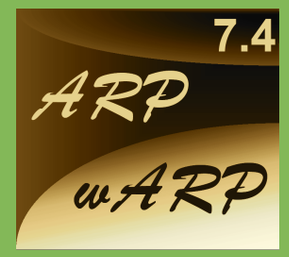


ARP/wARP

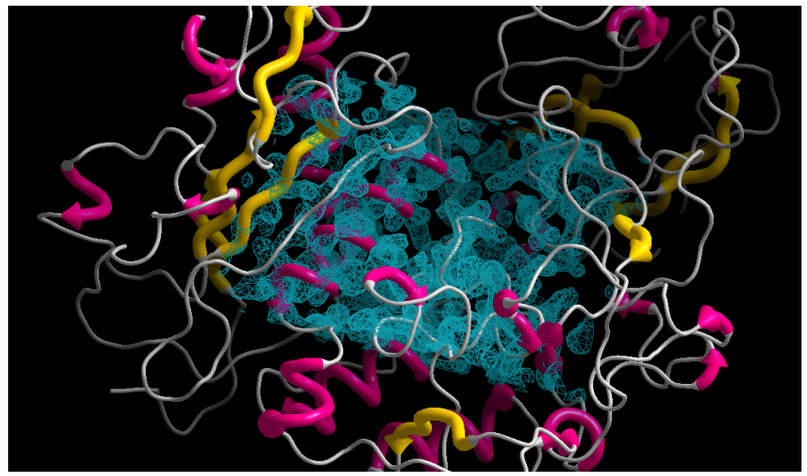
Hands-on Tutorial

Daria Beshnova and Joana Pereira

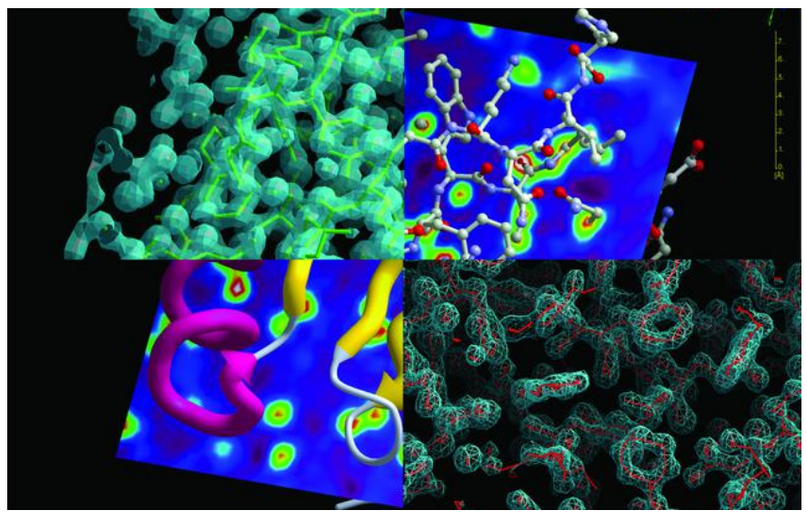
Lamzin Group, EMBL Hamburg

What will you learn?

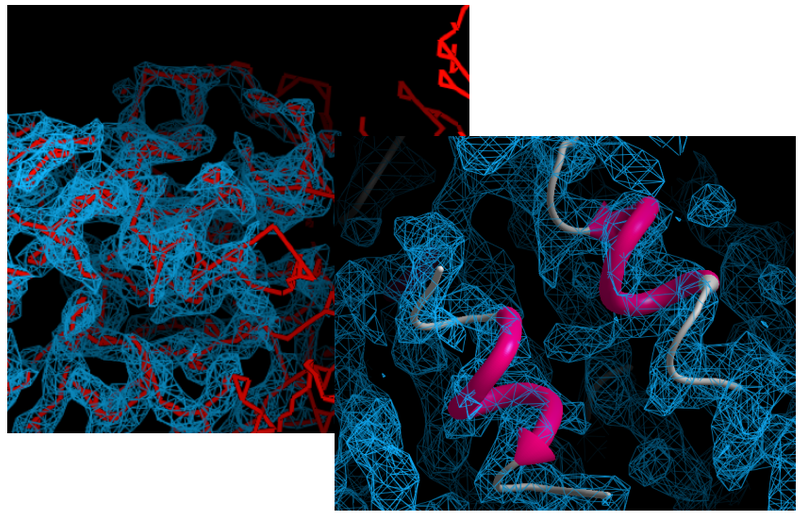
1. Automatically build a protein model from your electron density



2. Use several model-viewing options



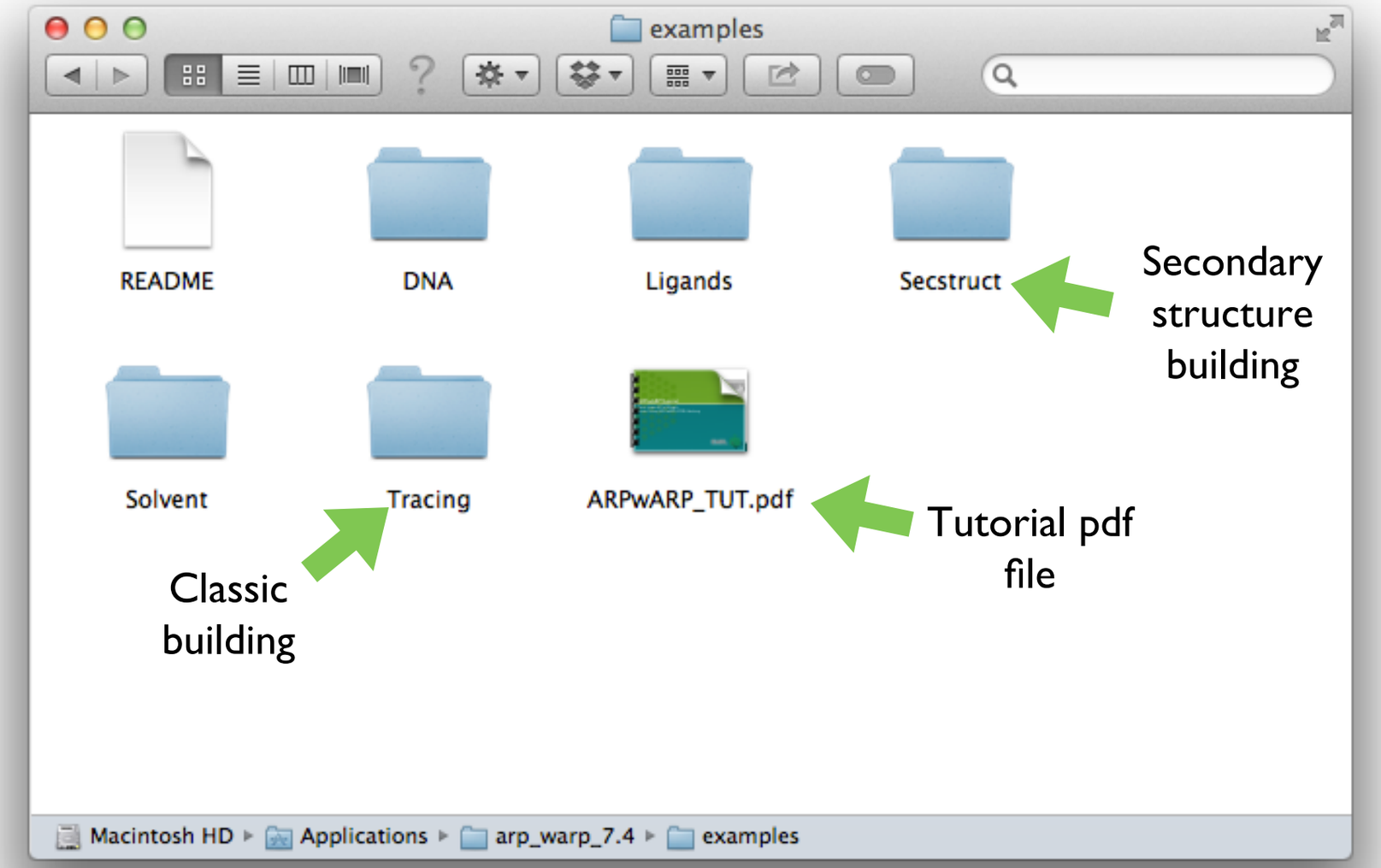
3. Build helices and skeletons for a quick quality assessment of the initial map



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
GPGSGPGRGFGKRRHPKKLTPLAYKQFIPNVAEKTLGASG
RYEGKITRNSERFKELTPNYNPDIIFKDEENTGADRLMTQ
RCKDKLNALAISVMNQWPGVKLRVTEGWDEDGHHSEESLH
YEGRAVDITTSDRDRSKYGMLARLAVEAGFDWVYYESKAH
IHCSVKAE

>Protein_B
GSTPITGPHIAYTEAVSDTQIMLKWTYIPSSNNNTPIQGF
YIYYRPTDSDNDSDYKRDVVEGSKQWHMIGHLQPETSYDI
KMQCFNEGGESEFSNVMICETK
```

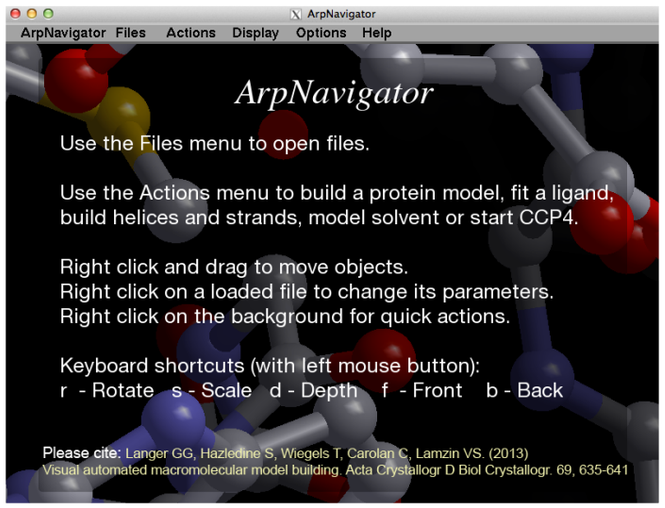
```
>Sequence

GPGSGPGRGFGKRRHPKKLTPLAYKQFIPNVAEKTLGASG
RYEGKITRNSERFKELTPNYNPDIIFKDEENTGADRLMTQ
RCKDKLNALAISVMNQWPGVKLRVTEGWDEDGHHSEESLH
YEGRAVDITTSDRDRSKYGMLARLAVEAGFDWVYYESKAH
