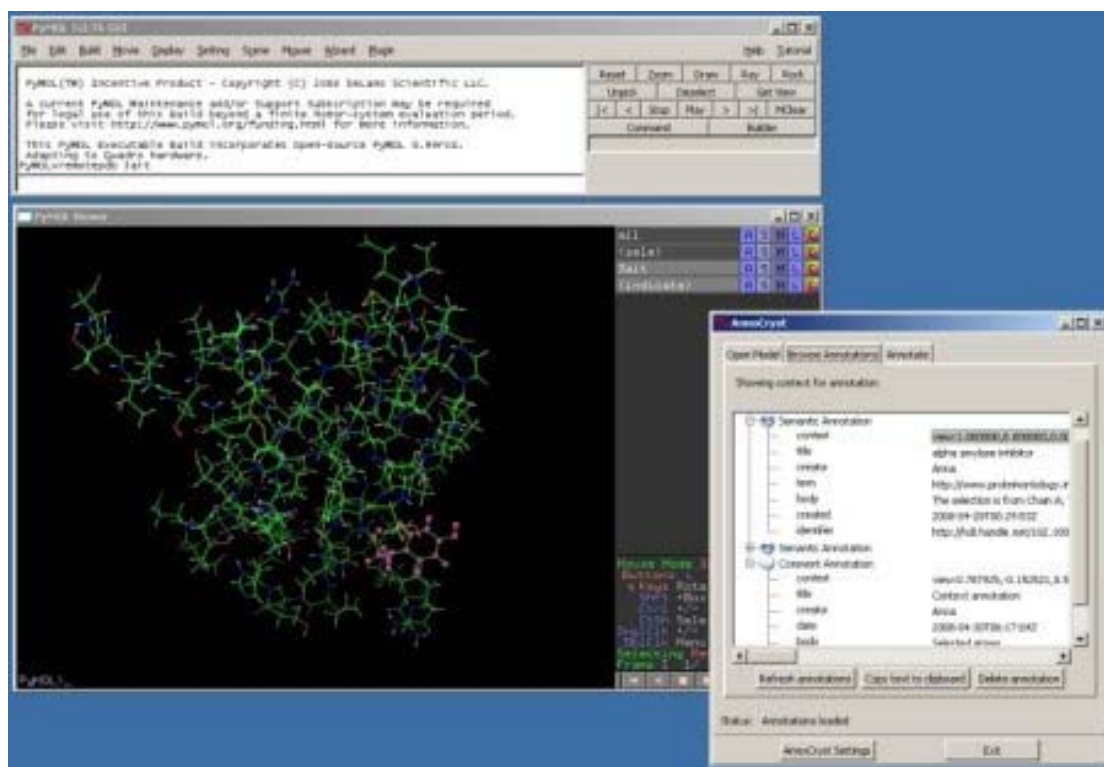


AnnoCryst for PyMOL User Guide

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Introduction



AnnoCryst for PyMOL

AnnoCryst for PyMOL extends the functionality of PyMOL to support collaborative annotation of 3D crystallographic models. It is implemented as a plugin to PyMOL that provides an interface to browse and create annotations on structures loaded from Protein Data Bank (PDB) files. The annotations are retrieved from and stored on an annotation server using the W3C's Annotea protocol.

