

PDIviz 1.2

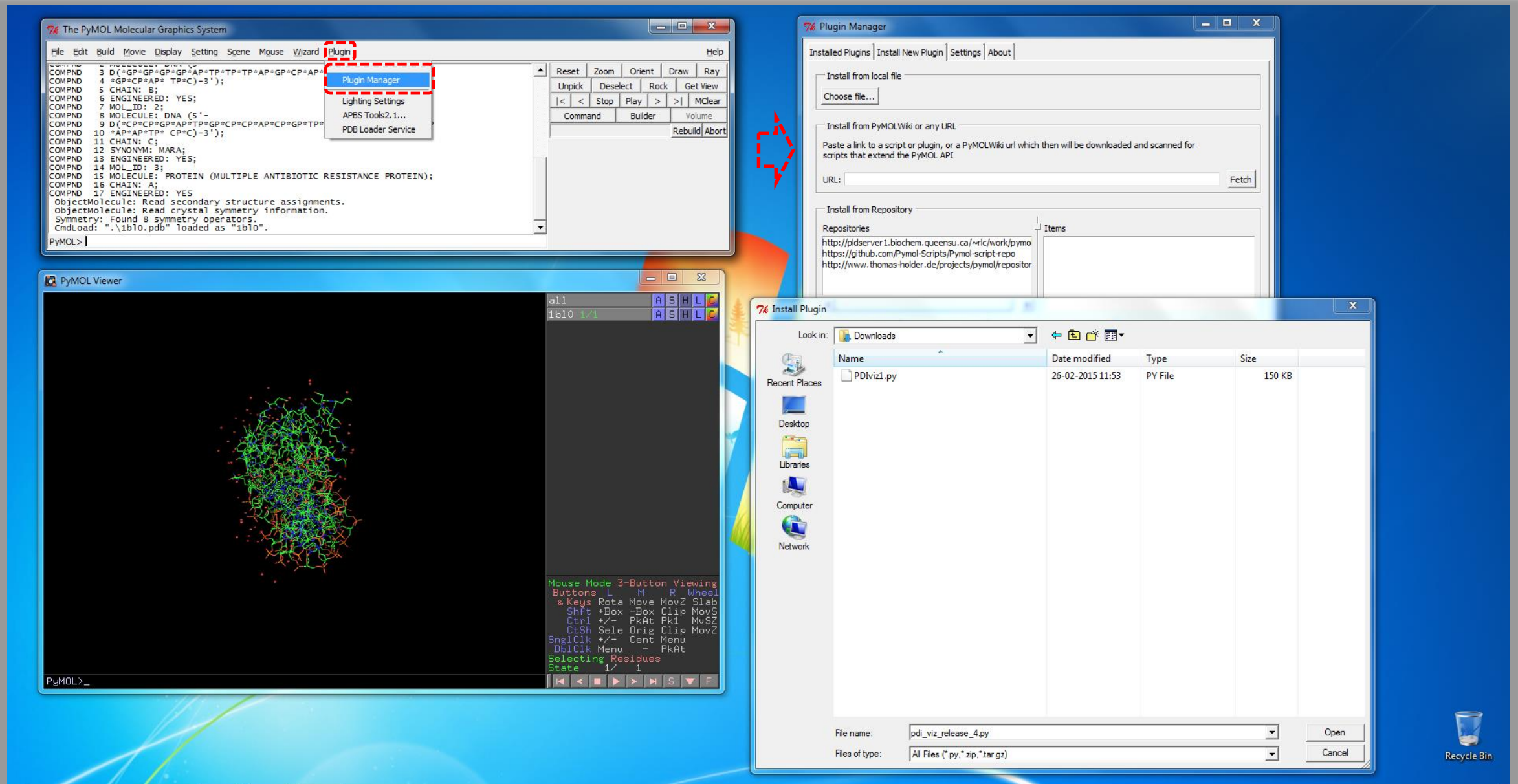
Quick Start Guide

Judemir Ribeiro, Francisco Melo and Andreas Schüller

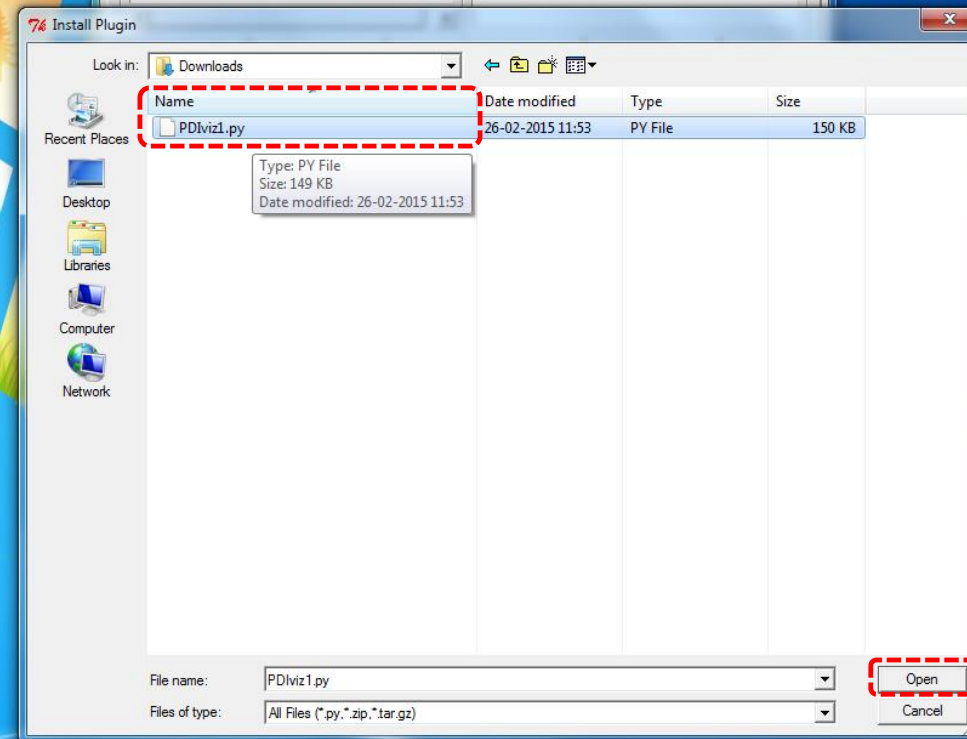
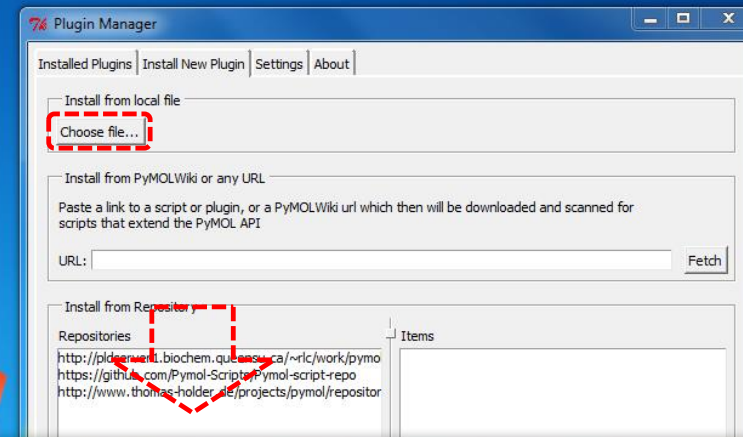
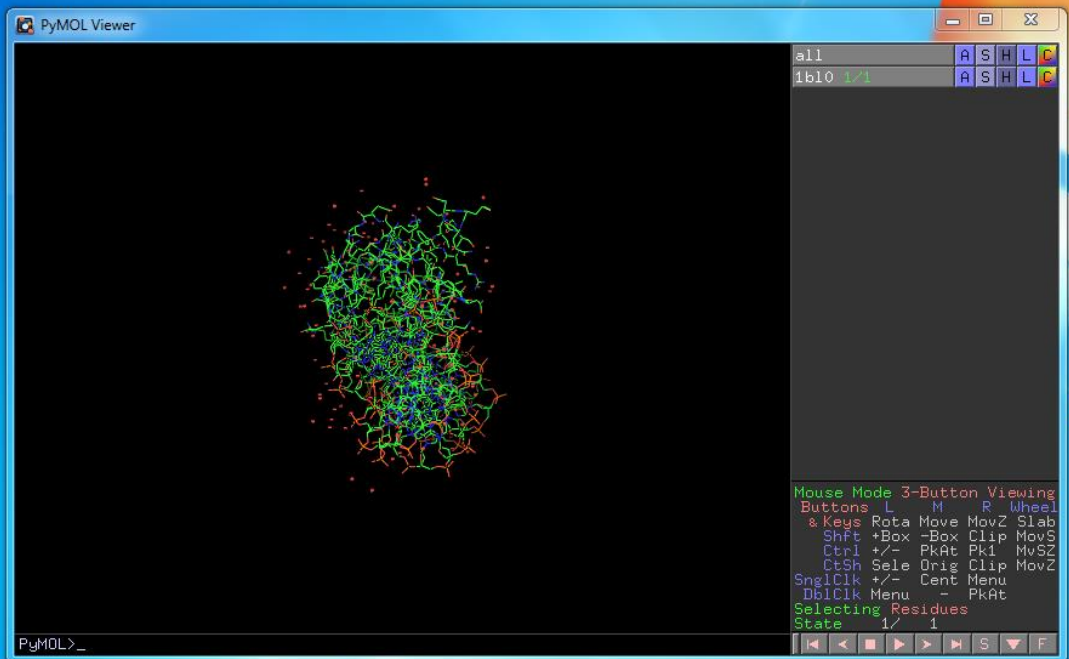
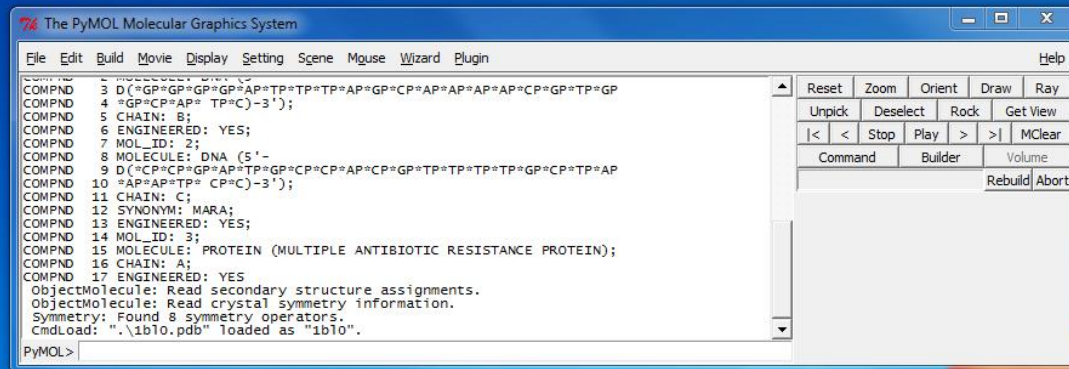
2016-04-07