IHCSVKAEAAAAAAAAAAAGSTPITGPHIAYTEAVSDTQI
MLKWTYIPSSNNNTPIQGFYIYYRPTDSDNDSDYKRDVVE
GSKQWHMIGHLQPETSYDIKMQCFNEGGESEFSNVMICET
K
```

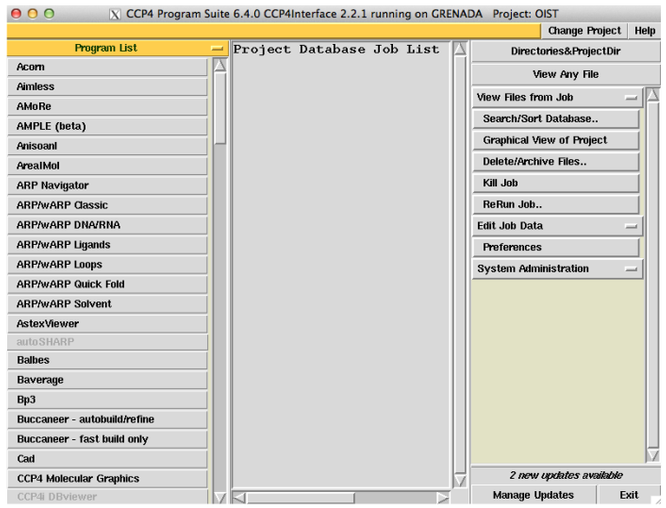
At least 10 alanines between both sequences!

How to start it?

3 ways:

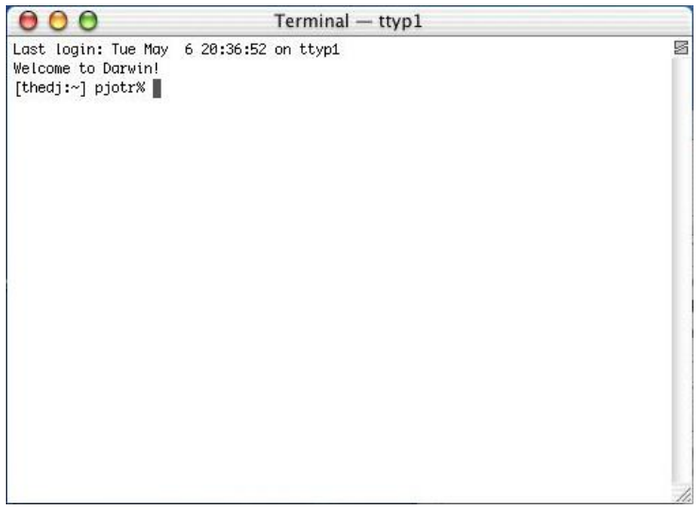


ArpNavigator



CCP4 Suite

This tutorial!



Terminal

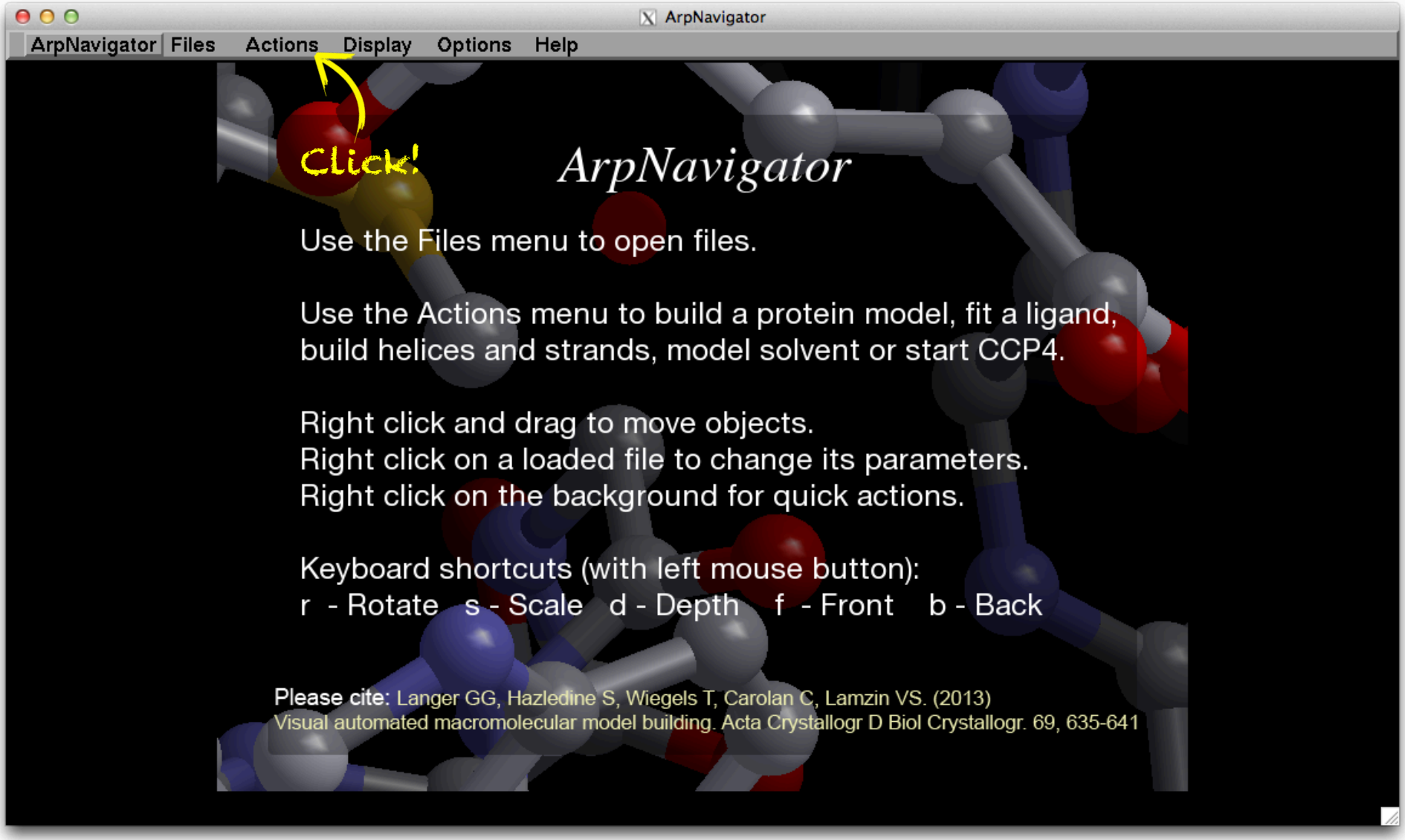
Check the user guide!

Classic Automated Model Building With ArpNavigator

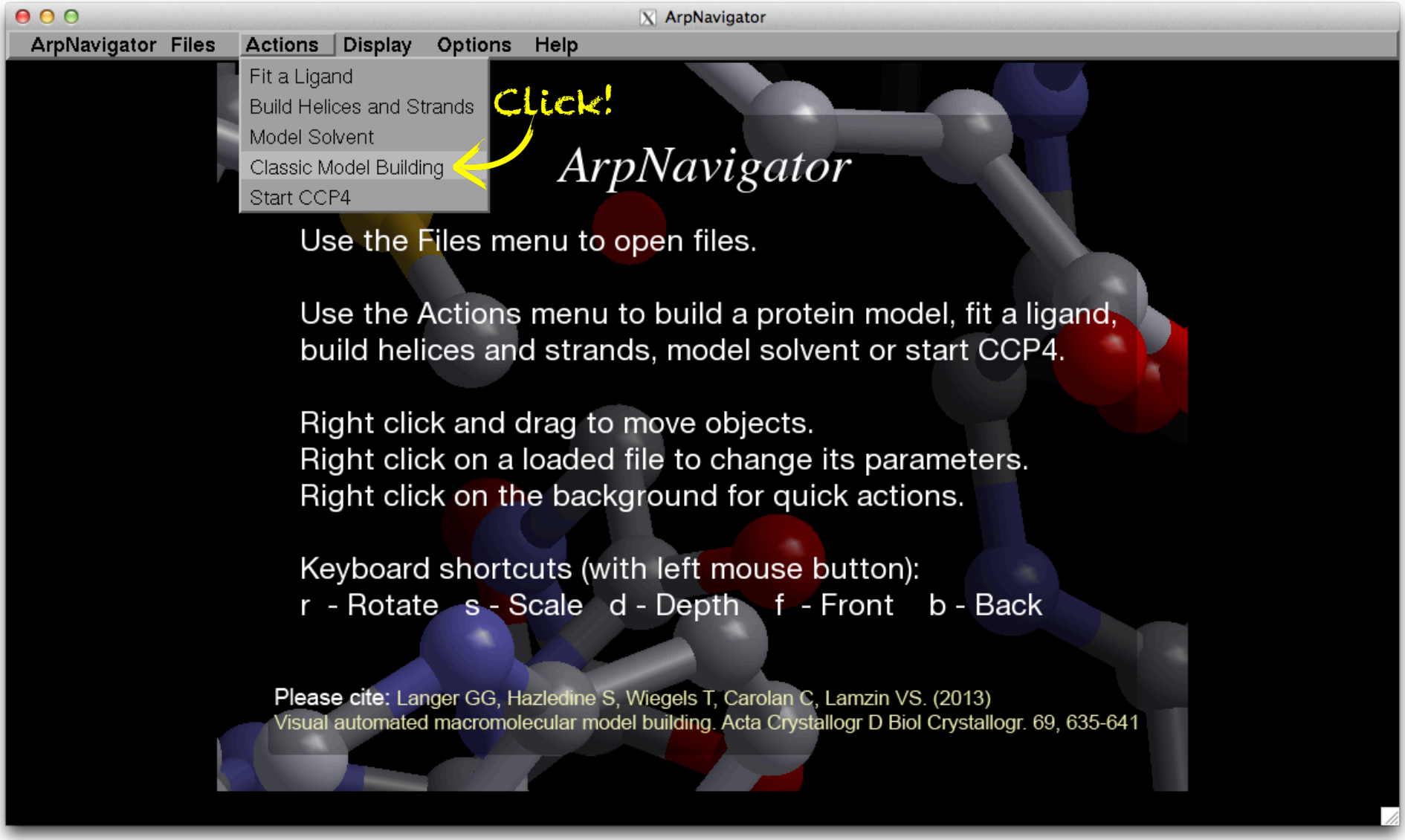
A Click-on Tutorial

EMBL
Hamburg

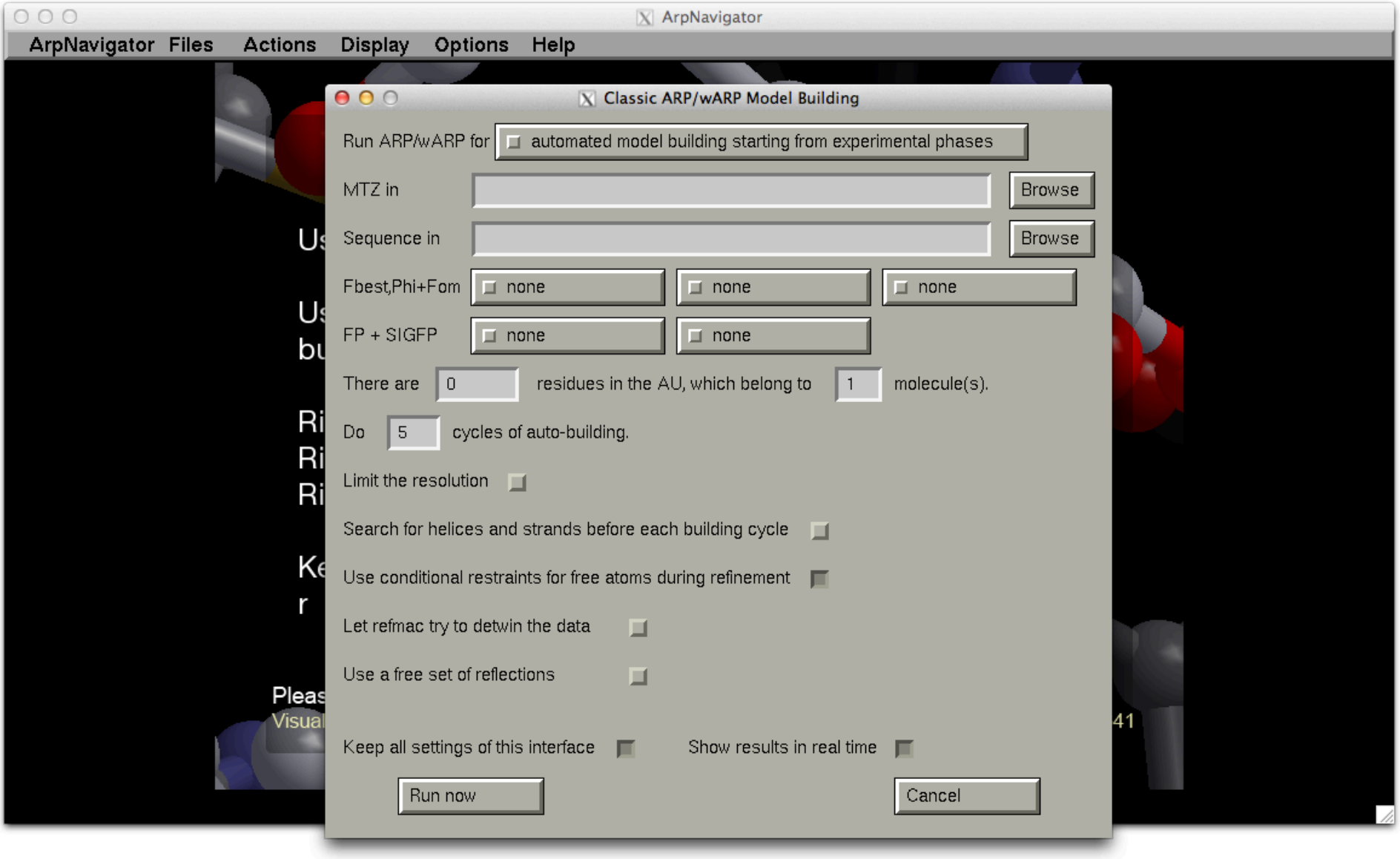
Where to go…


ArpNavigator
ArpNavigator Files Actions Display Options Help
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

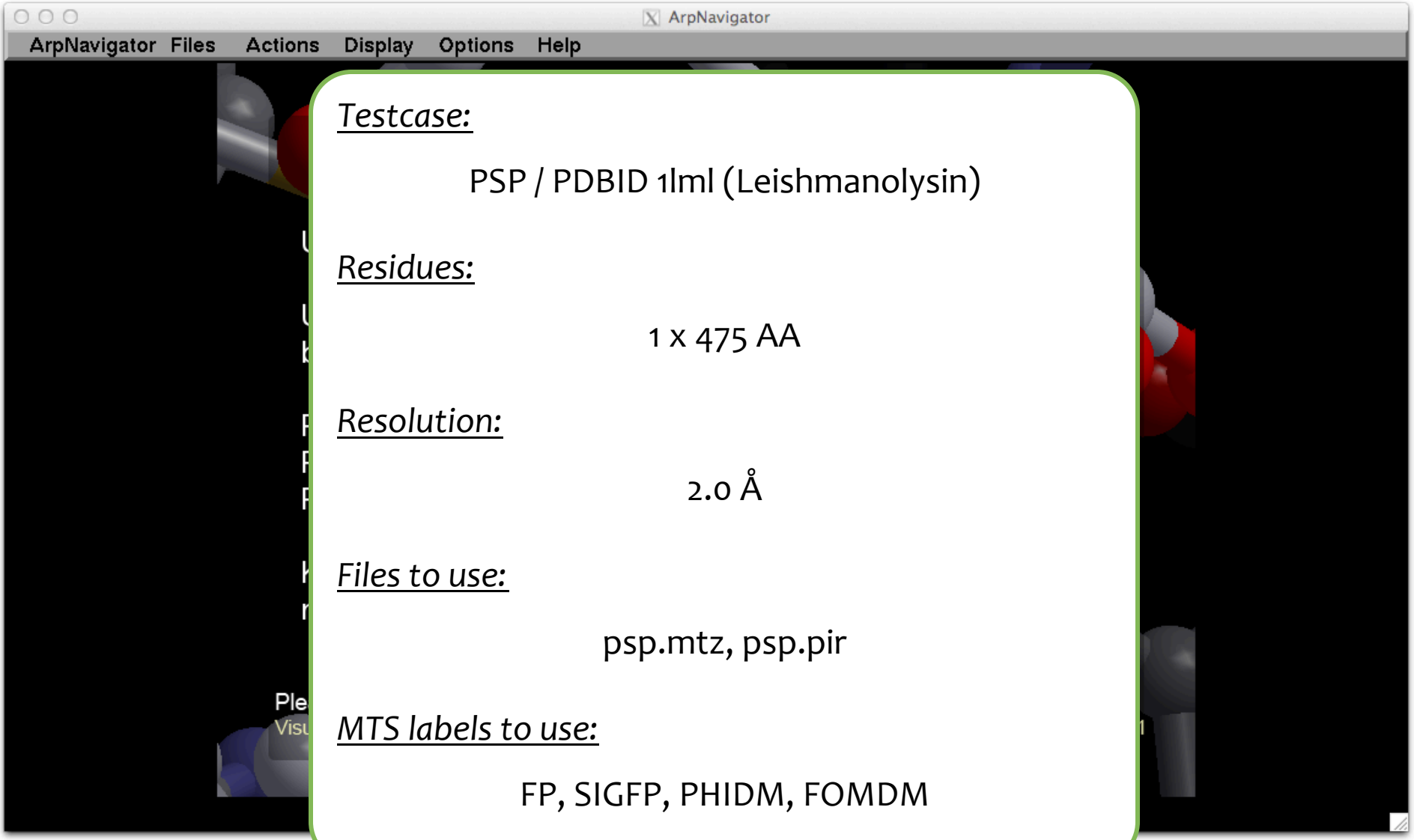
ARP/wARP: Classic Model Building (arp_tracing)



ARP/wARP: Classic Model Building (arp_tracing)



ARP/wARP: Classic Model Building (arp_tracing)



Testcase:

PSP / PDBID 1lml (Leishmanolysin)

Residues:

1 x 475 AA

Resolution:

2.0 Å

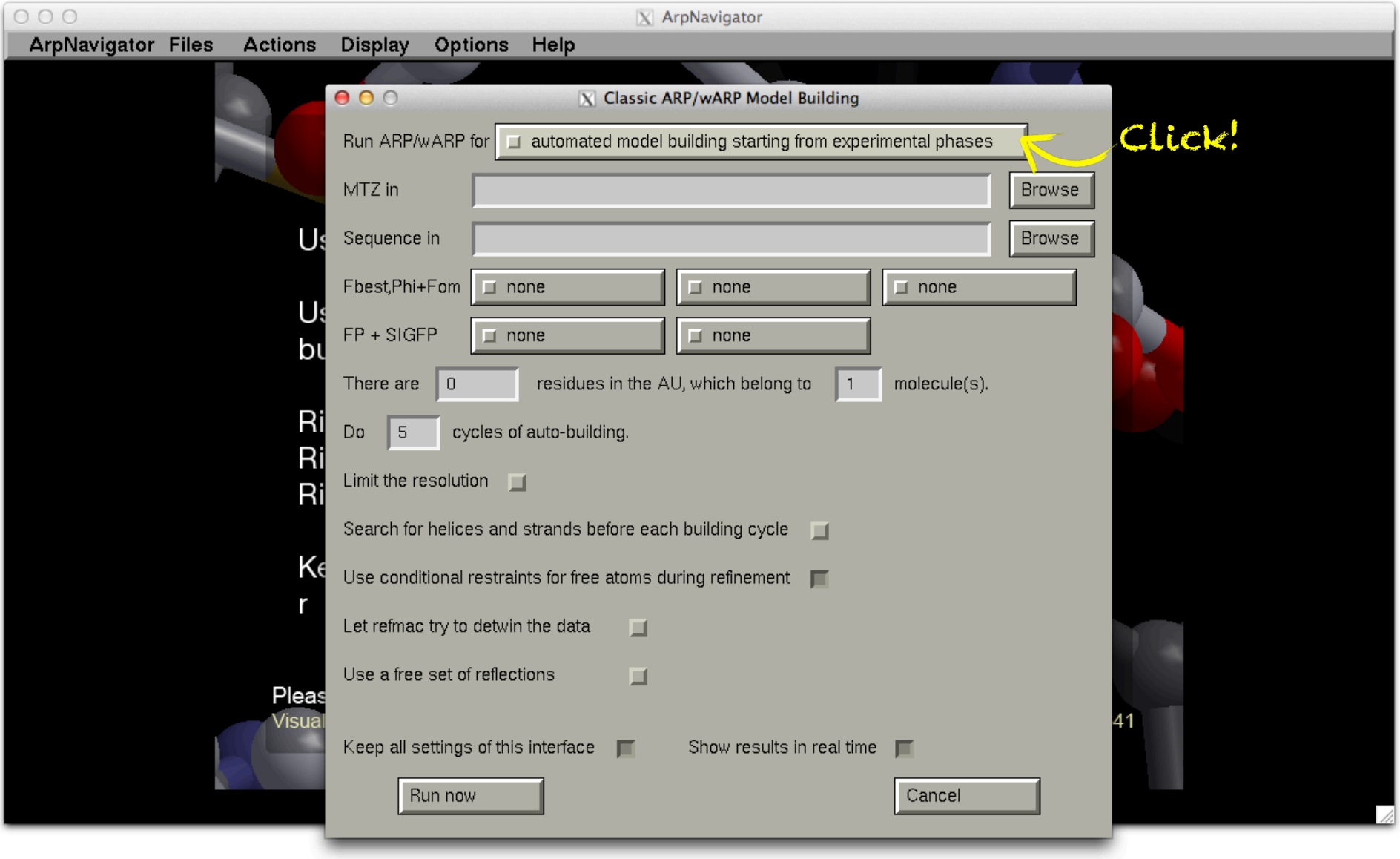
Files to use:

psp.mtz, psp.pir

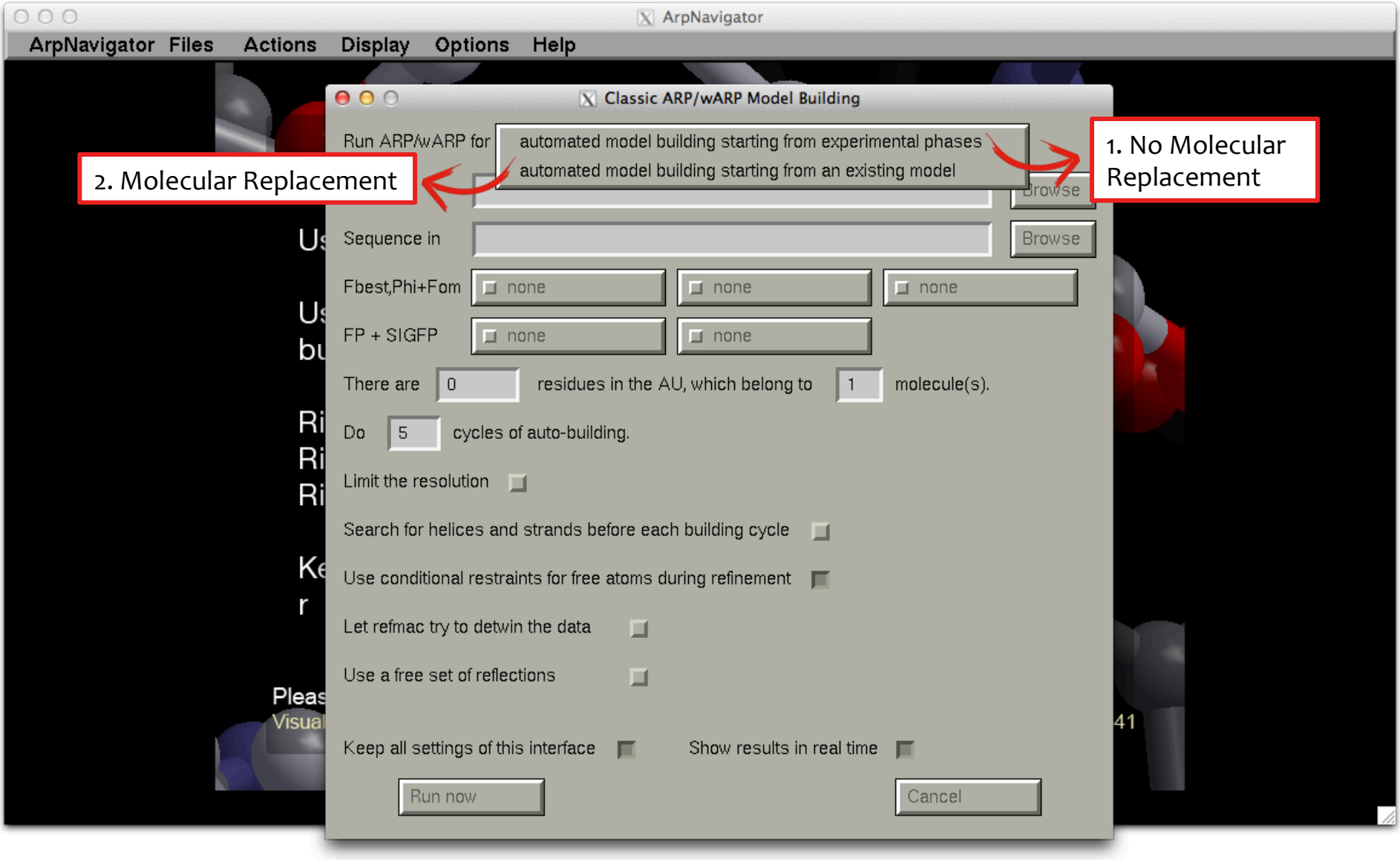