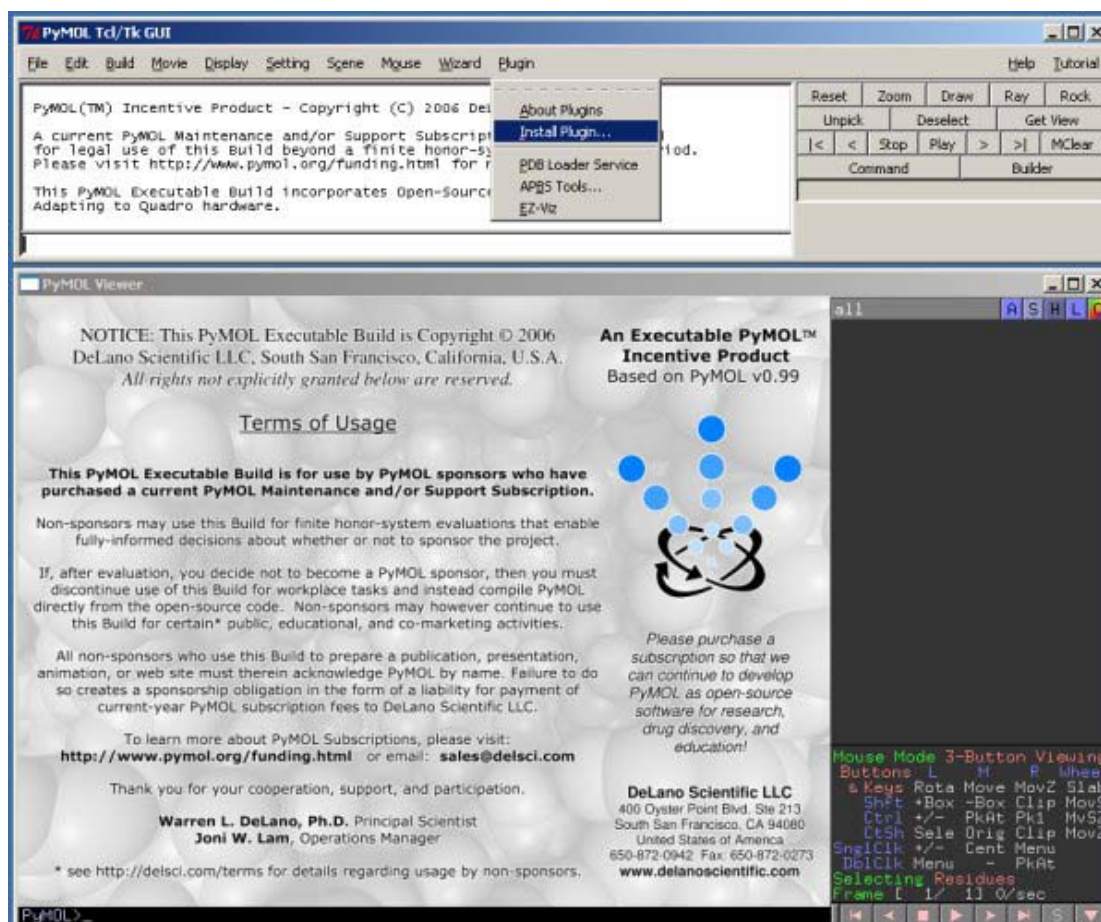
Technical Details

AnnoCryst for PyMOL requires the Tcl/Tk version of PyMOL that supports extension via plugins. This is the standard version of PyMOL for Windows. For Mac, you will need to use either the Fink or X11 hybrid versions of PyMOL. The plugin was developed against PyMOL v0.99rc6 for Windows using the Python programming language.

Installation

To install AnnoCryst for PyMOL:

- Download the plugin file (AnnoCryst.py) from the eResearch site.
- Select **Plugin > Install Plugin** from the PyMOL Tcl/Tk menu.

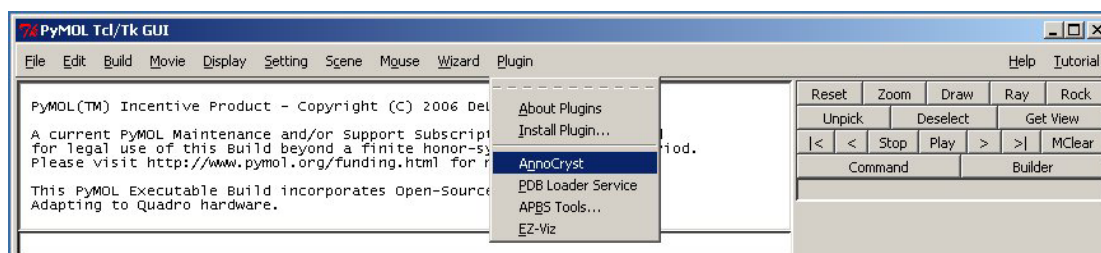


Installing AnnoCryst for PyMOL

- Browse to where you saved AnnoCryst.py and select **Open**.
- A dialog box will indicate that the plugin has been installed. Restart PyMOL to enable the plugin.