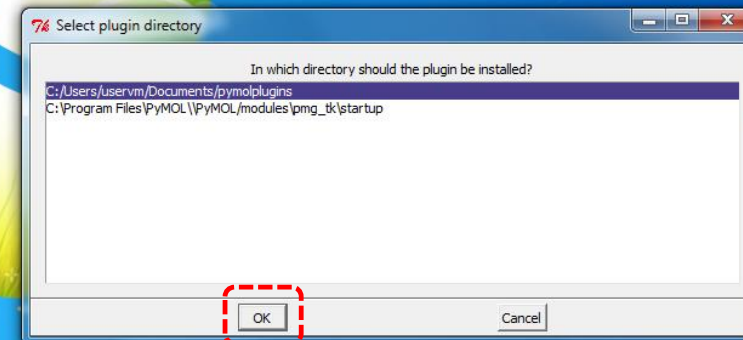
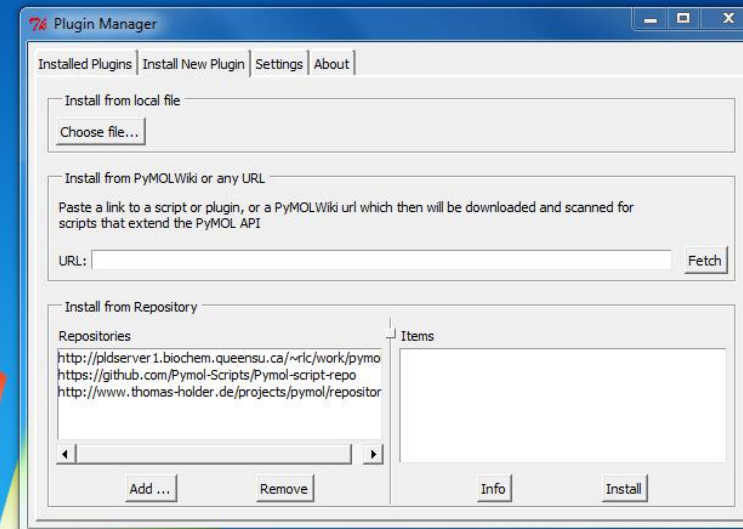
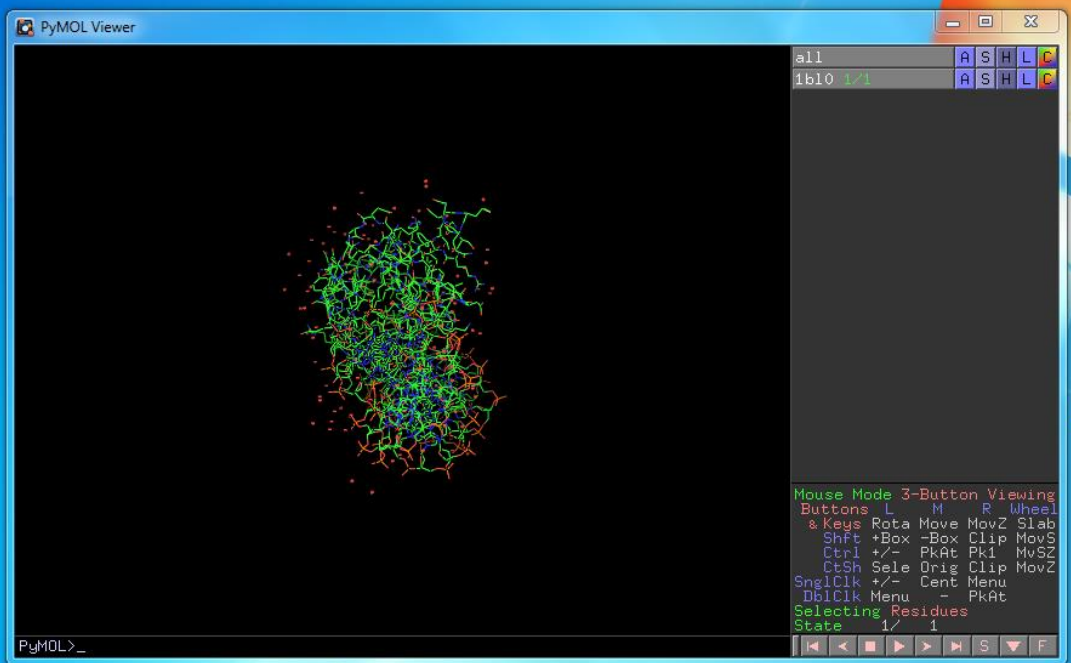
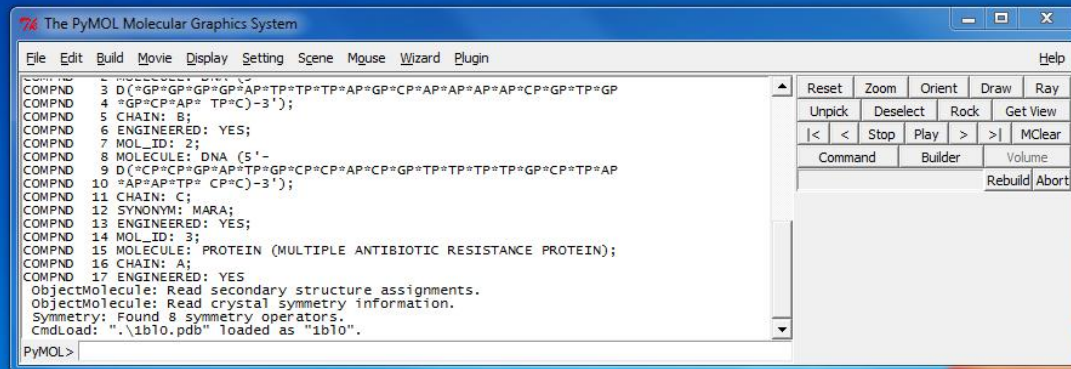
Windows Installation



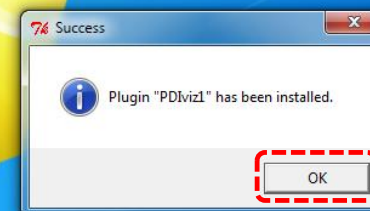
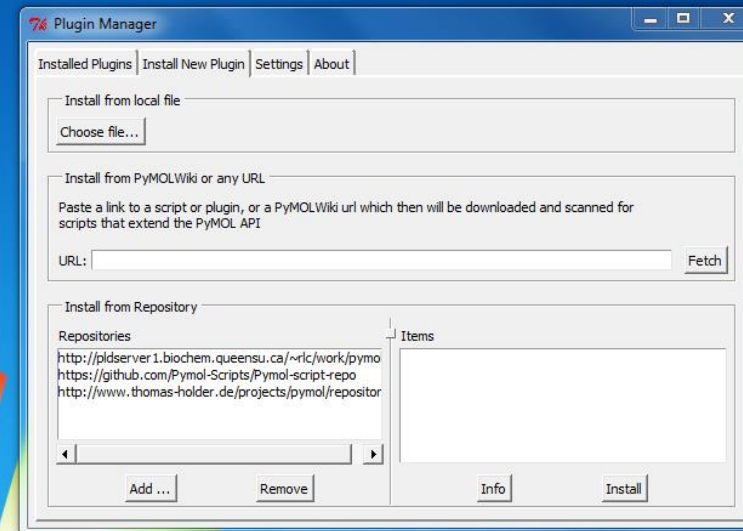
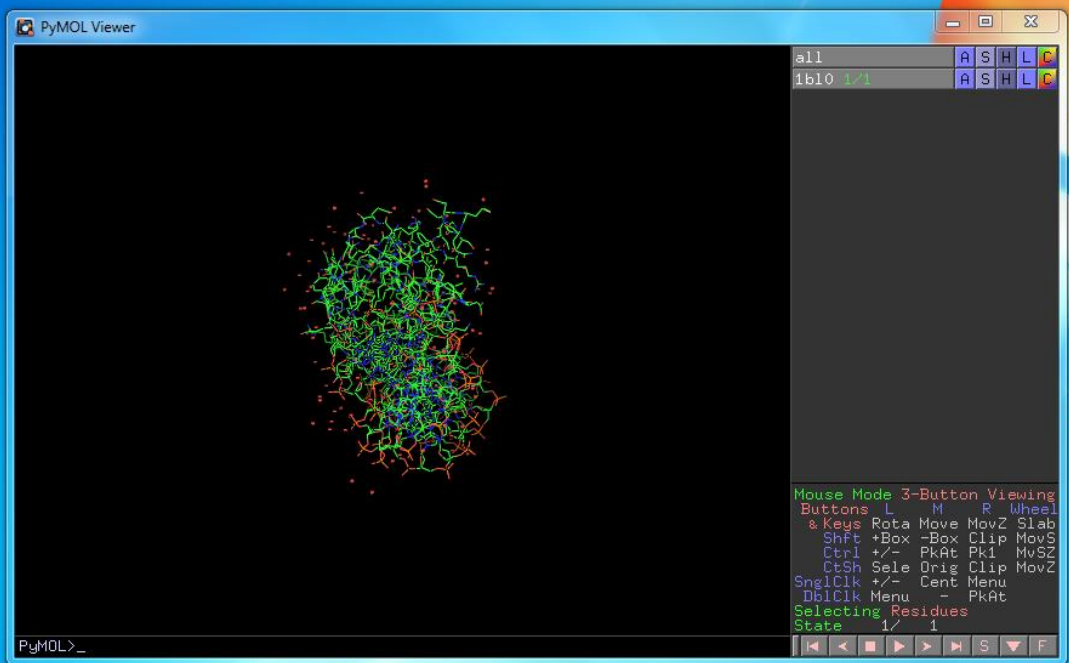
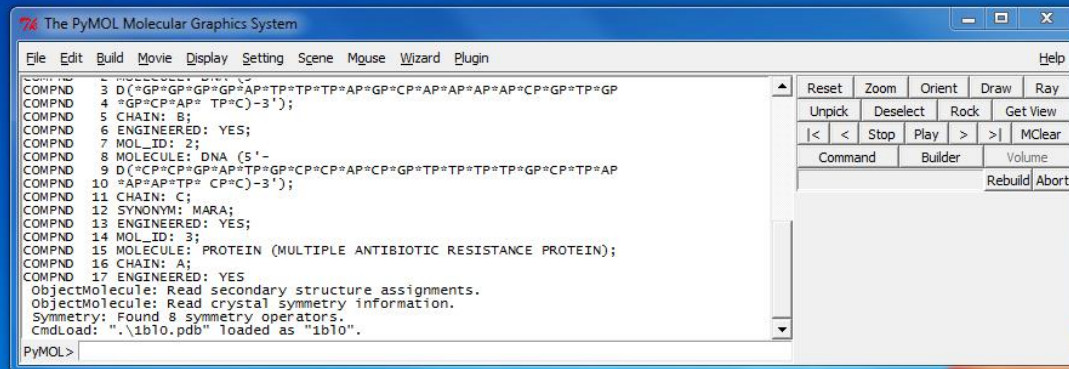
Step 1: Open PyMOL, then open the “Plugin” menu and click on “Plugin Manager”, as indicated by the red dashed rectangle. This will open the “Plugin Manager” window, as indicated by the dashed arrow.



Step 2: Click on the “Choose File” button in the Plugin Manager window, which will open the “Install Plugin” window, Indicated by the dashed arrow. Navigate to the folder where you downloaded the plugin, select it and click “Open”



Step 3: When asked to select the installation directory, confirm the default selection by clicking "OK".



Step 4: Click "OK" to dismiss the success popup and it's done! You may now close the "Plugin Manager" window, too. It is recommended to restart PyMOL, just to be sure. Earlier versions of PyMOL required this.

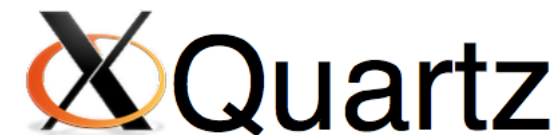
Mac OS X Installation

On Mac OS X the X11 version of PyMOL is required in order to run the PDIviz plugin.

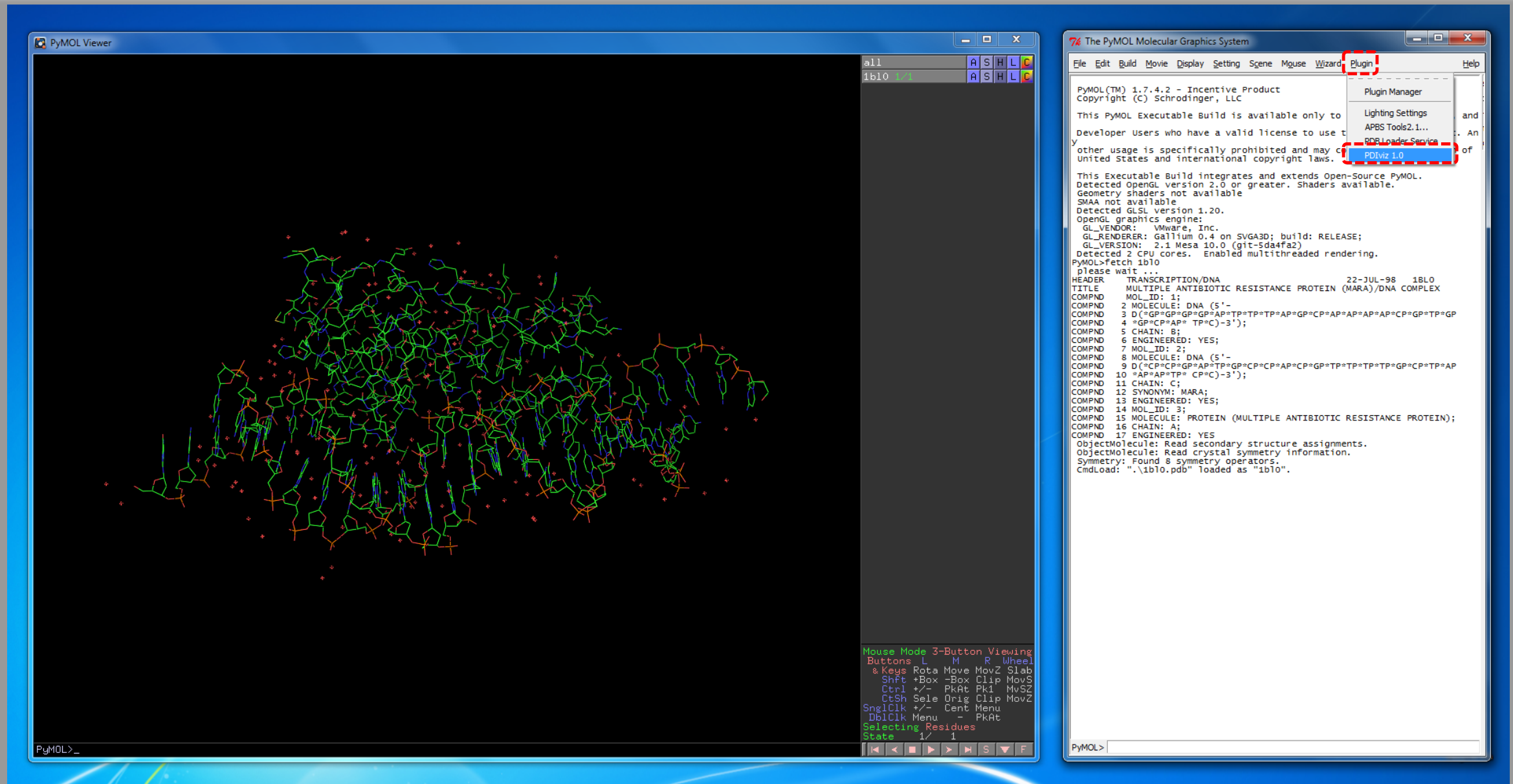
- If you have access to the latest incentive versions of PyMOL you may install the PyMOL version “[Mac alternative X11-only build](#)”.
- In addition, there is a trick to enable the X11 mode in normal MacPyMOL. All you need to do is to rename the application from “MacPyMOL” to “[MacPyMOLX11Hybrid](#)” or from “MacPyMOLEdu” to “[MacPyMOLX11Hybrid](#)”:



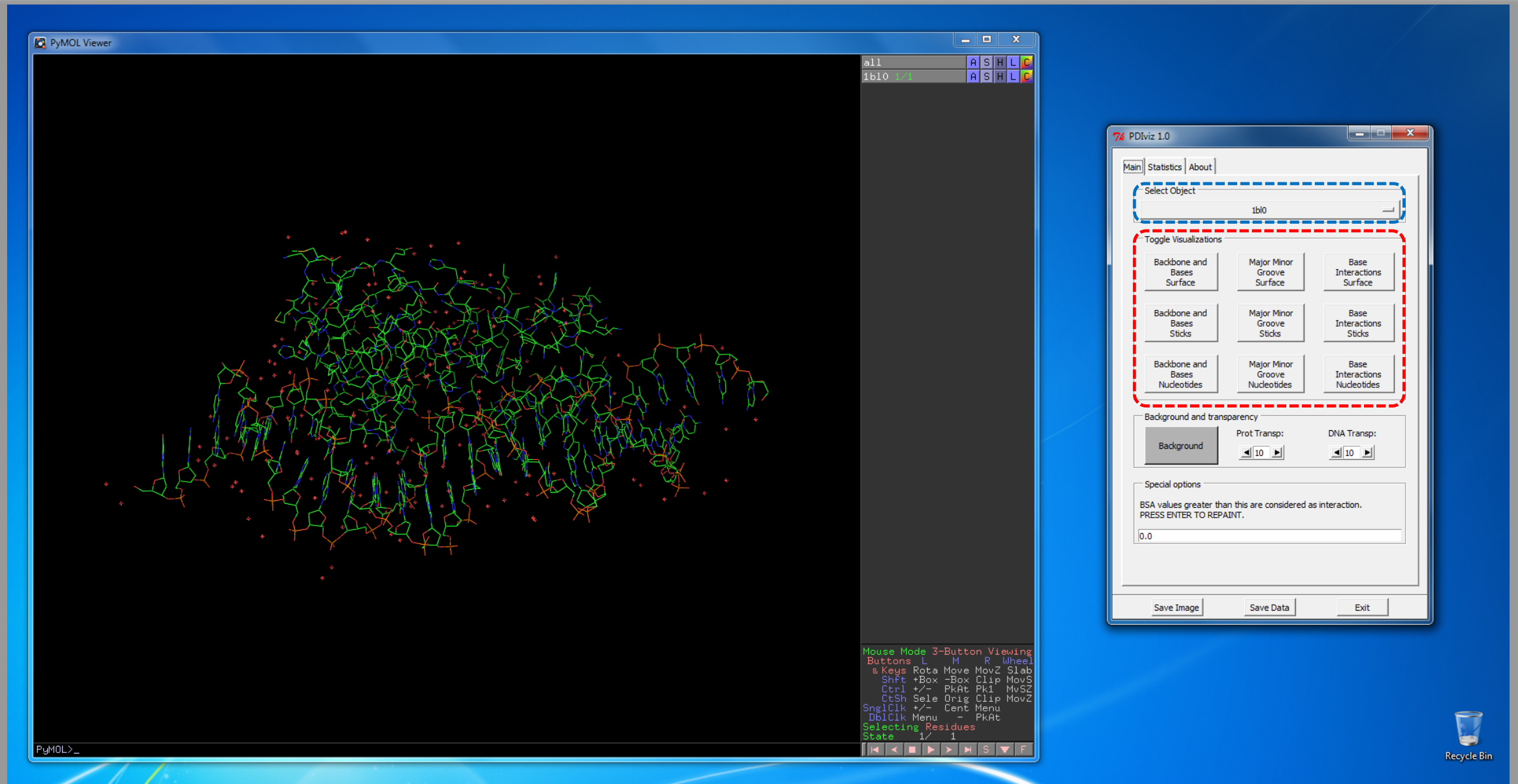
- To run X11 applications on Mac you need to install XQuartz, if you haven't done so, yet. It is available free of charge from <http://xquartz.macosforge.org/>.
- Once PyMOL runs with its X11 GUI on Mac, the installation of the plugin is equivalent to the Windows installation.



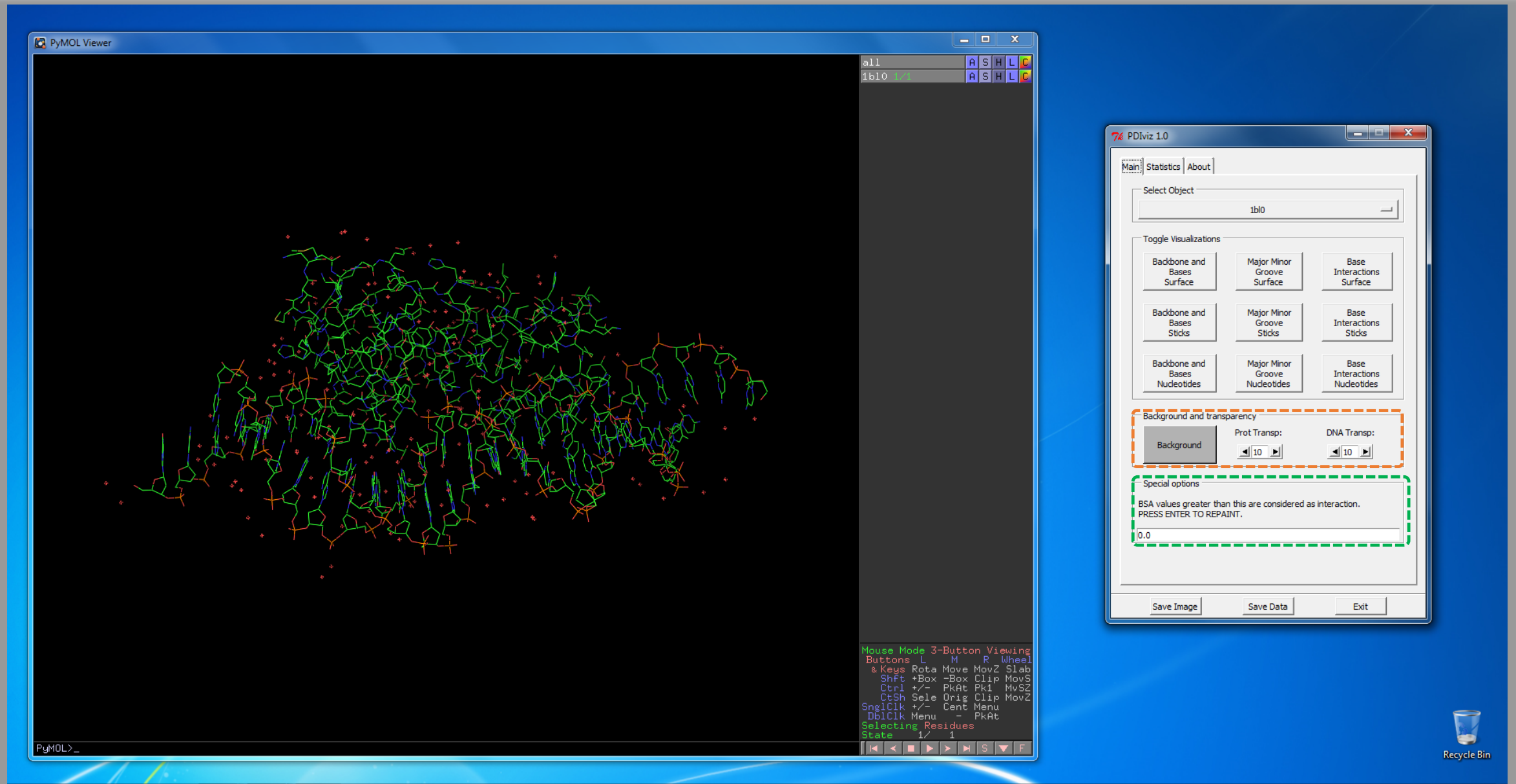
Basic Usage



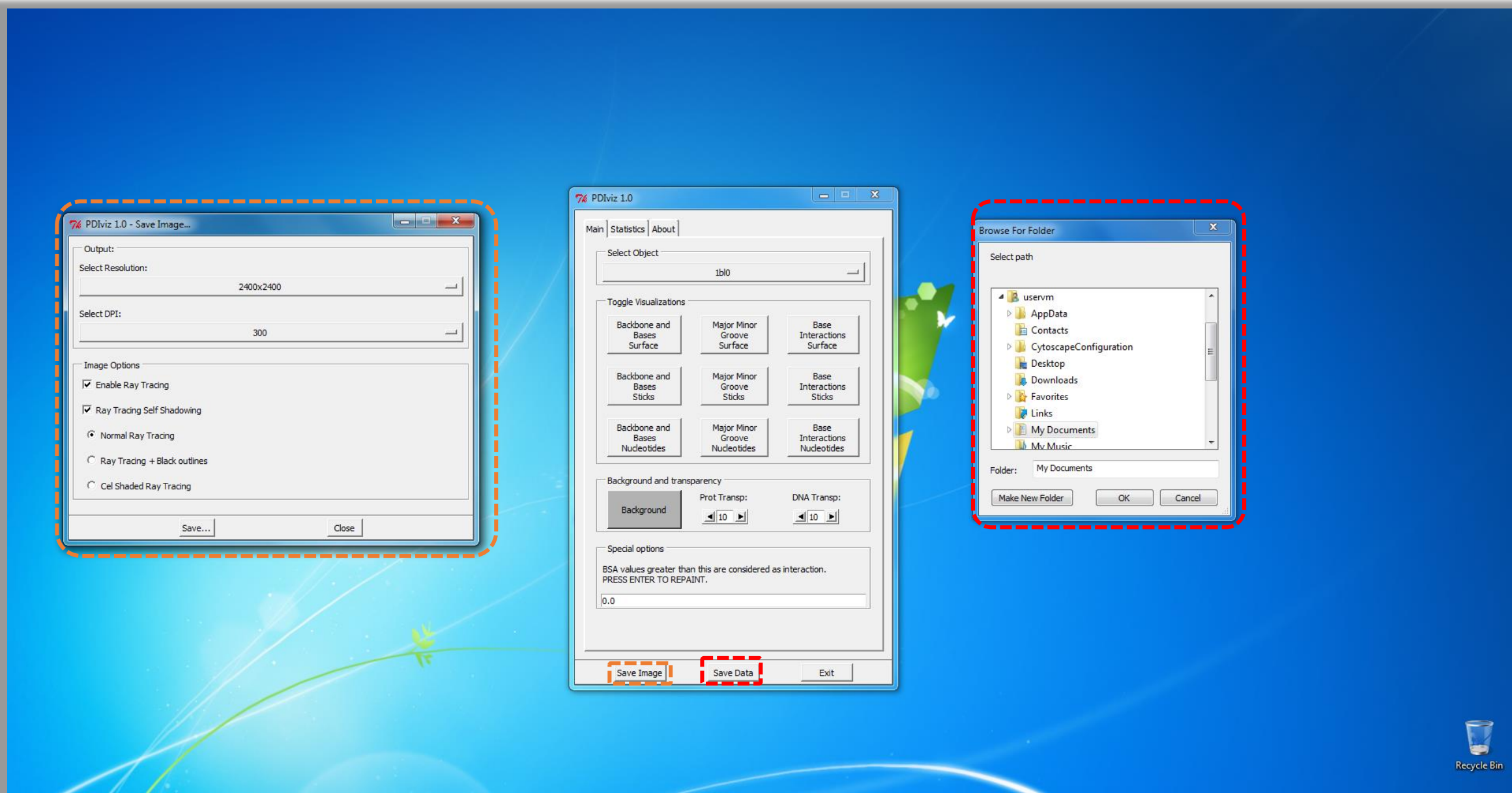
To start PDIviz, open the “Plugin” menu and select “PDIviz 1.0”.