MTS labels to use:

FP, SIGFP, PHIDM, FOMDM

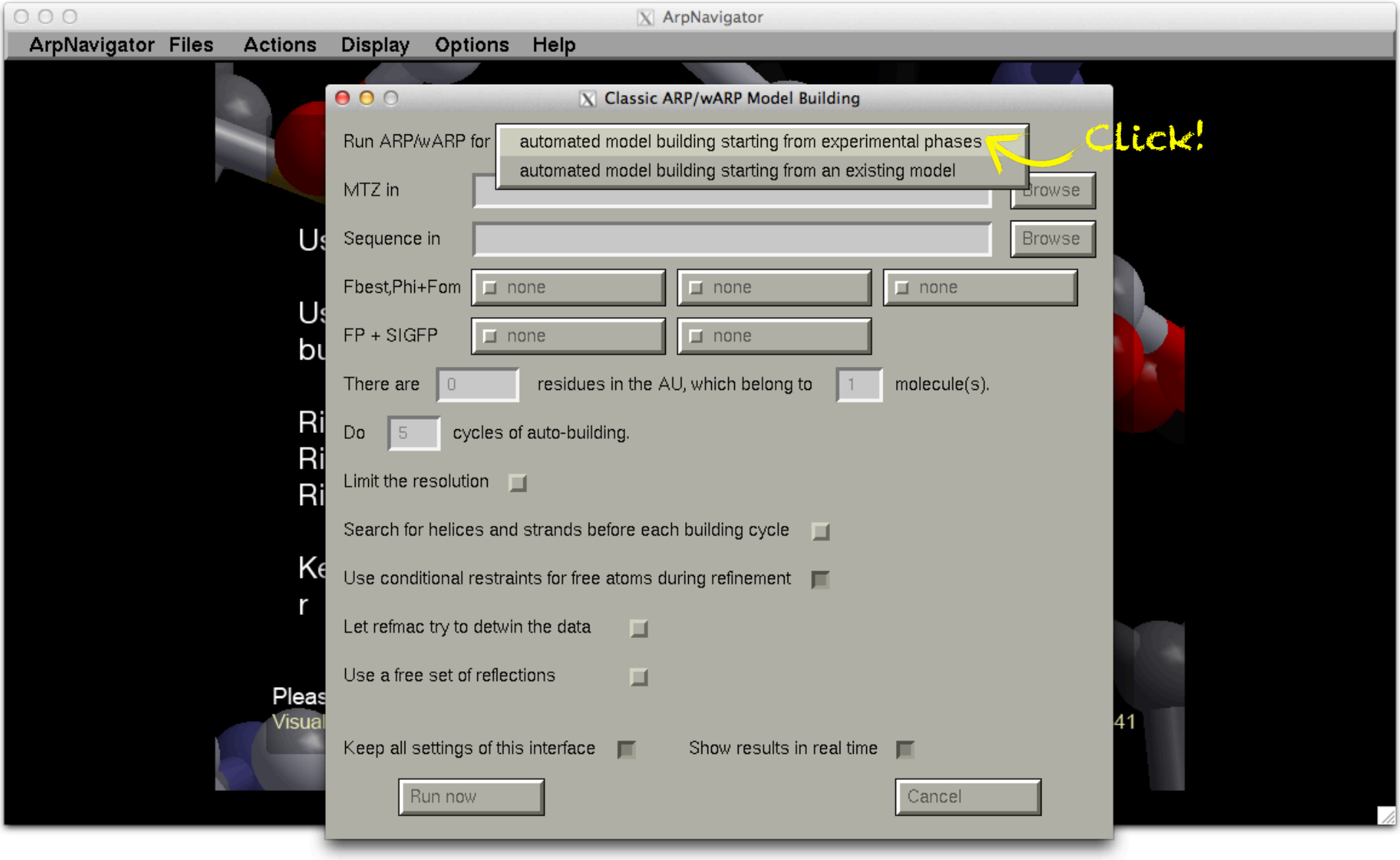
ARP/wARP: Classic Model Building (arp_tracing)



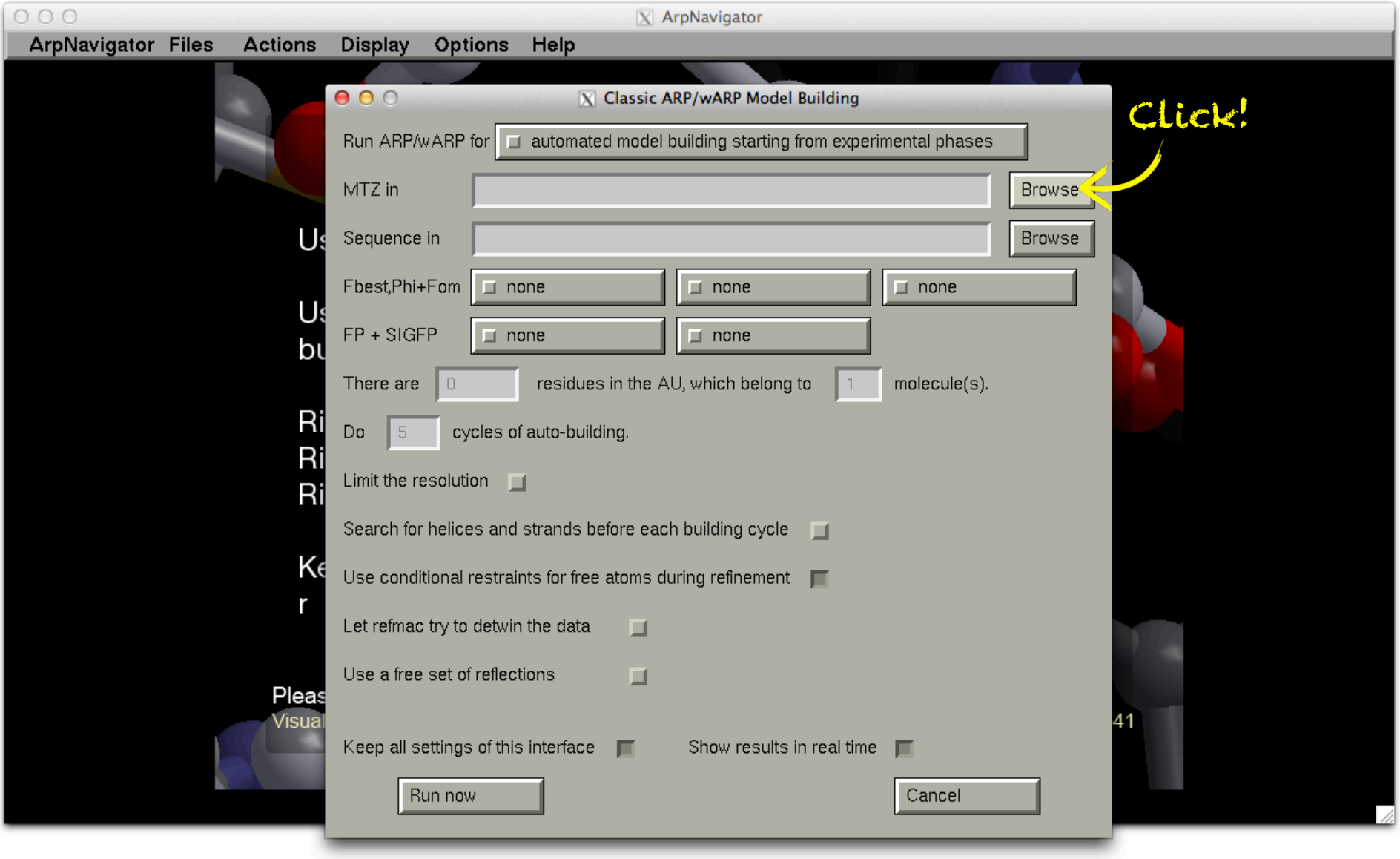
ARP/wARP: Classic Model Building (arp_tracing)



1. From Experimental Phases



1.1. Input Files: MTZ File



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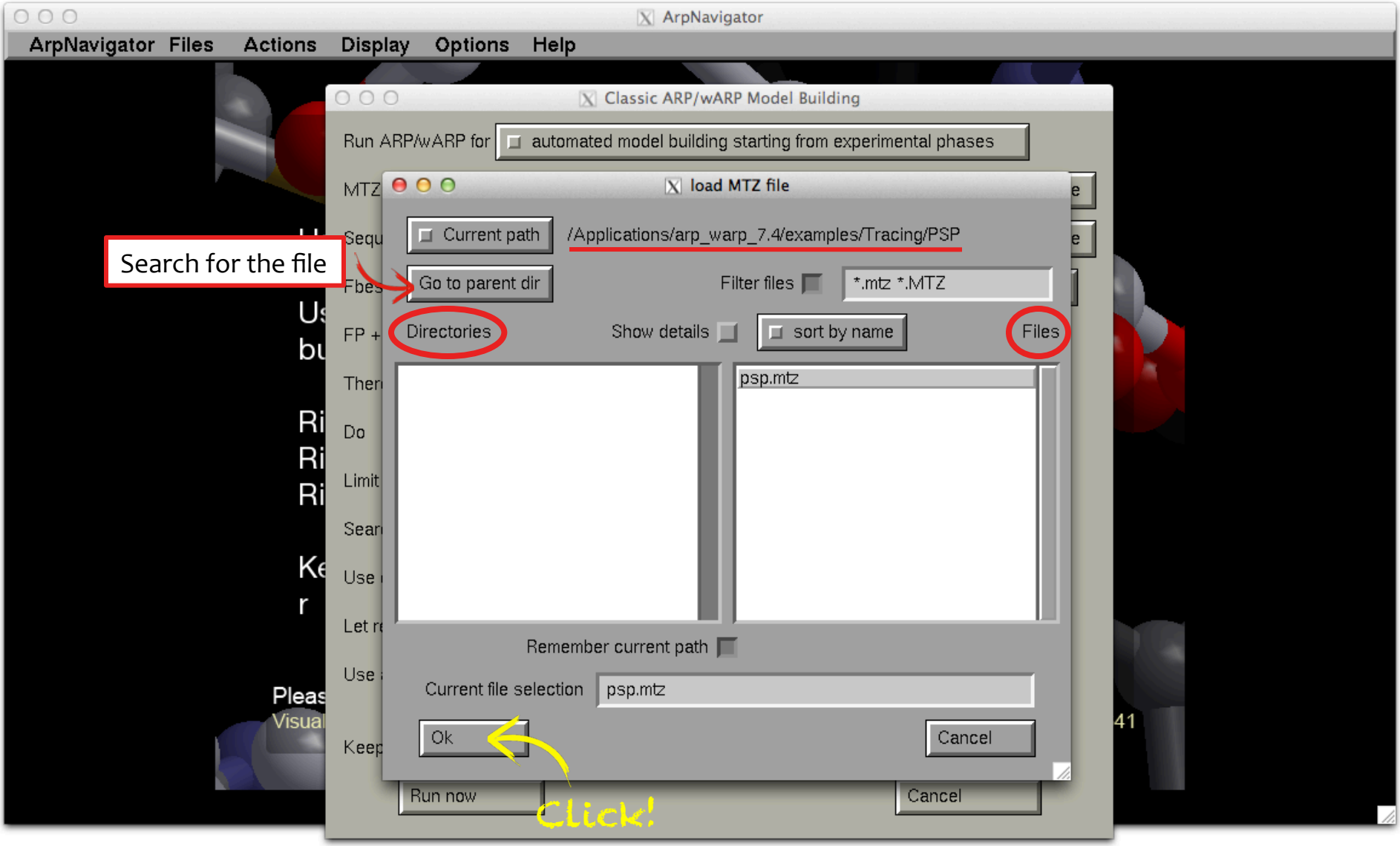
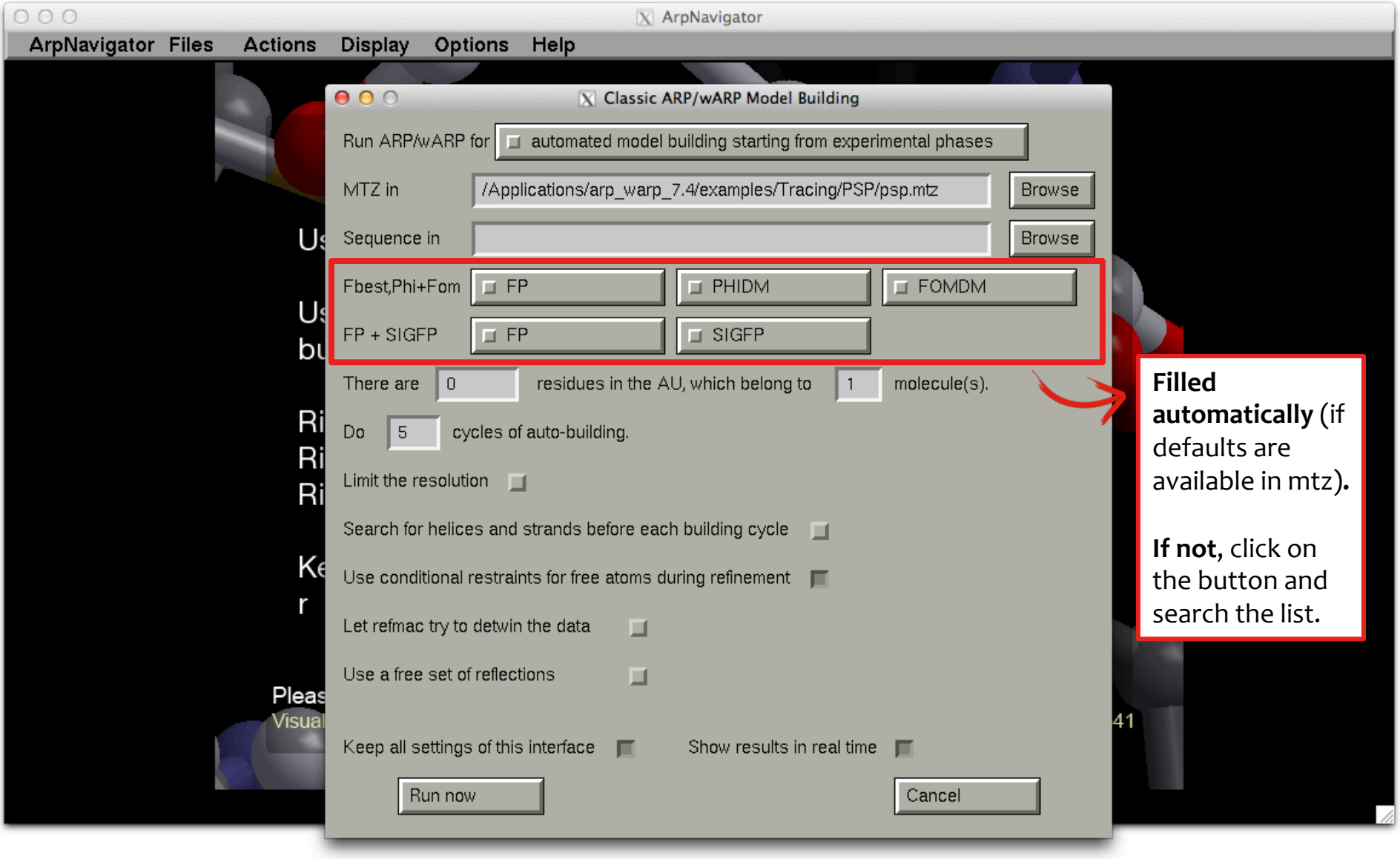
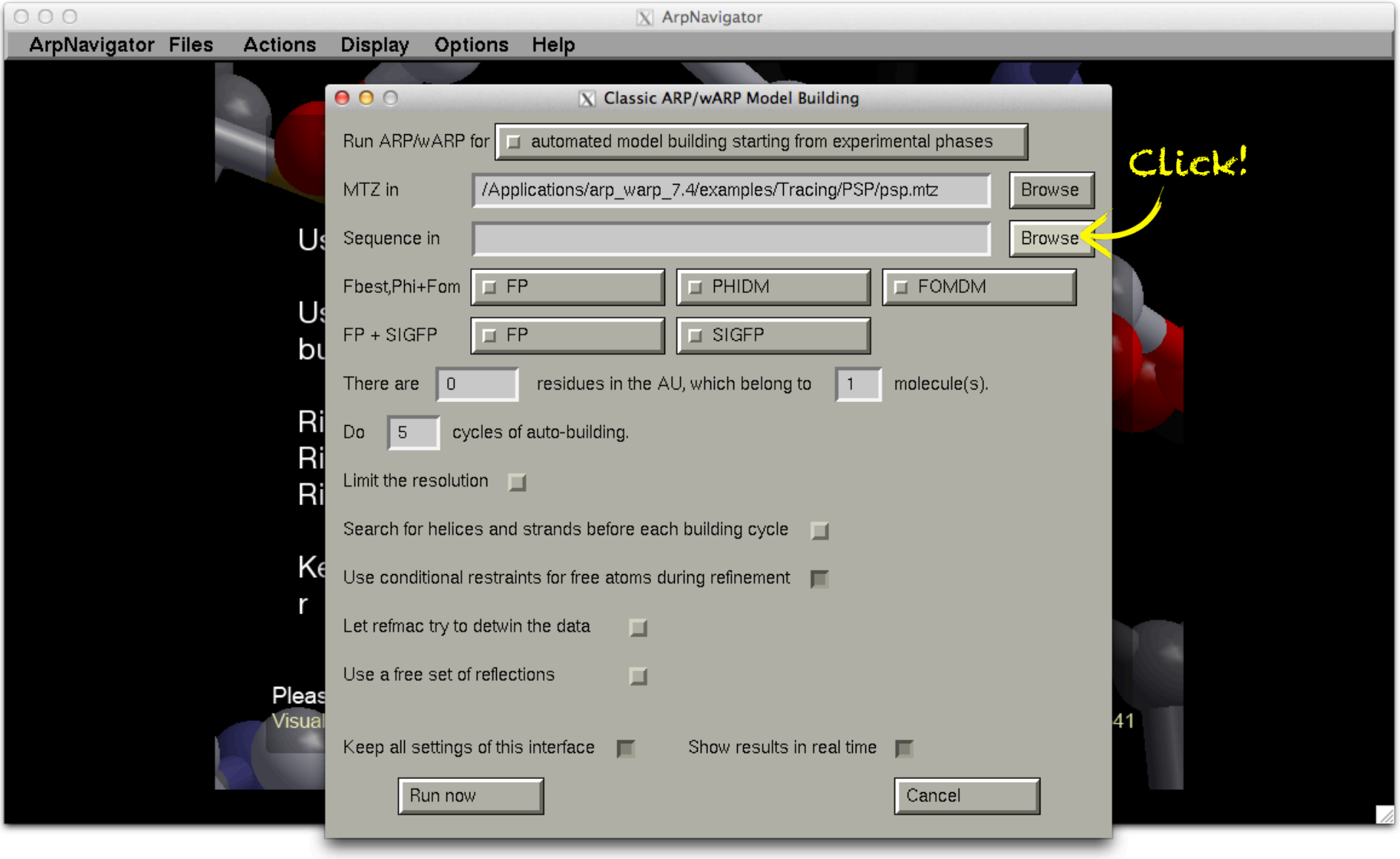


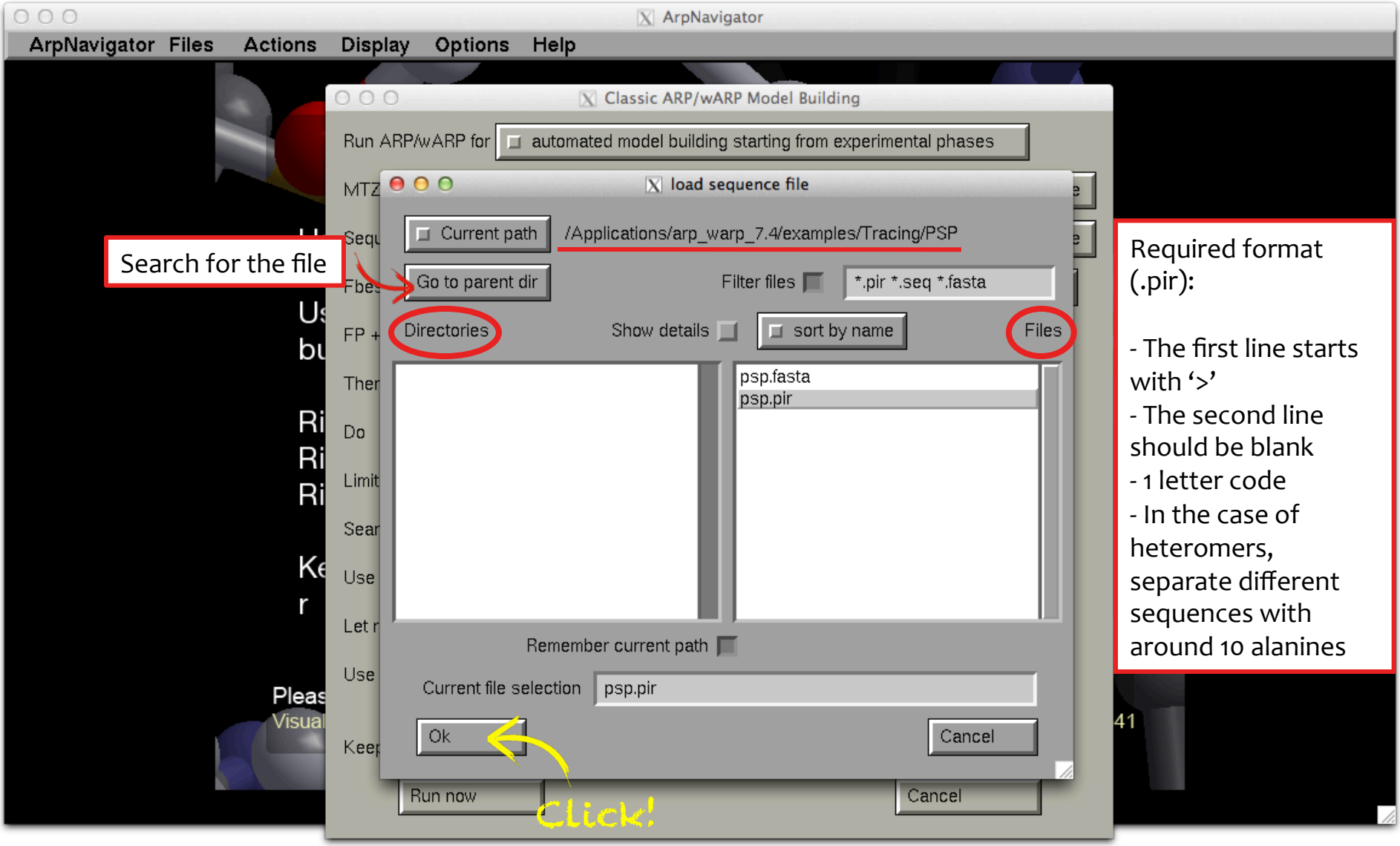
1.1. Input Files: MTZ File



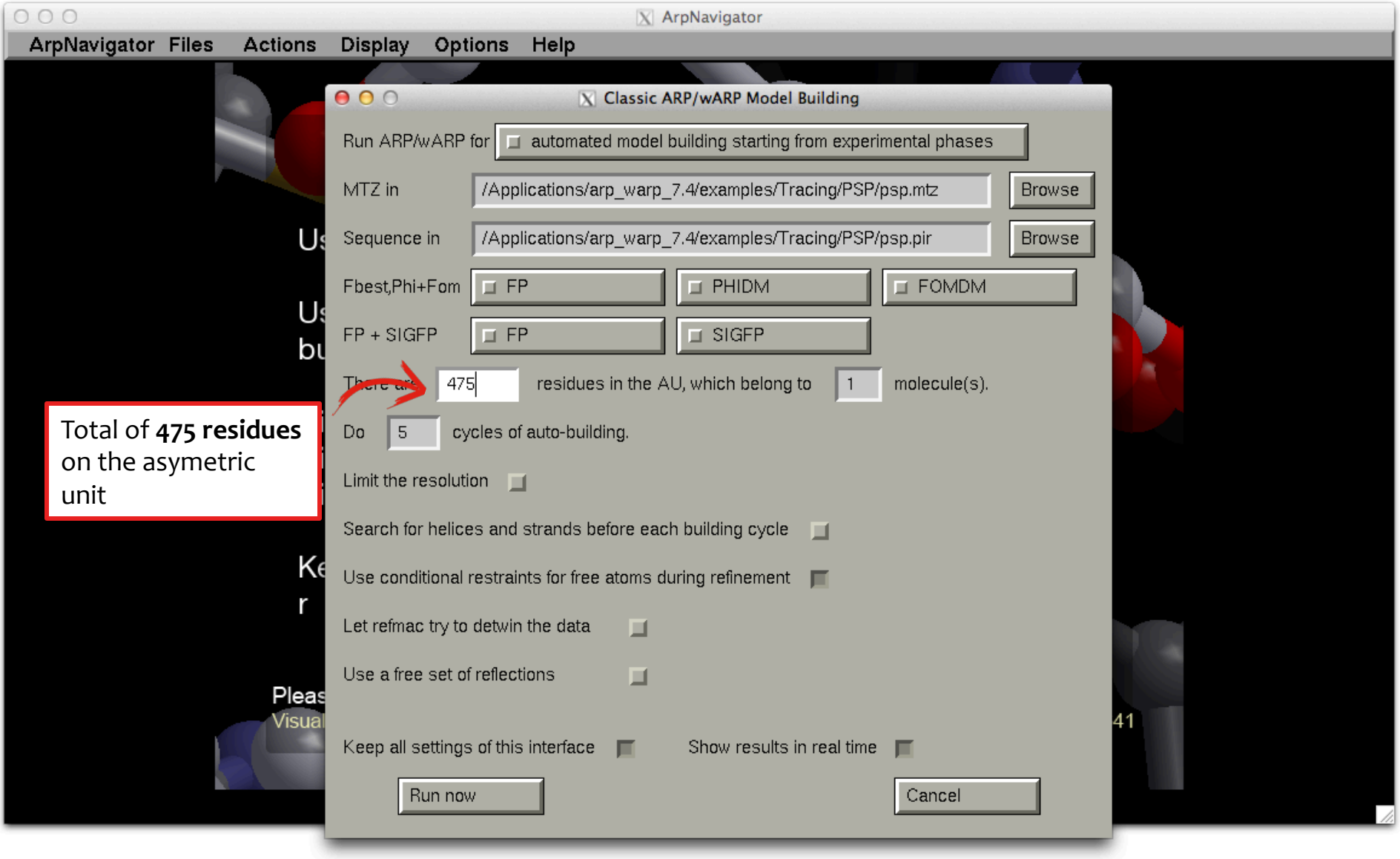
1.1. Input Files: Sequence



1.1. Input Files: Sequence

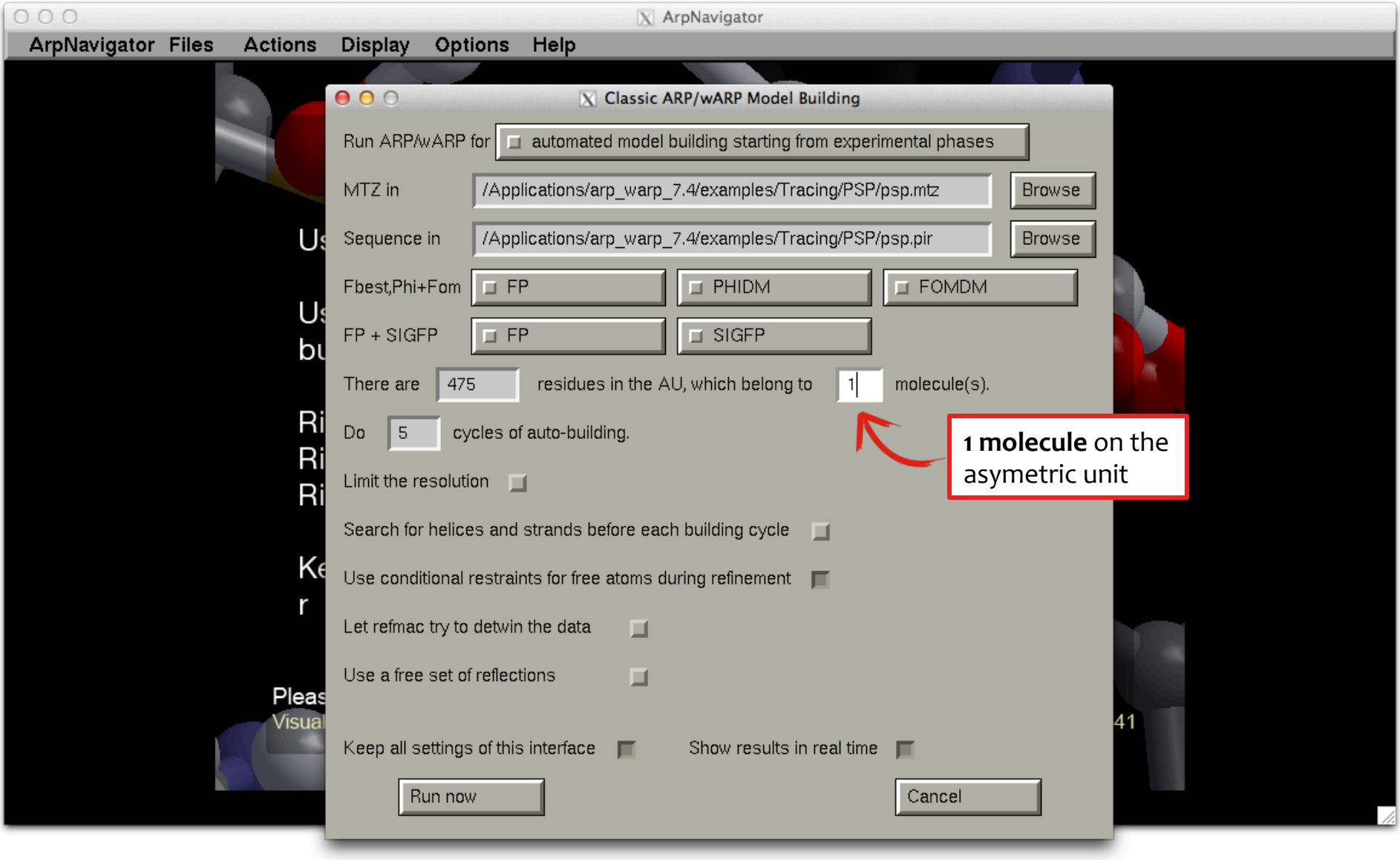


1.2. Required Parameters

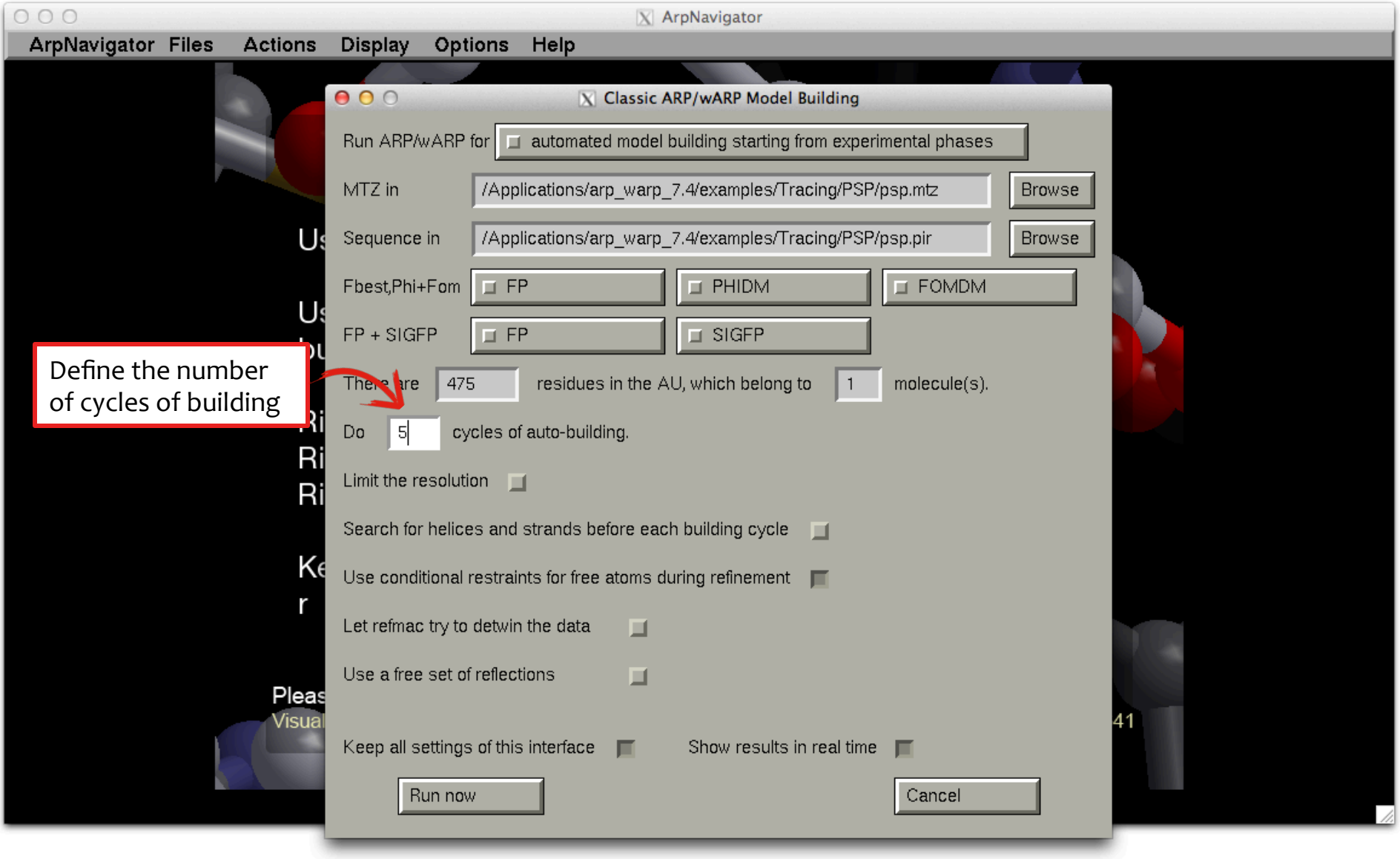


Total of **475 residues** on the asymetric unit

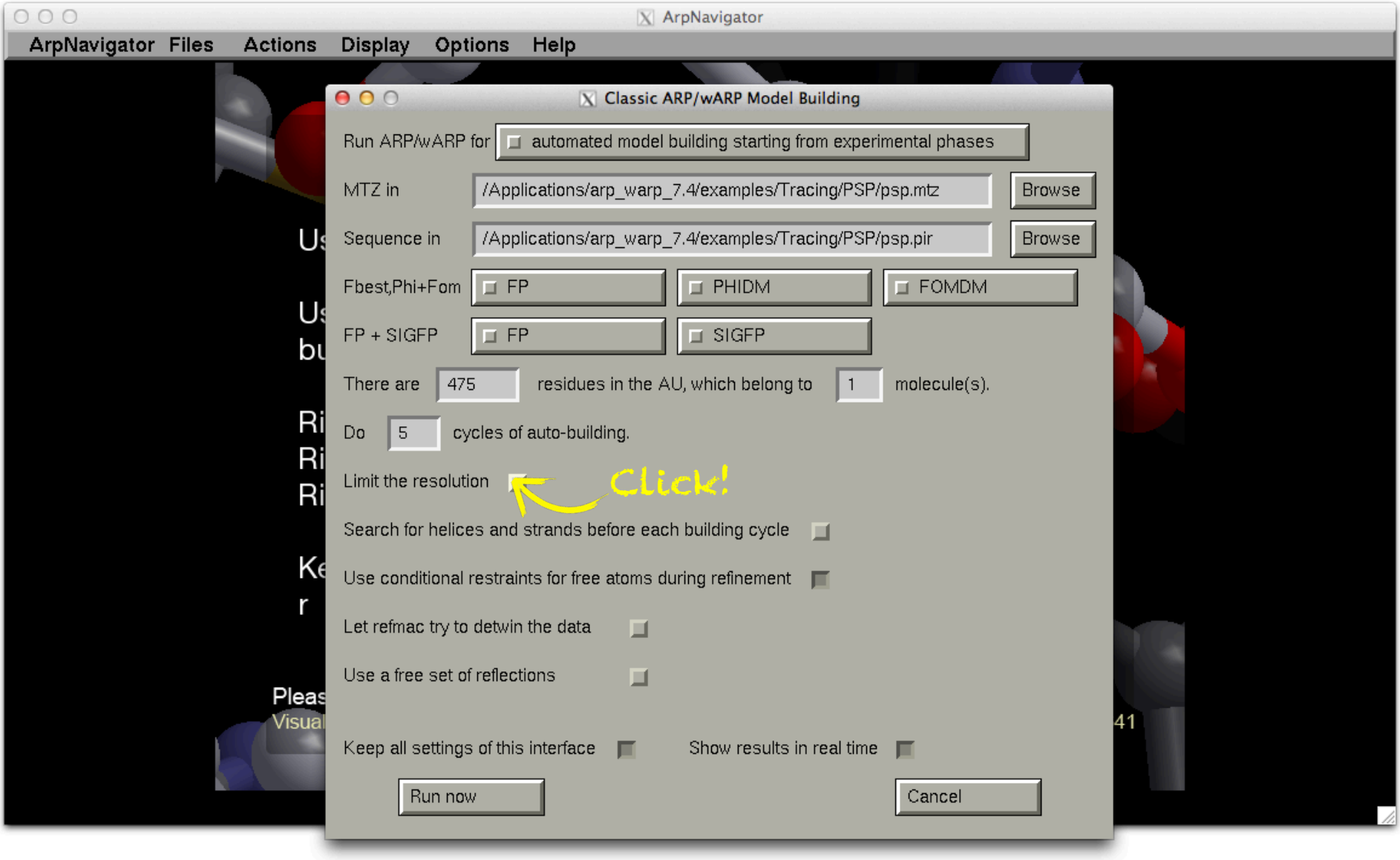
1.2. Required Parameters



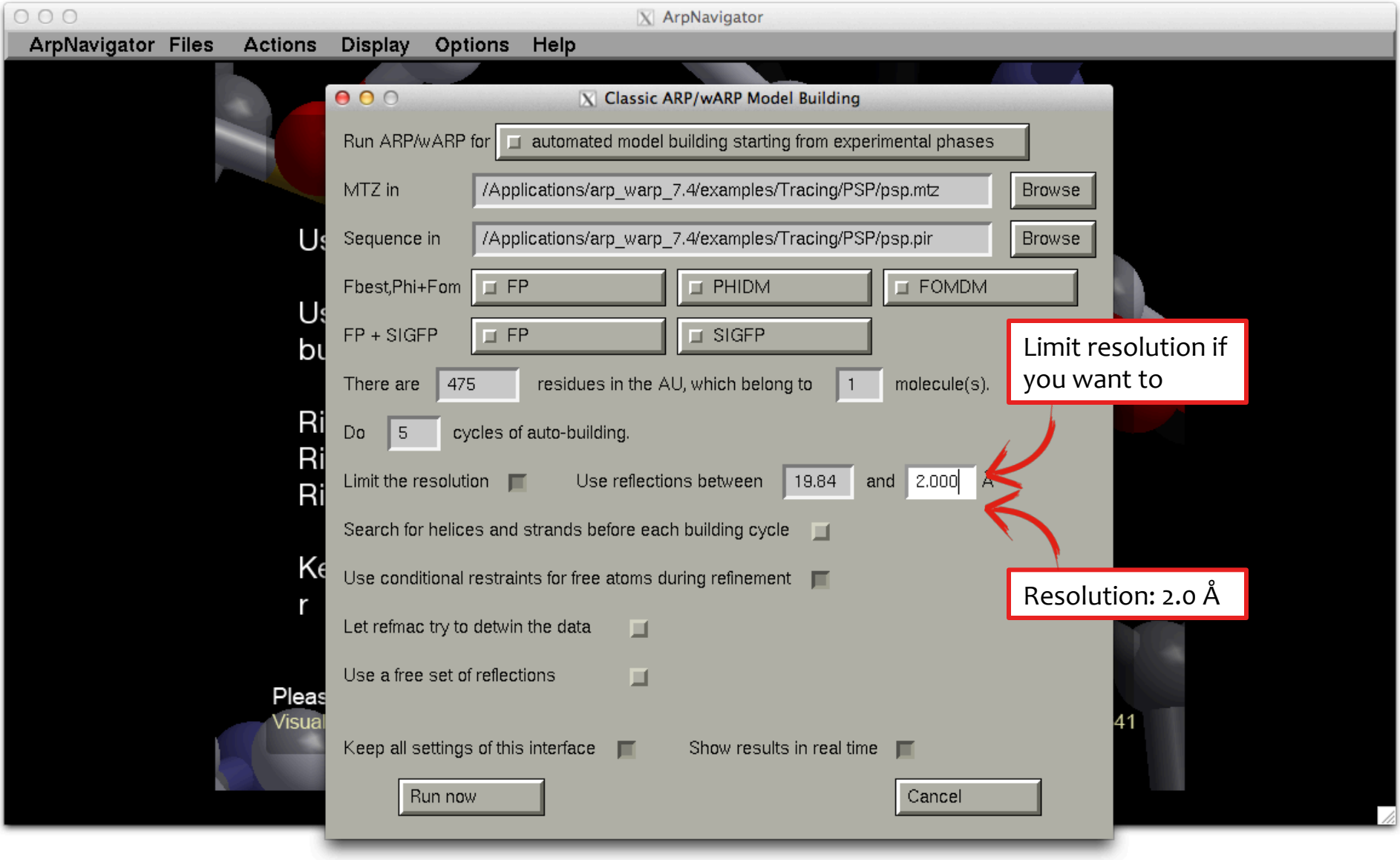
1.2. Required Parameters



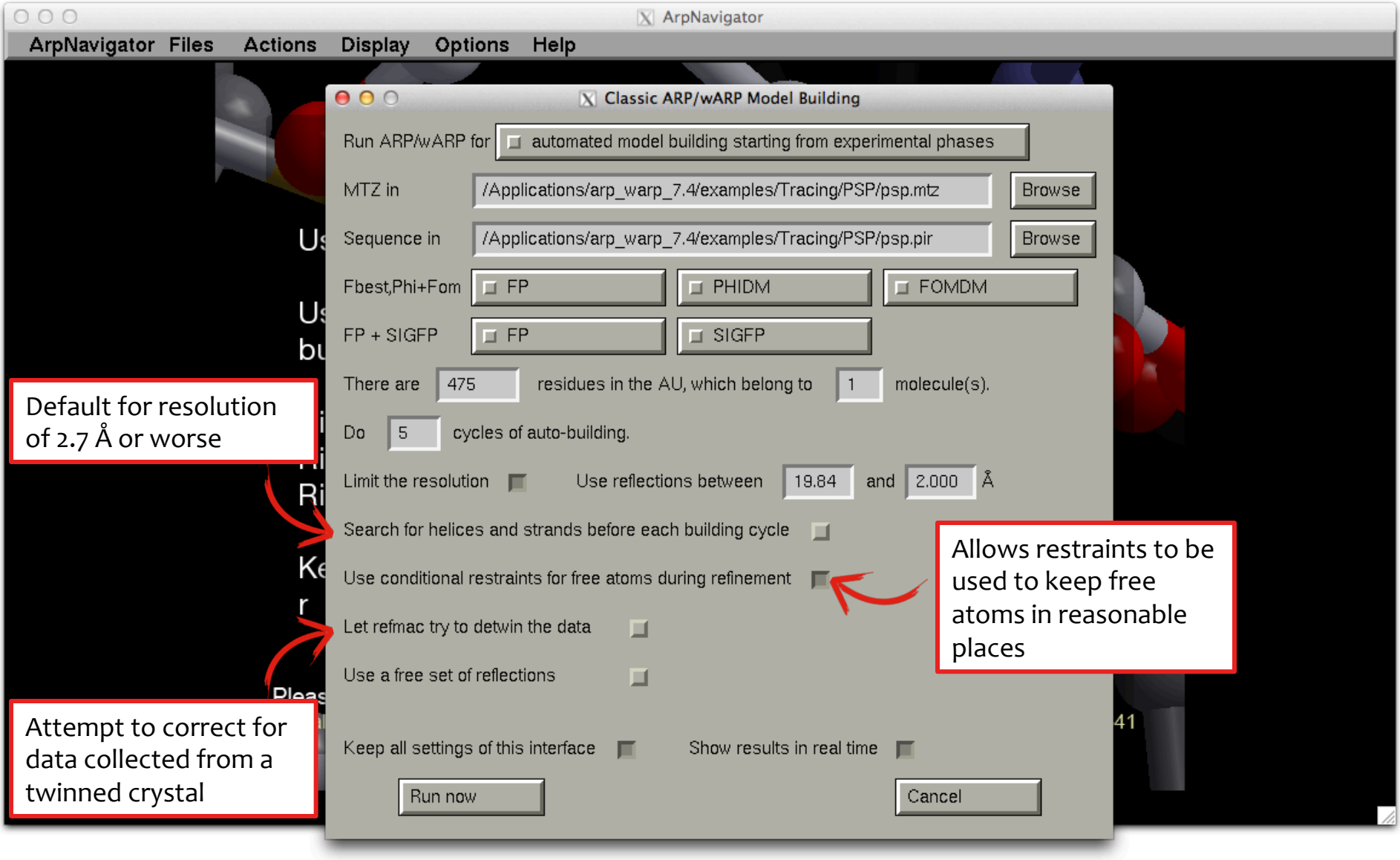
1.3. Resolution



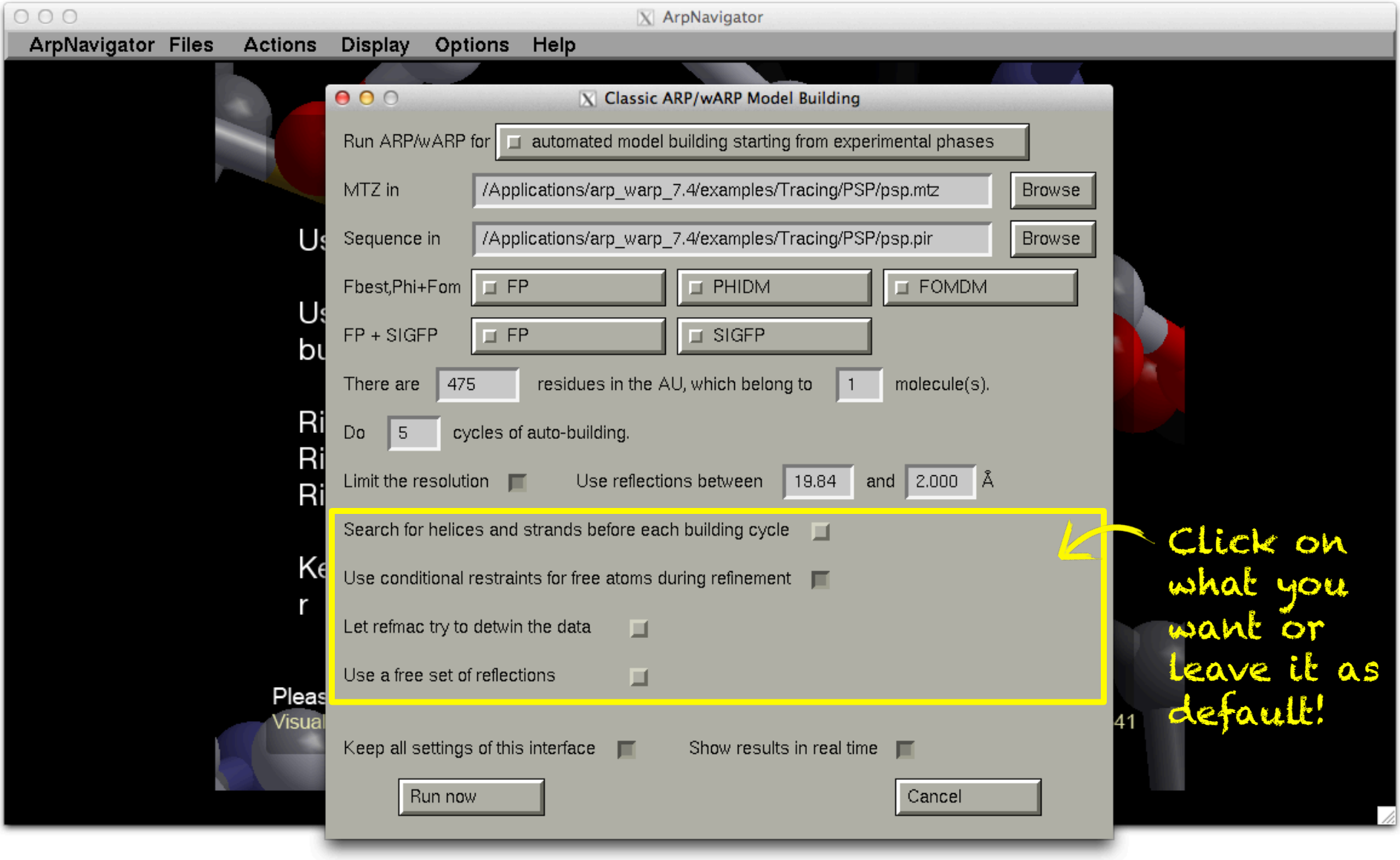
1.3. Resolution



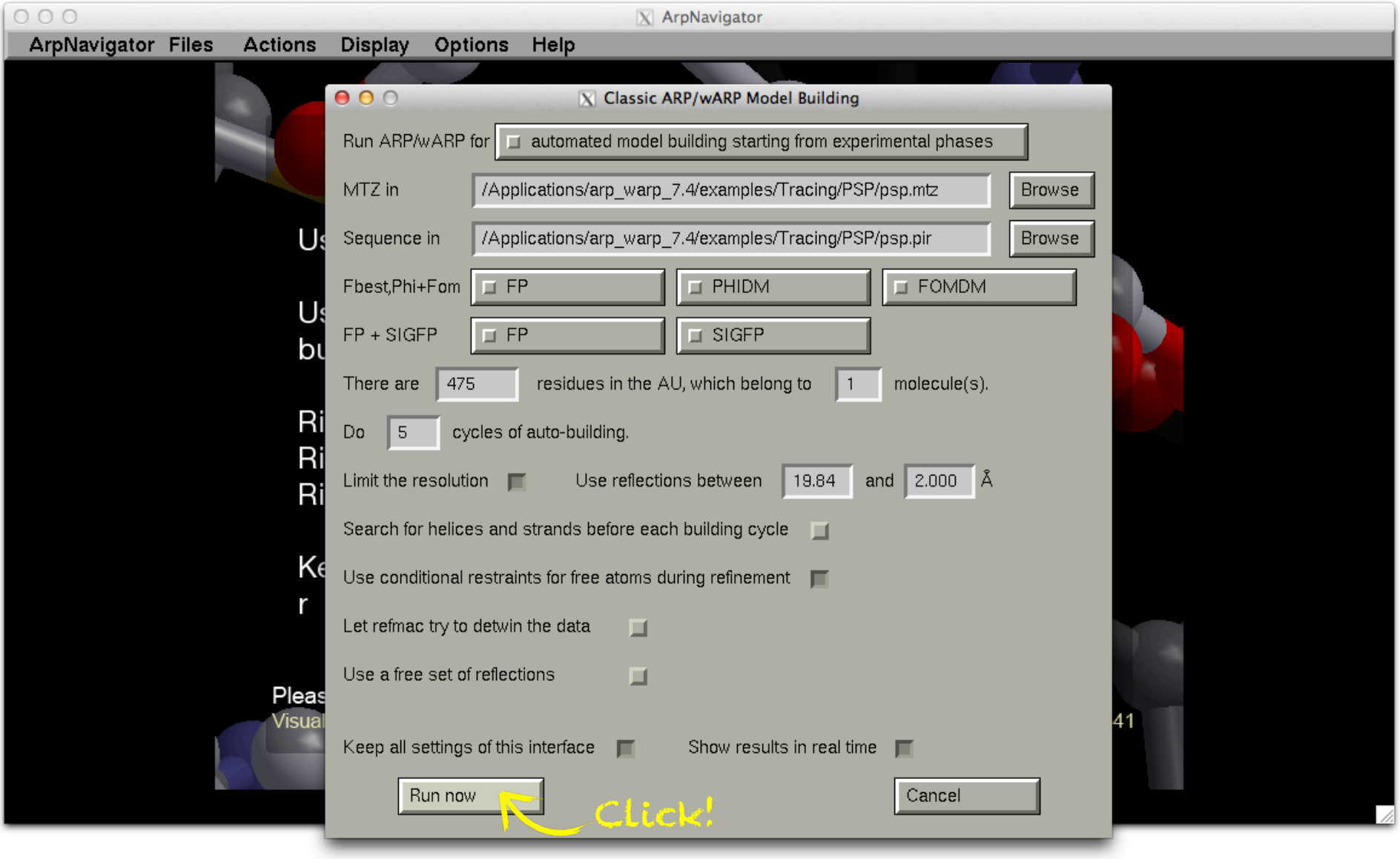