Launching AnnoCryst for PyMOL

To launch the plugin, select AnnoCryst from the Plugin menu.



Launching AnnoCryst for PyMOL

The tabs in the AnnoCryst User Interface (UI) facilitate loading a PDB model into AnnoCryst (Open Model), Browsing existing annotations (Browse Annotations) and creating new annotations (Annotate).



AnnoCryst UI

Configuring AnnoCryst

The first time you use the AnnoCryst plugin, you will need to customise the settings. The settings can be modified by selecting the AnnoCryst Settings button. The settings are saved in an XML file named `annocryst-settings.xml` in your home directory.

<code>annotationServerURL</code>	The server from which annotations are loaded and to which annotations are posted.
<code>keywordOntologyNamespace</code>	The URN indentifying the ontology used for keyword annotations
<code>keywordOntologyURL</code>	The URL from which the ontology can be retrieved (often the same as the <code>keywordOntologyNamespace</code>)
<code>pdbRepositoryURL</code>	Base URL for a repository of PDB files. This is used by the <code>remotepdb</code> command to load models by their PDB code.
<code>uploadServerURL</code>	For file attachments in annotations (not yet implemented)
<code>username</code>	Your name - used to identify the annotation creator (Also to be used in future to authenticate with Annotation Server).

Opening a Model in AnnoCryst

In order to browse or create annotations, a PDB model must first be opened via AnnoCryst. Models annotated using AnnoCryst are not opened from local files, but from URLs identifying online PDB resources. A preferred PDB repository can be configured in the settings so that models can be loaded by PDB code rather than having to enter the full URL every time.

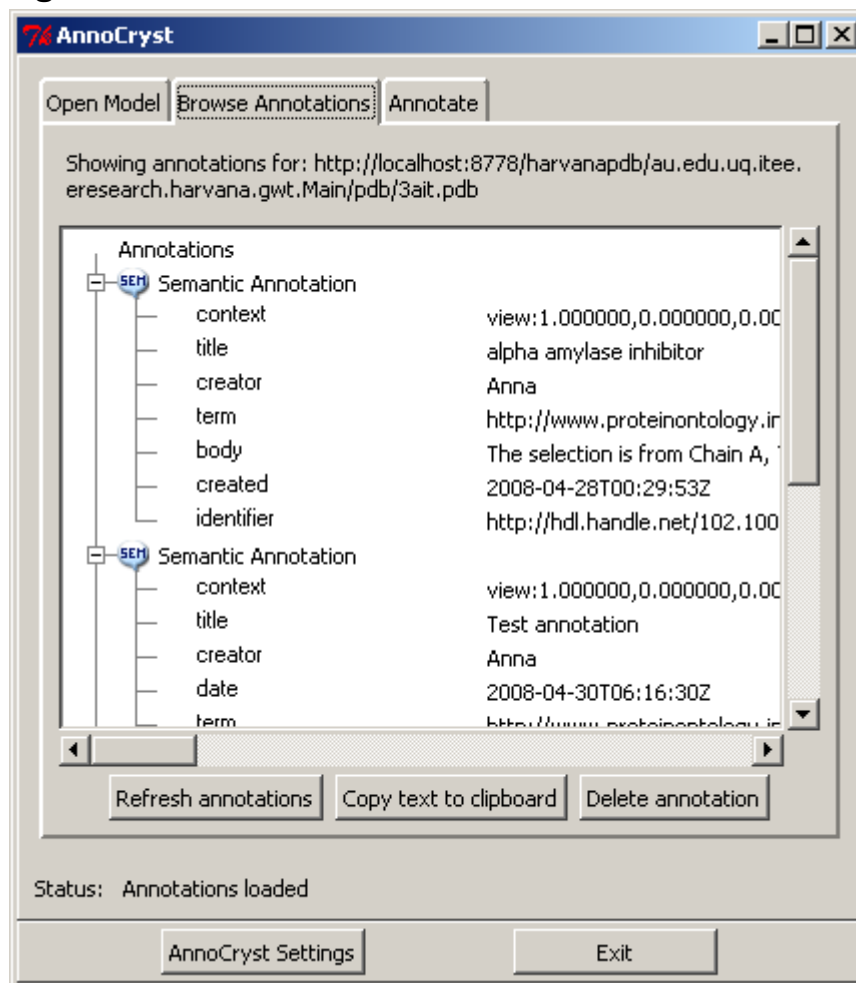
To load a model from the UI, select the `Open Model` tab, enter the full URL (including `http://`) of the PDB file in the text field and click `Open`.

