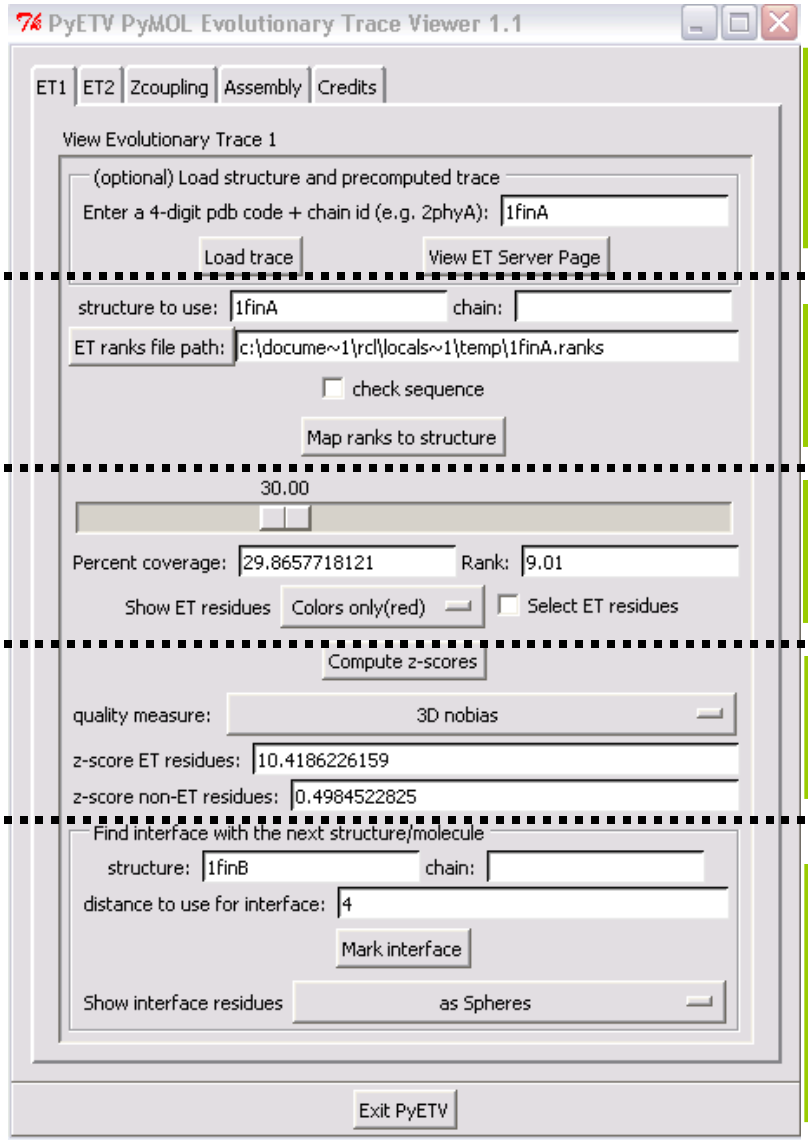
PyMOL Evolutionary Trace Viewer 1.1

Lichtarge Lab

Sept. 13, 2010

I. Basic sequence-evolution-structure analysis (ET1 or ET2)



Load trace with structure from the ET Server (Ref. 2)