You have now opened the PDiviz main window. The blue rectangle highlights the object selector, which lets you choose from a list of protein-DNA complexes currently loaded in PyMOL. *Note that objects with multiple states must be split first (command: split_states).* The red rectangle highlights the visualization selector buttons. They automatically begin the calculation once pressed.

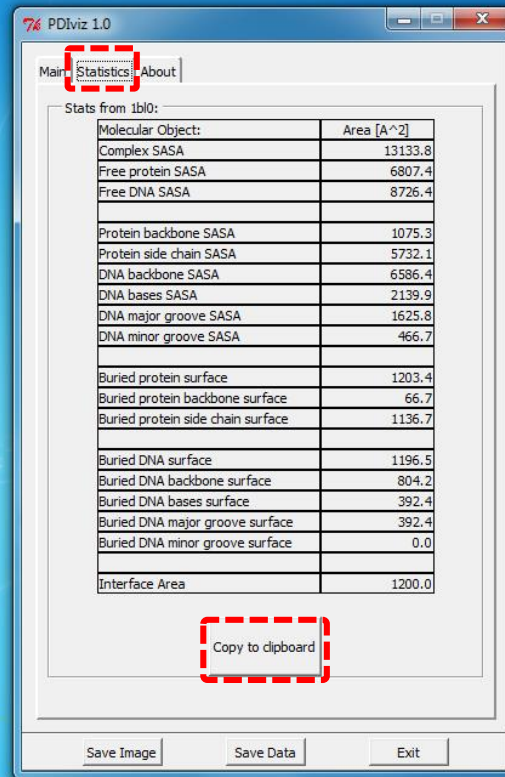


The orange rectangle highlights a background color setter, and two controls for the transparency of surface representations in proteins or DNA. Finally, the green rectangle emphasizes the buried surface area (BSA) cut-off field. Only atoms with a BSA value greater than the cutoff (A^2) will be considered as interaction.



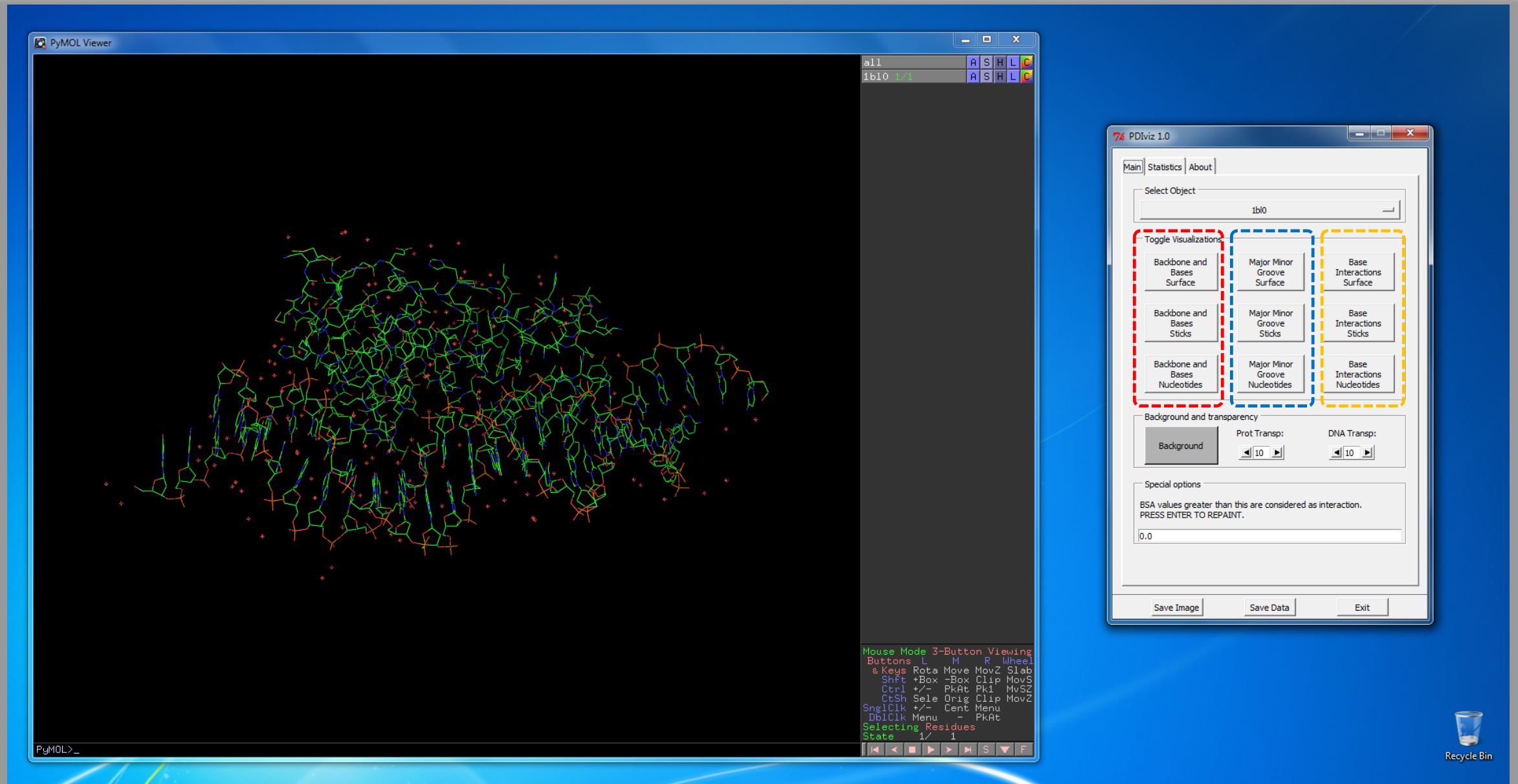
The orange boxes highlight the “Save Image” button and the “Save Image...” window. This provides more options for saving high-quality images than the native PyMOL menu.

The red boxes emphasize the “Save Data” button. This allows you to save the SASA/BSA calculation files in a selected folder.



The “Statistics” tab shows the SASA and BSA values of the various surface areas that compose the protein-DNA complex. This data can be copied to the clipboard with the “Copy to clipboard” button. It is also saved to a file when using “Save Data”.

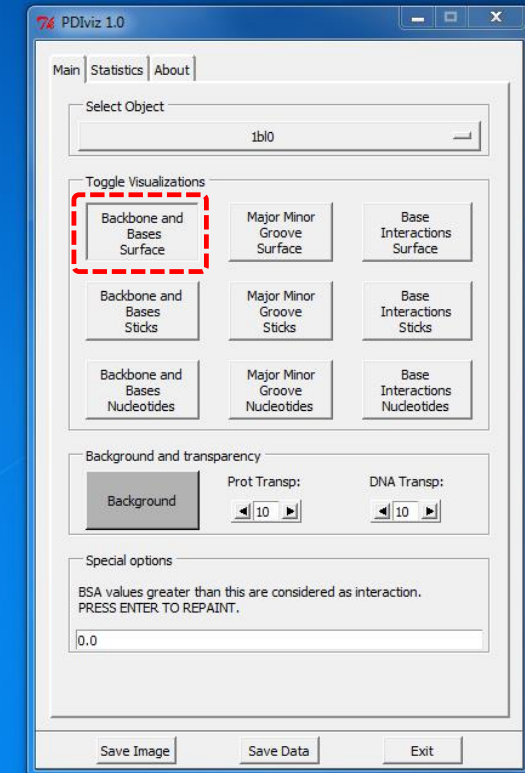
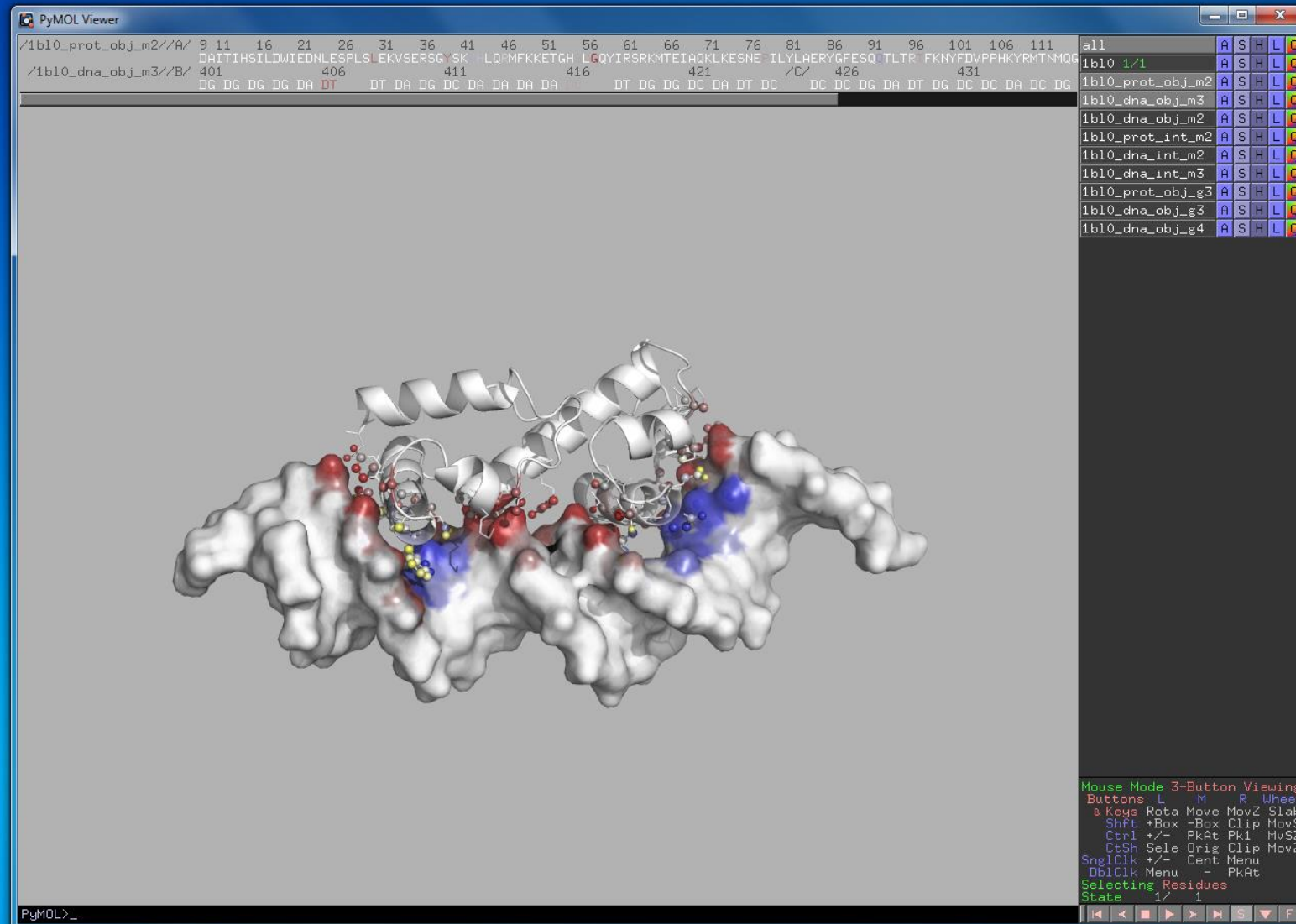
The Visualization Modes