1.4. Flow Parameters



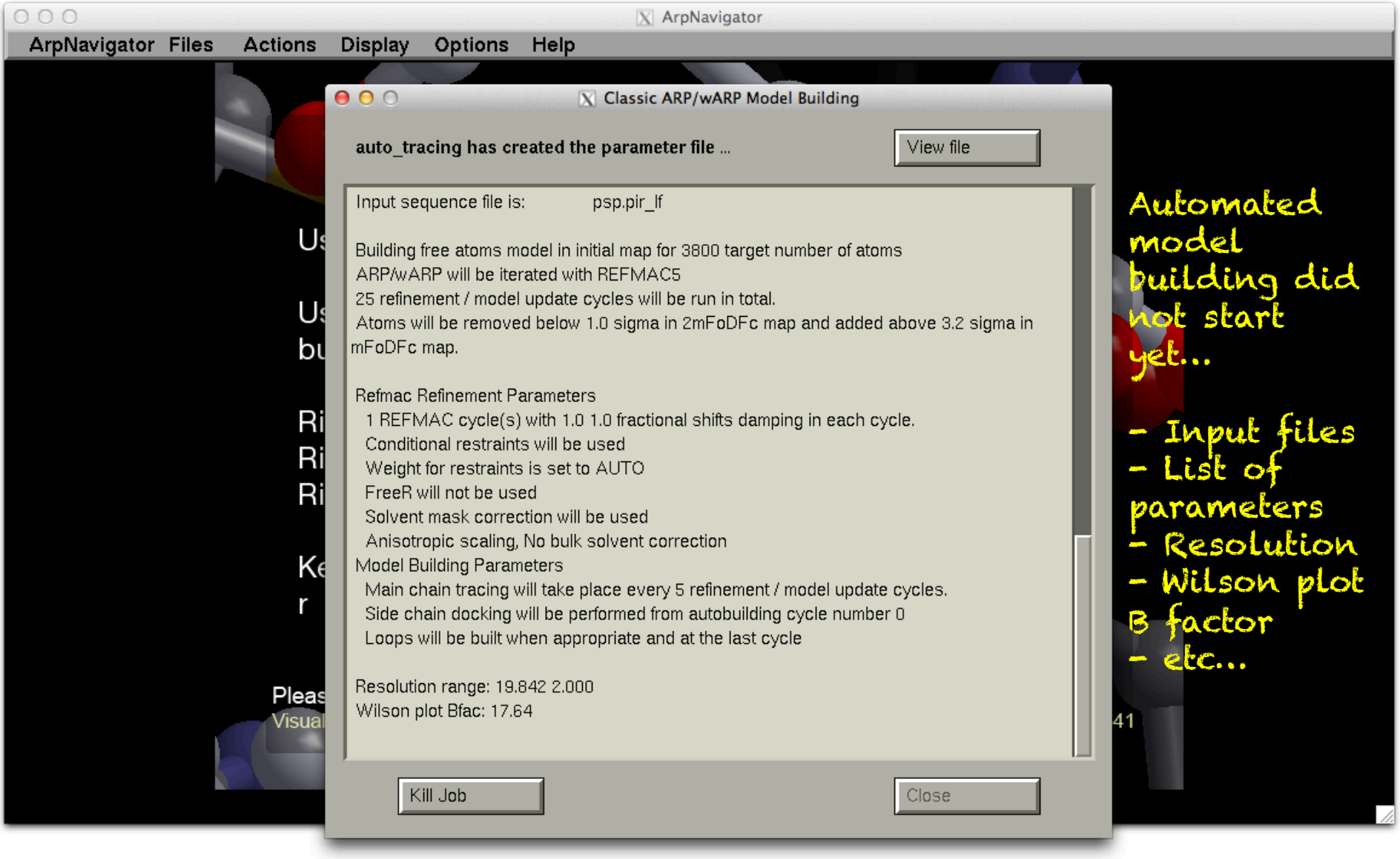
1.4. Flow Parameters



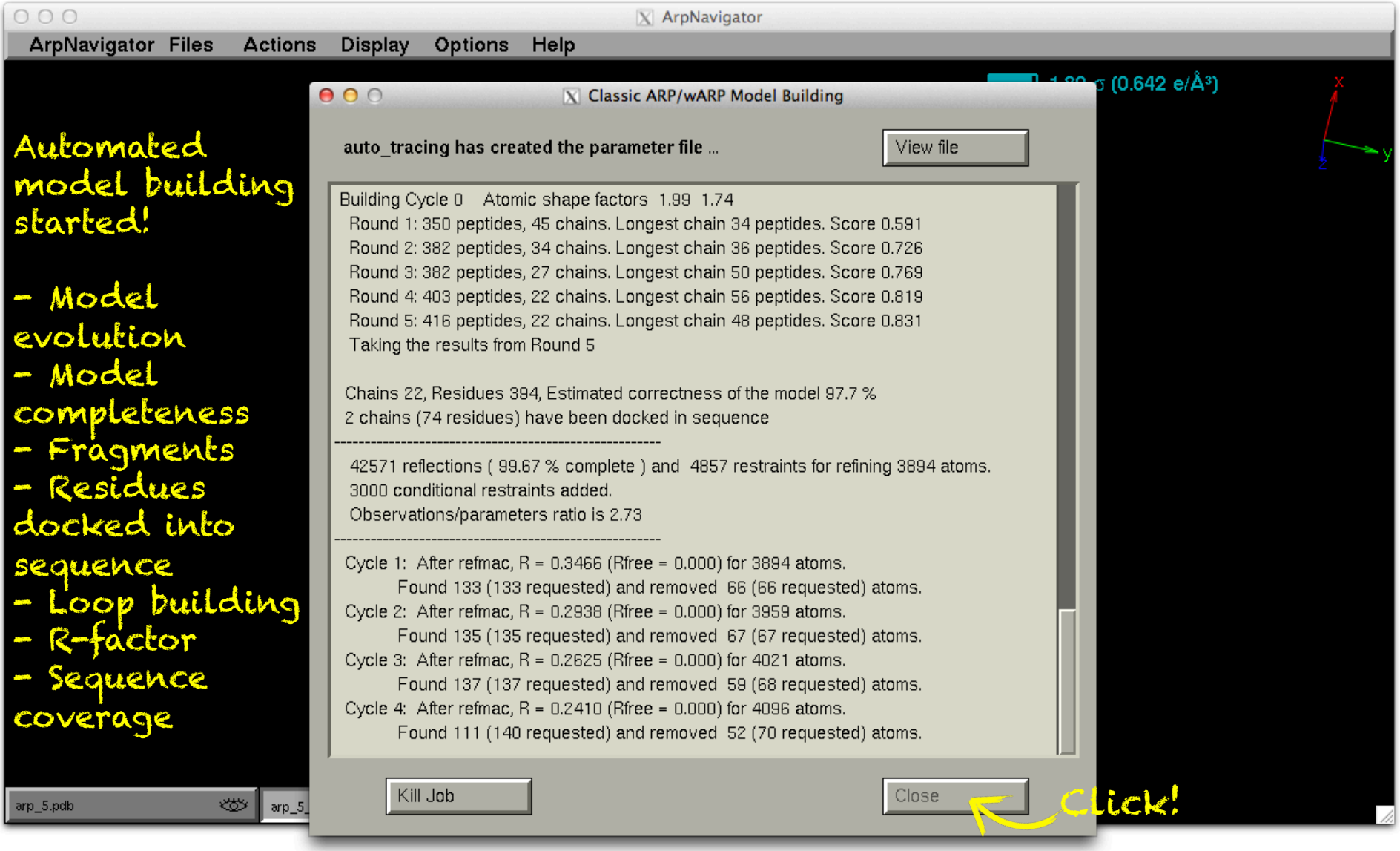
1.5. Run The Job



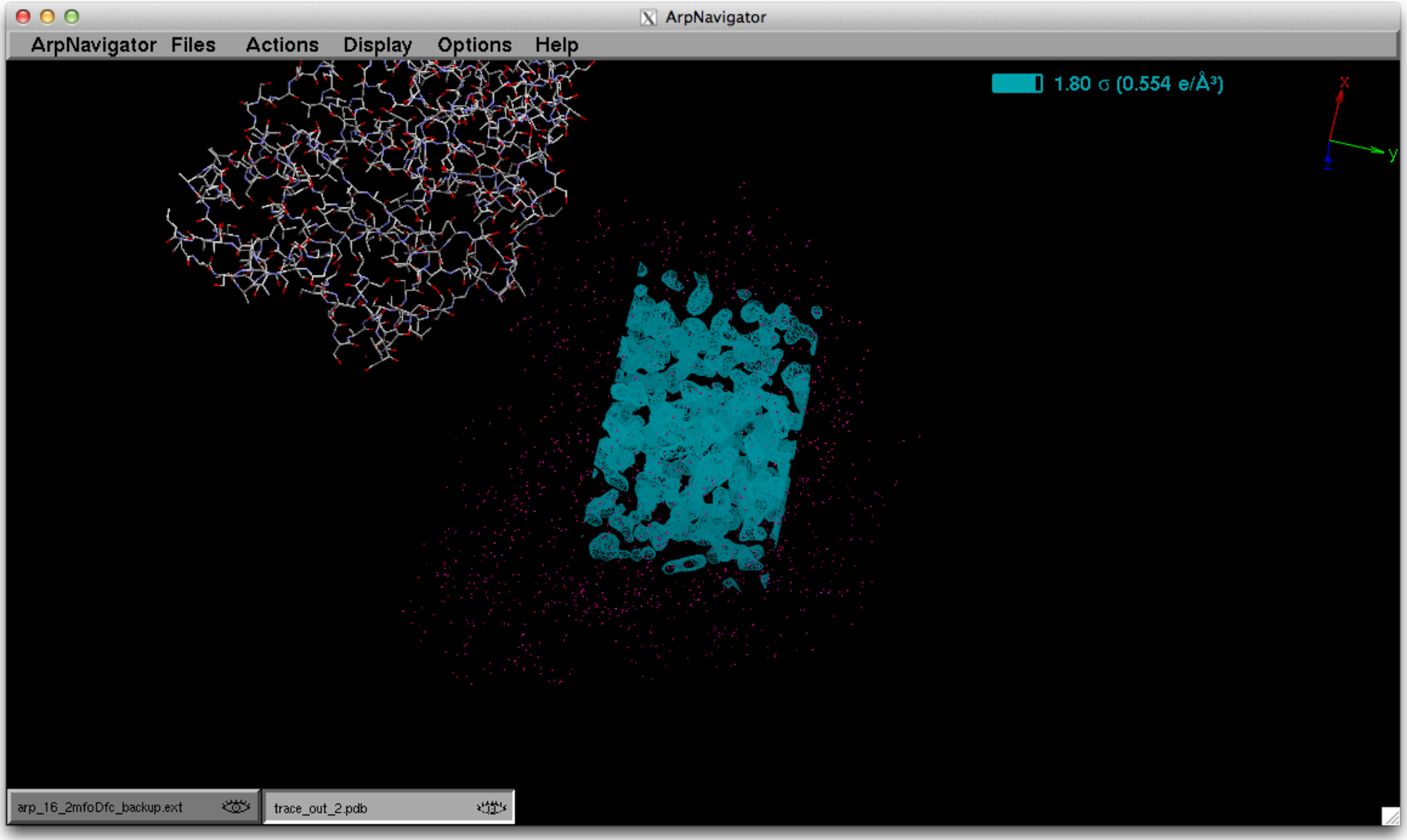
1.5. Run The Job – Log File



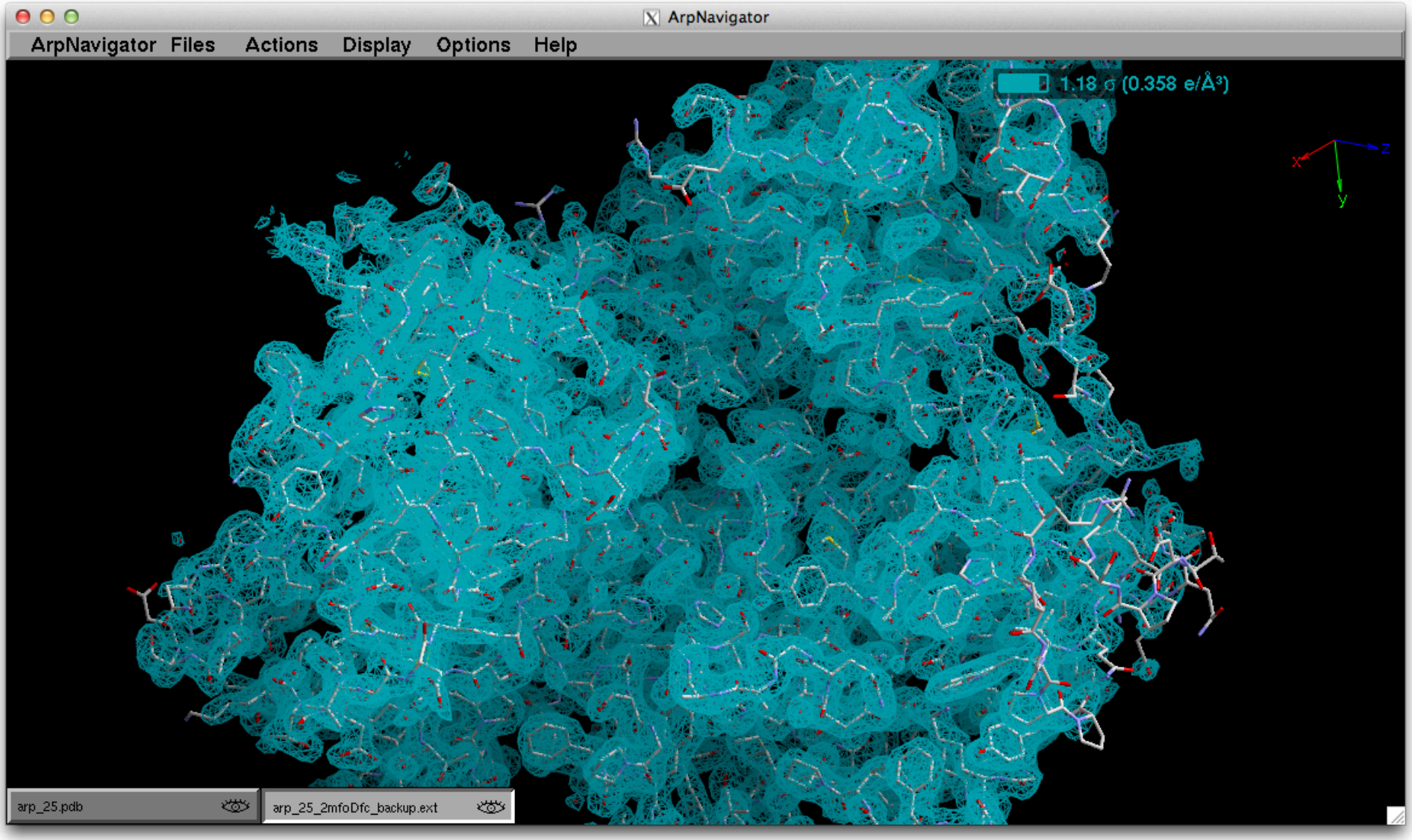
1.5. Run The Job – Log File



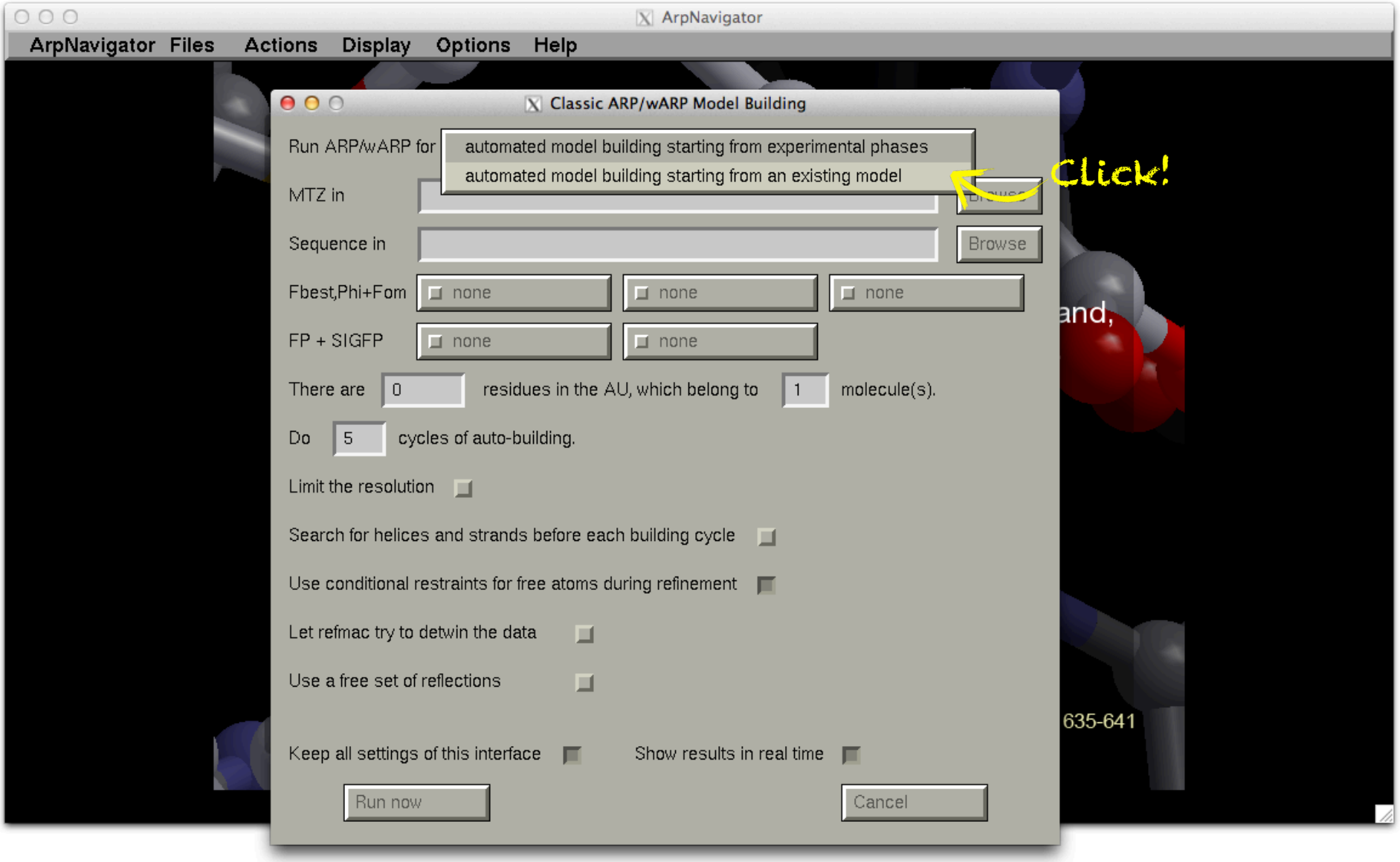
1.5. Run The Job – Live Model Building



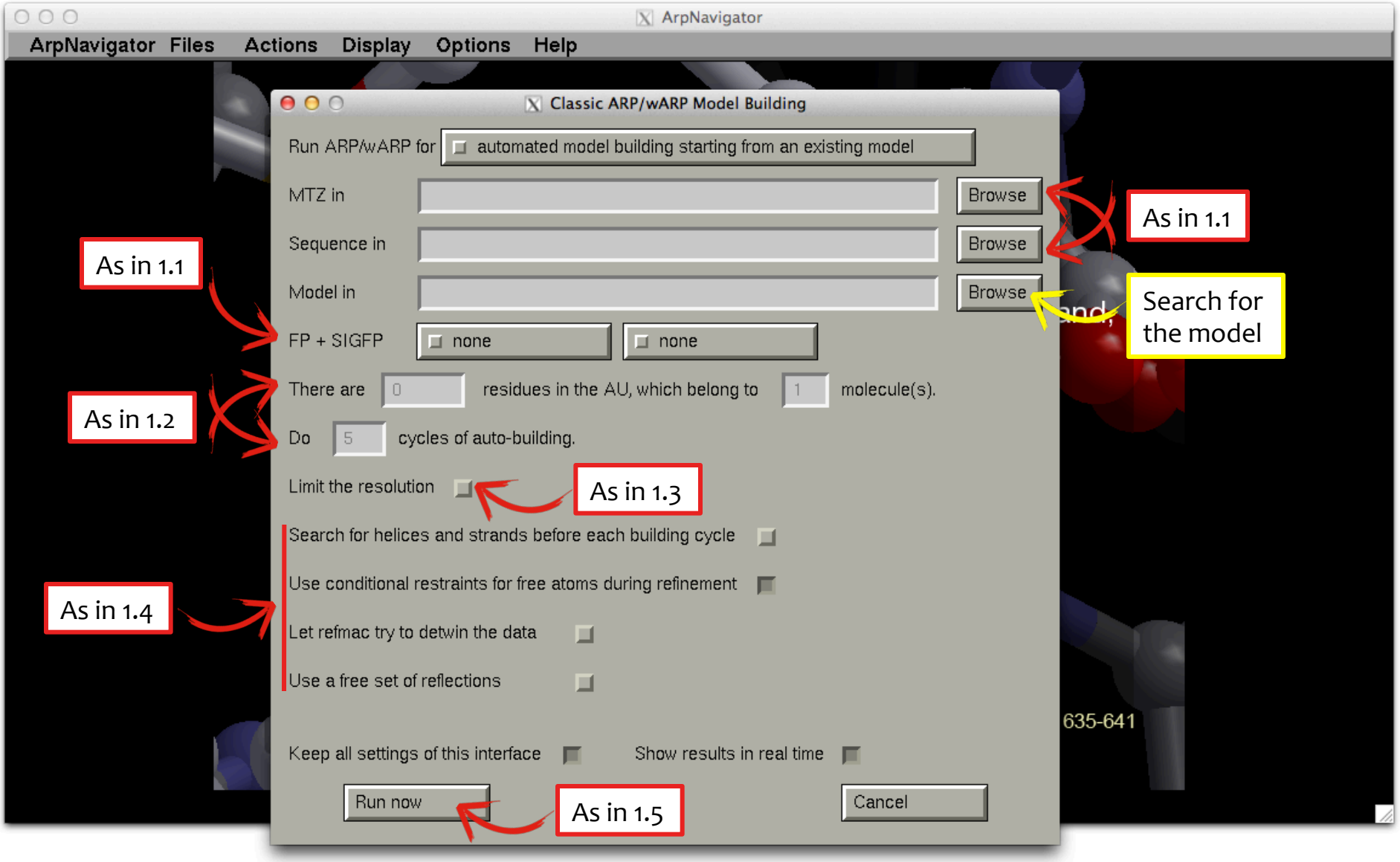
1.5. Run The Job – Live Model Building



2. Molecular Replacement



2. Molecular Replacement



For any questions…

EMBL

The Developers

Contact us anytime!

Victor Lamzin — Philipp Heuser

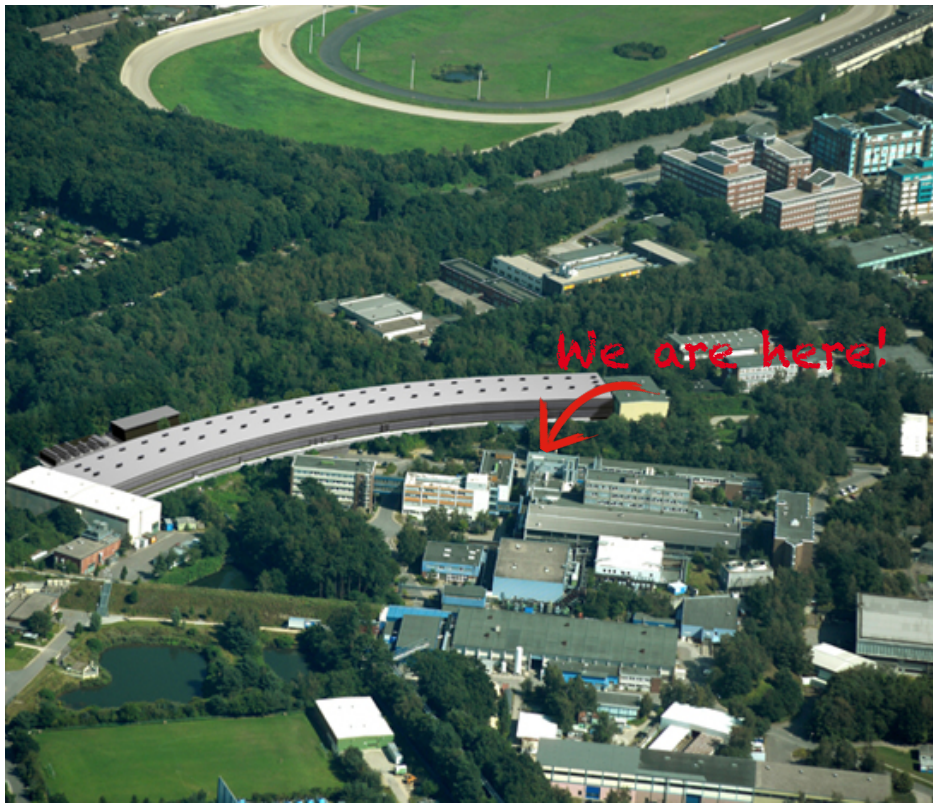
Ioan Vancea — Joana Pereira

Daria Beshnova

Or just visit our website!

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

User guide
Frequently asked questions
Tutorials



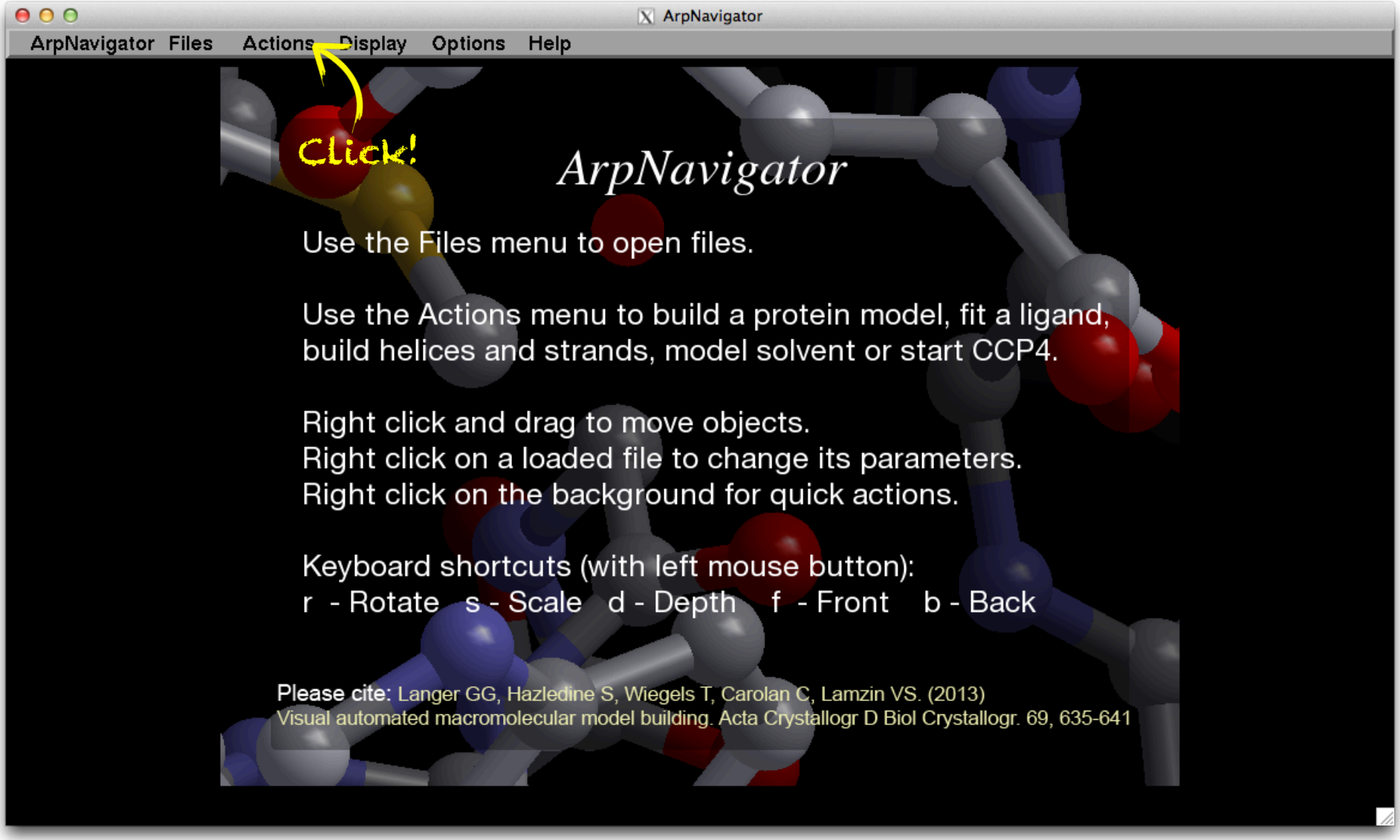
EMBL @ Desy Hamburg

Automated Building of Secondary Structure Elements With ArpNavigator

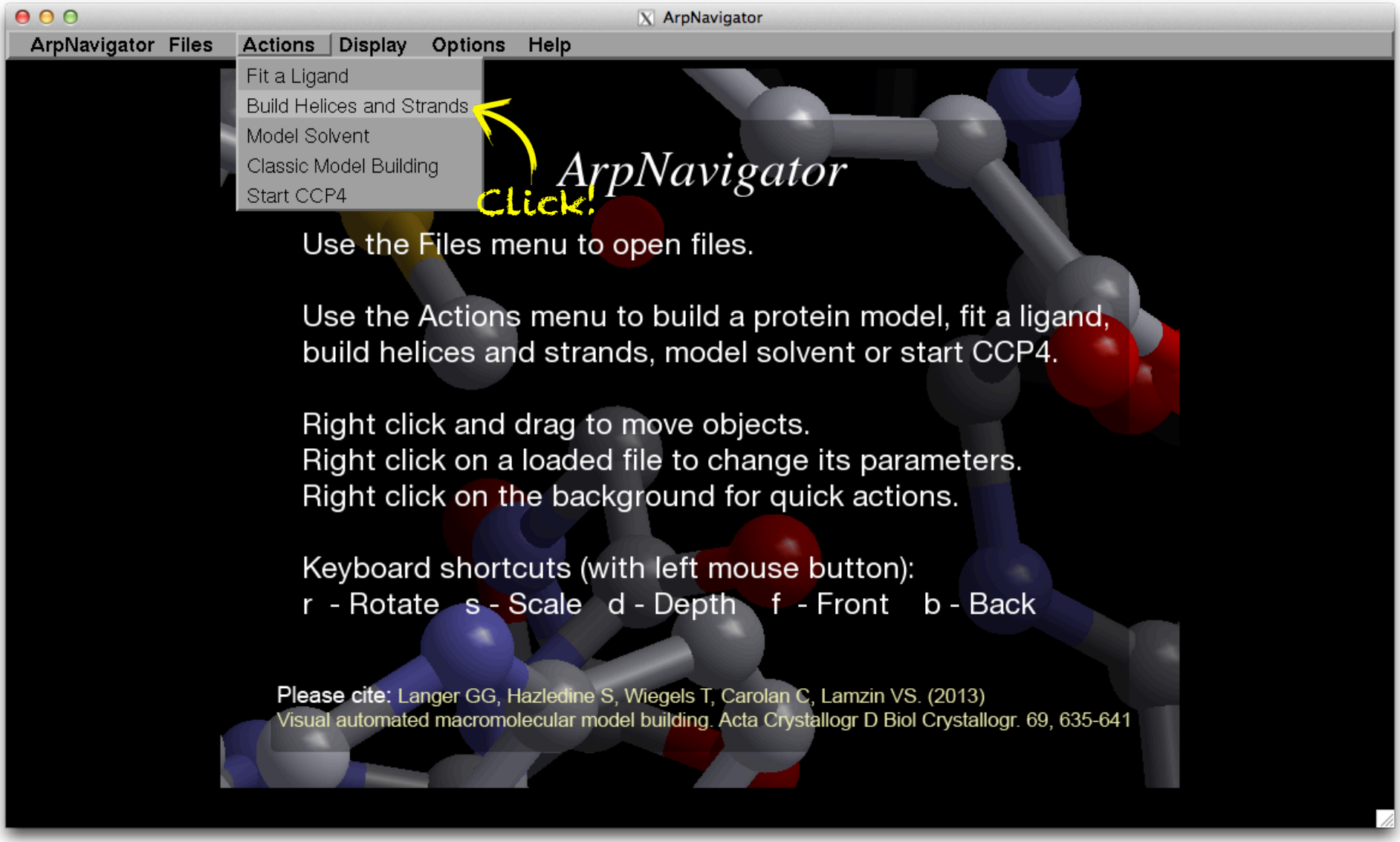
A Click-on Tutorial

EMBL
Hamburg

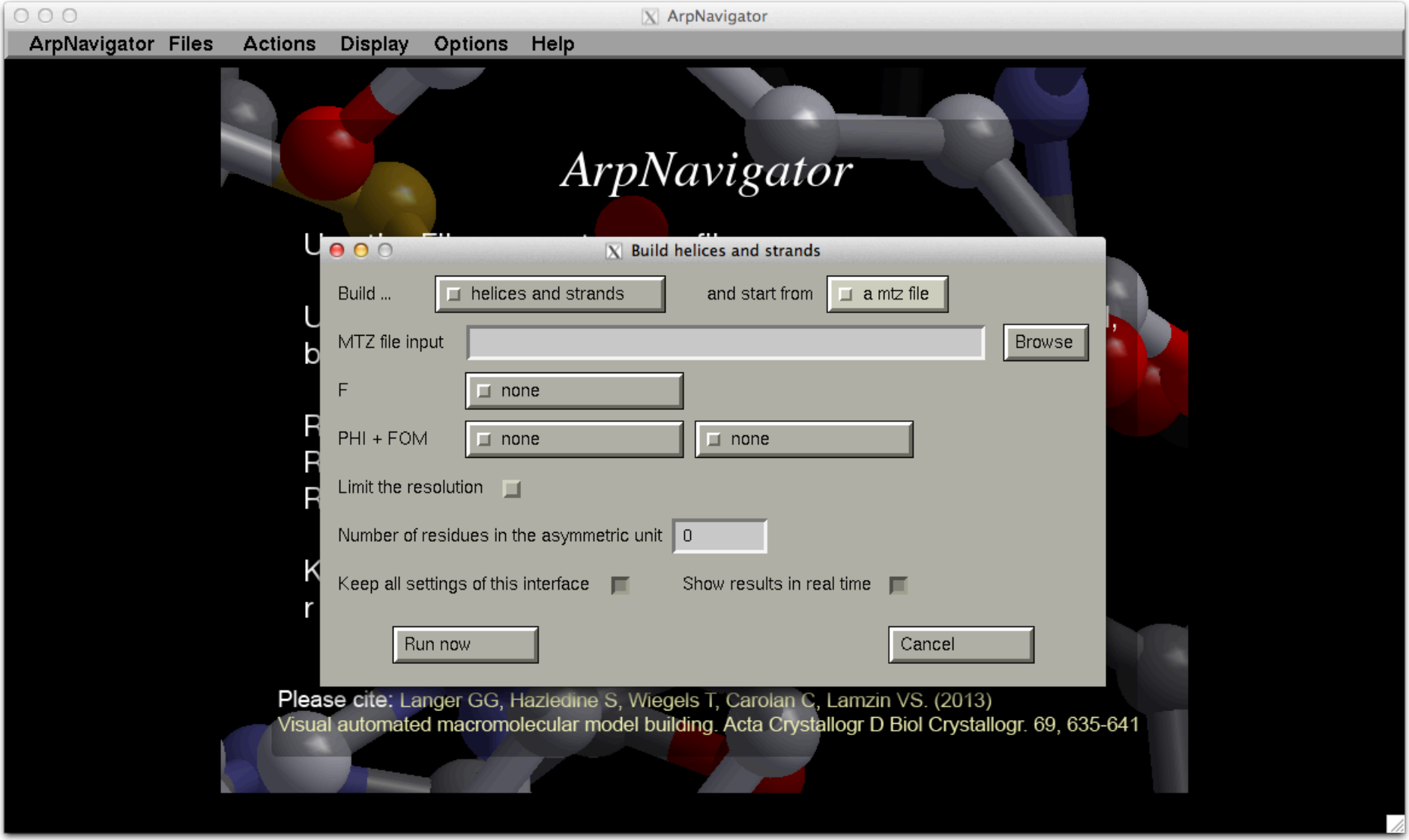
Where to go…


ArpNavigator