Map ET rank data to a PyMOL structure

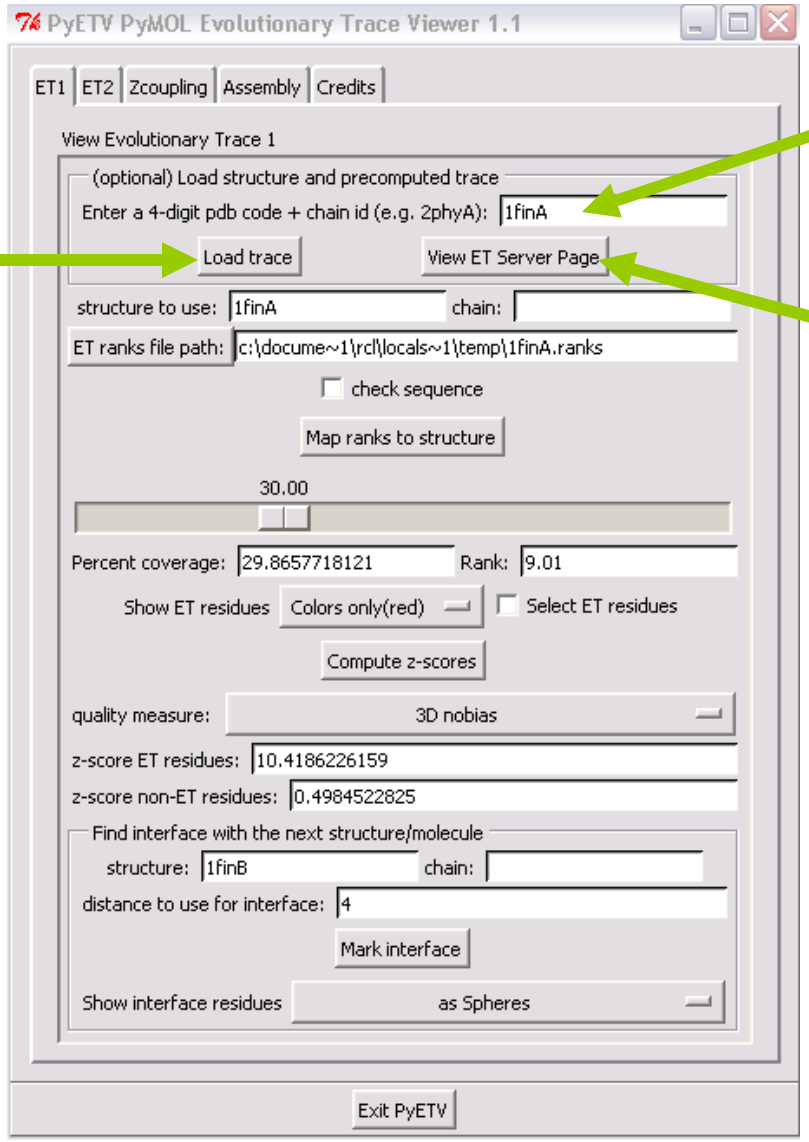
Vary the selection of ET residues

Assess clustering of ET residues

Mark interface of the structure with another PyMOL structure or ligand

I.1 Load trace with structure from the ET server (Ref. 2)

This will download a PDB chain into PyMOL and an ET ranks file. The boxes below automatically get filled with the correct information.



Enter a single PDB code with chain indicator.

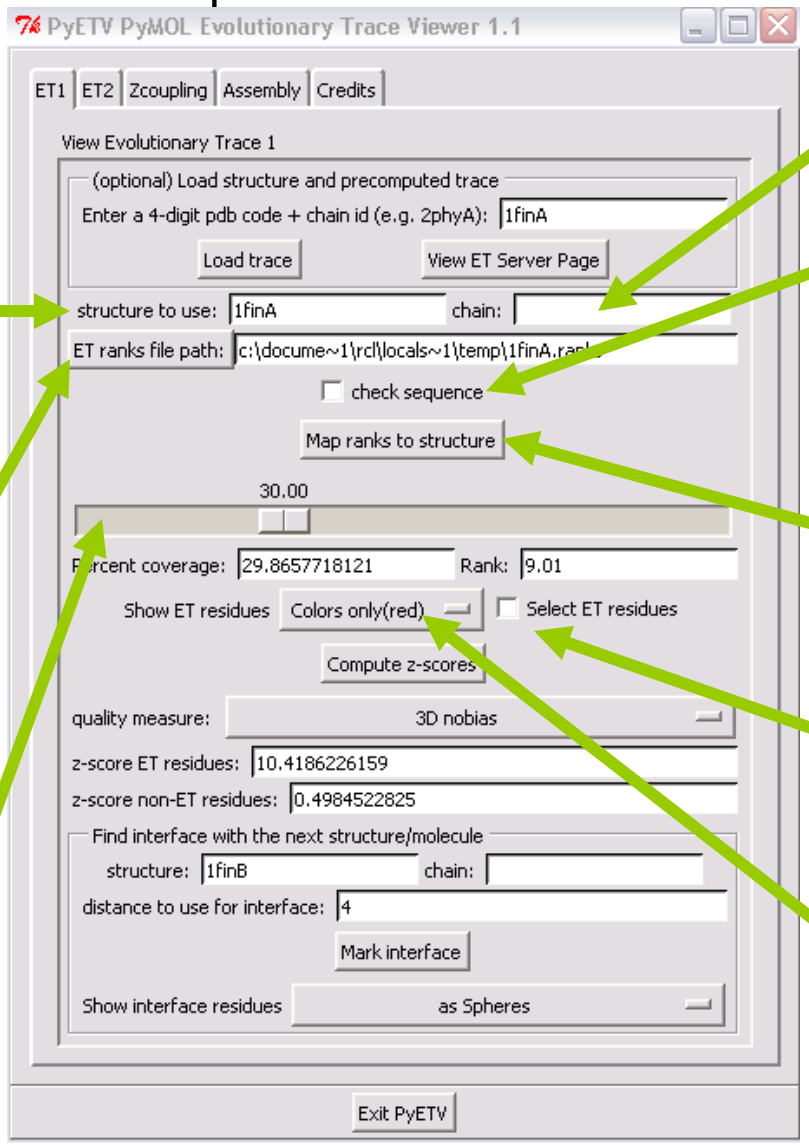
This will open an internet browser and take the user to the ET Server search results.