Alternatively, the PyMOL command line can be used. The command `remoteurl` loads a PDB file from URL and `remotepdb` loads using the PDB code from the PDB repository in the AnnoCryst settings. For example:

```
remoteurl http://www.rcsb.org/pdb/files/3ait.pdb
remotepdb 3ait
```

Both of the above commands load the same model when the `pdbRepositoryURL` is set to `http://www.rcsb.org/pdb/files/`

Browsing Annotations



AnnoCryst Annotation Browser

Selecting the `Browse Annotations` tab displays any annotations stored for the model that has been opened in AnnoCryst. If multiple models have been opened, the browser displays annotations for model at the URL shown on the `Open Model` tab (usually the most recently loaded), or on the structure currently selected in the PyMOL UI (as long as it was loaded by AnnoCryst and not from the local file system or by other means).

Clicking on any context of a displayed Annotation will cause the PyMOL UI to highlight and rotate and zoom to the atoms in the annotation context.

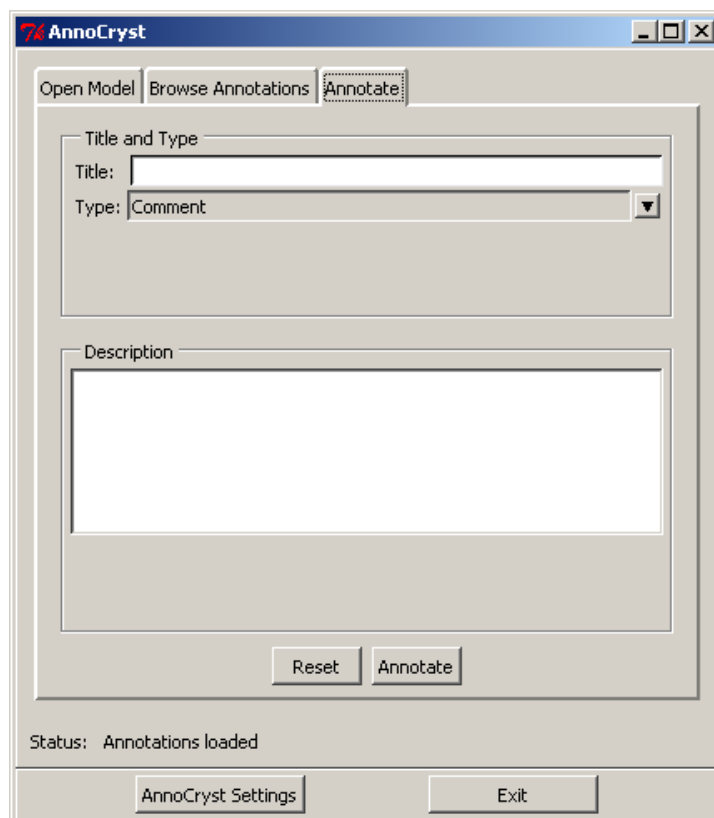
Clicking on the URL in a SeeAlso annotation will load that URL in the default system web browser.

Annotations can be expanded or collapsed using the plus and minus buttons within the tree view. The `Copy text to clipboard` button copies the text of the currently selected item in the annotation tree view to the clipboard for use in other applications. The `Delete annotation` button removes the currently selected Annotation from the server. The delete operation can not be undone.