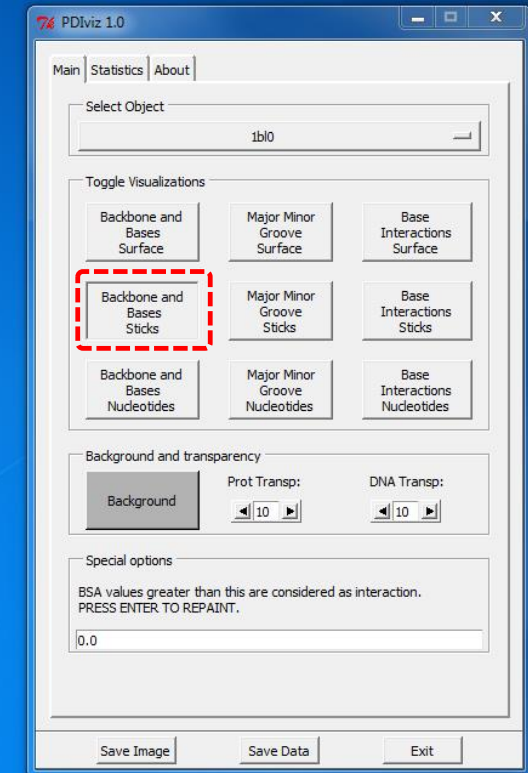
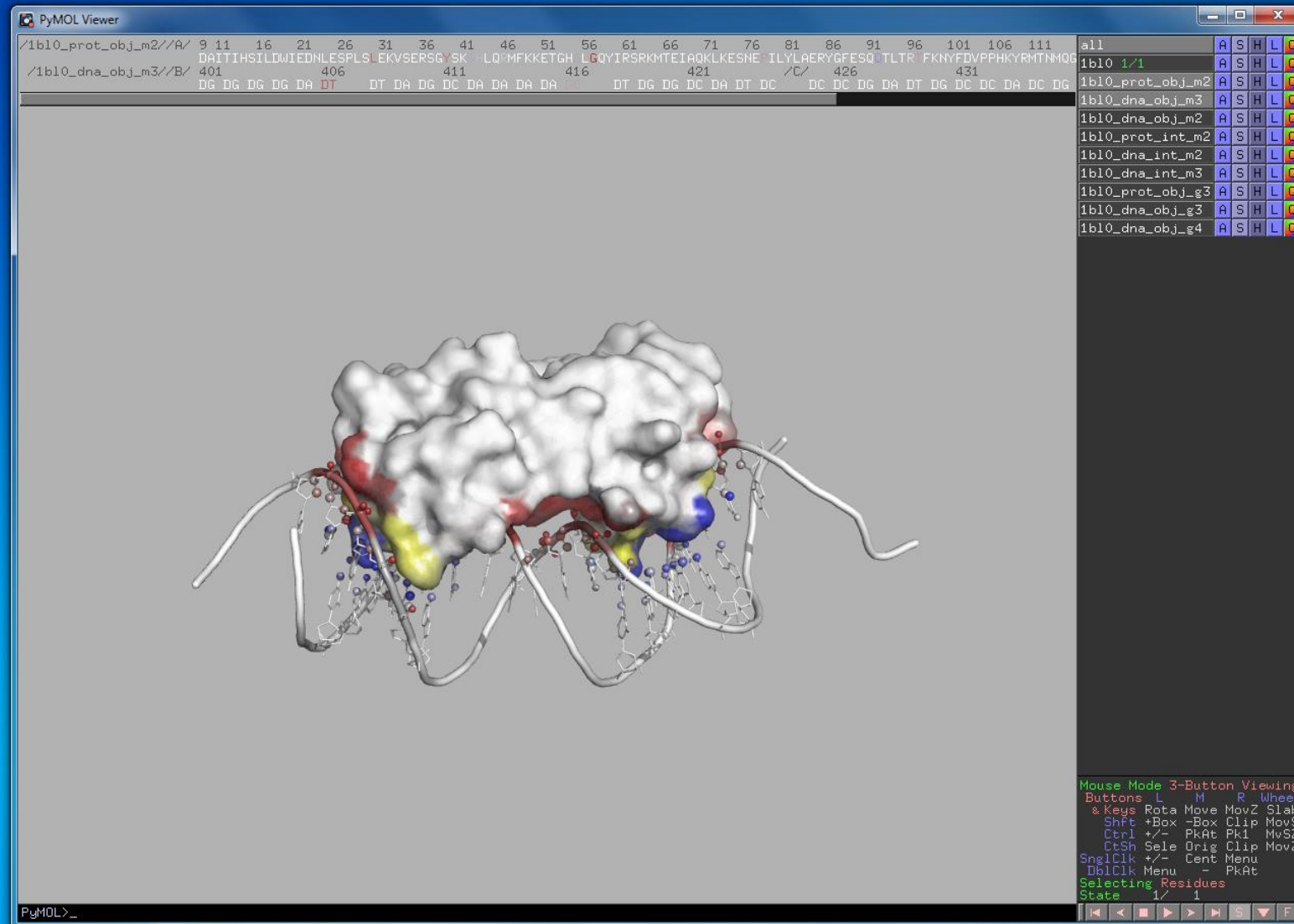
PDIviz has nine visualization modes, organized in 3 columns and 3 rows. The column marked in red shows the interactions of the protein with the DNA backbone and bases, the blue column shows the interactions with the minor and major grooves, and the orange column shows a pharmacophoric interaction map.

The Visualization Modes

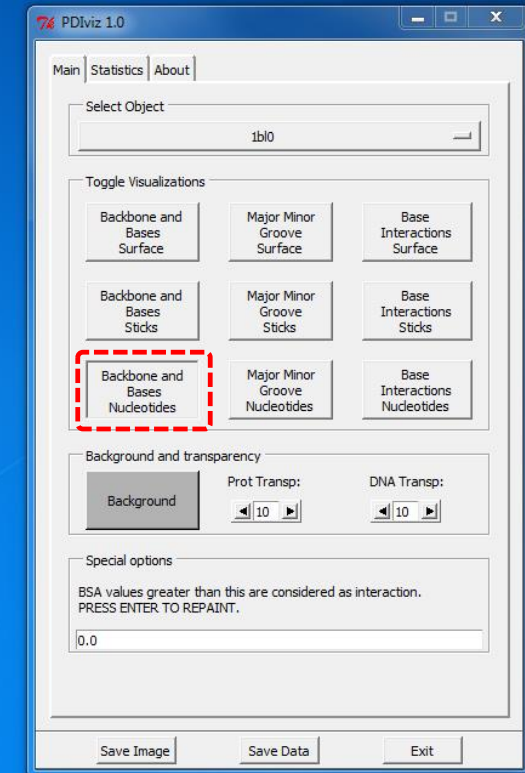
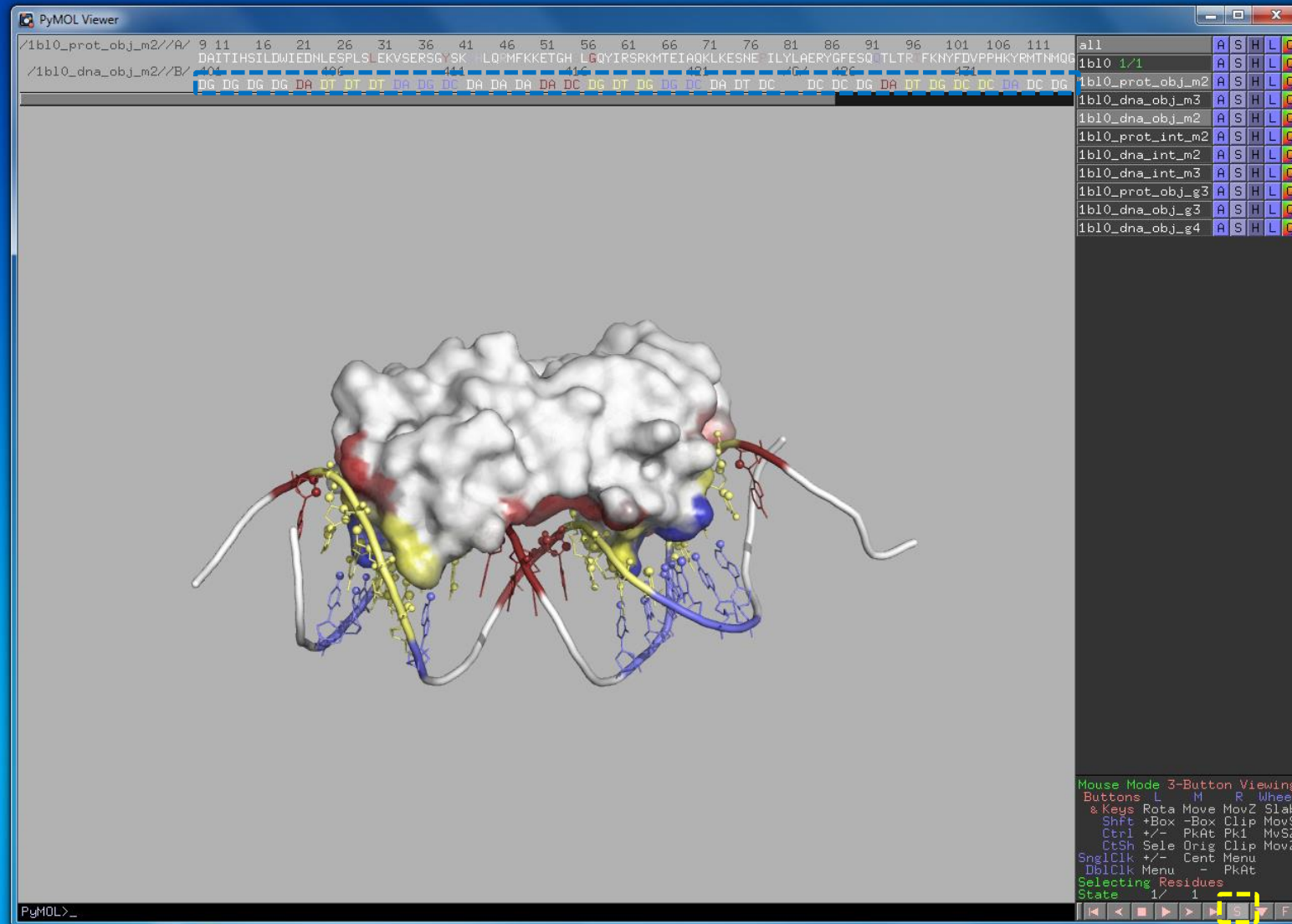
DNA bases and backbone



In this mode, the DNA is shown in a surface representation. Each atom is painted red (backbone atom) or blue (base atom) if they have a BSA greater than the cut-off. In the protein, atoms are painted red if they only interact with backbone atoms, blue if only with base atoms, and yellow if they interact with both types. Color intensities correspond with the BSA of the atoms. All atoms with surface contacts are shown as colored spheres.