ArpNavigator Files Actions Display Options Help
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

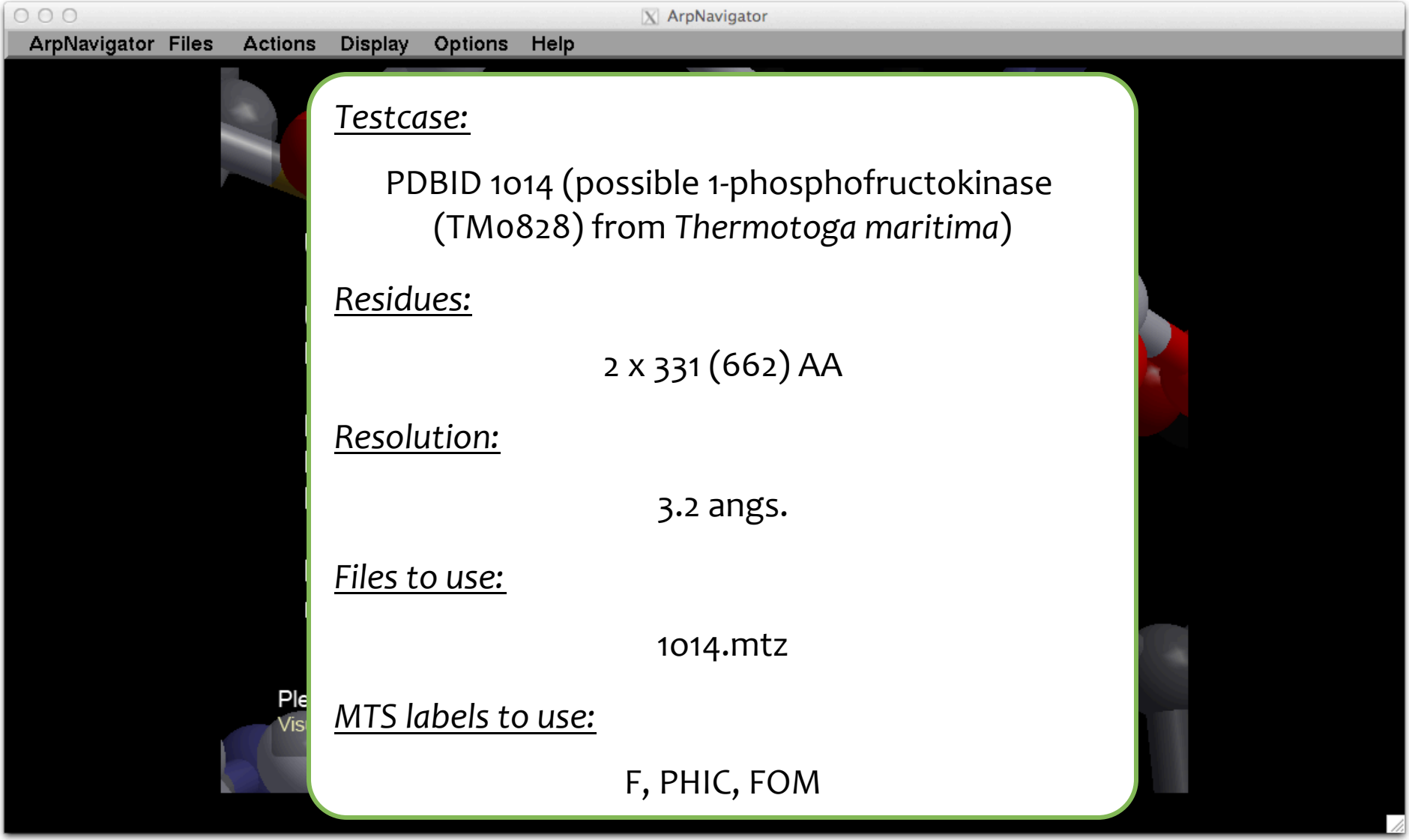
ARP/wARP: Secondary Structure (albe)



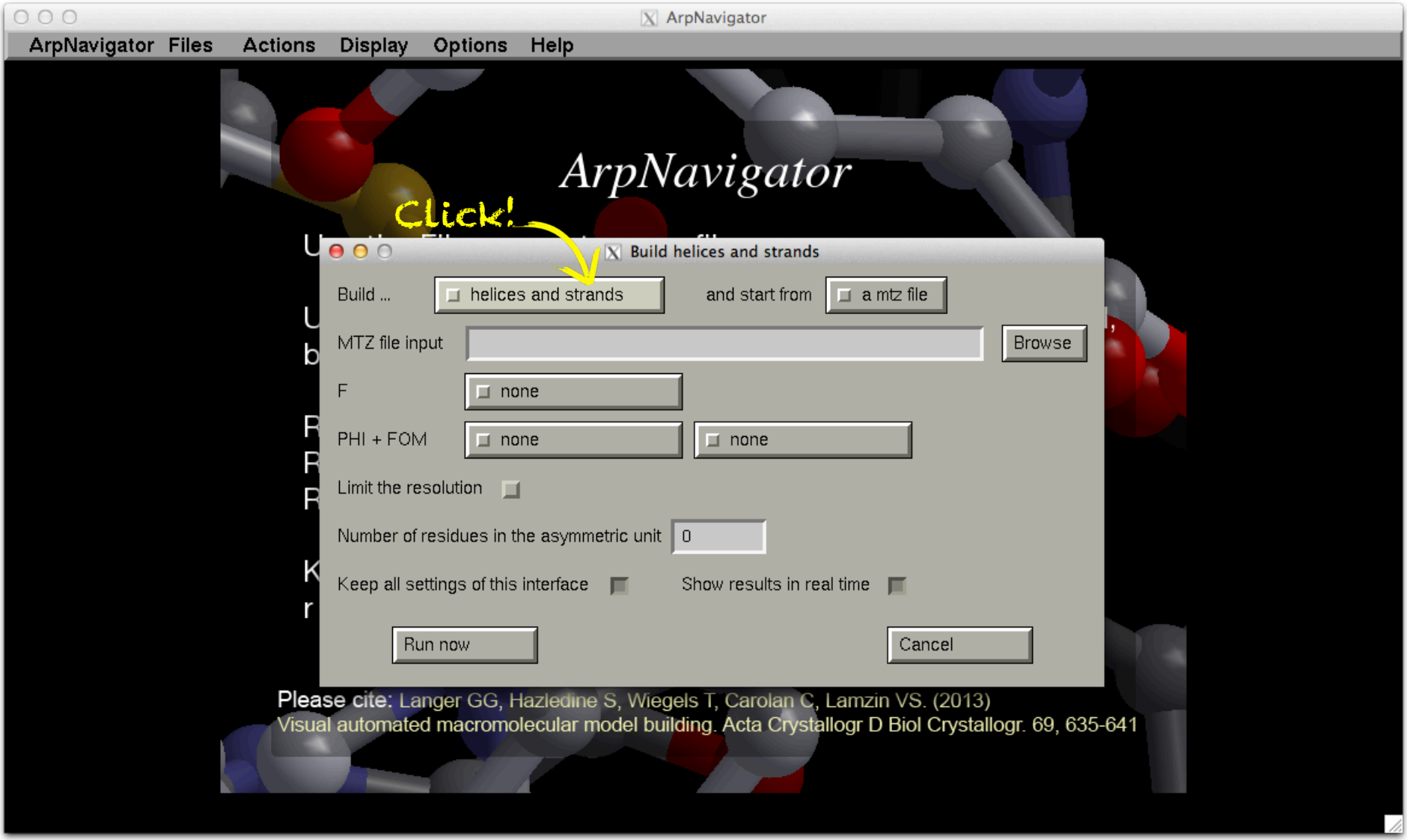
ARP/wARP: Secondary Structure (albe)



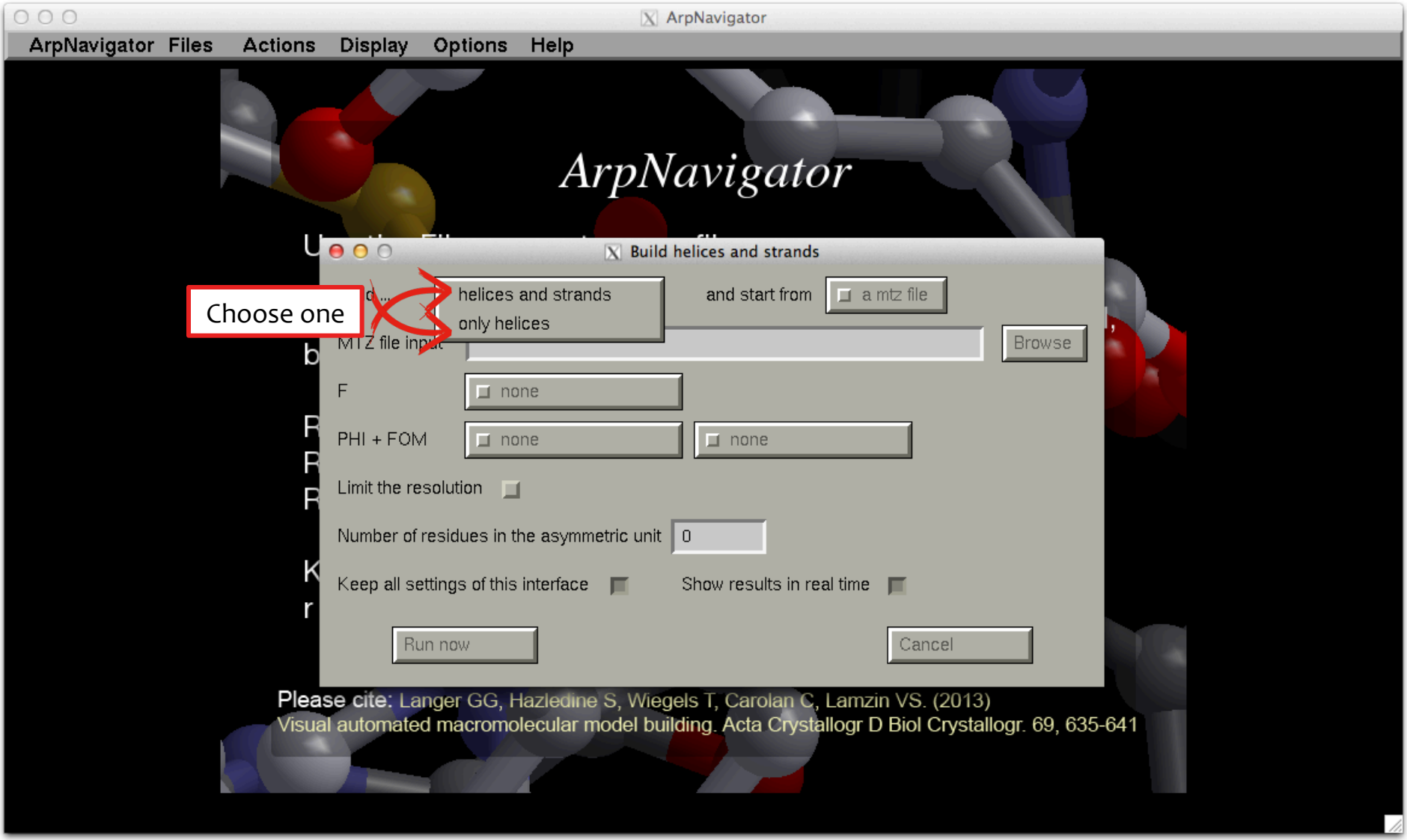
ARP/wARP: Secondary Structure (albe)



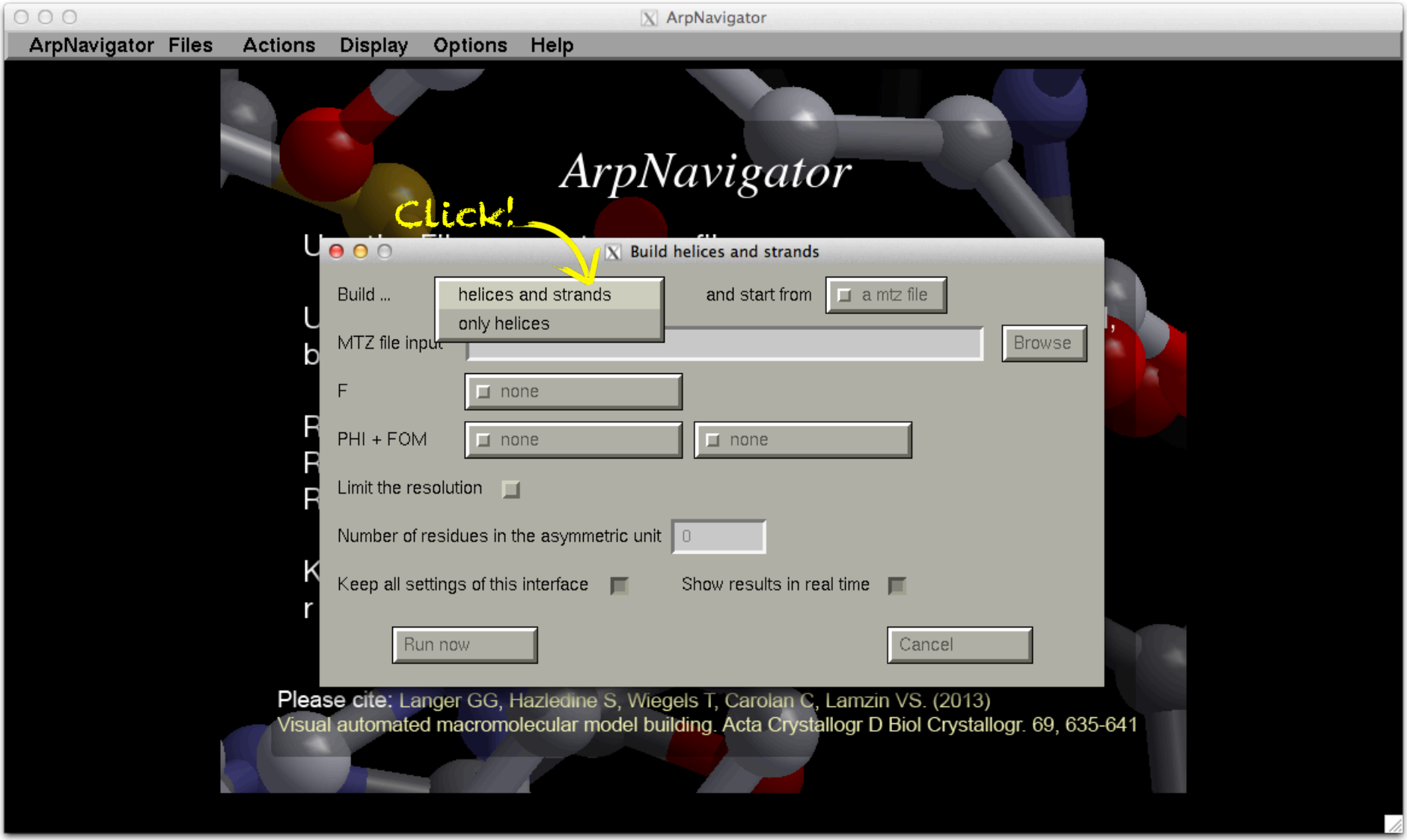
ARP/wARP: Secondary Structure (albe)



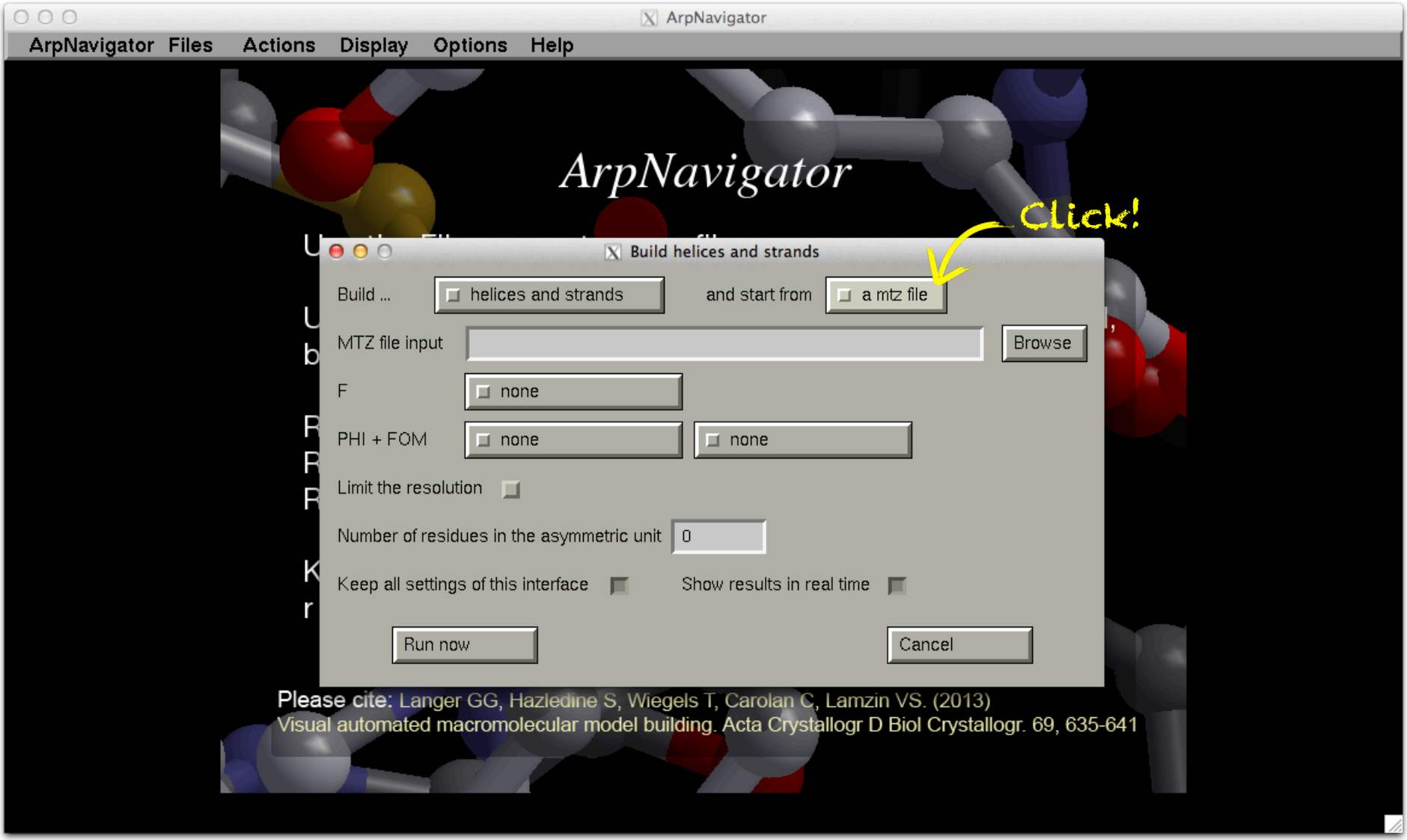
ARP/wARP: Secondary Structure (albe)



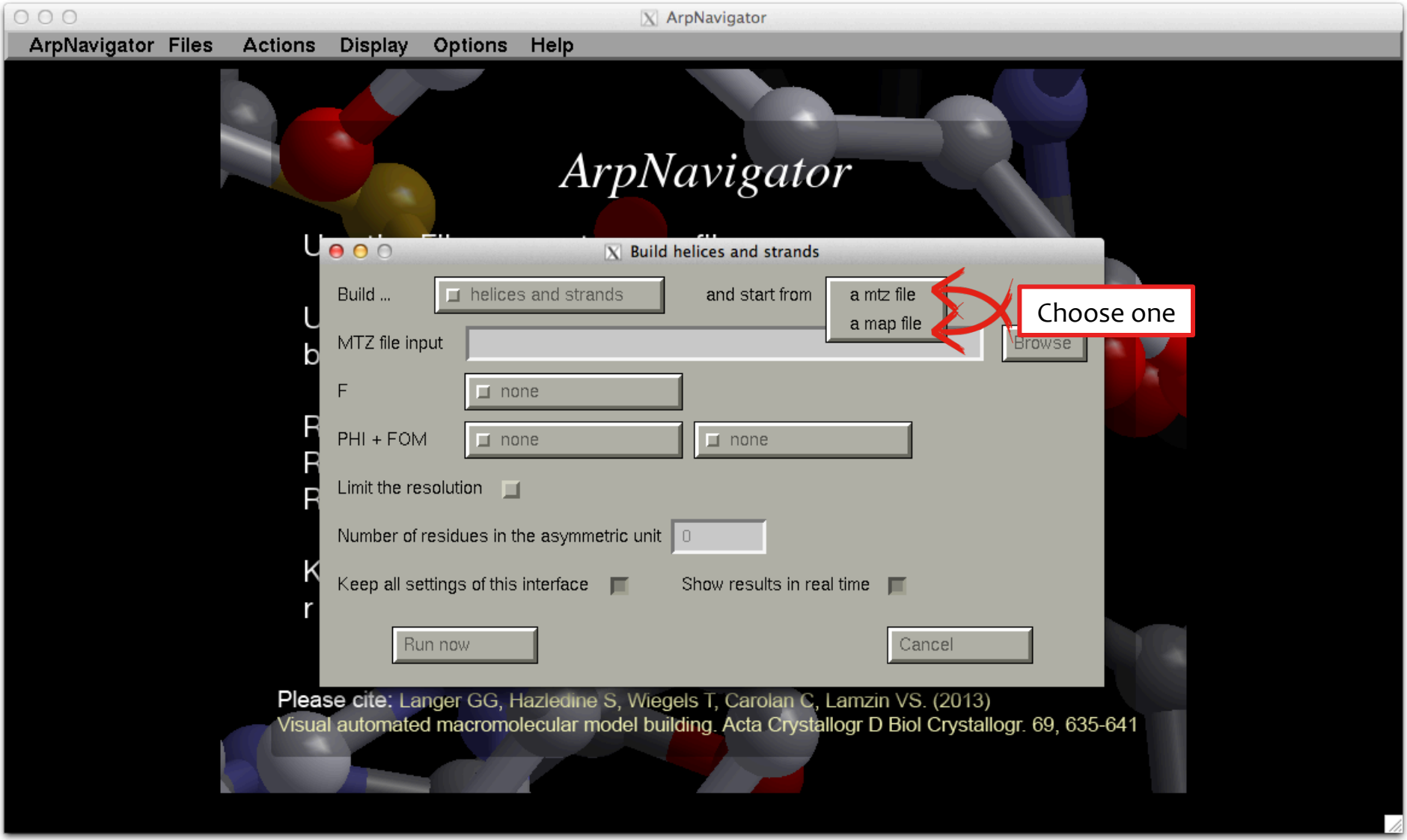
1. Building of Helixes and Strands



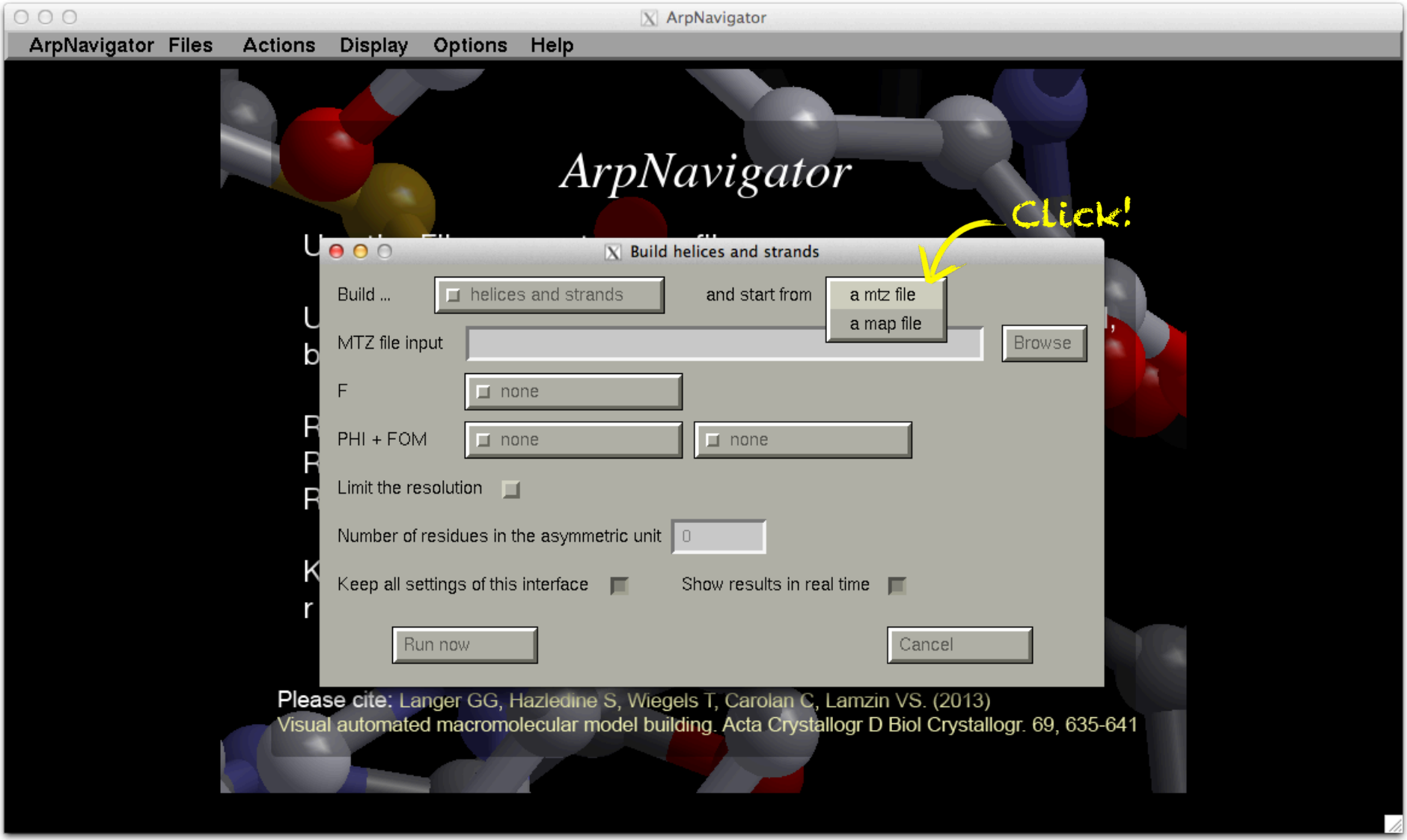
1. Building of Helixes and Strands



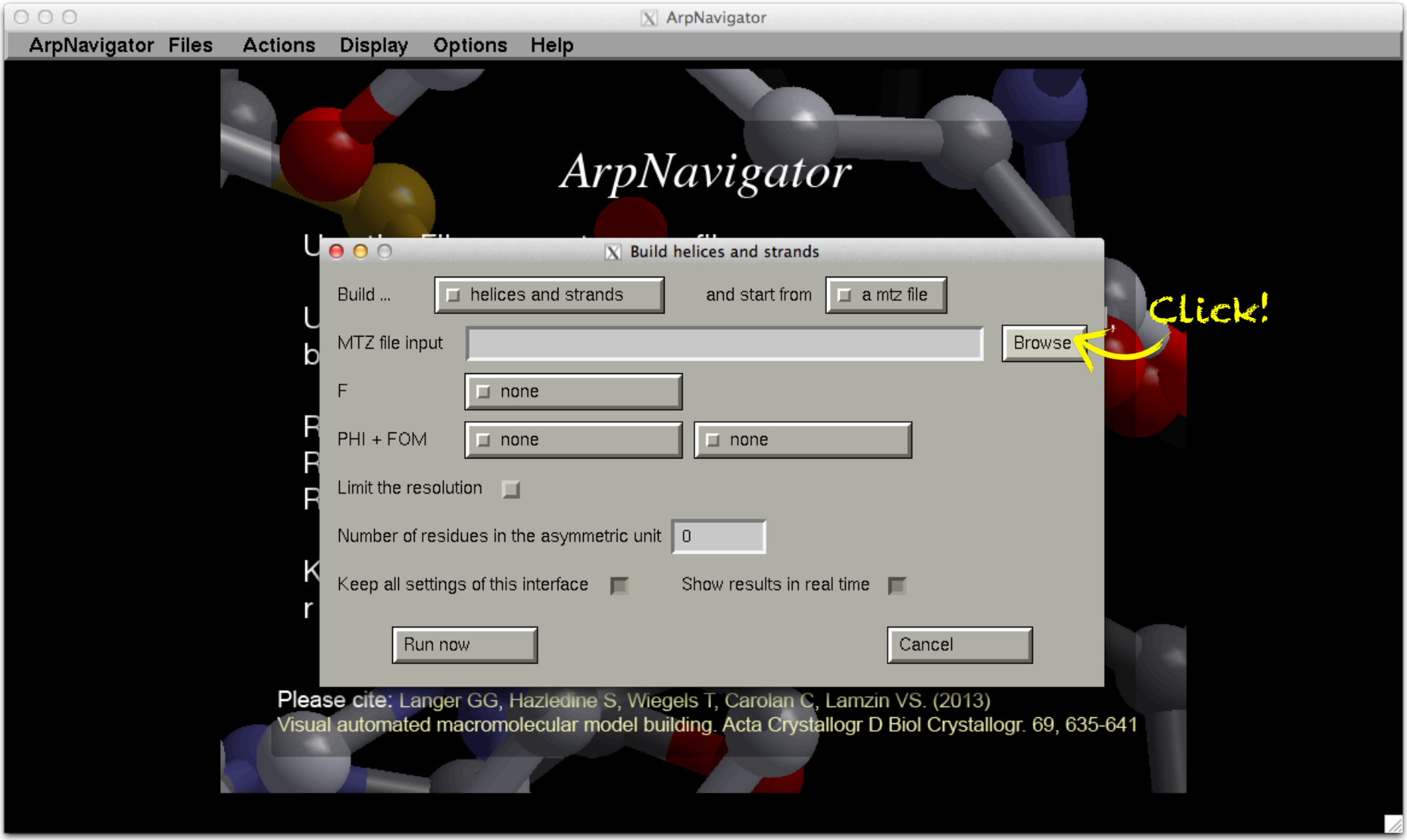
1. Building of Helixes and Strands



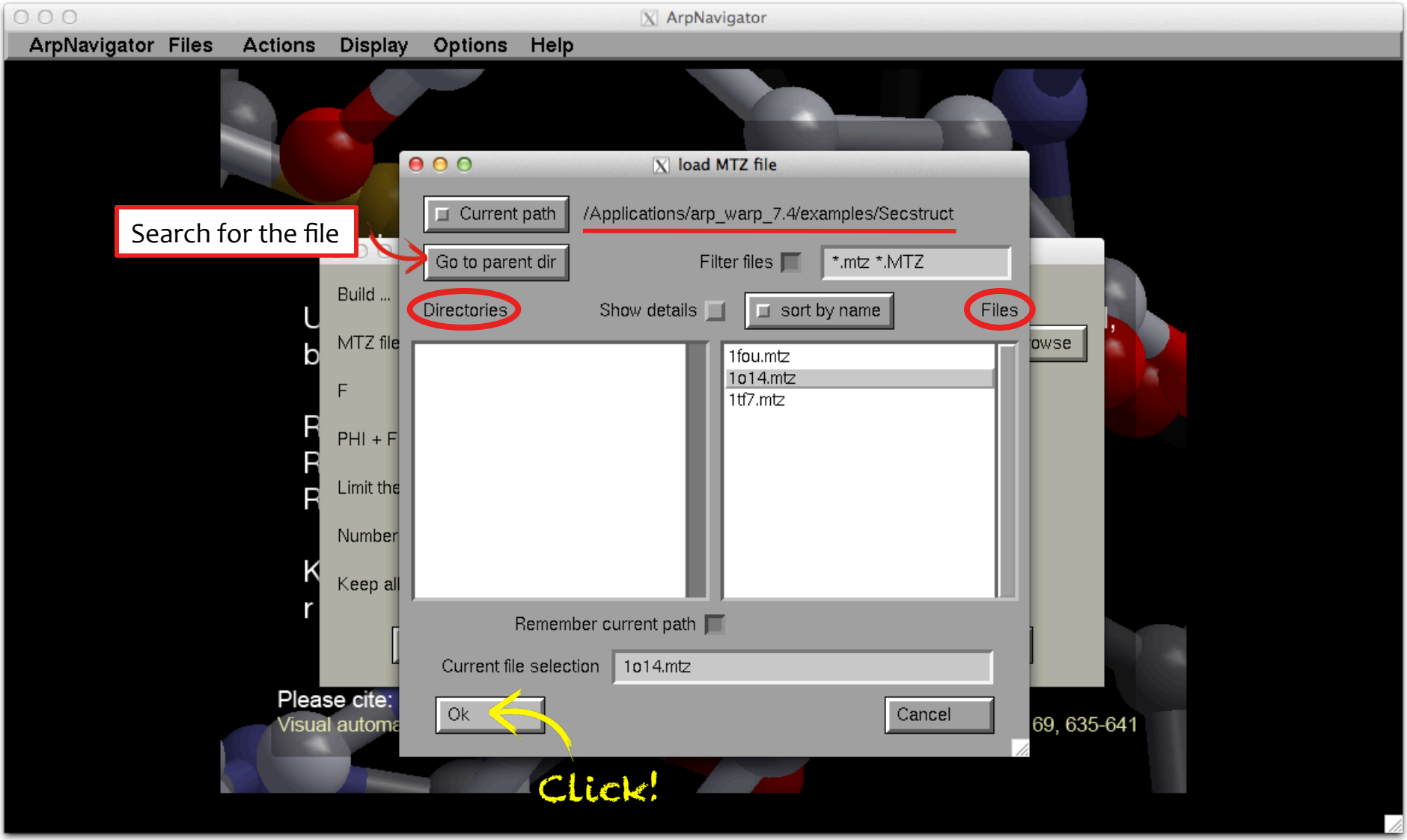
1.1. Start From MTZ File



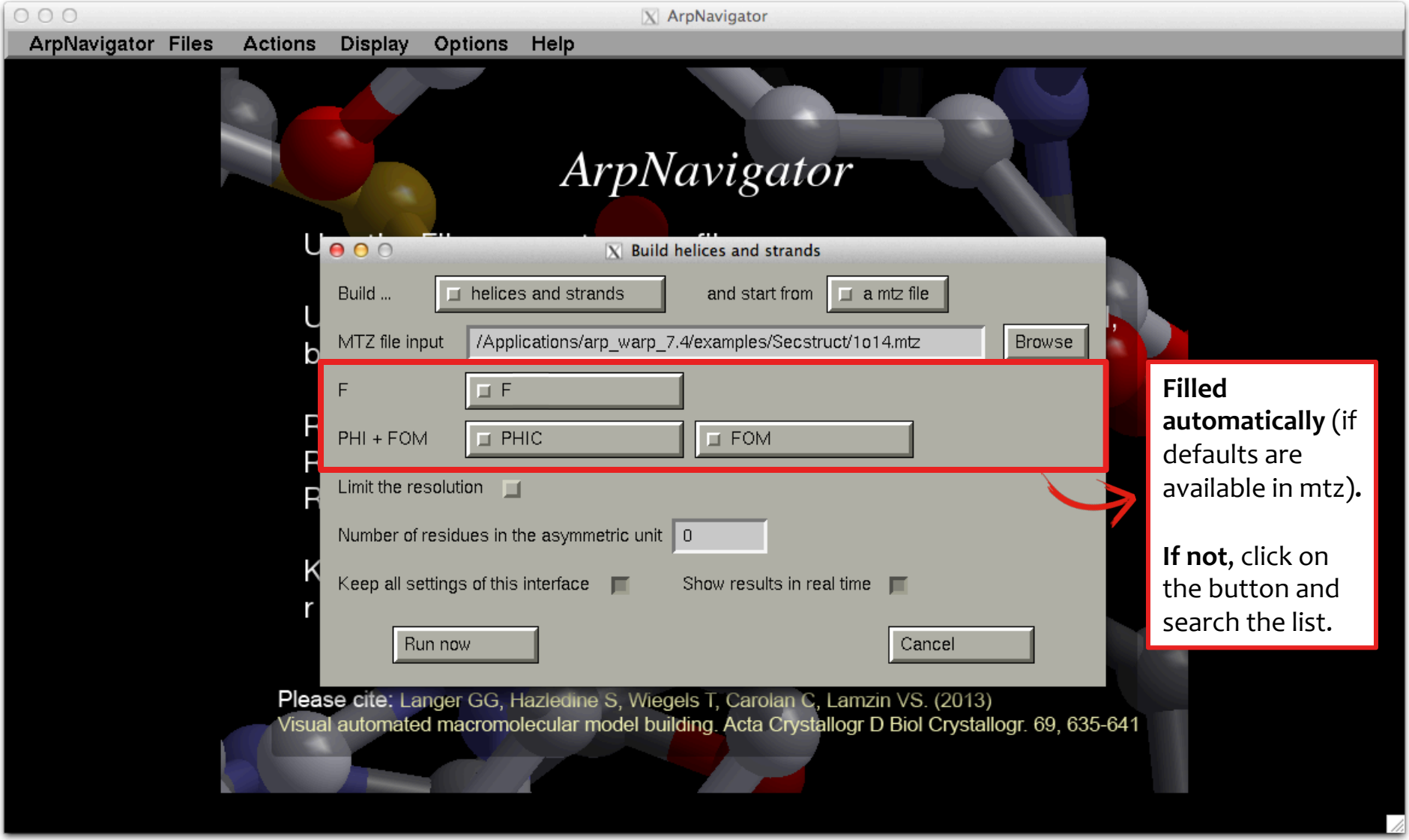
1.1.1. Input Files: MTZ File



1.1.1. Input Files: MTZ File



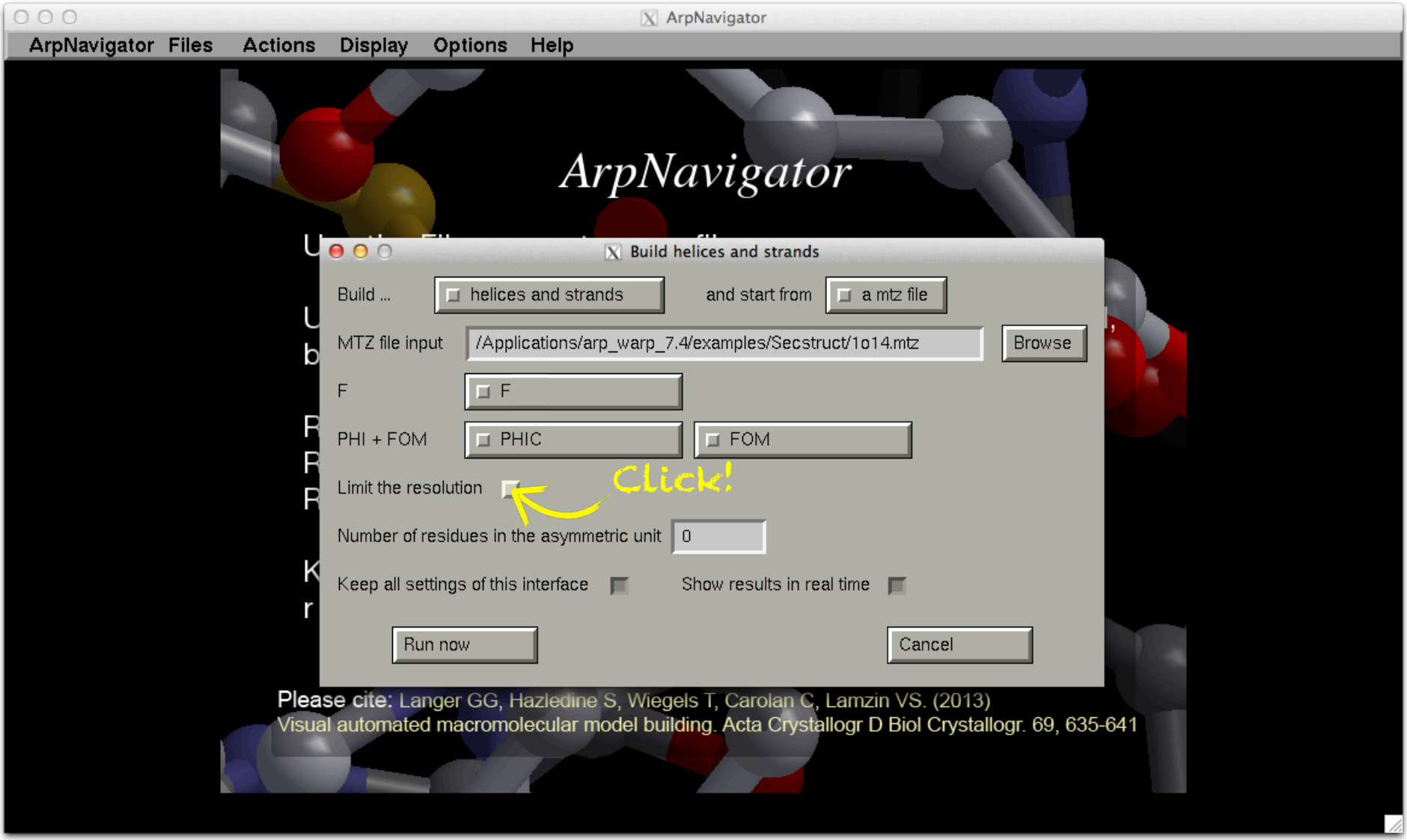
1.1.1. Input Files: MTZ File



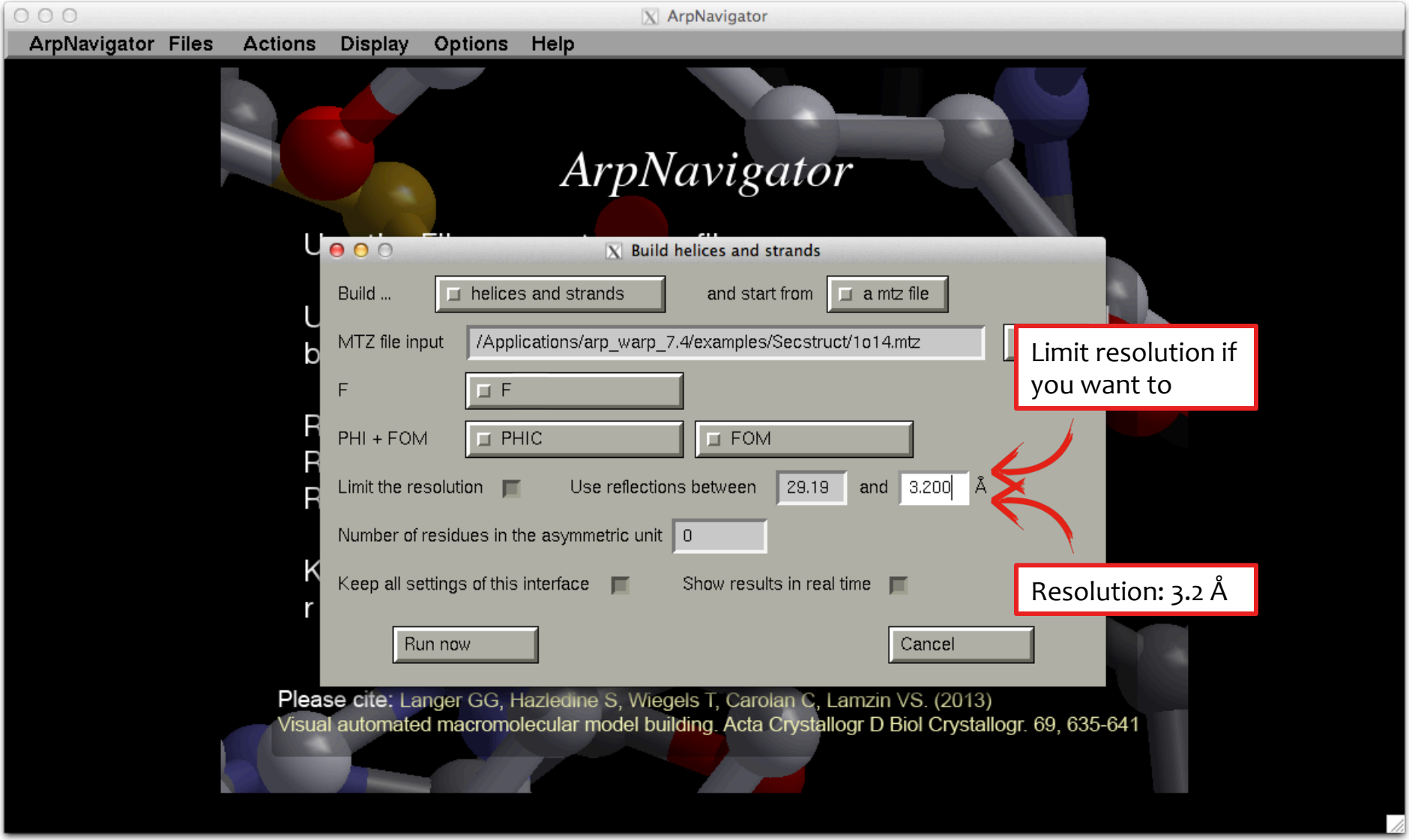
Filled automatically (if defaults are available in mtz).