I.2 Map ET rank data to a PyMOL structure and vary the selection of top ET-ranked residues

Enter the PyMOL name of the structure. This structure must be present in the PyMOL graphics window.

Select an ET ranks file. The button opens a file selection window.

Vary selection of ET residues (Left mouse click, drag, then release). The slider value corresponds to a percent coverage.



Optional chain indicator

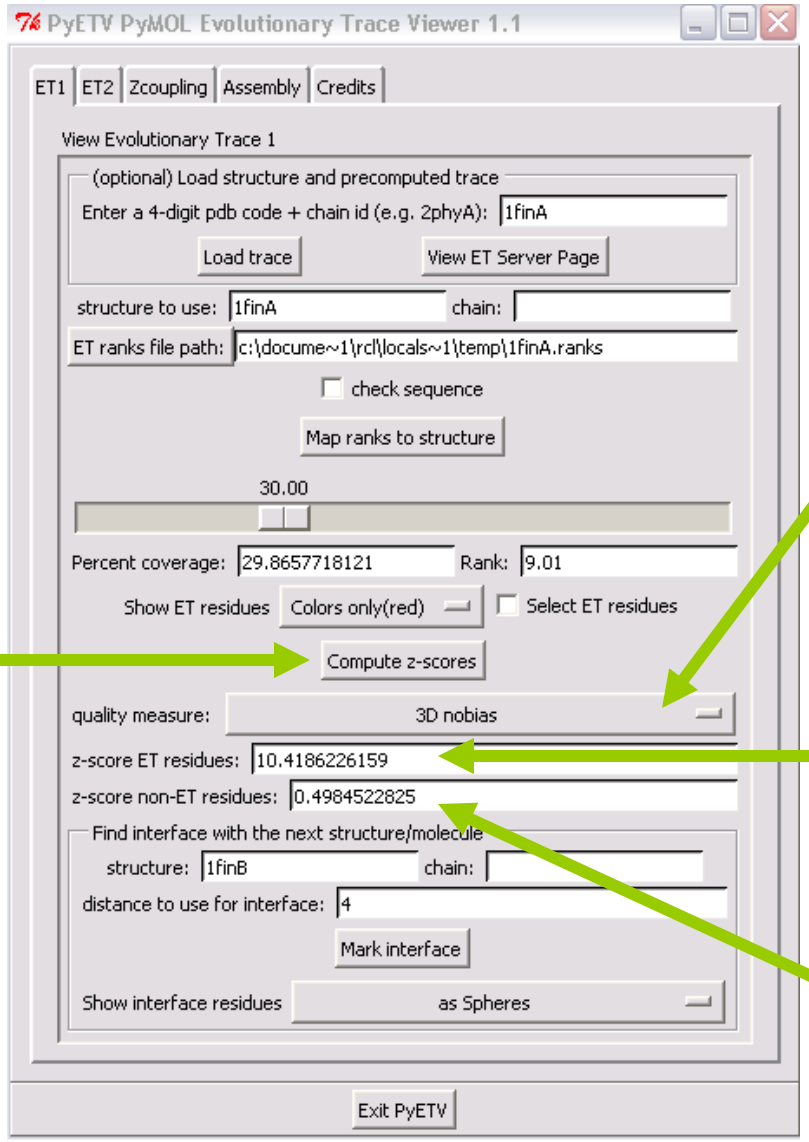
Check the box to compare the sequences between the structure and ET ranks file.