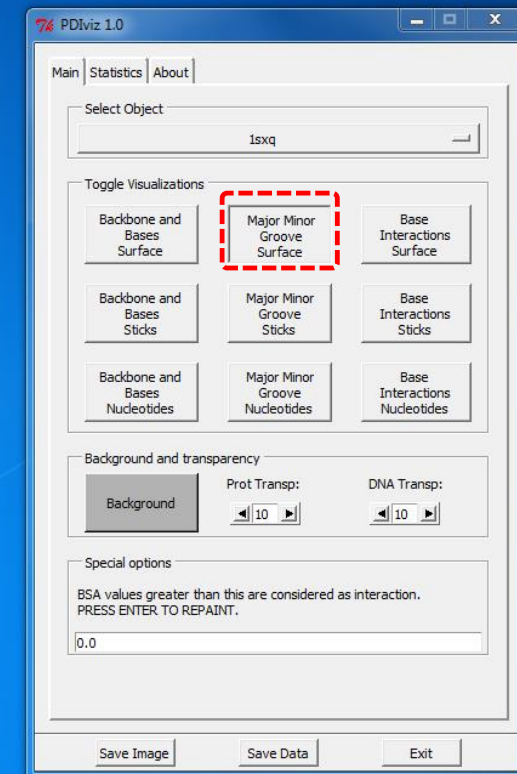
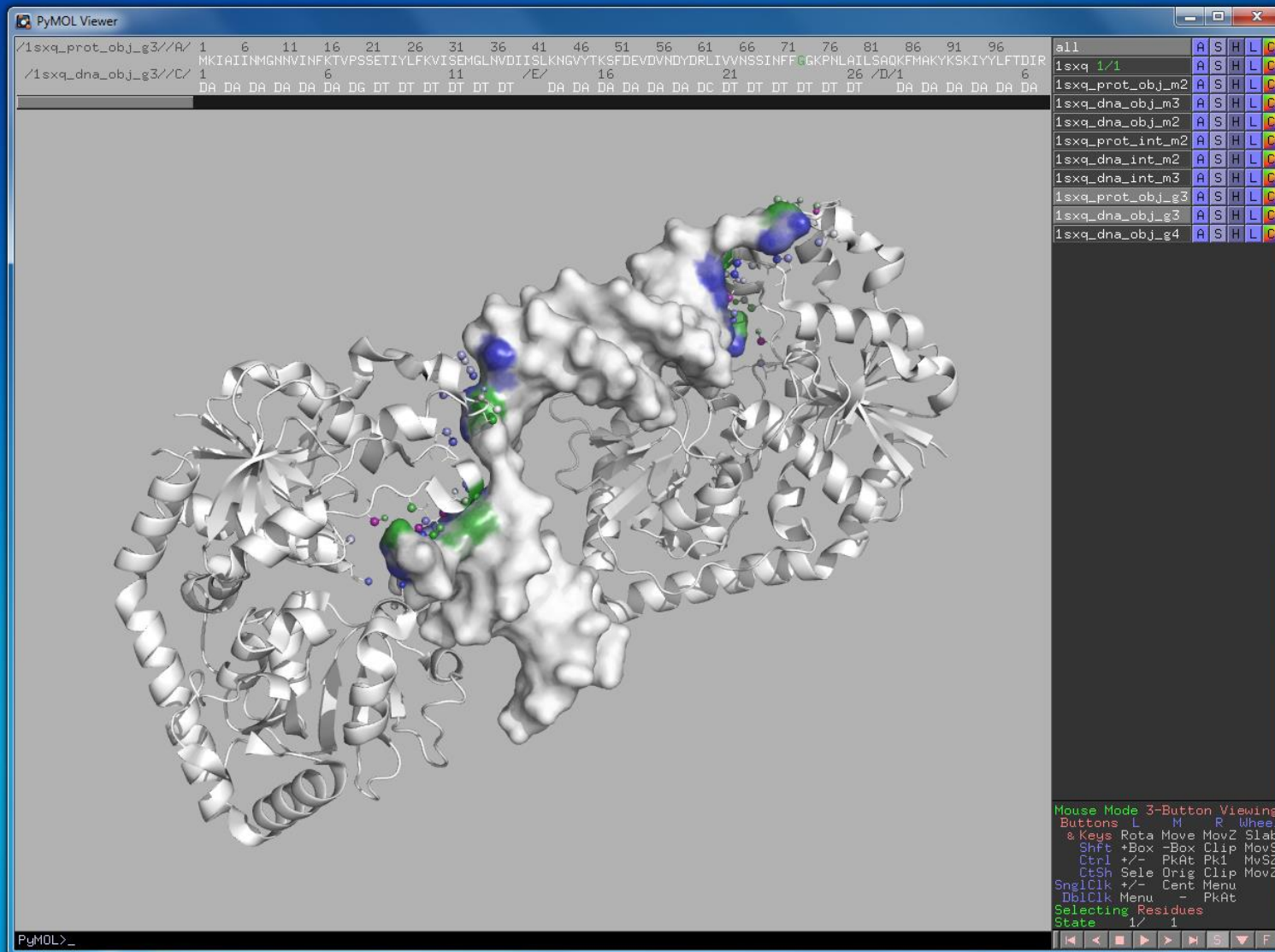
This mode keeps the same coloring pattern, but changes the protein to the surface representation and the DNA to stick representation. Colored spheres show interacting atoms.



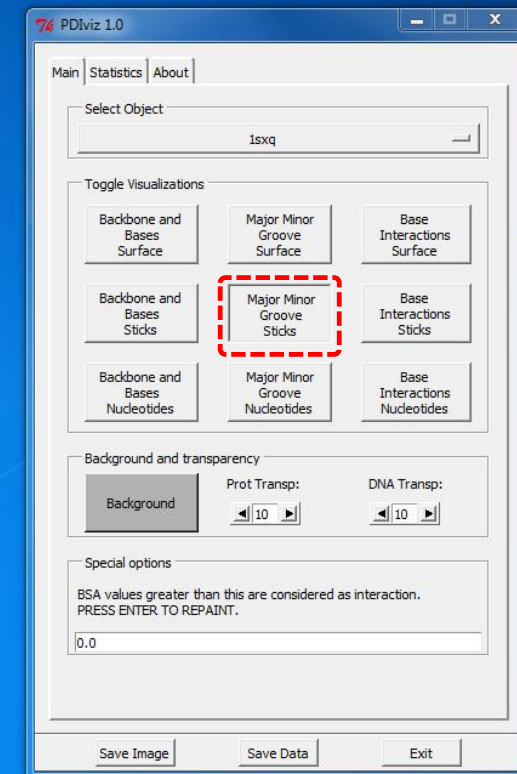
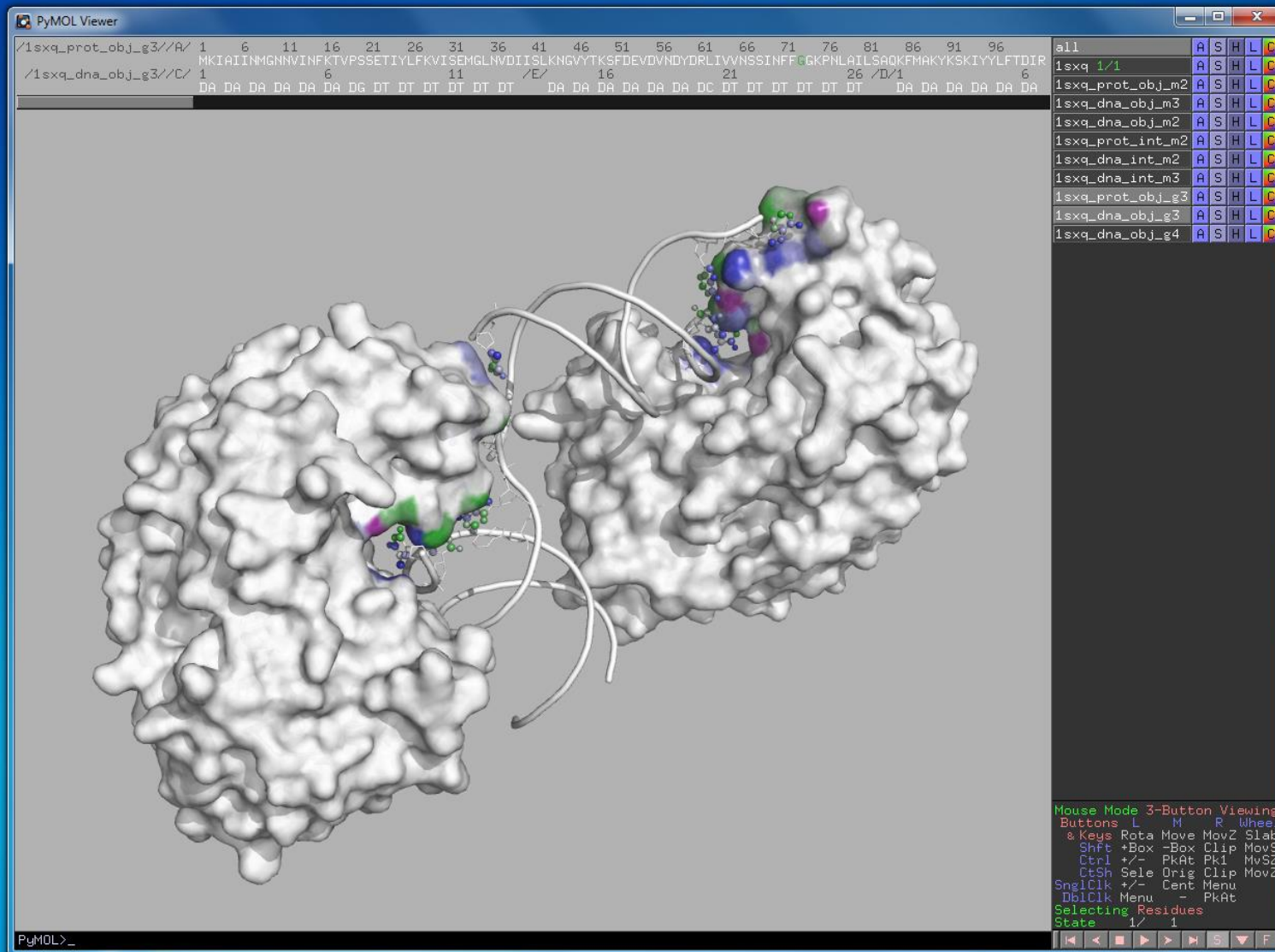
This mode colors the DNA by nucleotide, which allows you to identify the type of interactions of nucleotide without looking at the structure. This can also be seen in sequence viewer (blue highlight), opened in the PyMOL main window by clicking in the “S” button (yellow box). Red nucleotides interact with the protein only via the DNA backbone, blue ones interacts only via DNA base atoms, and yellow nucleotides interact with both types of atoms.

The Visualization Modes

DNA minor and major grooves



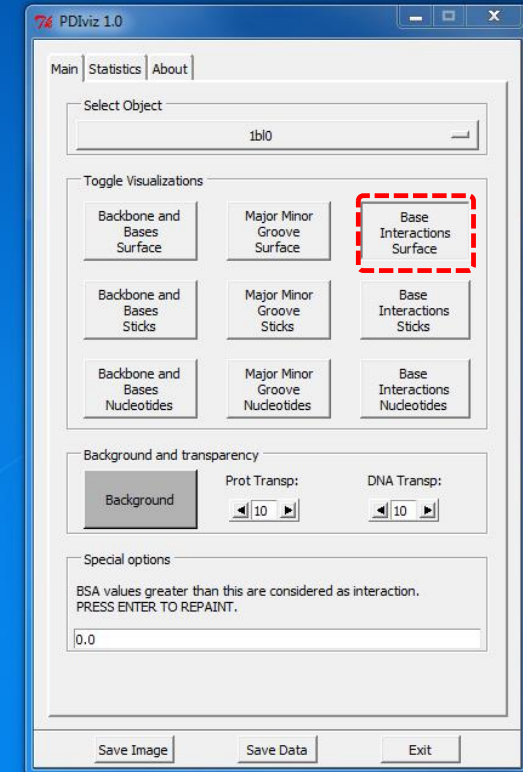
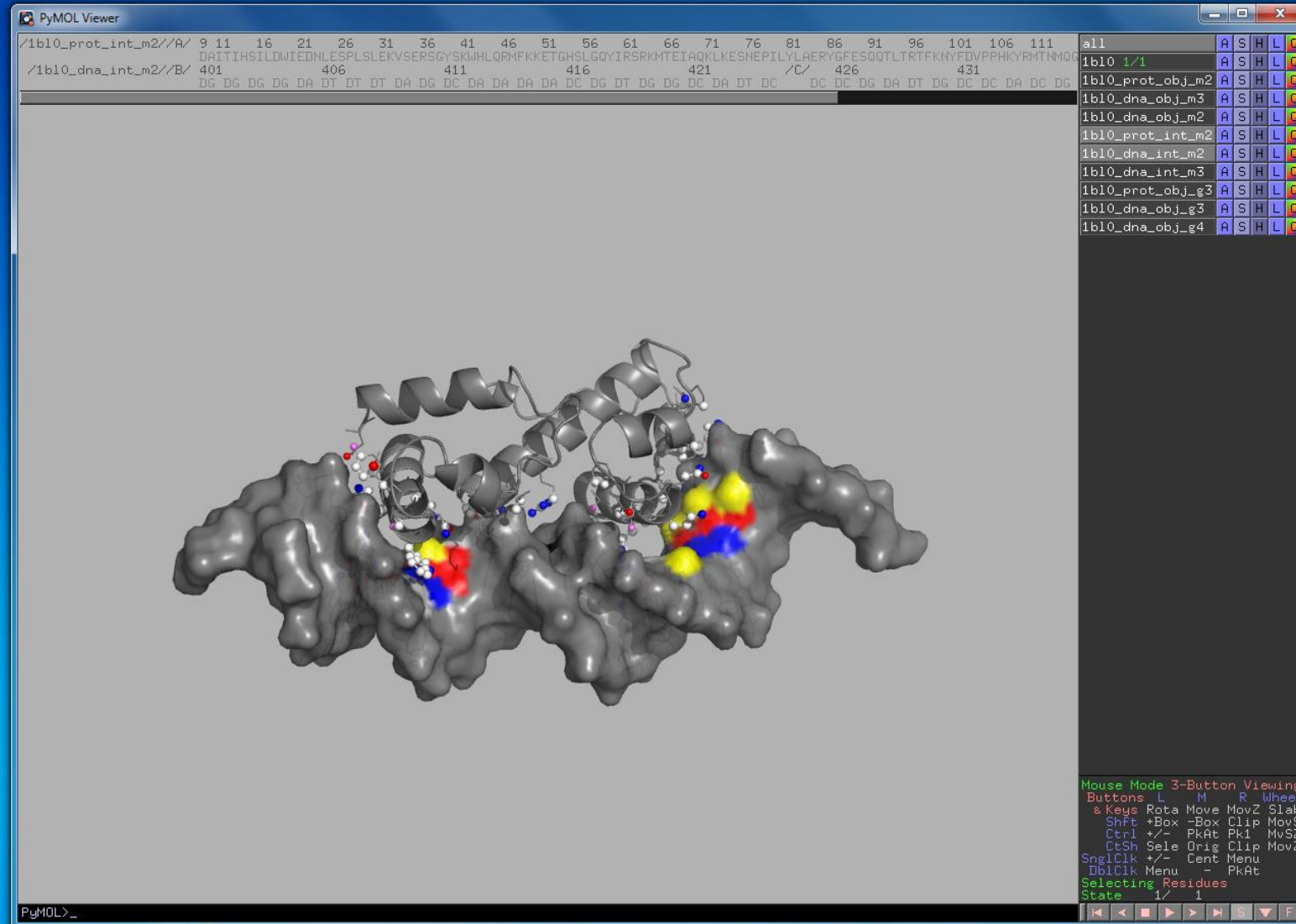
In this mode, the DNA is shown in a surface representation. Each atom is painted blue (major groove atom) or green (minor groove atom) if they have a BSA greater than the cut-off. In the protein, atoms are painted blue if they only interact with major groove atoms, green if only with minor groove atoms, and purple if they interact with both types. Colors intensities correspond to the BSA values of the atoms.