Creating an Annotation

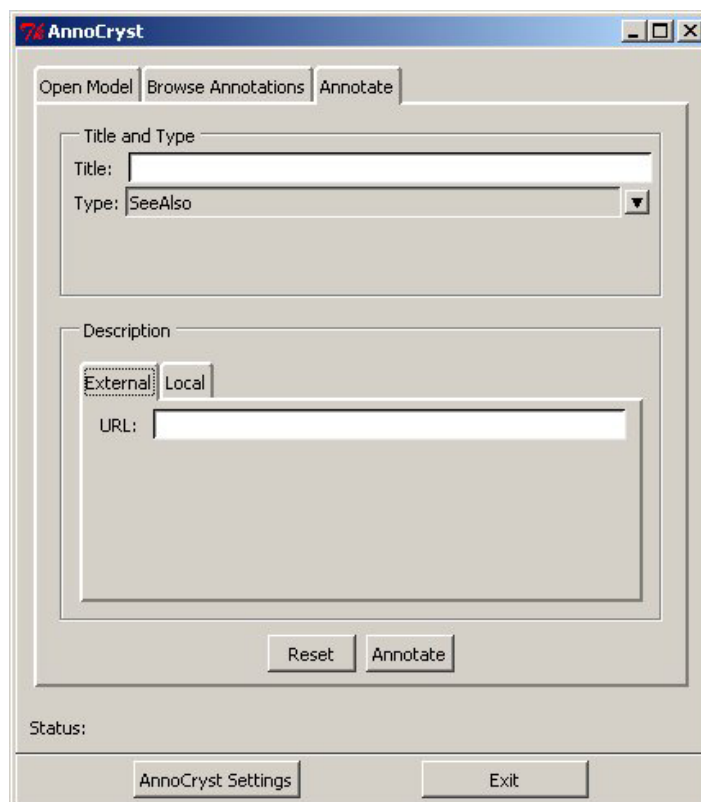
Once a model has been opened in AnnoCryst, annotations can be created from the `Annotate` tab in the AnnoCryst UI. The fields that make up an annotation change depending on the type of the annotation. AnnoCryst can create Comment, Rating, Question, SeeAlso, Feedback, Reference or Keyword annotations.

For Comment, Rating, Question, Feedback and Reference annotations, the textual annotation content should be entered in the Description field, as well as an optional Title.



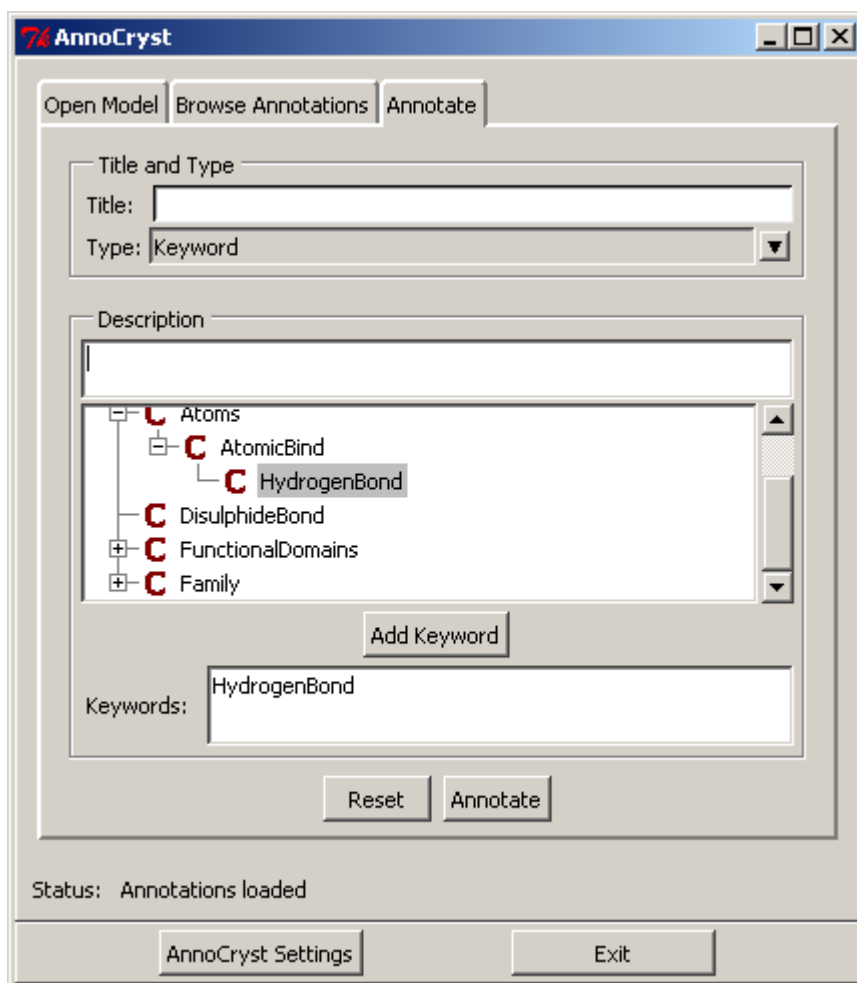
Creating an annotation with a description