Map ET rank data to the residues in the structure.

Check the box to create a PyMOL selection of the ET residues.

Select display options to distinguish ET residues from the rest of the structure.

I.3 Assess the statistical significance of the spatial clustering of top ET-ranked residues



Start computation of the ET clustering z-scores

Select clustering measure (nobias, or with bias for residues more distant in sequence (Ref. 3))

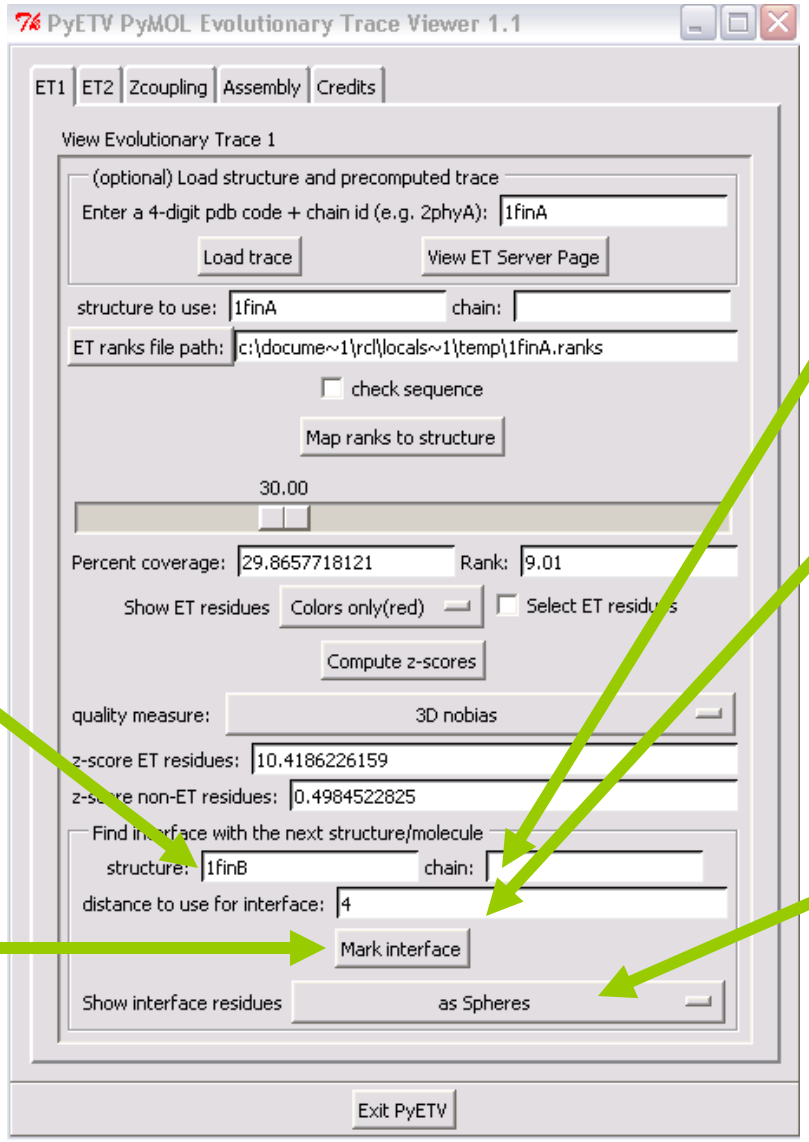
Clustering z-score of the top-ranked residues at the current ET rank threshold.

Clustering z-score of the rest of the residues in the structure

I.4 Find interface residues on main ET1 structure

Enter the PyMOL name of the partner structure. A structure with this name must be present in the PyMOL graphics window.

