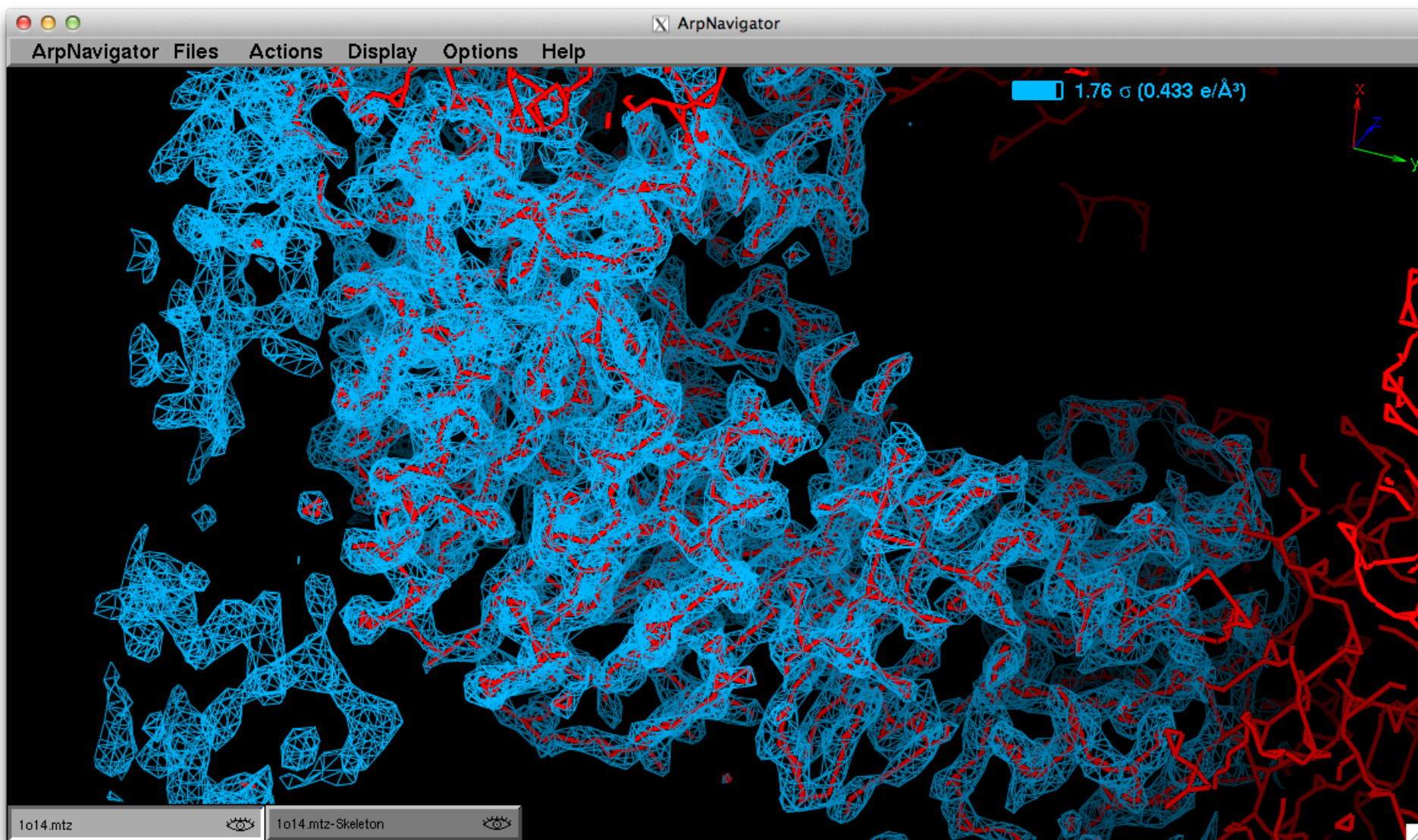
2.1. Build Helices (Only)



2.2. Build Skeletons



2.2. Build Skeletons



For any questions...

The Developers

Contact us anytime!

Victor Lamzin Philipp Heuser

Ioan Vancea Joana Pereira

Daria Beshnova

Or just visit our website!

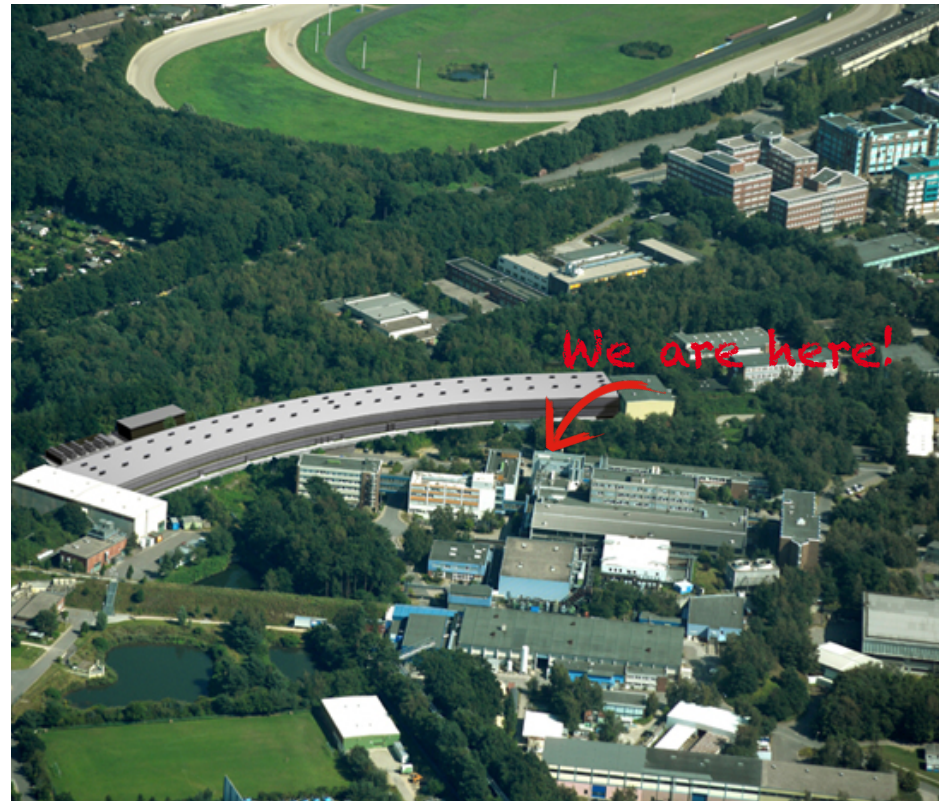
<http://www.embl-hamburg.de/ARP/>



User guide

Frequently asked questions

Tutorials



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