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

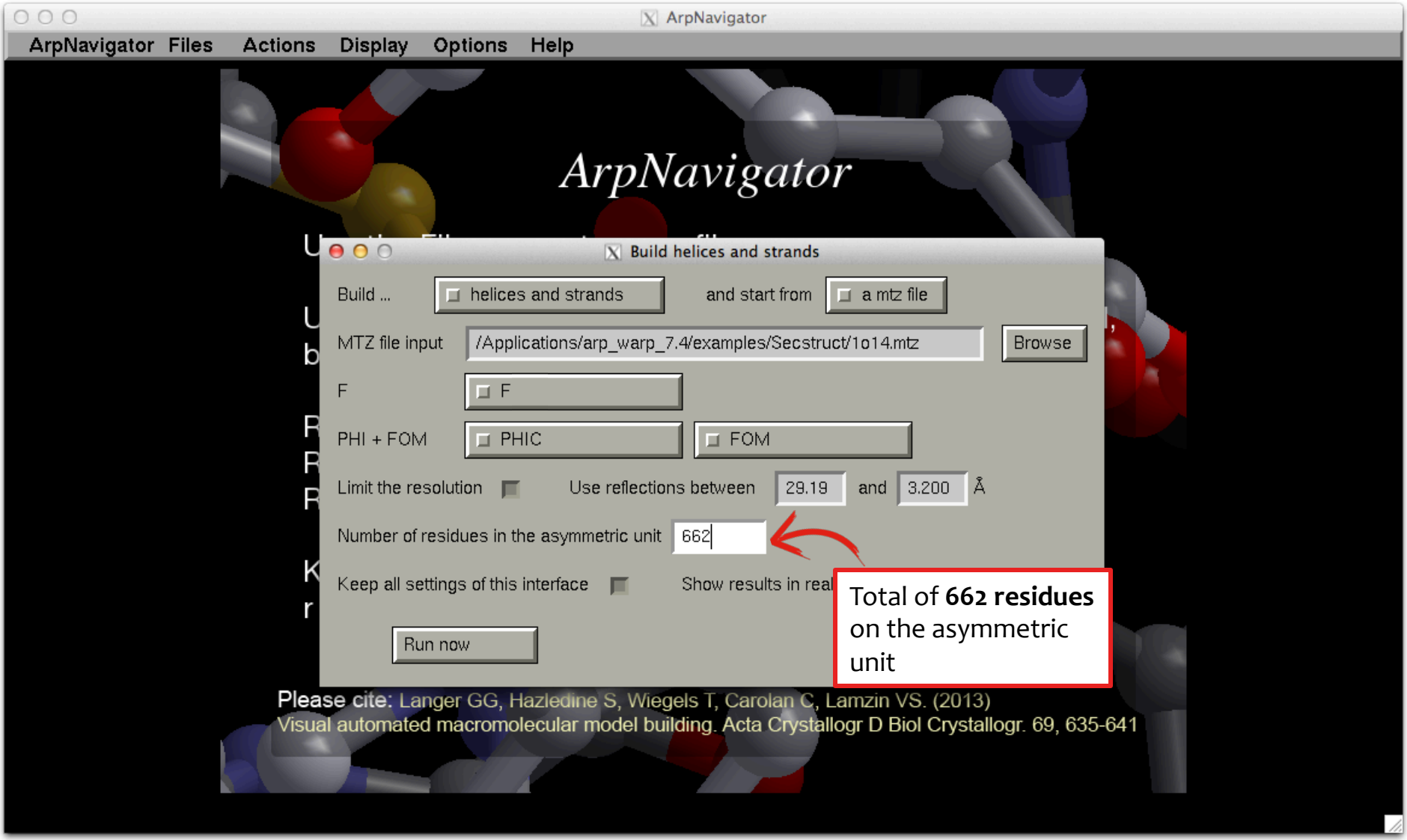
1.1.2. Resolution



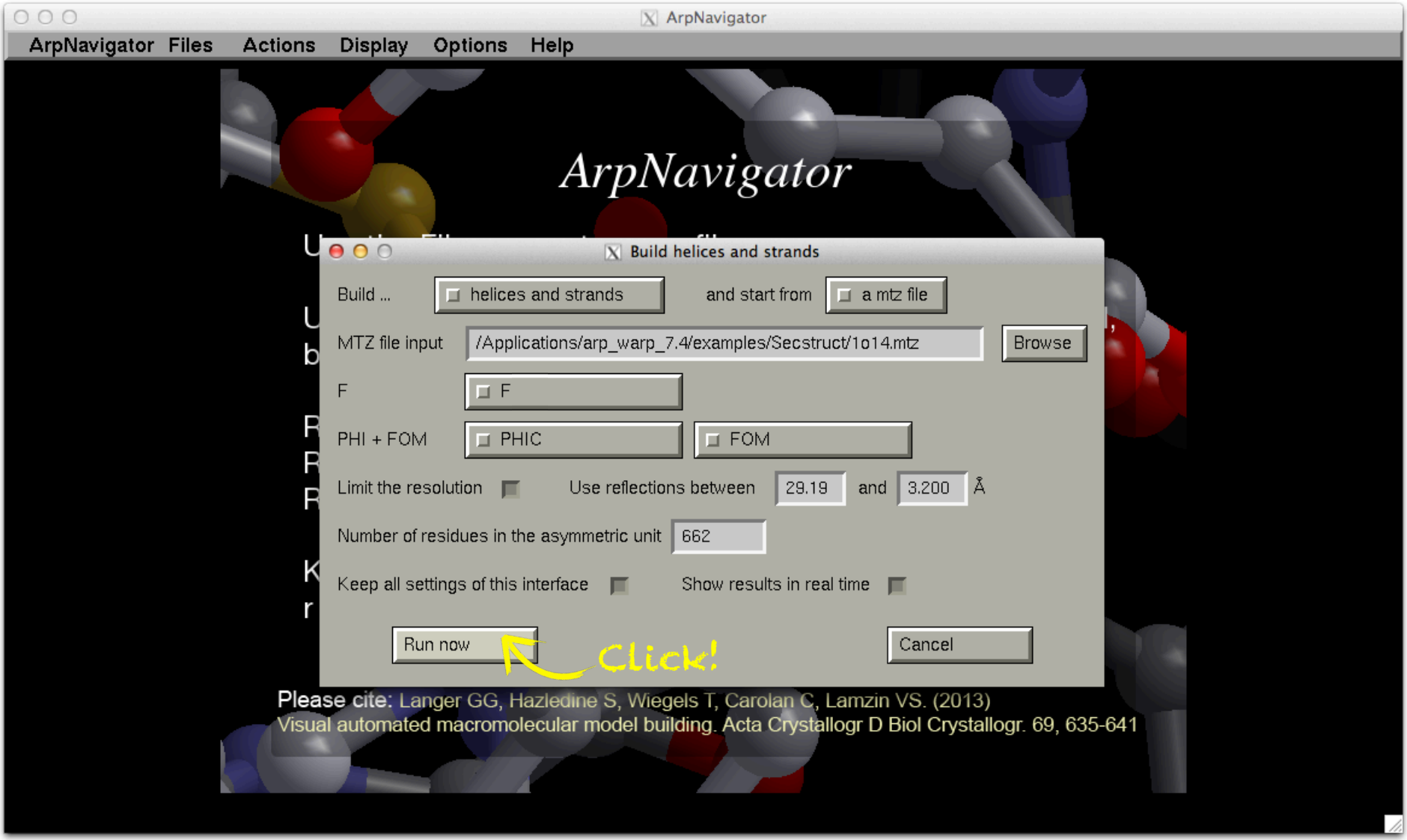
1.1.2. Resolution



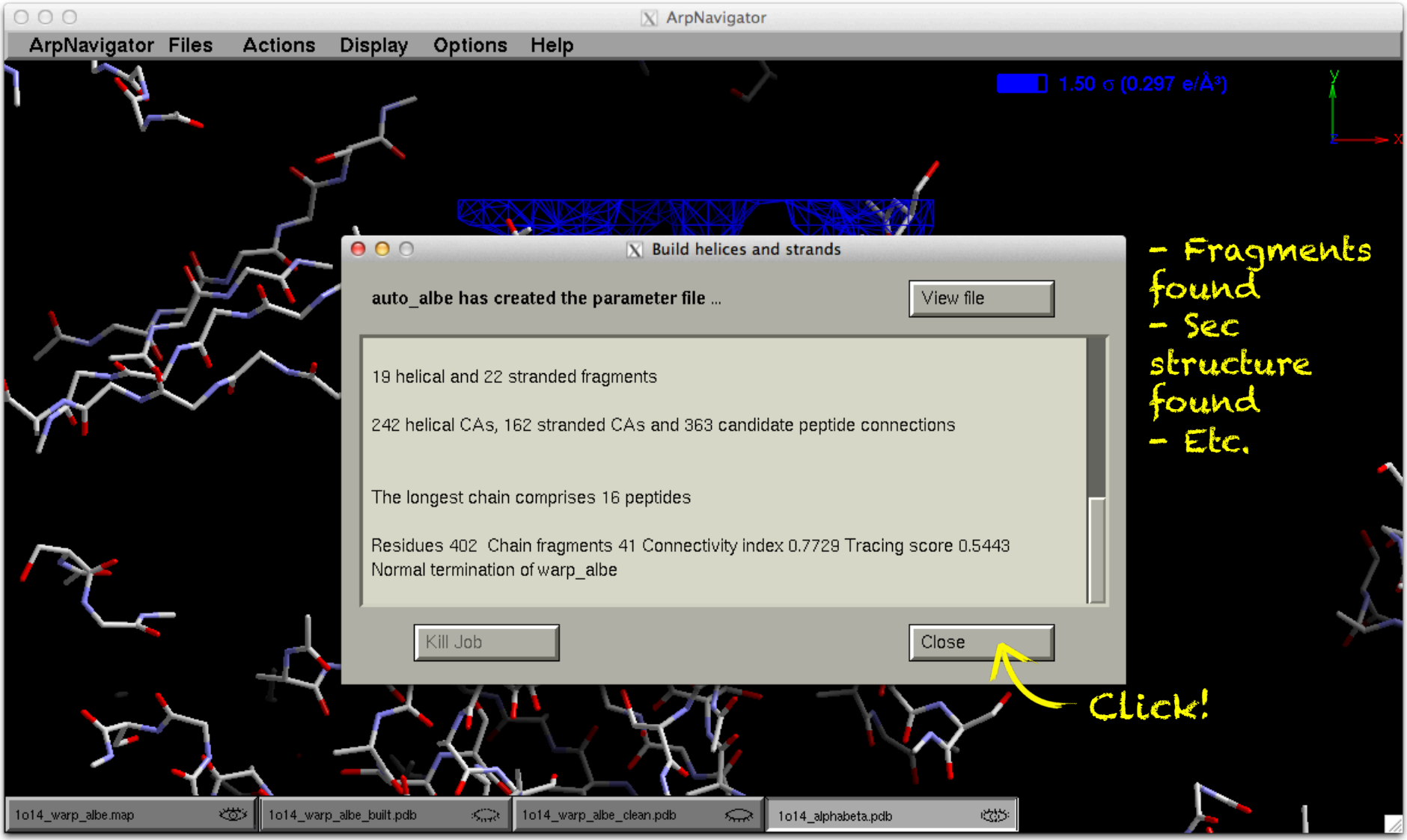
1.1.3. Required Parameters



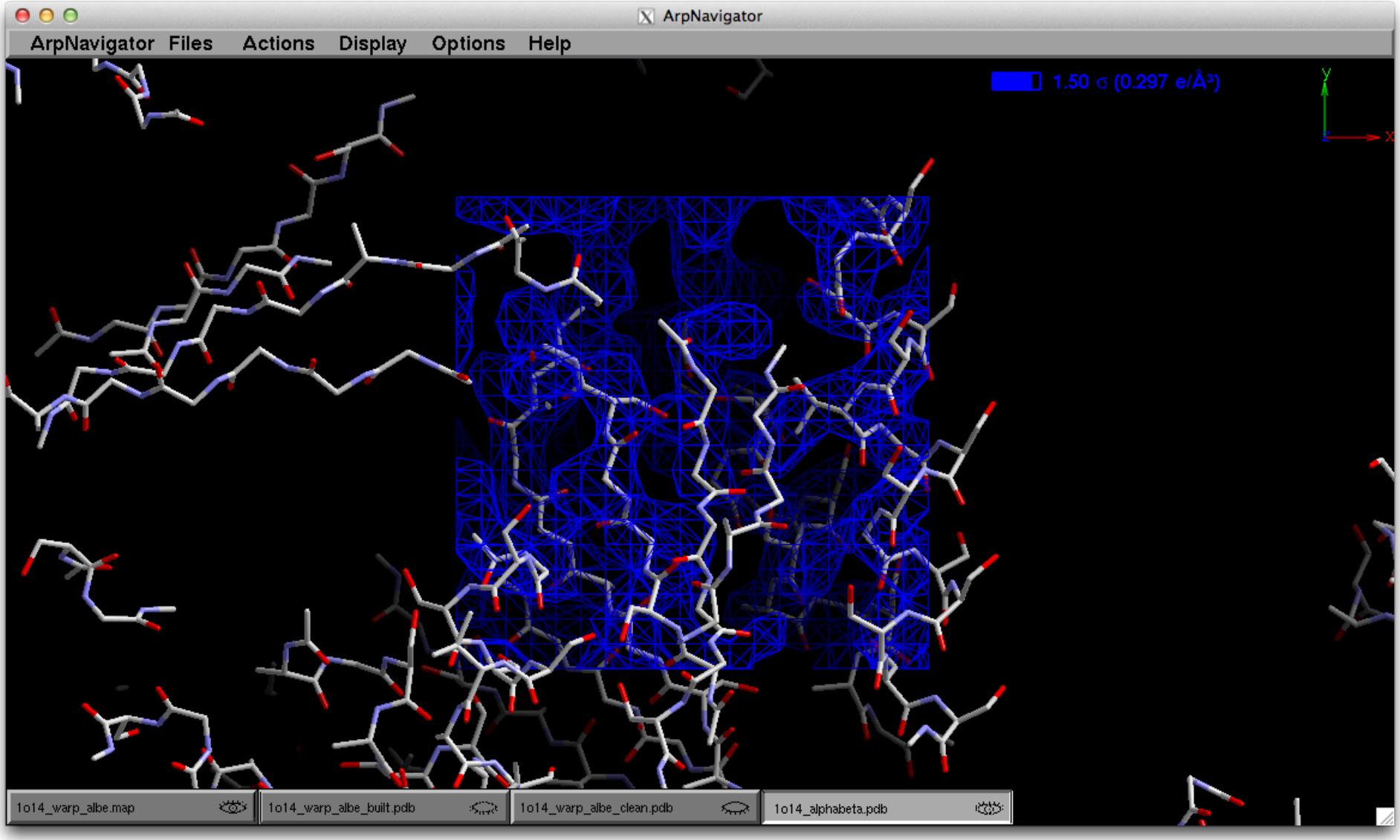
1.1.4. Run The Job



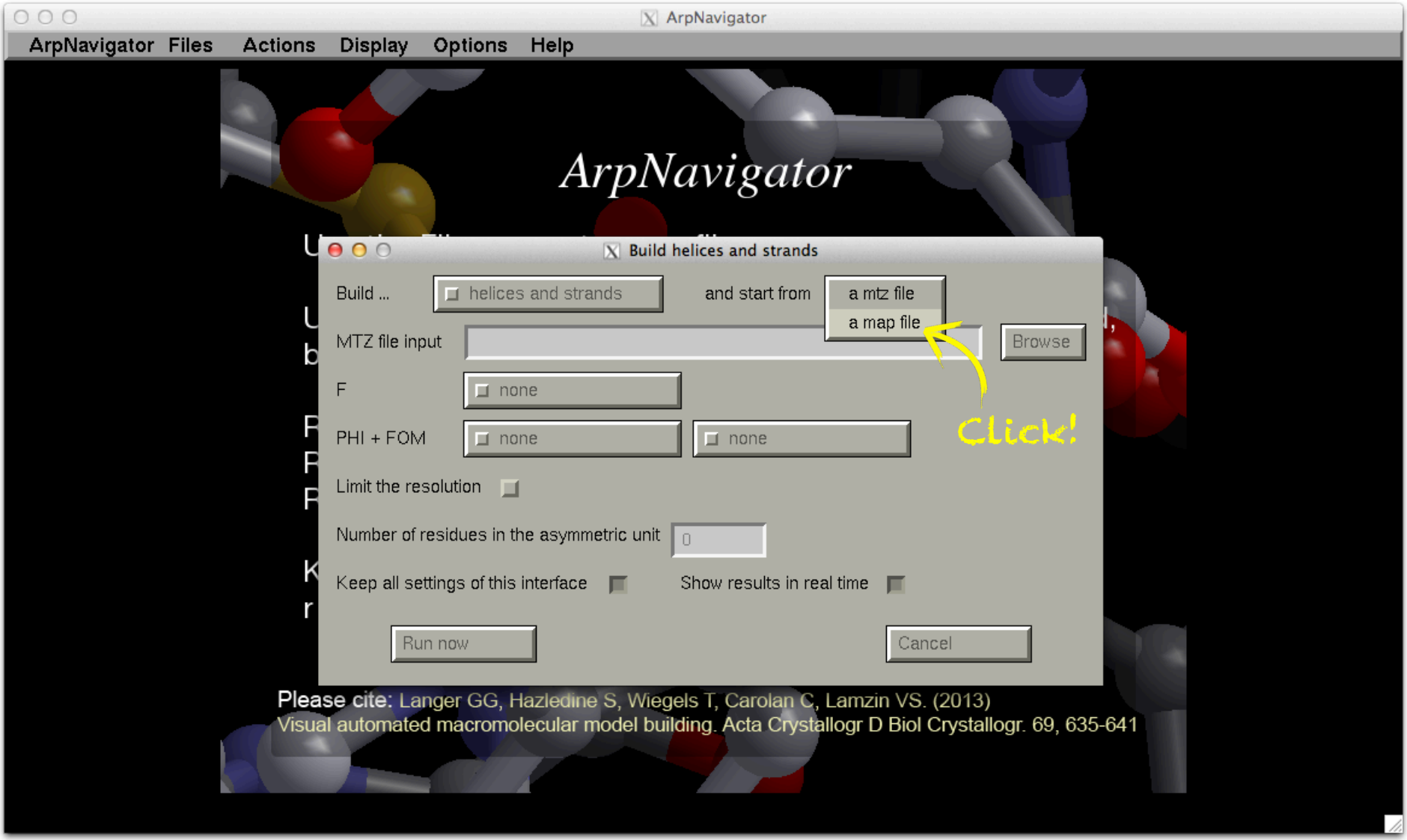
1.1.4. Run The Job – Log File



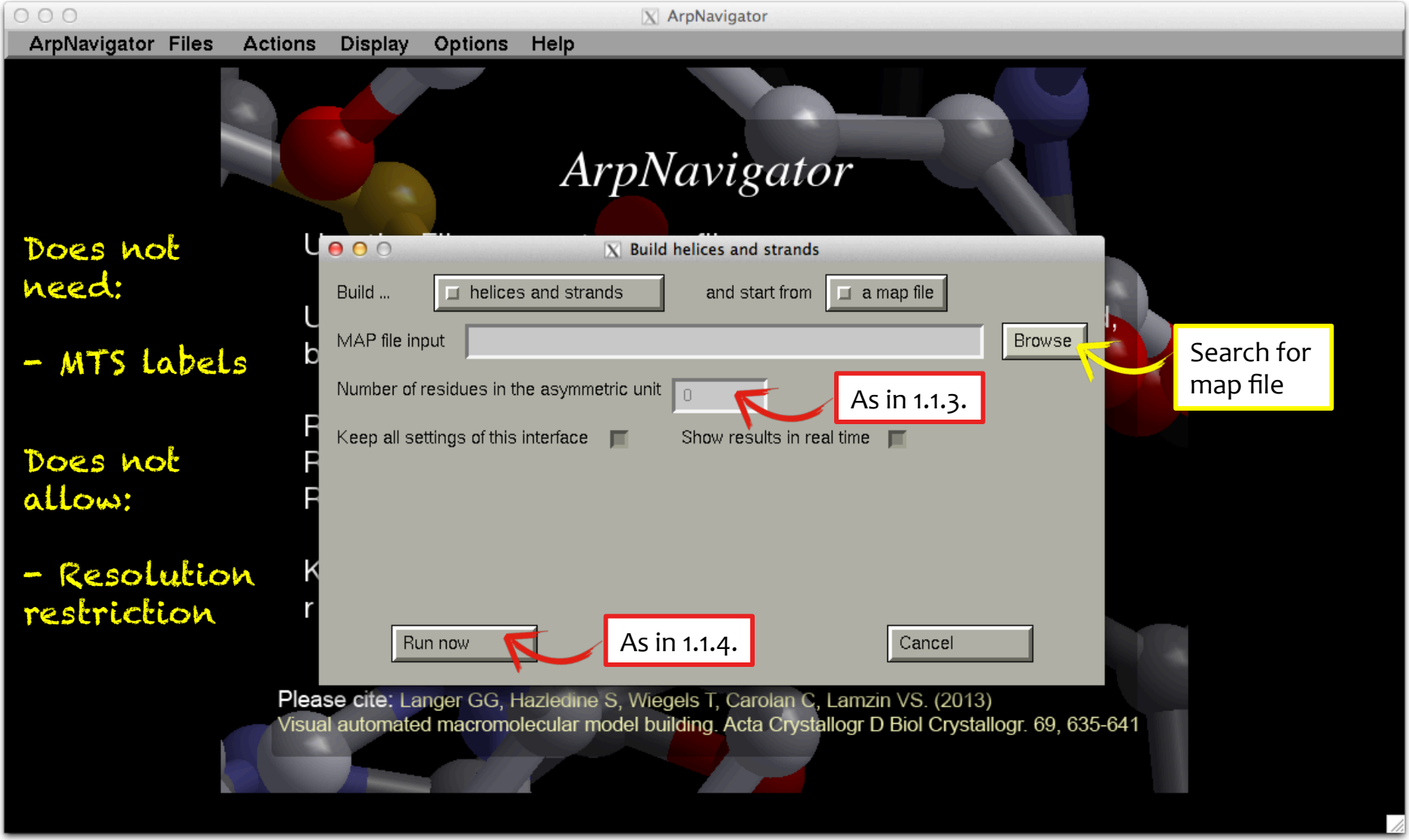
1.1.4. Run The Job – Live Model Building



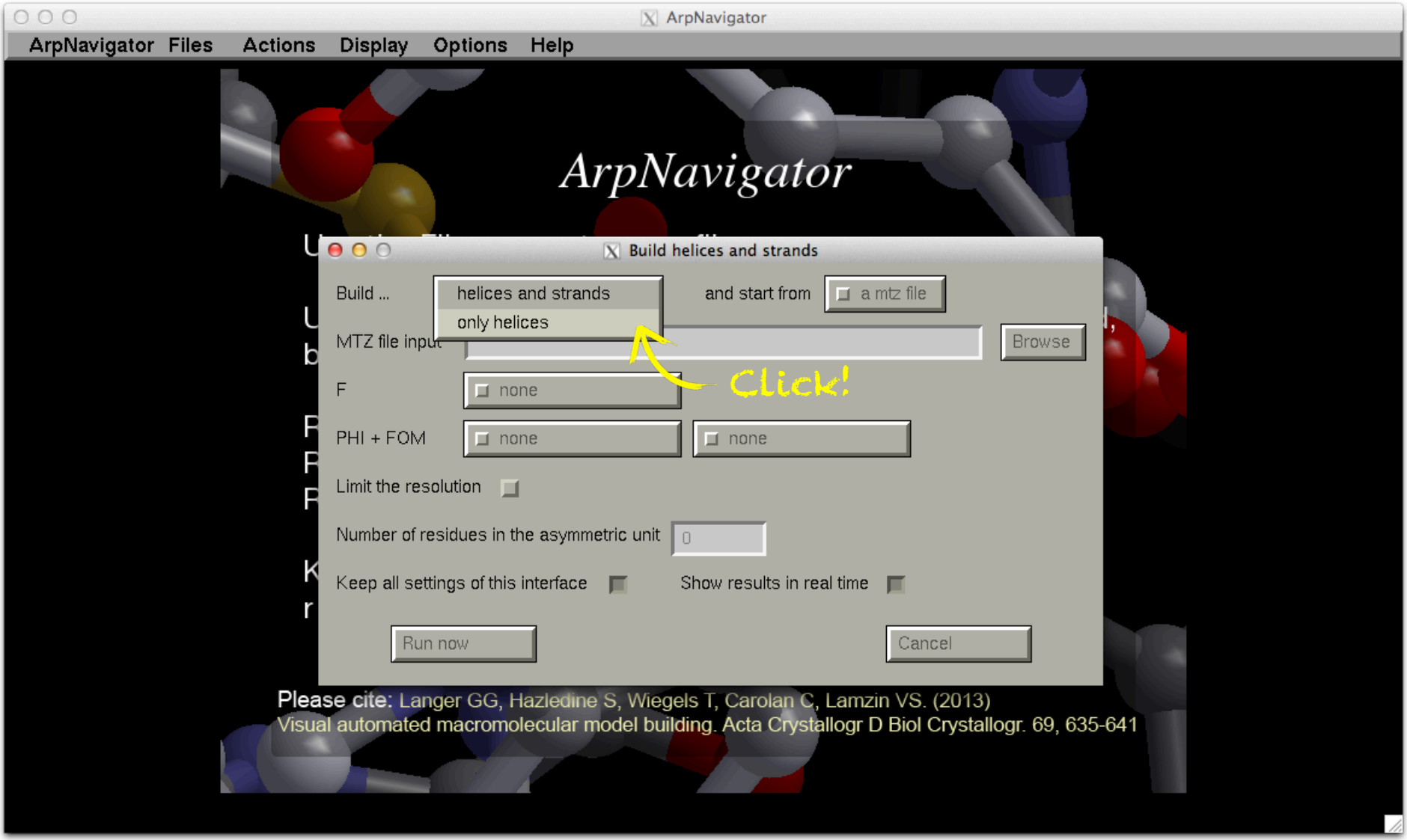
1.2. Start From MAP File



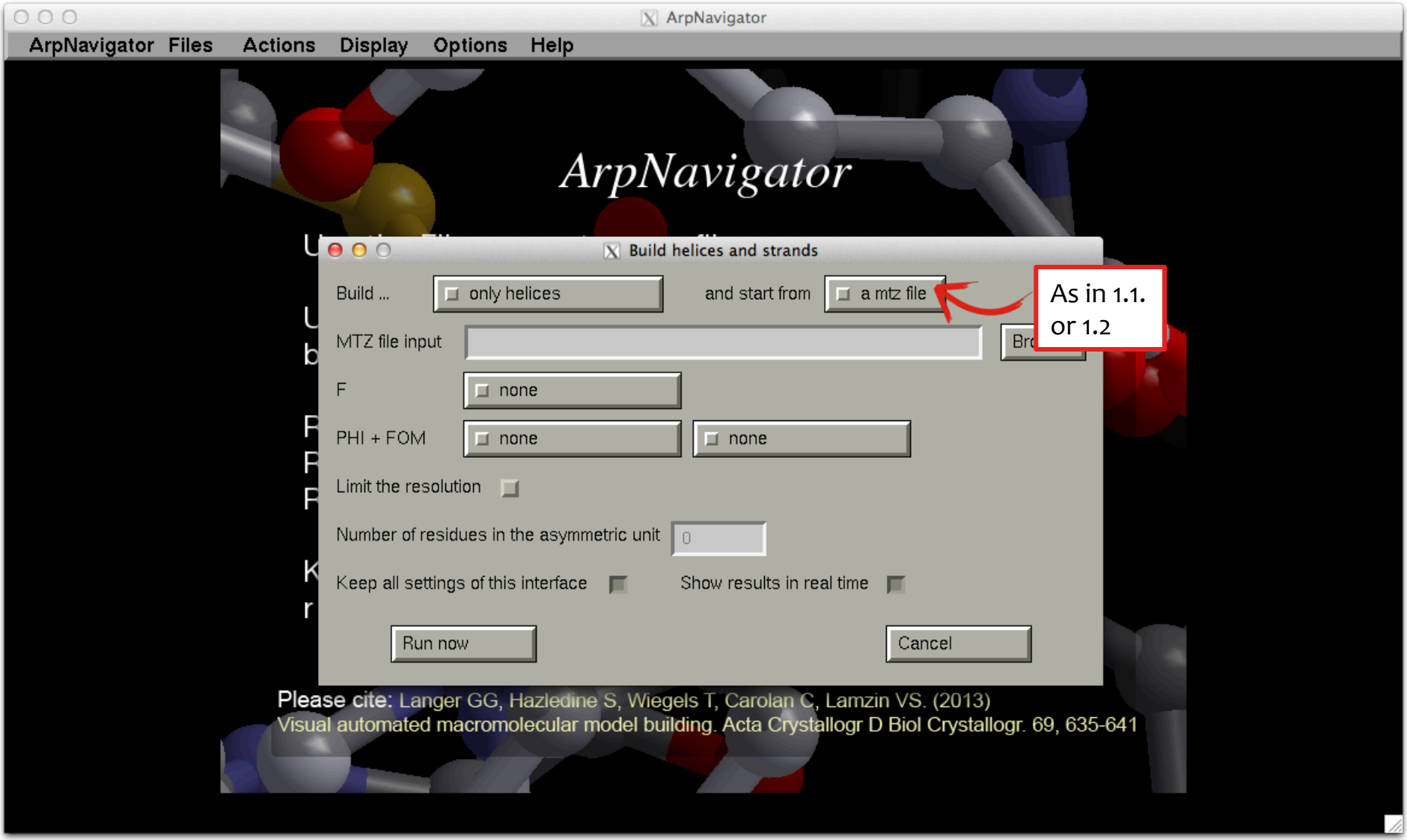
1.2.1. Input Files: MAP File



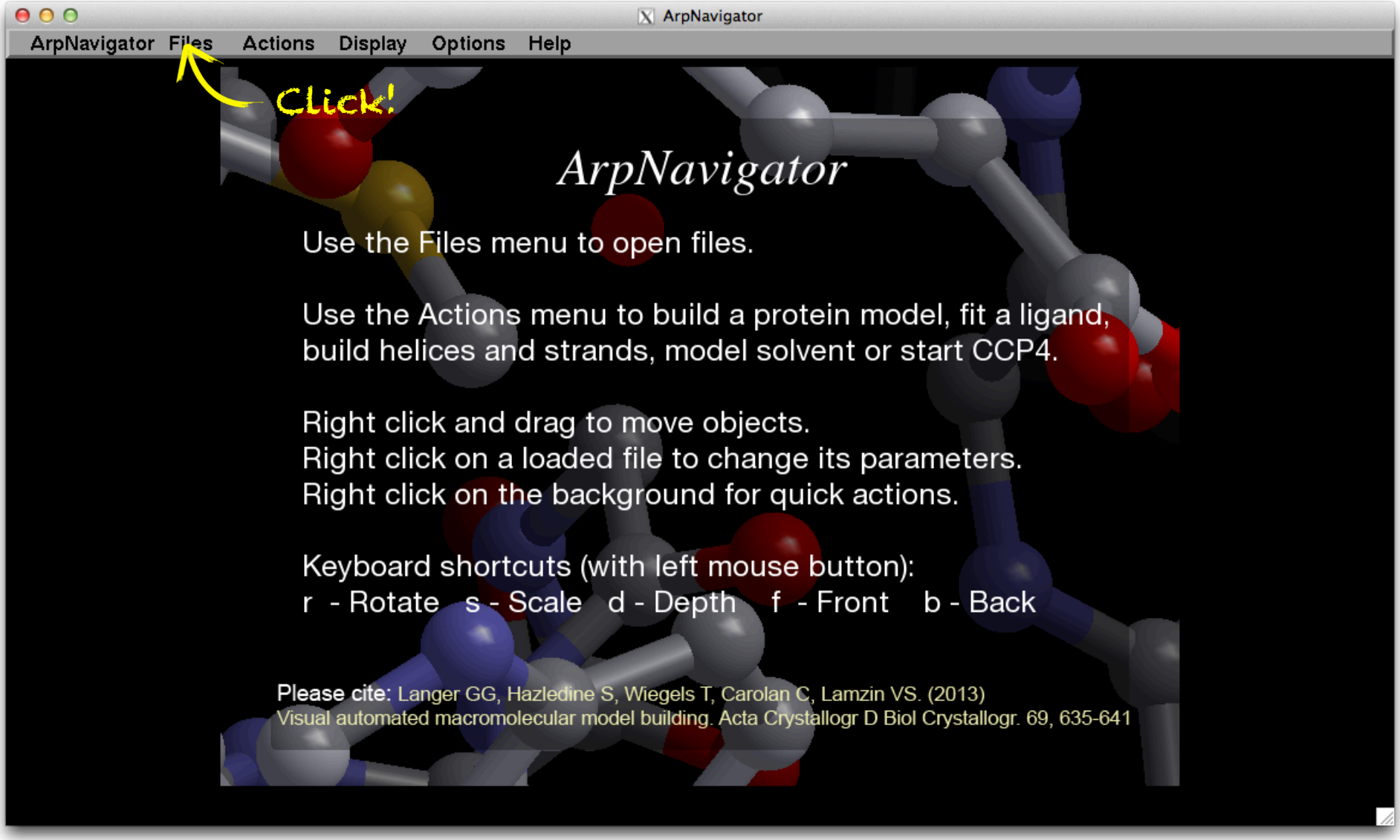
2. Building of Helixes Only



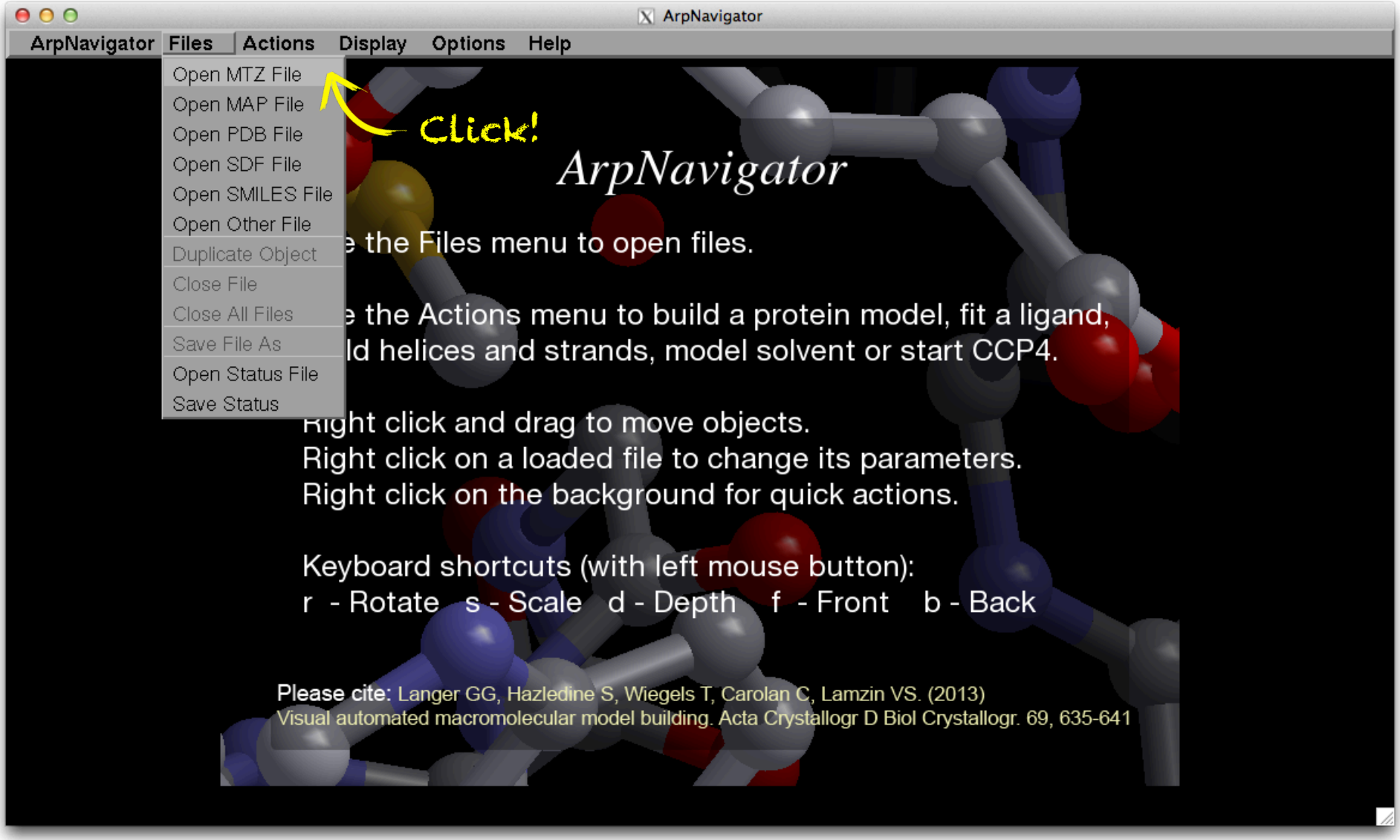