Start finding the interface residues between the main **ET1** structure (e.g. 1finA) and the partner structure (e.g. 1finB)

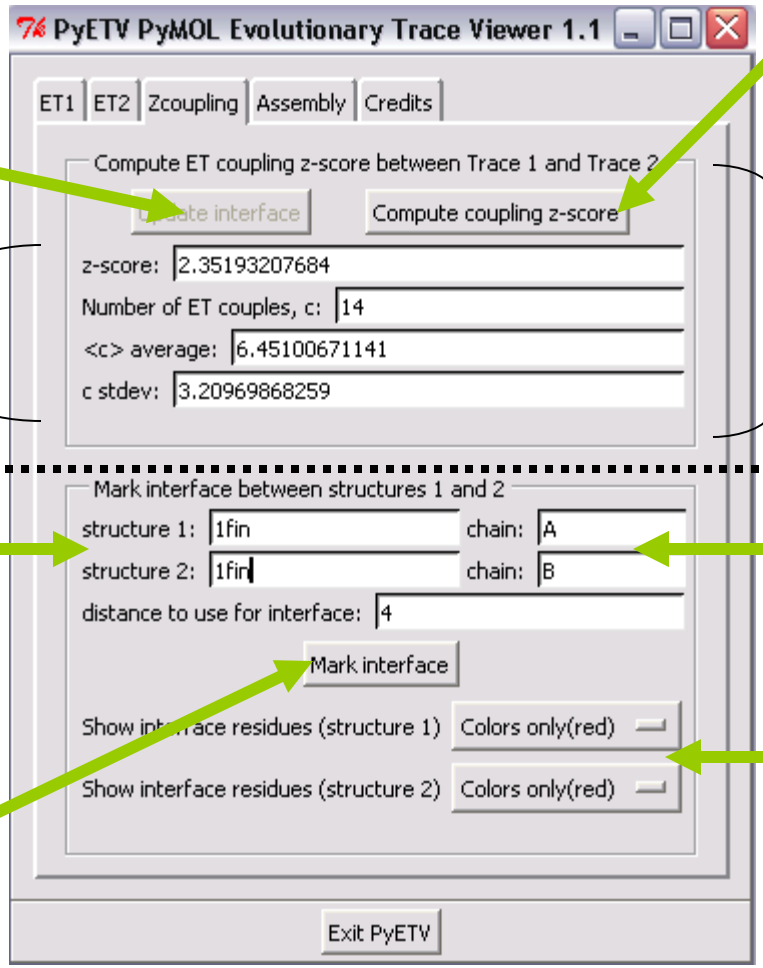


Optional chain indicator

This input distance refers to the atom-atom distance (Å) threshold between the interface residues of the partners.

Select display option for interface residues (Color(red), Spheres, Sticks, PyMOL selection)

II. Zcoupling – ET coupling z-score computation (dependent on ET1 and ET2 pages) and interface selection (bottom)



Start computation

Currently disabled

Computes the ET coupling z-score of the structures and current ET selections made with **ET1** and **ET2**.

The z-score and its components; Z=(c-<c>)/stdev (Ref. 5)

Specify PyMOL structures. Must be present in the PyMOL graphics window.

chain indicators (optional)