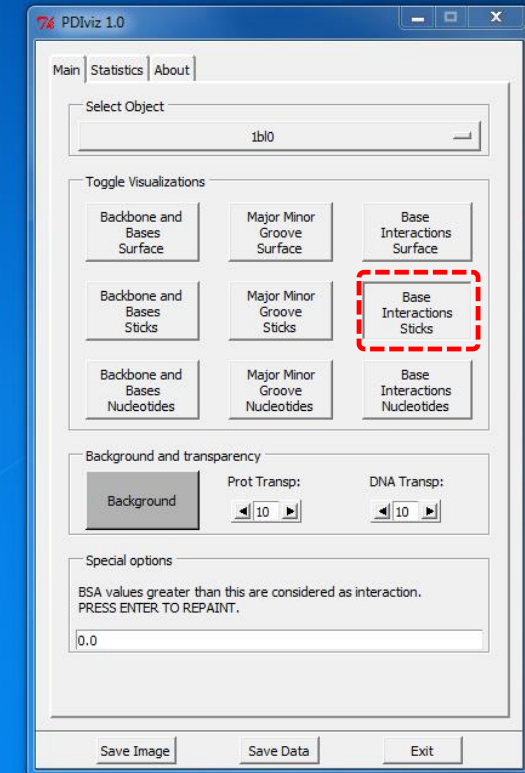
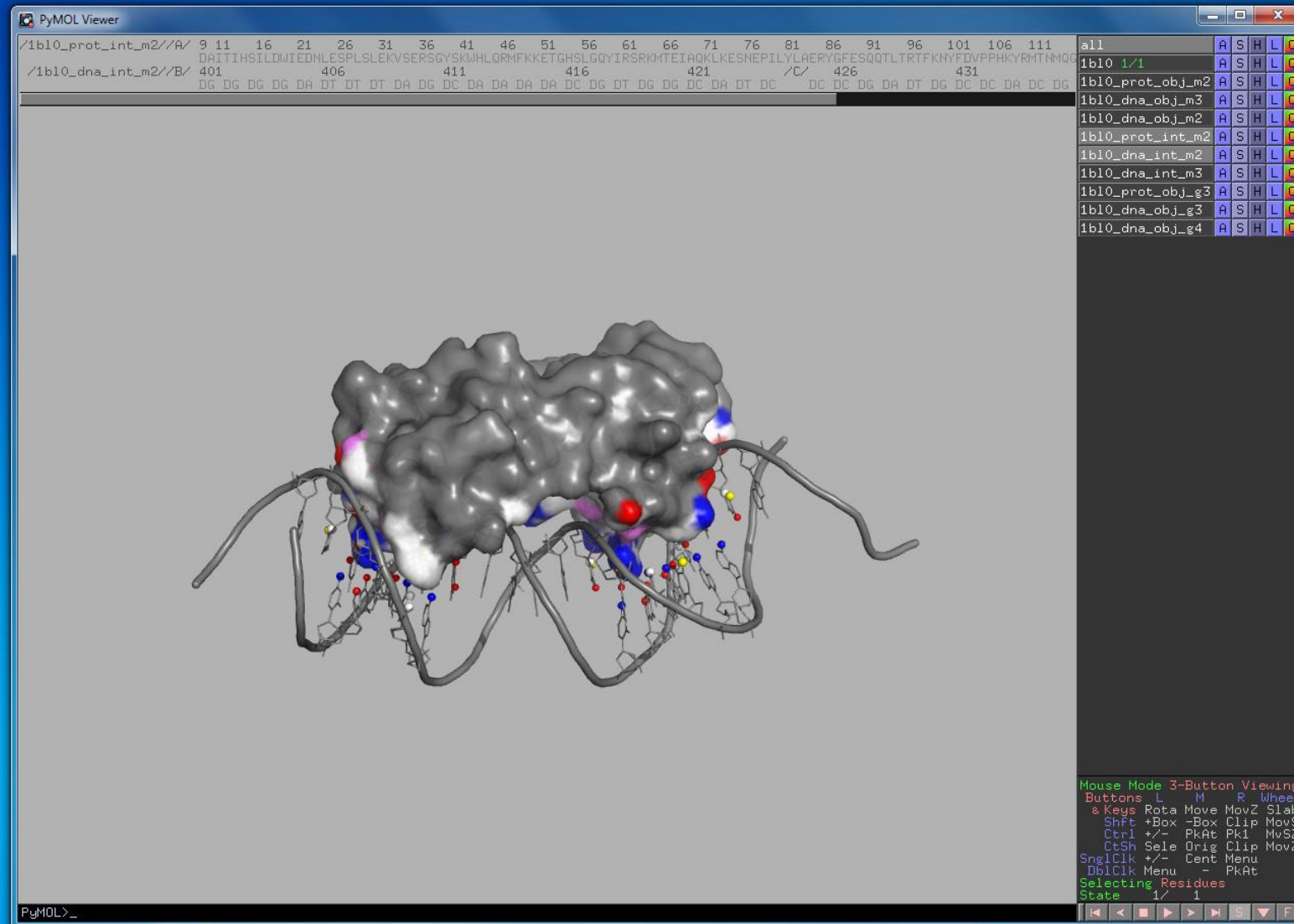
This mode keeps the same coloring pattern, but changes the protein to the surface representation and the DNA to stick representation. Colored spheres show interacting atoms.

The Visualization Modes

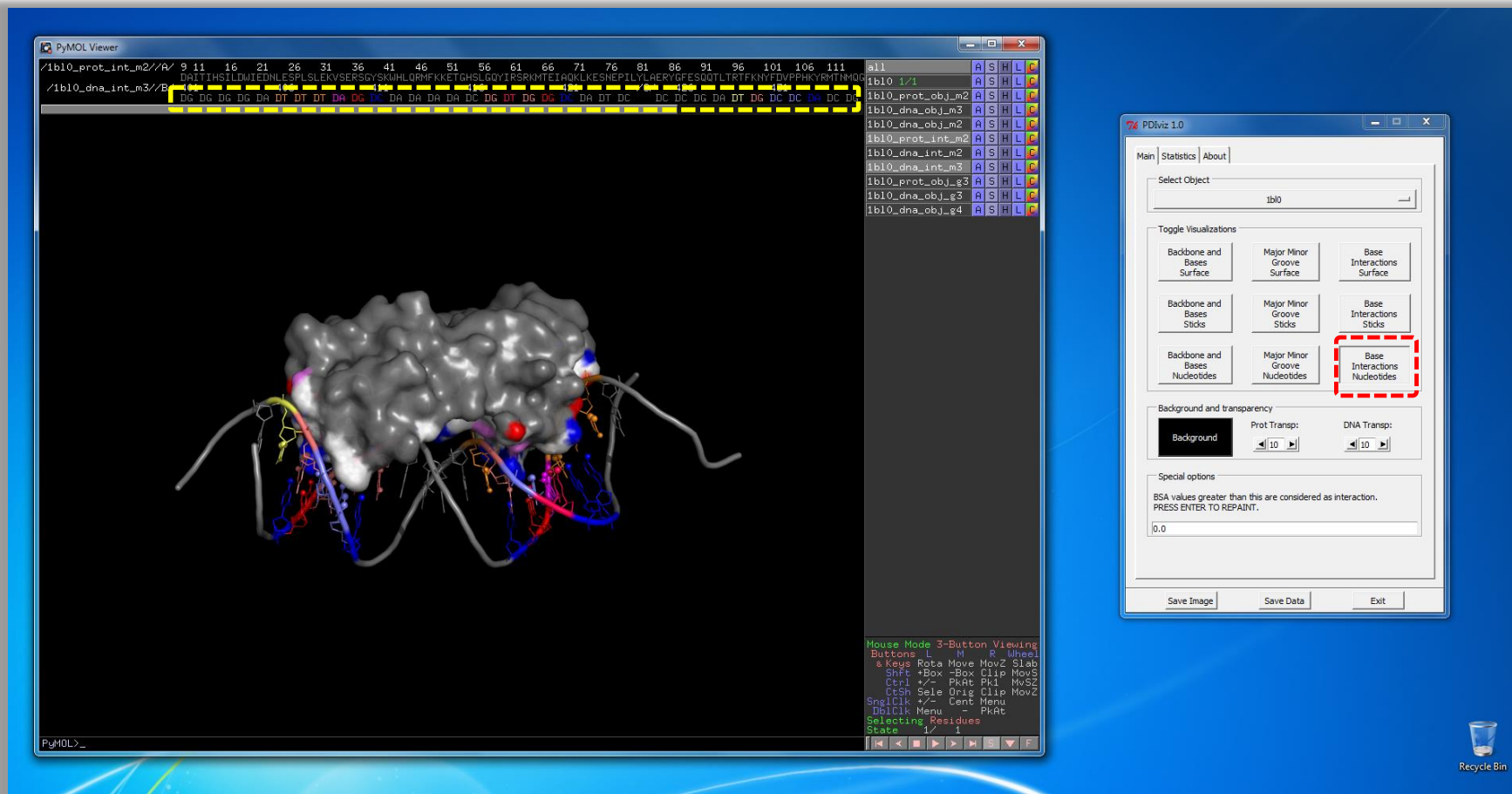
DNA and protein pharmacophoric visualization



In this mode, the DNA is shown with a surface representation. Atoms are painted blue (H-bond donor), red (H-bond acceptor), white (neutral carbon) and yellow (thymine methyl) if they have a BSA greater than the cut-off. In the protein, atoms with a BSA value greater than the cut-off are painted in the same scheme, with the addition of purple for atoms that can be both, donors and acceptors of H-bonds. The colors are shaded according to the BSA value of the atom.



This mode keeps the same coloring pattern, but changes the protein to the surface representation and the DNA to stick representation. Colored spheres show interacting atoms.



In this mode, the nucleotides are painted in one of 15 colors, according to the combination of interactions of its atoms. The types in the table are as follows: **D**, H-bond donor; **A**, H-bond acceptor; **H**, neutral carbon (C-H); and **T**, thymine methyl. An interacting nucleotide will have one of the combinations in the table, and will be painted with respective color.

In the yellow box you can see how the DNA sequence is painted according to this scheme. The types highlighted in light yellow only occur on Thymine nucleotides.