2. Building of Helixes Only



Build Secondary Structure and Skeletons Quickly



1. Load MTZ File



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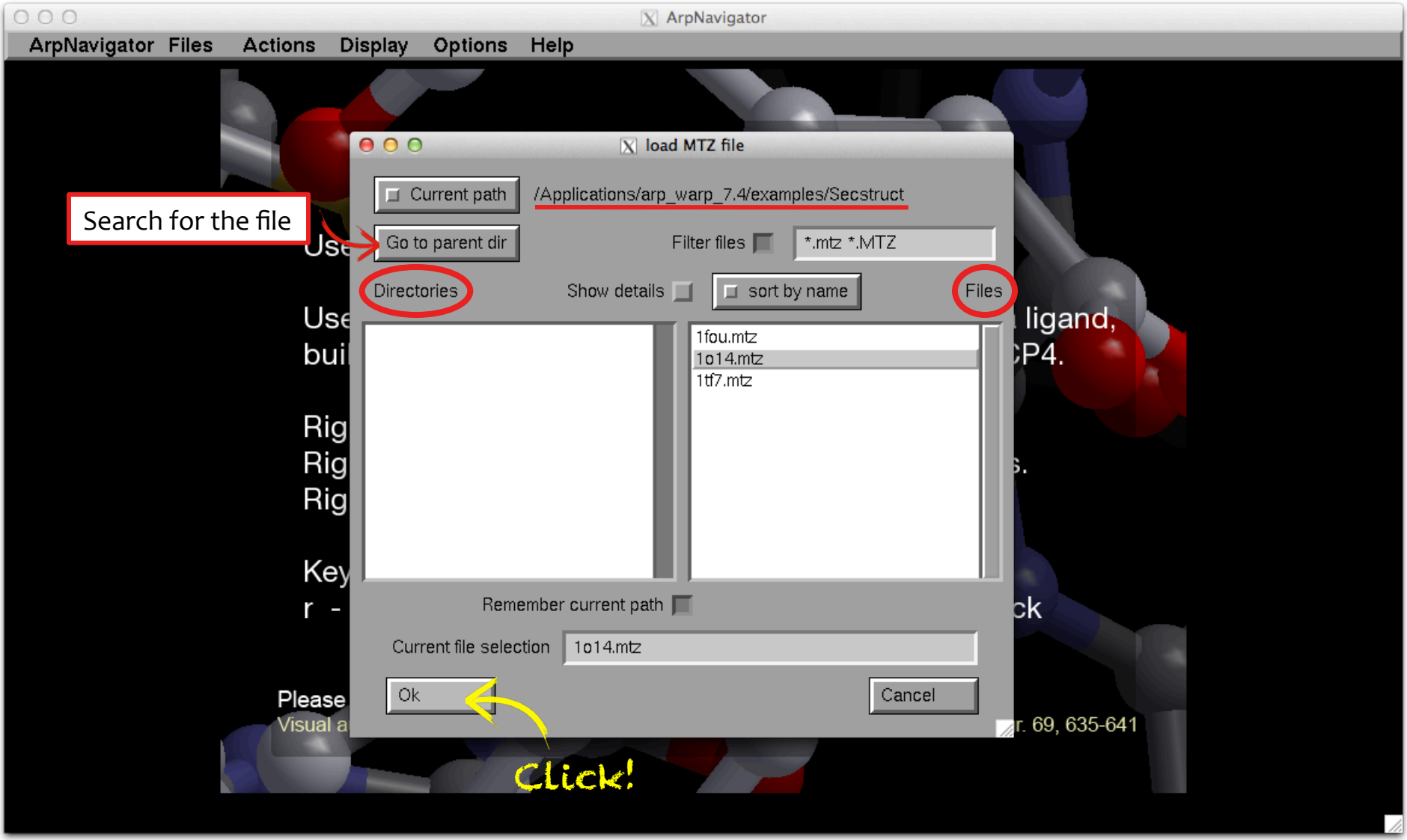

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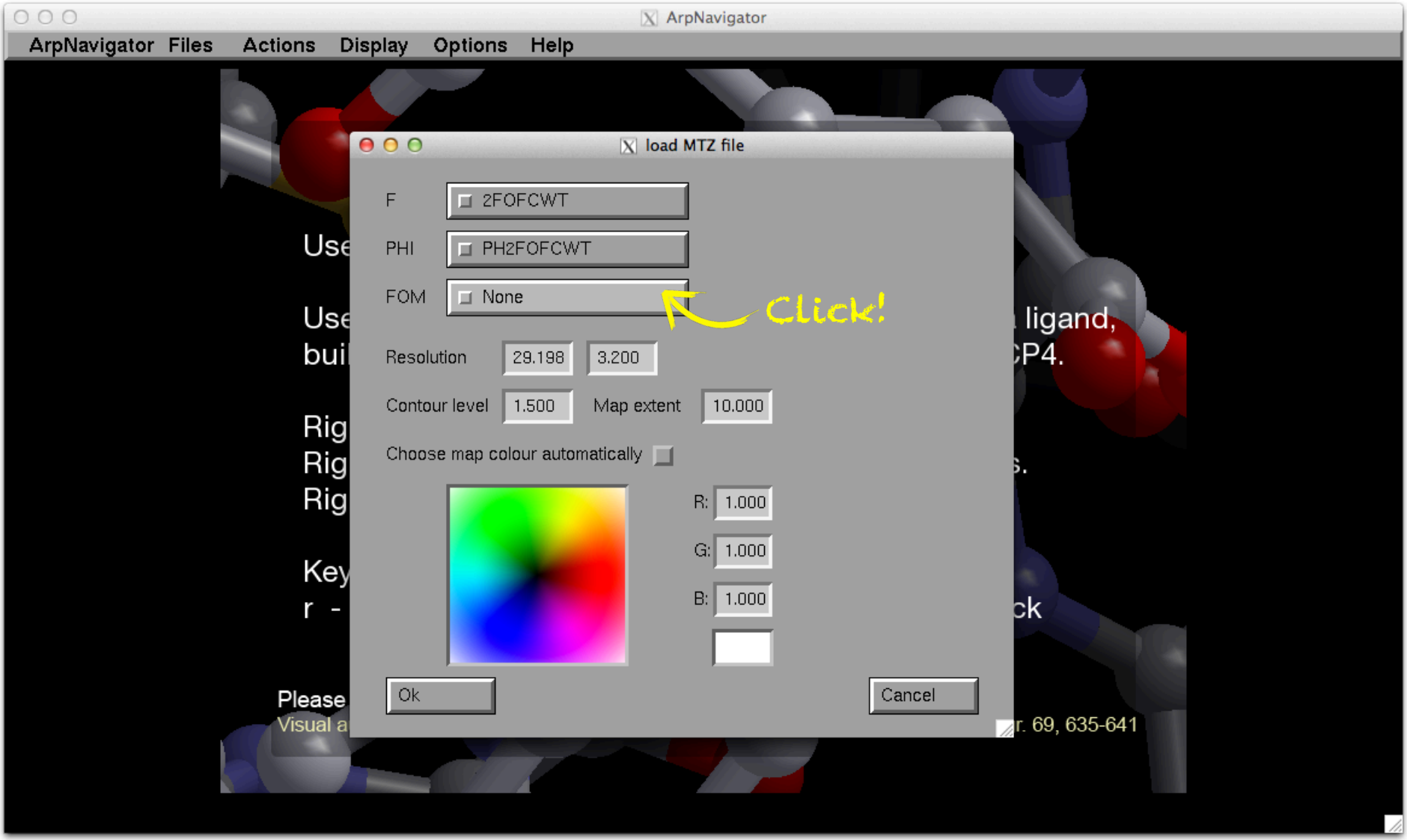

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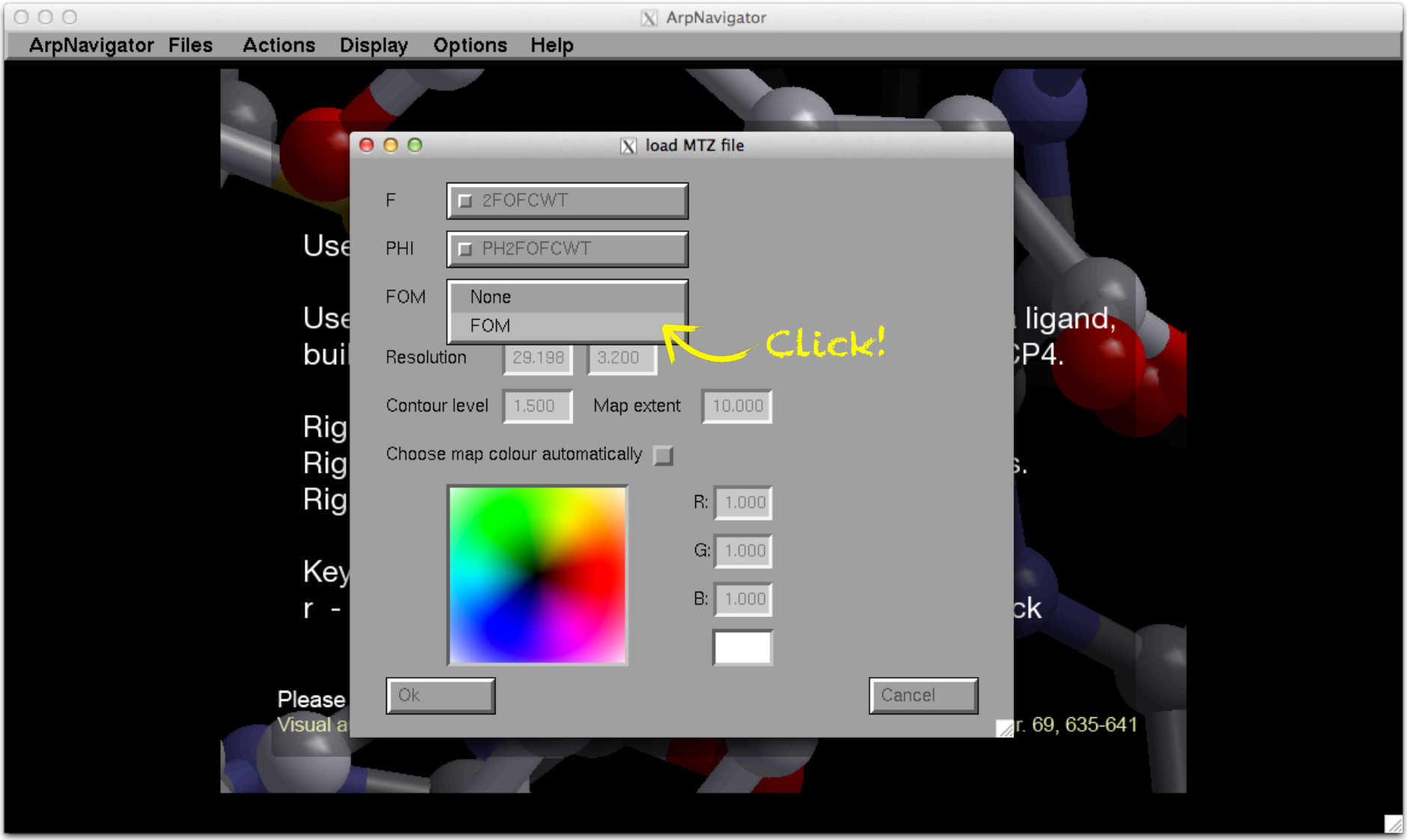
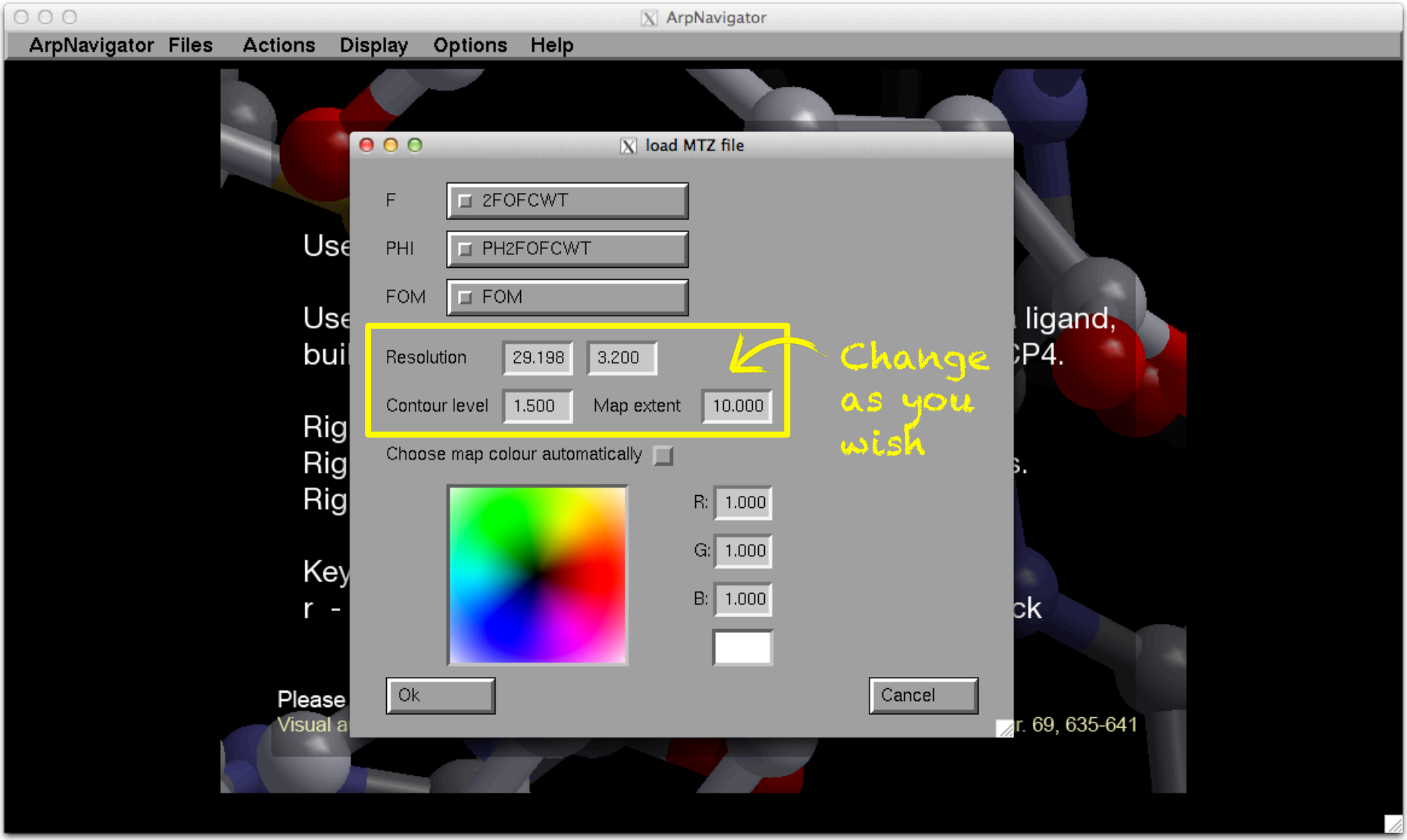
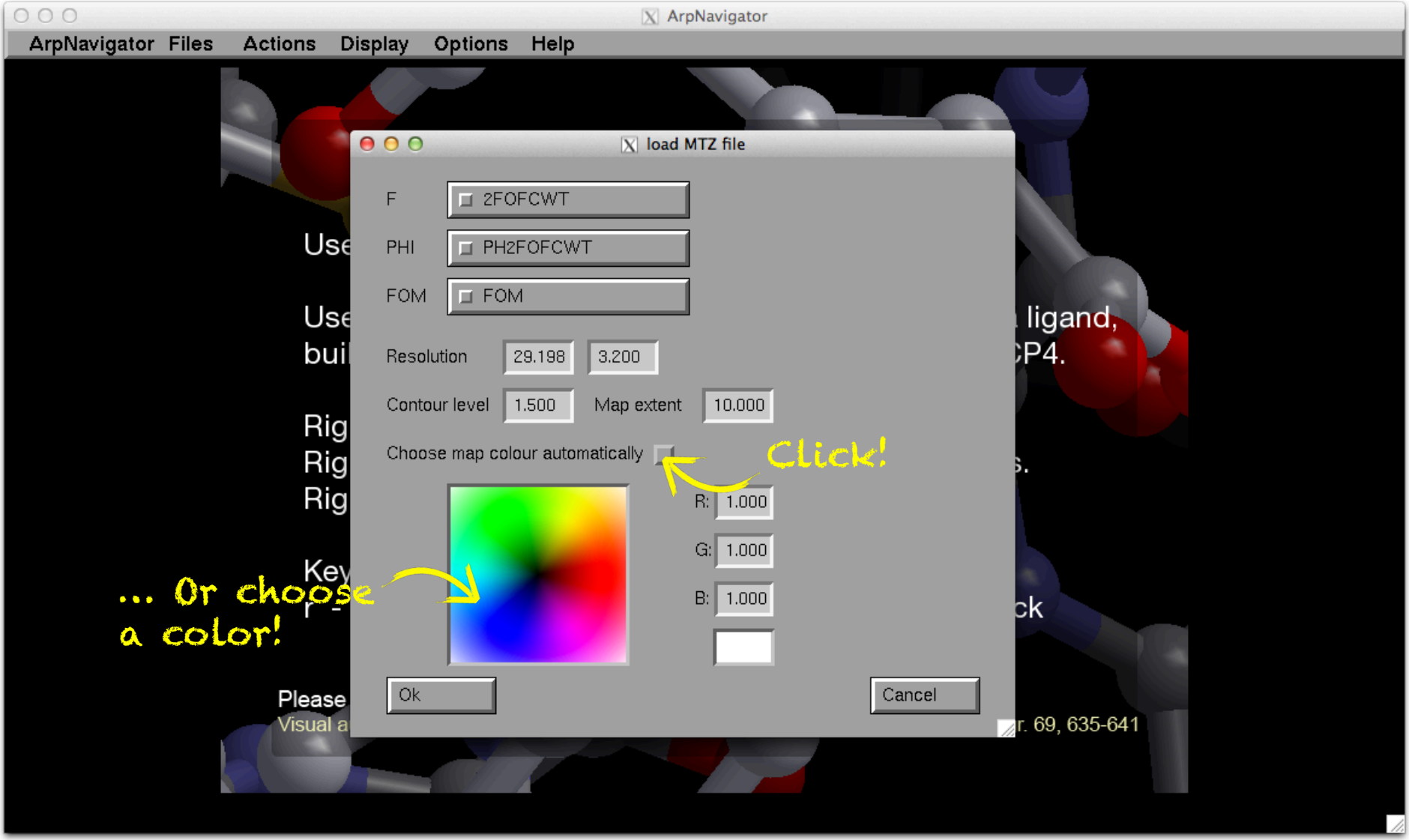


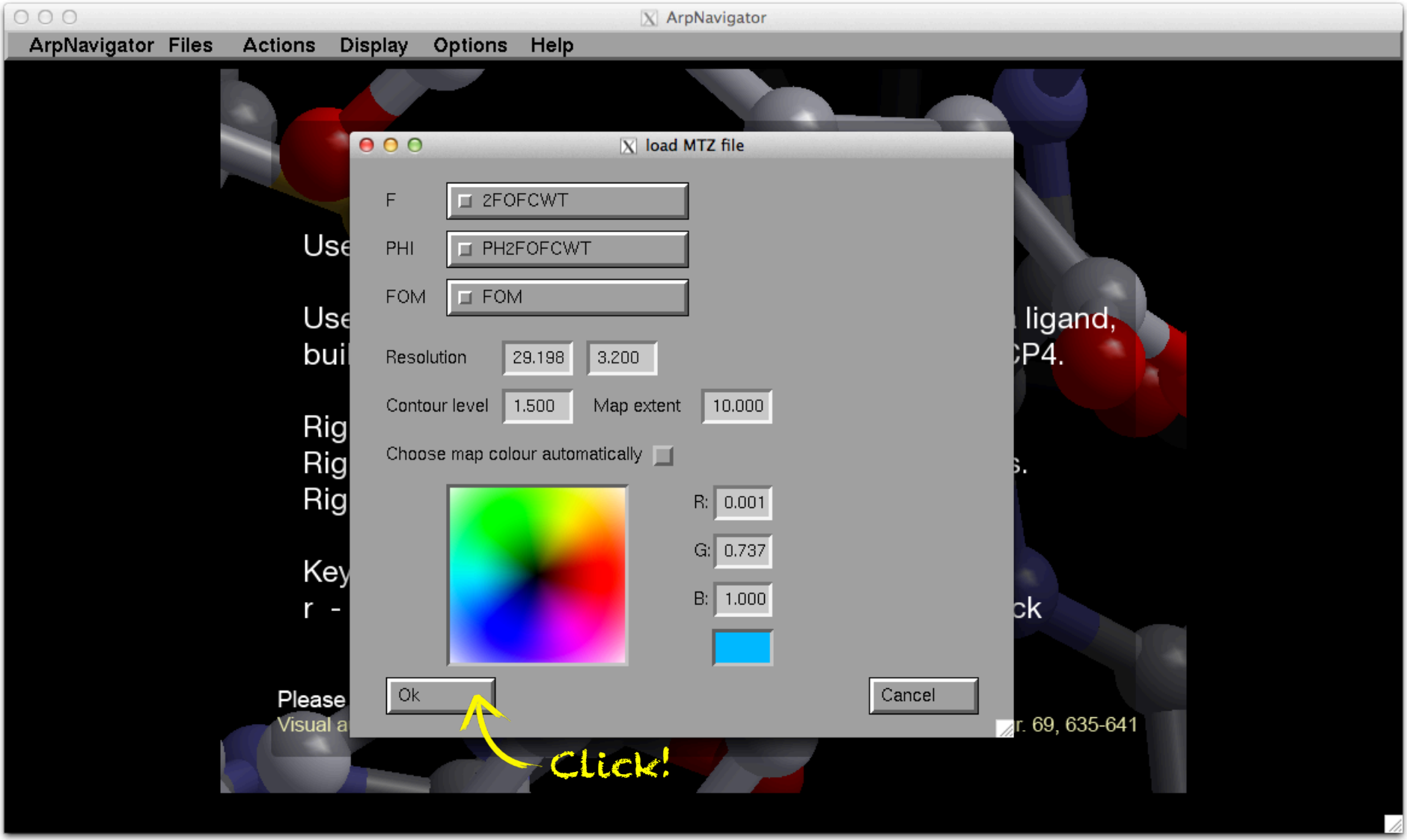
1. Load MTZ File



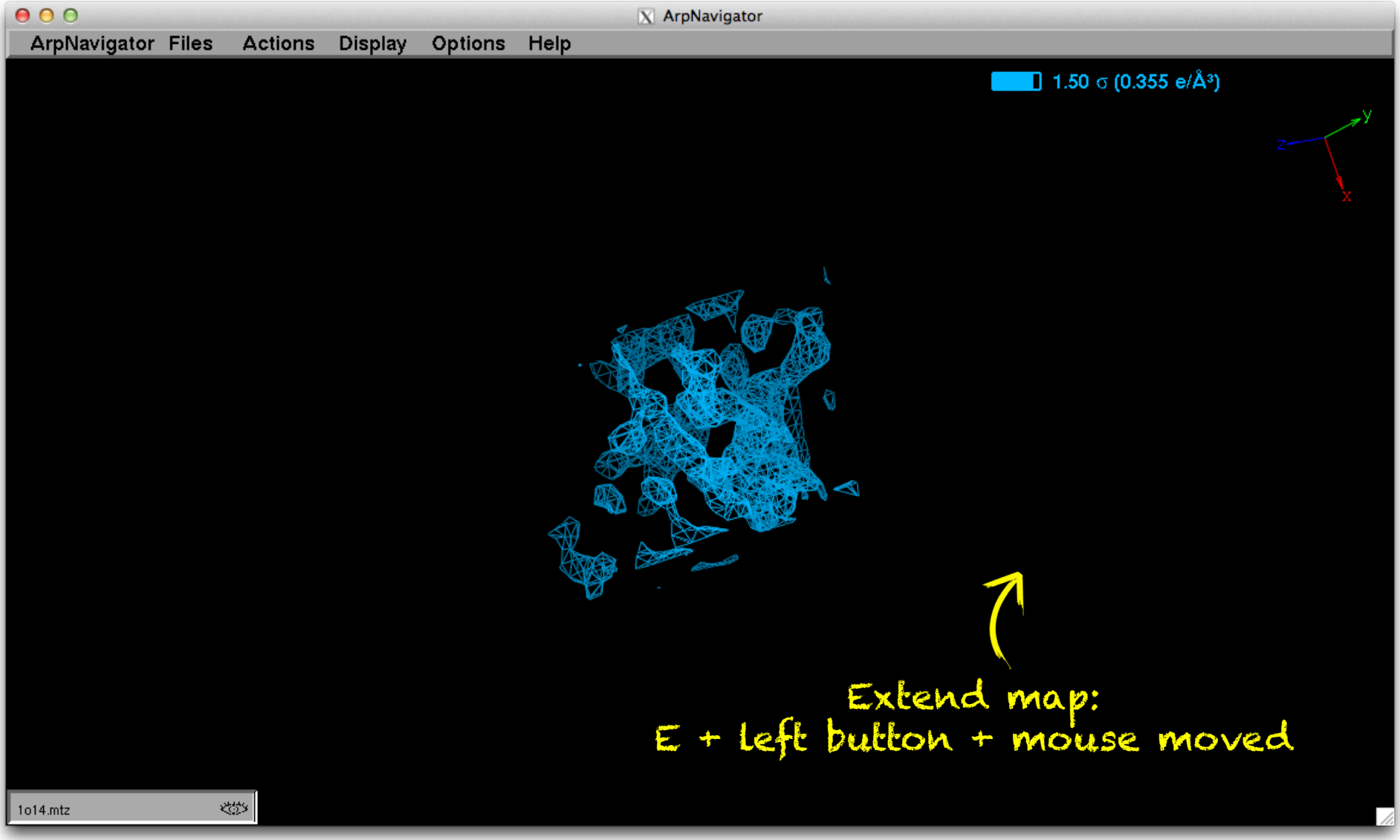
1. Loading MTZ File



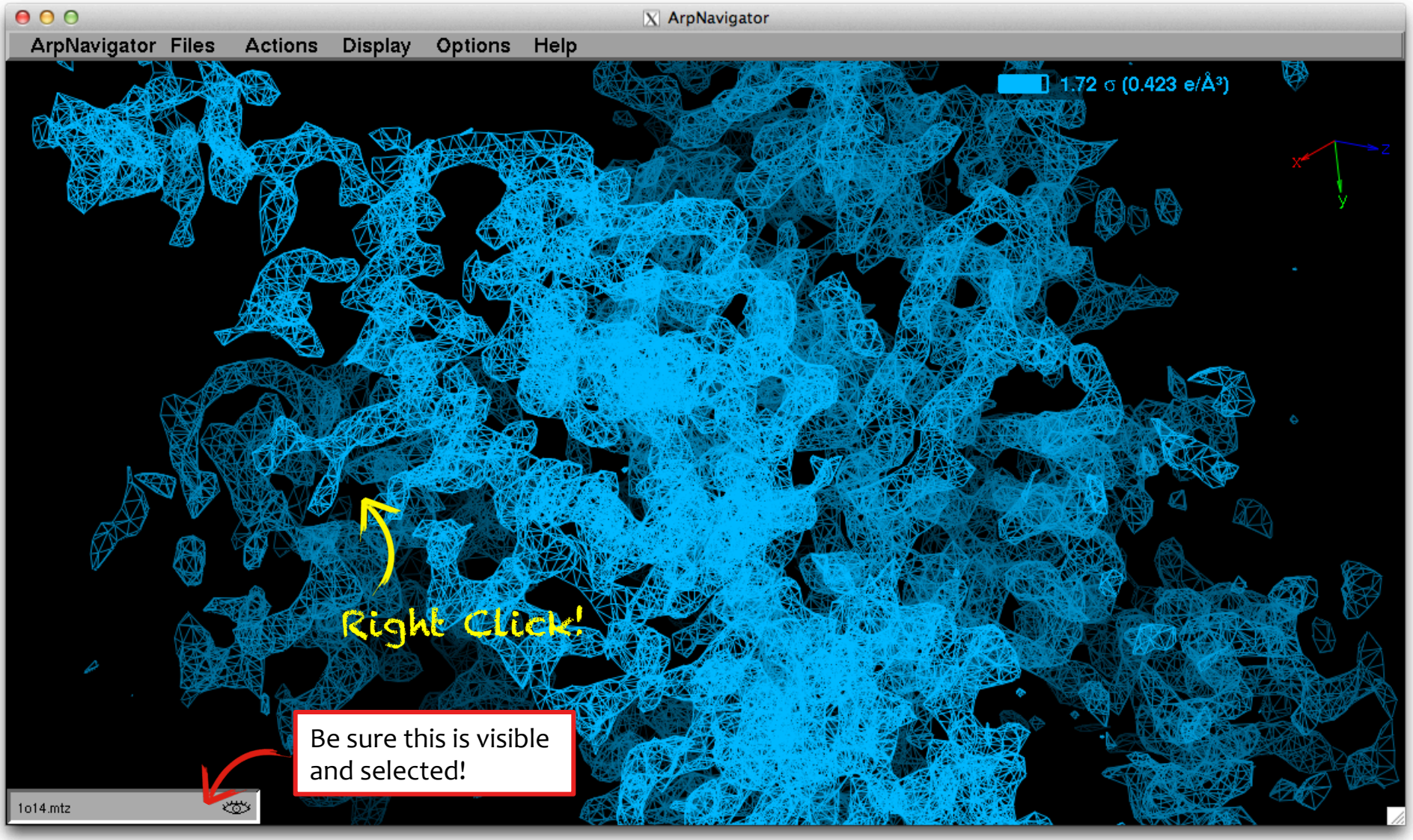
1. Load MTZ File



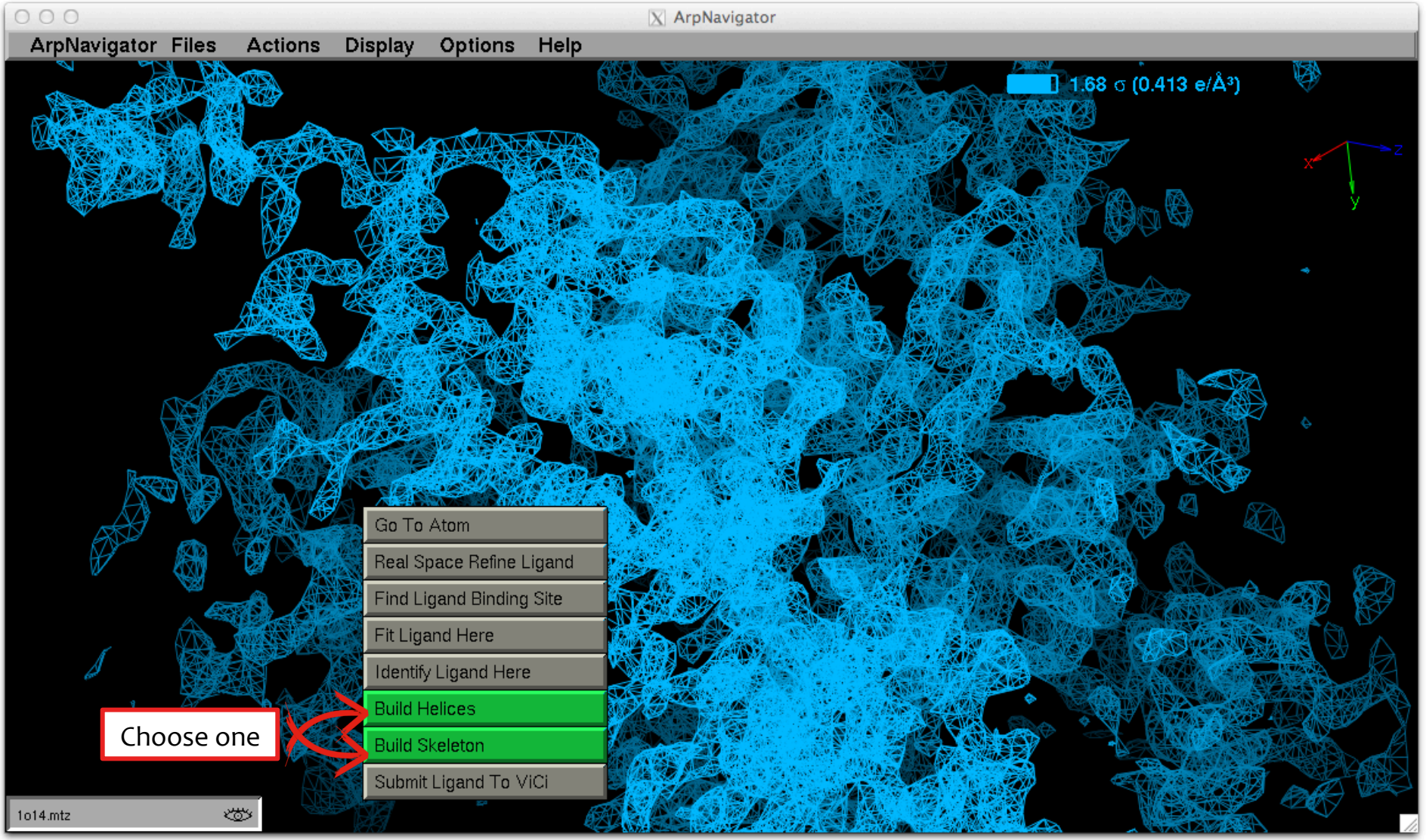
1. Load MTZ File