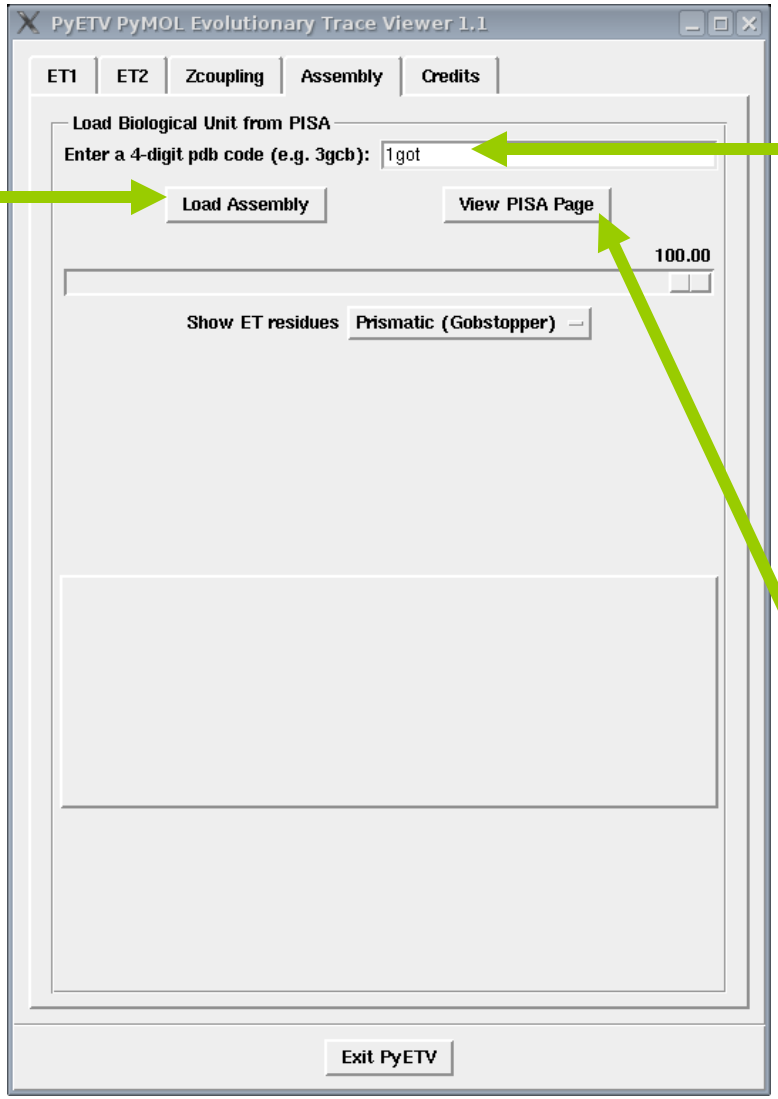
Start interface computation

Select display option for interface residues (Color(red), Spheres, Sticks, PyMOL selection)

Interface selection is independent of the z-score computation.

III. Assembly tool – loading and viewing a PISA assembly (Ref. 6)

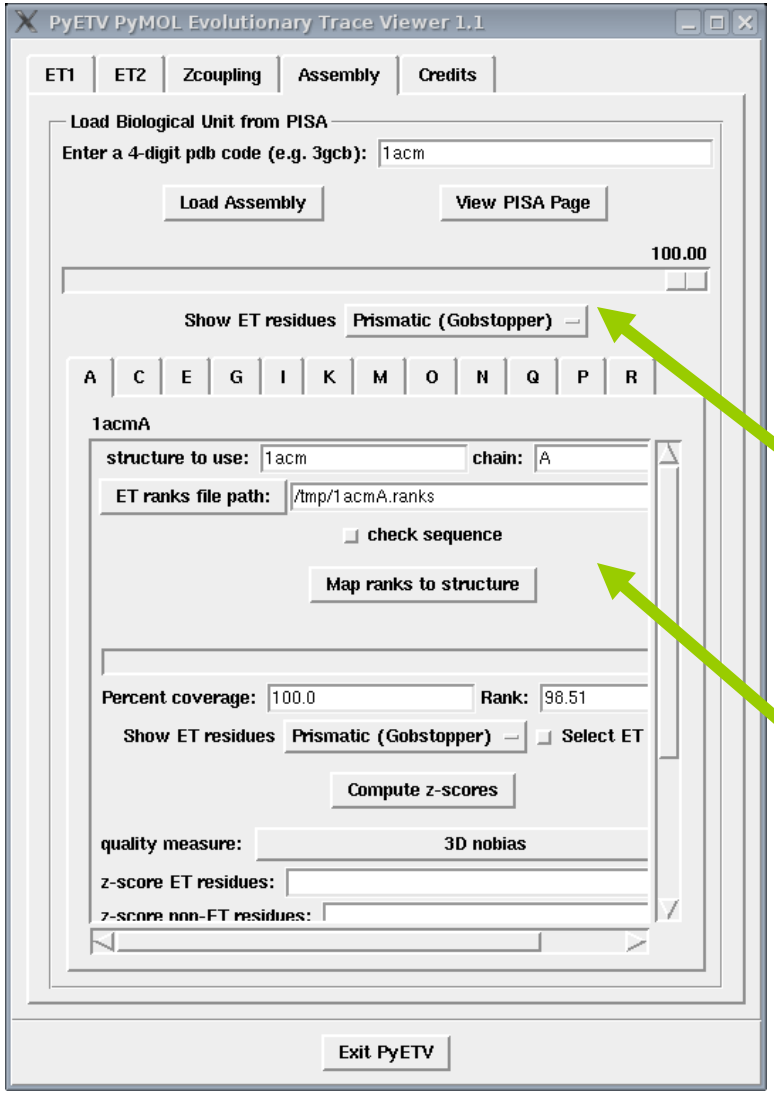
This will start the download of the multimer into PyMOL. PyETV will also attempt to match ET rank data from the ET server to each chain in the assembly. A page for each chain will be created below the **Assembly** page, organized into a tabbed folder.