For a SeeAlso annotation, the related URL should be entered in the URL field in the External tab. The Local tab will be for file attachments, which are not currently implemented.



Creating a SeeAlso annotation

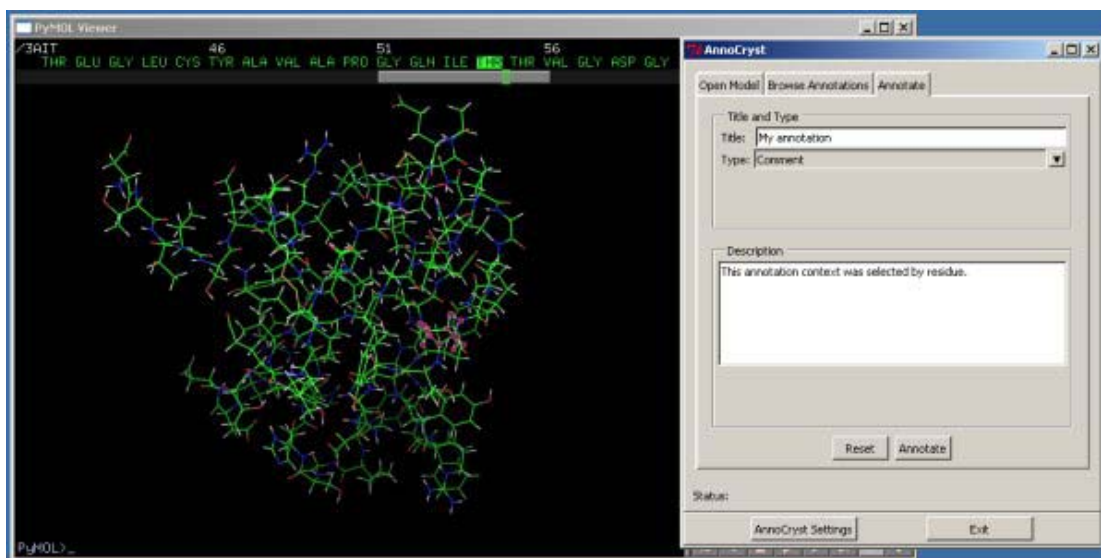
For Keyword annotations, the annotation consists of an optional Title and Description, as well as any number of keywords selected from the ontology specified in the settings. To add a keyword, select it in the tree view, then click Add keyword, which will copy it to the keywords field. Keywords can also be added by typing directly in the Keywords field. Use commas to separate each keyword.



Creating a keyword Annotation

The `Reset` button can be used at any time to clear all of the fields.

The annotation context will be set automatically from the PyMOL Viewer display. The rotation and zoom currently used to display the model that has been loaded by AnnoCryst will be stored with the annotation. The most recent selection, '(sele)' made in the PyMOL Viewer will also be stored as part of the context. Context atoms can be selected by any means through the PyMOL UI (e.g. command line, mouse selection via sequence display or structure), and can be selected by Residue, Chain, C-Alpha etc.



Annotation context selection

After filling in the fields, select the `Annotate` button to store the annotation on the annotation server.

Current Limitations

AnnoCryst for PyMOL does not currently support file attachments for annotations, replying to annotations or user authentication for secure annotations.