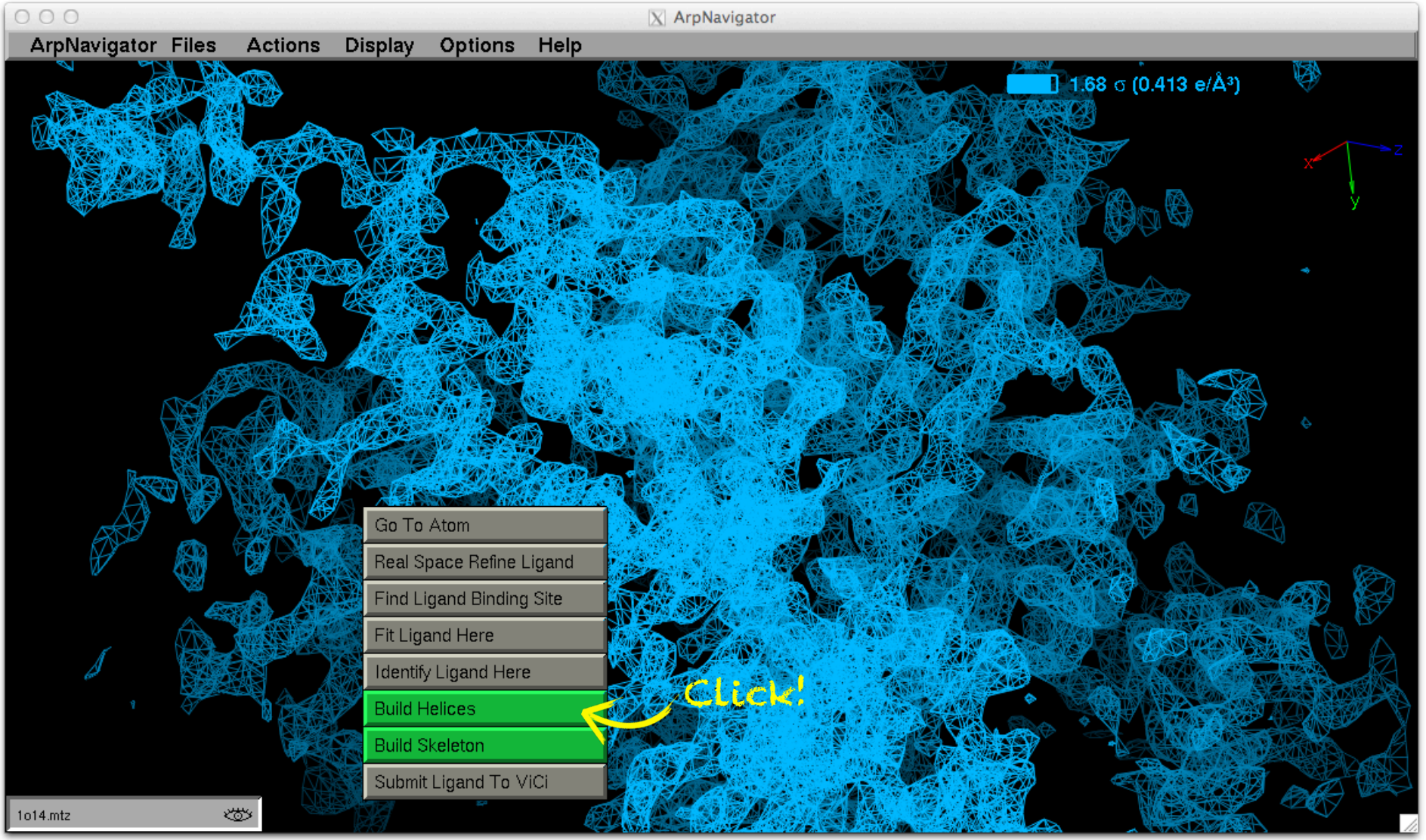
2. Build Helices (Only) or Skeletons



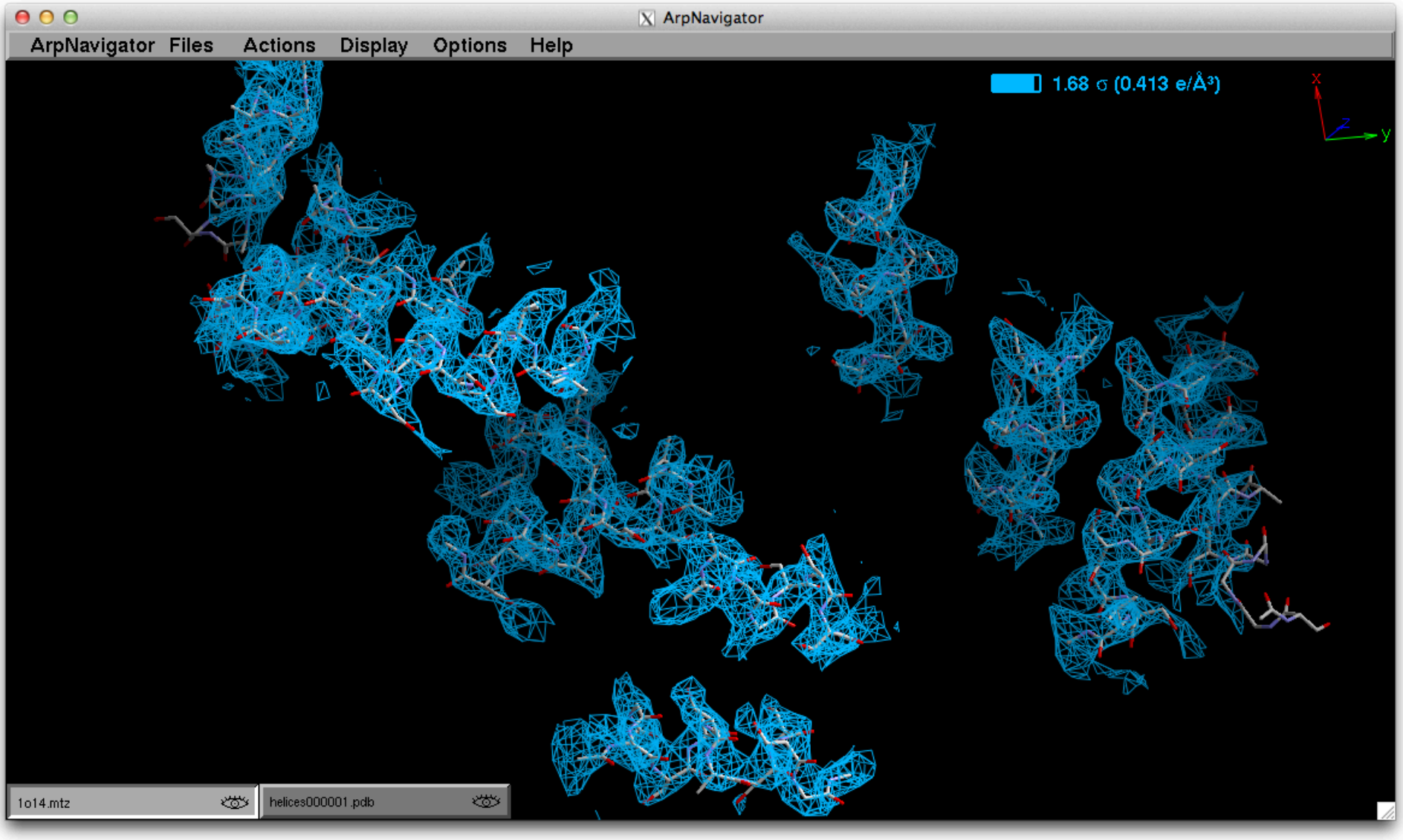
2. Build Helices (Only) or Skeletons



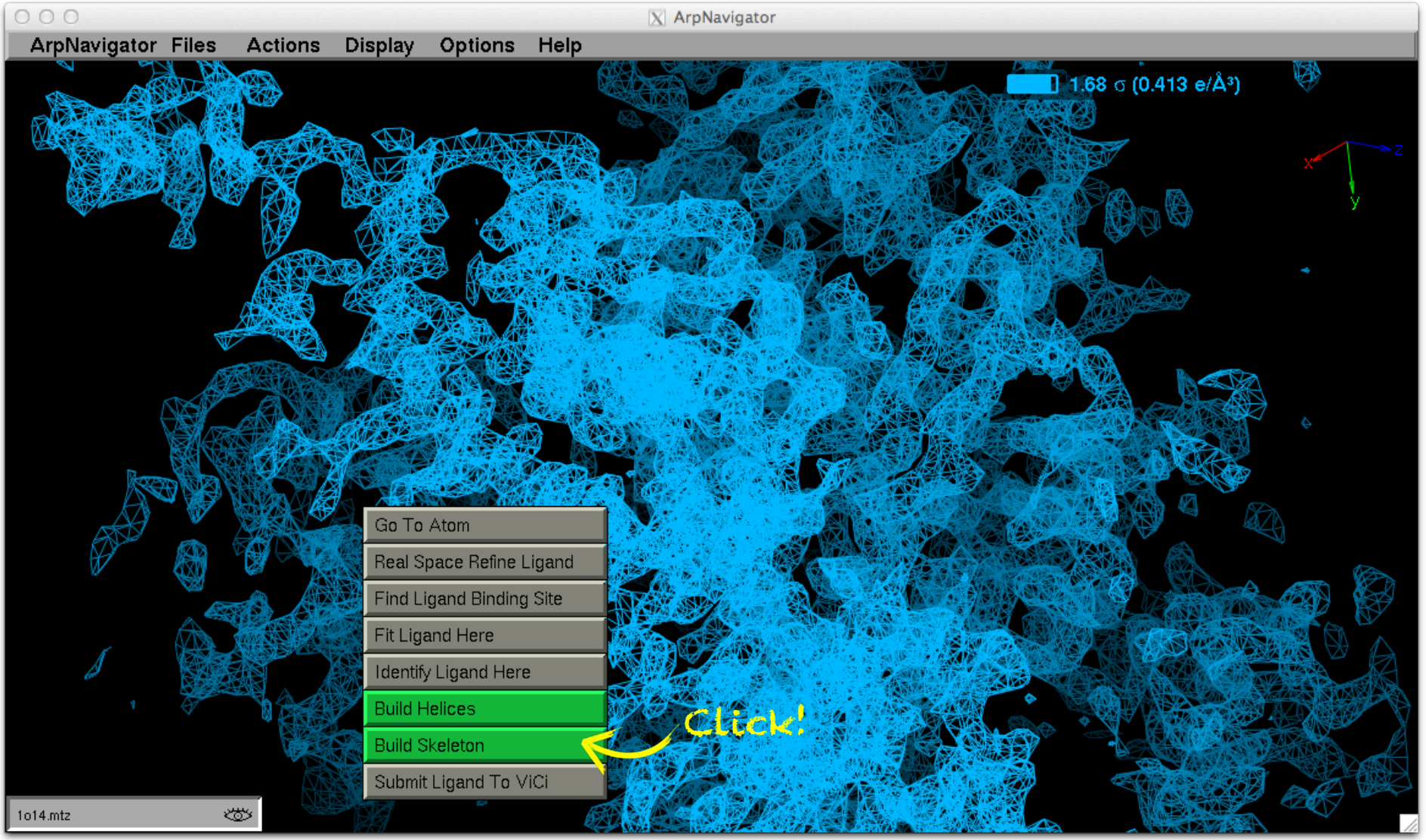
2.1. Build Helices (Only)



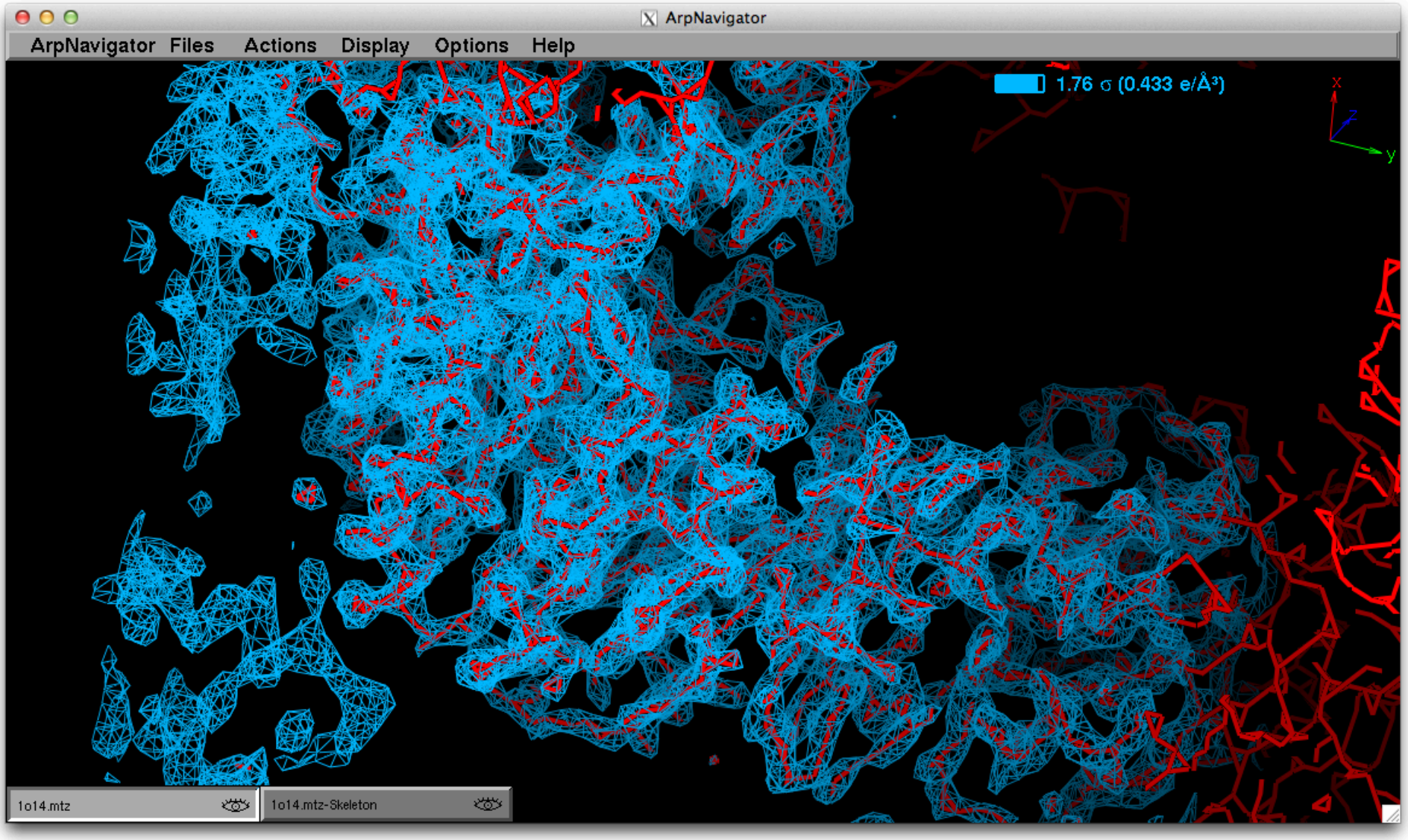
2.1. Build Helices (Only)



2.2. Build Skeletons



2.2. Build Skeletons



For any questions…

EMBL

The Developers

Contact us anytime!

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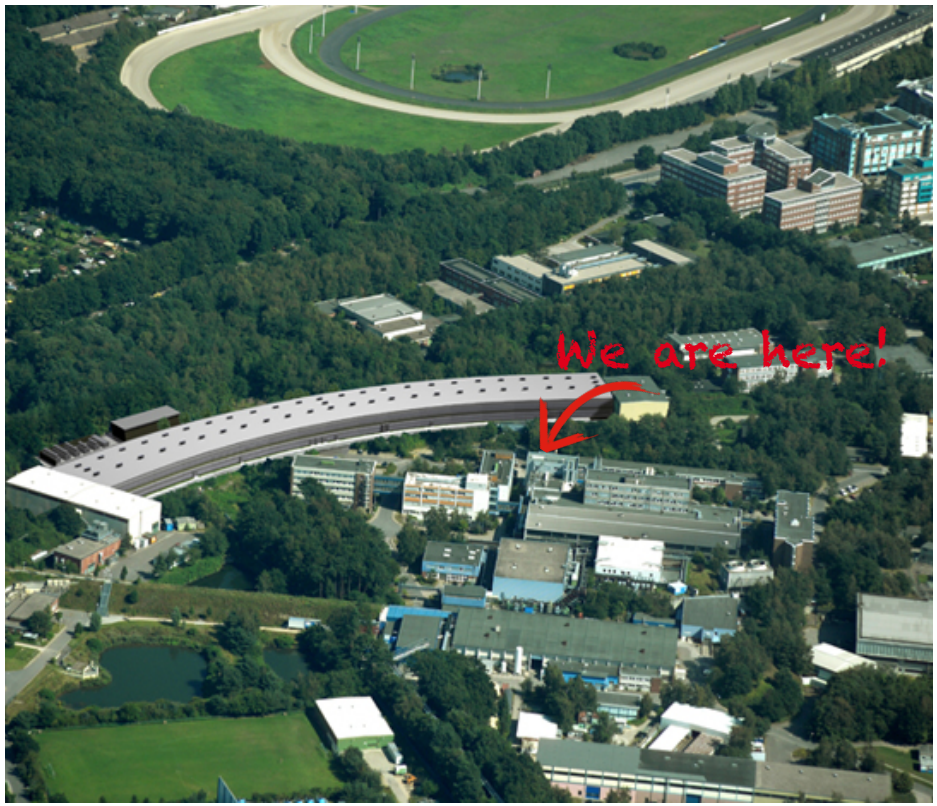
Ioan Vancea — Joana Pereira

Daria Beshnova

Or just visit our website!

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

User guide
Frequently asked questions
Tutorials



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