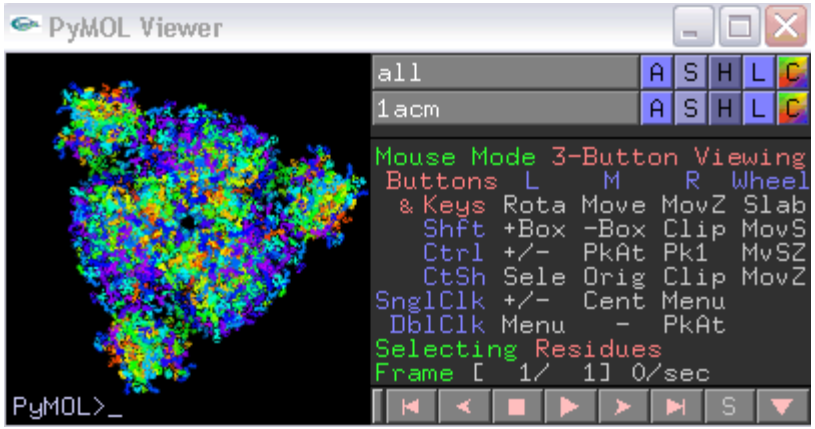


Enter a single PDB code (e.g. *1got*) to get the most probable PISA solution, or a PDB code with PISA assembly numbers (e.g. *1got:1,1* for the top solution).

This will open an internet browser and take the user to the PISA search results.

III.1 Assembly tool – completion of Load Assembly





Use the slider and select options to modify the ET residue selections for all chains in the assembly

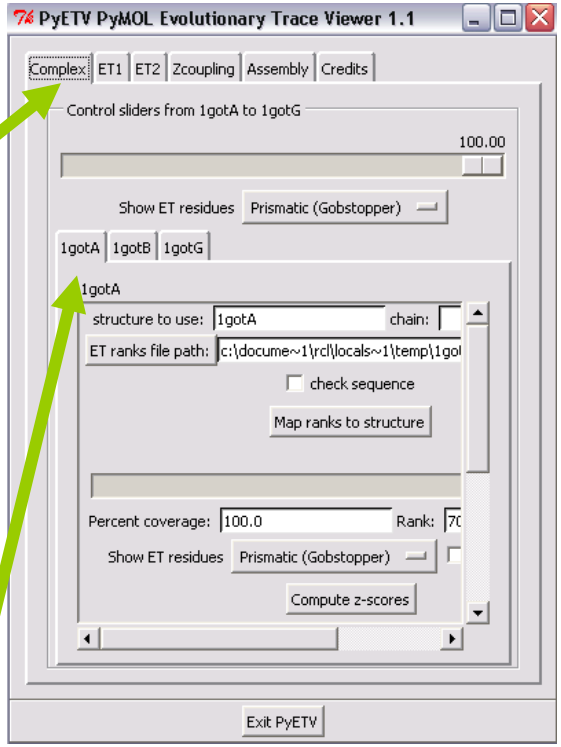
The page for each chain (**A**,**C**,**E**,…) operates like **ET1** or **ET2** (without the **Load Trace** feature)

IV. New tab created when traces are loaded via PyMOL scripts

Case 1: More than one trace

Complex tab created after running a PyMOL script and opening the plugin. This tab is similar to **Assembly.**

Three chains loaded

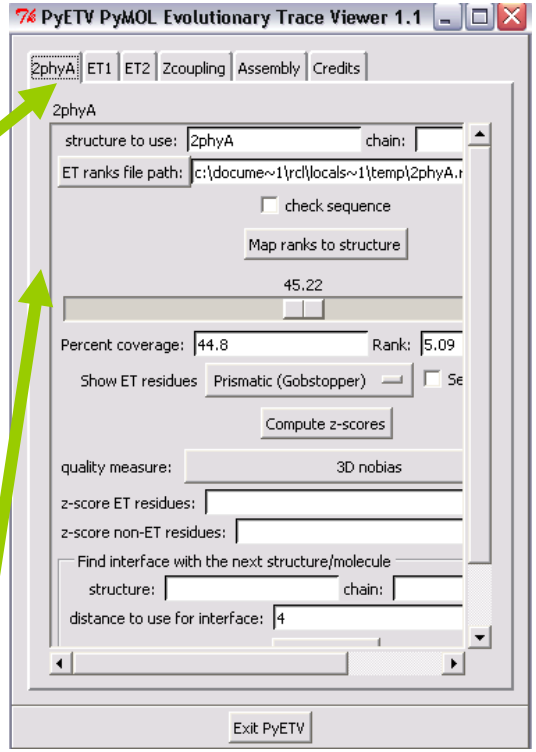


PyMOL script:
http://mammoth.bcm.tmc.edu/ETserver2/pdbeasytrace/pmlFiles/1got.pml

Case 2: One trace

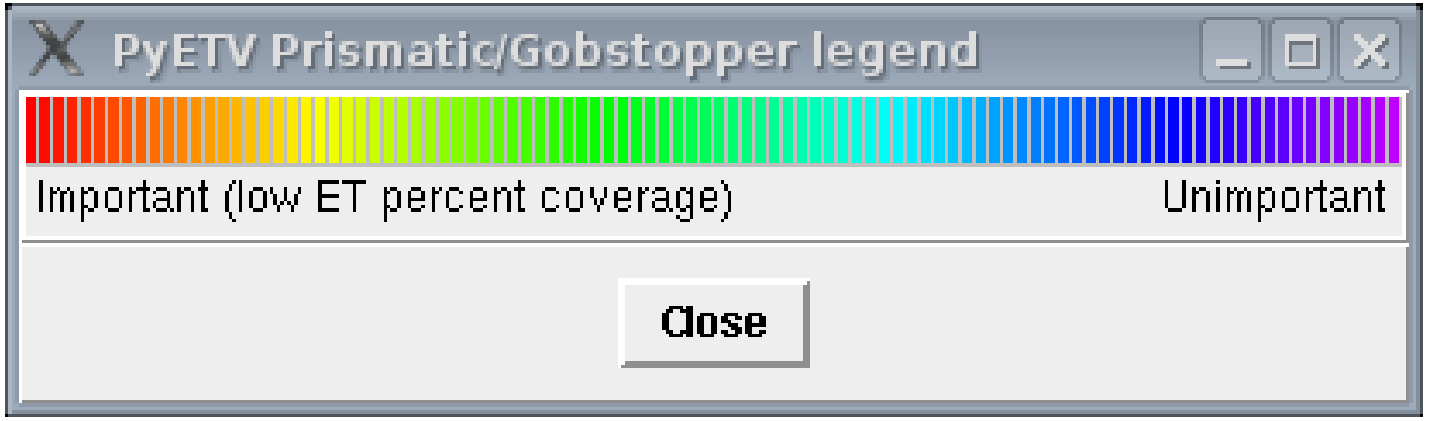
Tab created after running a PyMOL script and opening the plugin. This tab is similar to **ET1**.

One chain loaded



PyMOL script:
http://mammoth.bcm.tmc.edu/ETserver2/pdbeasytrace/pmlFiles/2phy.pml

V. Prismatic (Gobstopper) color ramp



This box appears whenever **Prismatic (Gobstopper)** is selected as the display option for the currently selected top ET-ranked residues.

References

1. Warren L. DeLano "The PyMOL Molecular Graphics System." DeLano Scientific LLC, San Carlos, CA, USA. http://www.pymol.org; The PyMOL Molecular Graphics System, Version 1.2r3pre, Schrödinger, LLC
2. http://mammoth.bcm.tmc.edu/ETserver.html; Mihalek, I., I. Res, et al. (2006). "Evolutionary trace report_maker: a new type of service for comparative analysis of proteins." Bioinformatics **22**(13): 1656-7.
3. Mihalek, I., I. Res, et al. (2003). "Combining inference from evolution and geometric probability in protein structure evaluation." J Mol Biol **331**(1): 263-79.
4. Wilkins, A. D., R. Lua, et al. (2010). "Sequence and Structure Continuity of Evolutionary Importance Improves Protein Functional Site Discovery and Annotation." Protein Science
5. http://mammoth.bcm.tmc.edu/wiki/index.php/Zcoupling
6. Krissinel, E. and K. Henrick (2007). "Inference of macromolecular assemblies from crystalline state." J Mol Biol **372**(3): 774-97.