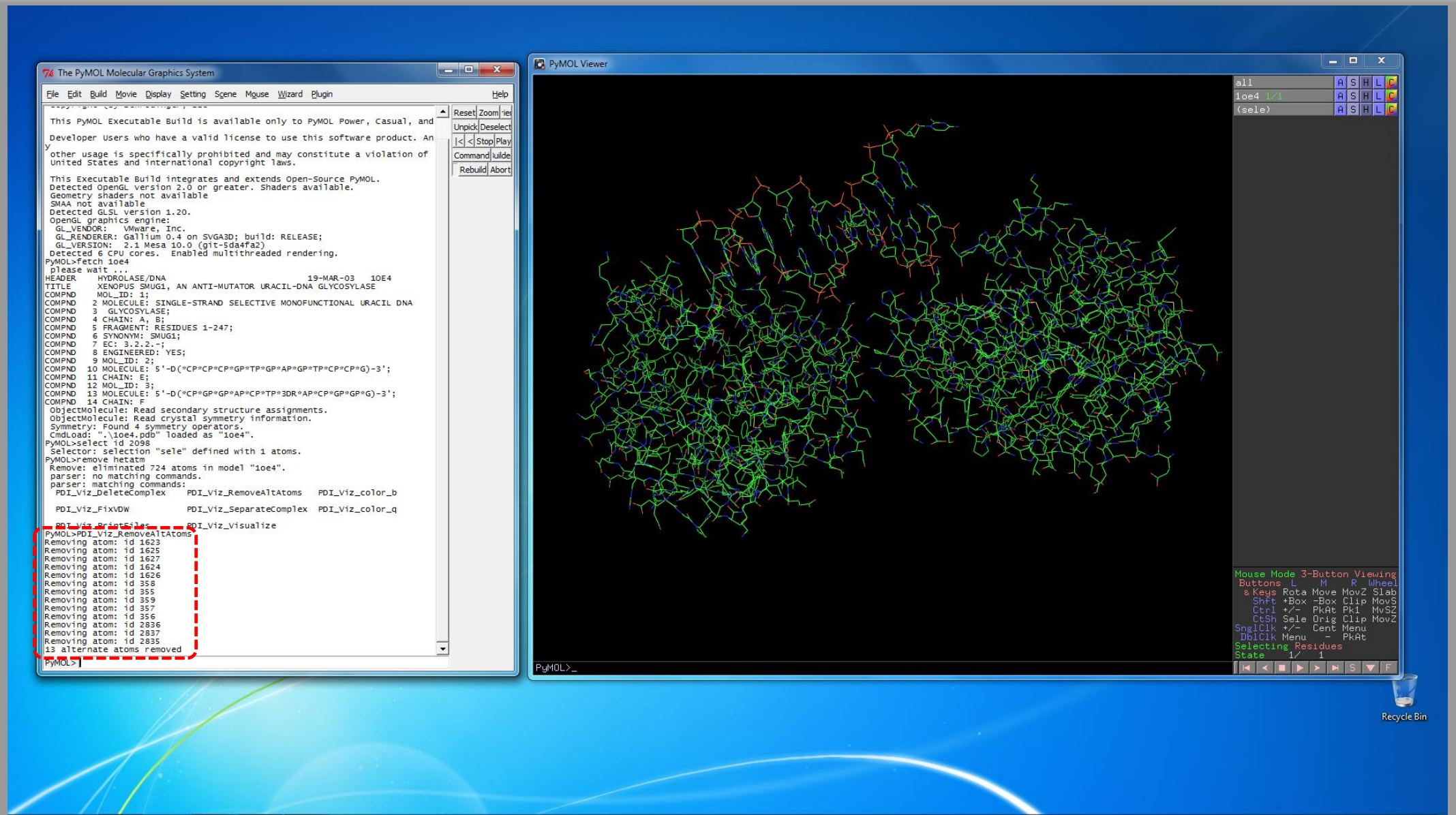
Type	Color
D	Blue
A	Red
H	
T	Yellow
DA	Magenta
DH	Light Blue
AH	Light Red
DAH	Light Purple
DT	Light Yellow
AT	Light Red
HT	Light Yellow
ATH	Light Orange
DAT	Light Green
DTH	Light Red
DAHT	Light Green

Command Line Functions

PDI_Viz_SeparateComplex and PDI_Viz_DeleteComplex

Command Line Functions

PDI_Viz_RemoveAltAtoms and PDI_Viz_FixVDW



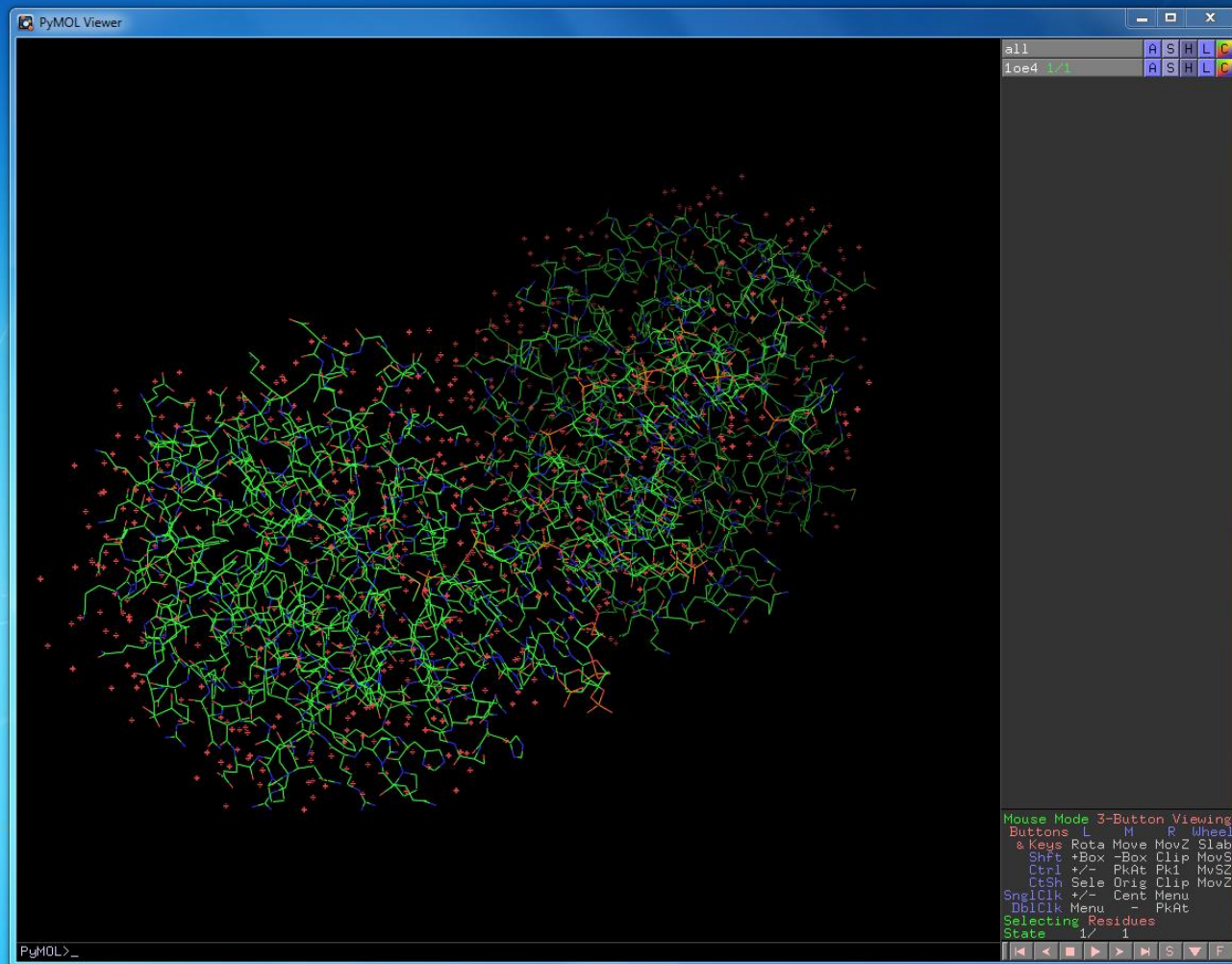
The `PDI_Viz_RemoveAltAtoms` function removes alternative positions (altloc). It removes the standard “alternative atom locations” and non-standard “alternative chain locations”. The red box highlights the ID of the removed atoms. Its only optional argument is an object name.


```
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File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

PyMOL(TM) 1.7.4.2 - Incentive Product
Copyright (C) Schrodinger, LLC

This PyMOL Executable Build is available only to PyMOL Power, Casual, and
Developer Users who have a valid license to use this software product. Any
other usage is specifically prohibited and may constitute a violation of
United States and international copyright laws.

This Executable Build integrates and extends Open-Source PyMOL.
Detected OpenGL version 2.0 or greater. Shaders available.
Geometry shaders not available
SMAA not available
Detected GLSL version 1.20.
OpenGL graphics engine:
GL_VENDOR: VMware, Inc.
GL_RENDERER: Gallium 0.4 on SVGA3D; build: RELEASE;
GL_VERSION: 2.1 Mesa 10.0 (git-sda4fa2)
Detected 6 CPU cores. Enabled multithreaded rendering.
PyMOL>load 1oe4.pdb
HEADER HYDROLASE/DNA 19-MAR-03 1OE4
TITILE XENOPUS SMUG1, AN ANTI-MUTATOR URACIL-DNA GLYCOSYLASE
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL DNA
COMPND 3 GLYCOSYLASE;
COMPND 4 CHAIN: A, B;
COMPND 5 FRAGMENT: RESIDUES 1-247;
COMPND 6 SYNONYM: SMUG1;
COMPND 7 EC: 3.2.2.-;
COMPND 8 ENGINEERED: YES;
COMPND 9 MOL_ID: 2;
COMPND 10 MOLECULE: 5'-D(*CP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*G)-3';
COMPND 11 CHAIN: E;
COMPND 12 MOL_ID: 3;
COMPND 13 MOLECULE: 5'-D(*CP*GP*GP*AP*CP*TP*3DR*AP*CP*GP*GP*G)-3';
COMPND 14 CHAIN: F
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 4 symmetry operators.
PyMOL>PDI_Viz_FixVDW
Atom radii fixed.
PyMOL>get_area
Cmd.get_area: 76310.609 Angstroms^2.
PyMOL>PDI_Viz_RemoveAltAtoms
Removing atom: id 1623
Removing atom: id 1625
Removing atom: id 1627
Removing atom: id 1624
Removing atom: id 1626
Removing atom: id 358
Removing atom: id 355
Removing atom: id 359
Removing atom: id 357
Removing atom: id 356
Removing atom: id 2836
Removing atom: id 2837
Removing atom: id 2835
13 alternate atoms removed
PyMOL>get_area
Cmd.get_area: 74334.500 Angstroms^2.
PyMOL>
```



The `PDI_Viz_FixVDW` function redefines the van der Waals (vdW) radii of all atoms in an object. As can be see in the red box, fixing the vdW radii has a great effect on SASA calculations. Removing alternate locations also has an effect. It only has a single argument, the object name. If no argument is given, the vdW radii of all atoms will be redefined.

Command Line Functions

PDI_Viz_PrintFiles

```
PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin Help

TITLE XENOPUS SMUG1, AN ANTI-MUTATOR URACIL-DNA GLYCOSYLASE
COMPND 1 MOLECULE: SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL-DNA GLYCOSYLASE
COMPND 2 MOLECULE: SINGLE-STRAND SELECTIVE MONOFUNCTIONAL URACIL-DNA GLYCOSYLASE
COMPND 3 GLYCOSYLASE;
COMPND 4 CHAIN: A, B;
COMPND 5 FRAGMENT: RESIDUES 1-247;
COMPND 6 SYNONYM: SMUG1;
COMPND 7 EC: 3.2.2.-;
COMPND 8 ENGINEERED: YES;
COMPND 9 MOL_ID: 2;
COMPND 10 MOLECULE: 5'-D-(CP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*G)-3';
COMPND 11 CHAIN: E;
COMPND 12 MOL_ID: 3;
COMPND 13 MOLECULE: 5'-D-(CP*GP*GP*AP*CP*TP*3DR*AP*CP*GP*GP*G)-3';
COMPND 14 CHAIN: F;
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 4 symmetry operators.
PyMOL>PDI_Viz_PrintFiles 10e4
Saving data for 10e4
Begin file output for 10e4
Removing atom: 10e4 and id 1623
Removing atom: 10e4 and id 1625
Removing atom: 10e4 and id 1627
Removing atom: 10e4 and id 1624
Removing atom: 10e4 and id 1626
Removing atom: 10e4 and id 358
Removing atom: 10e4 and id 355
Removing atom: 10e4 and id 359
Removing atom: 10e4 and id 357
Removing atom: 10e4 and id 356
Removing atom: 10e4 and id 2836
Removing atom: 10e4 and id 2837
Removing atom: 10e4 and id 2835
13 alternate atoms removed
Atom radii fixed.
Complex SASA: 25618.6
Free protein SASA: 22087.5
Free DNA SASA: 4897.9
Protein backbone SASA: 4139.3
Protein side chain SASA: 17948.2
DNA backbone SASA: 3402.0
DNA bases SASA: 1495.9
Buried protein surface: 636.0
Buried protein backbone surface: 57.8
Buried protein side chain surface: 578.2
Buried DNA surface: 730.8
Buried DNA backbone surface: 535.4
Buried DNA bases surface: 195.4
DNA major groove surface: 991.6
DNA minor groove surface: 456.0
Buried DNA major groove surface: 105.4
Buried DNA minor groove surface: 79.3
Interface Area: 683.4
10e4 done.
DATA SAVED!
PyMOL>
```

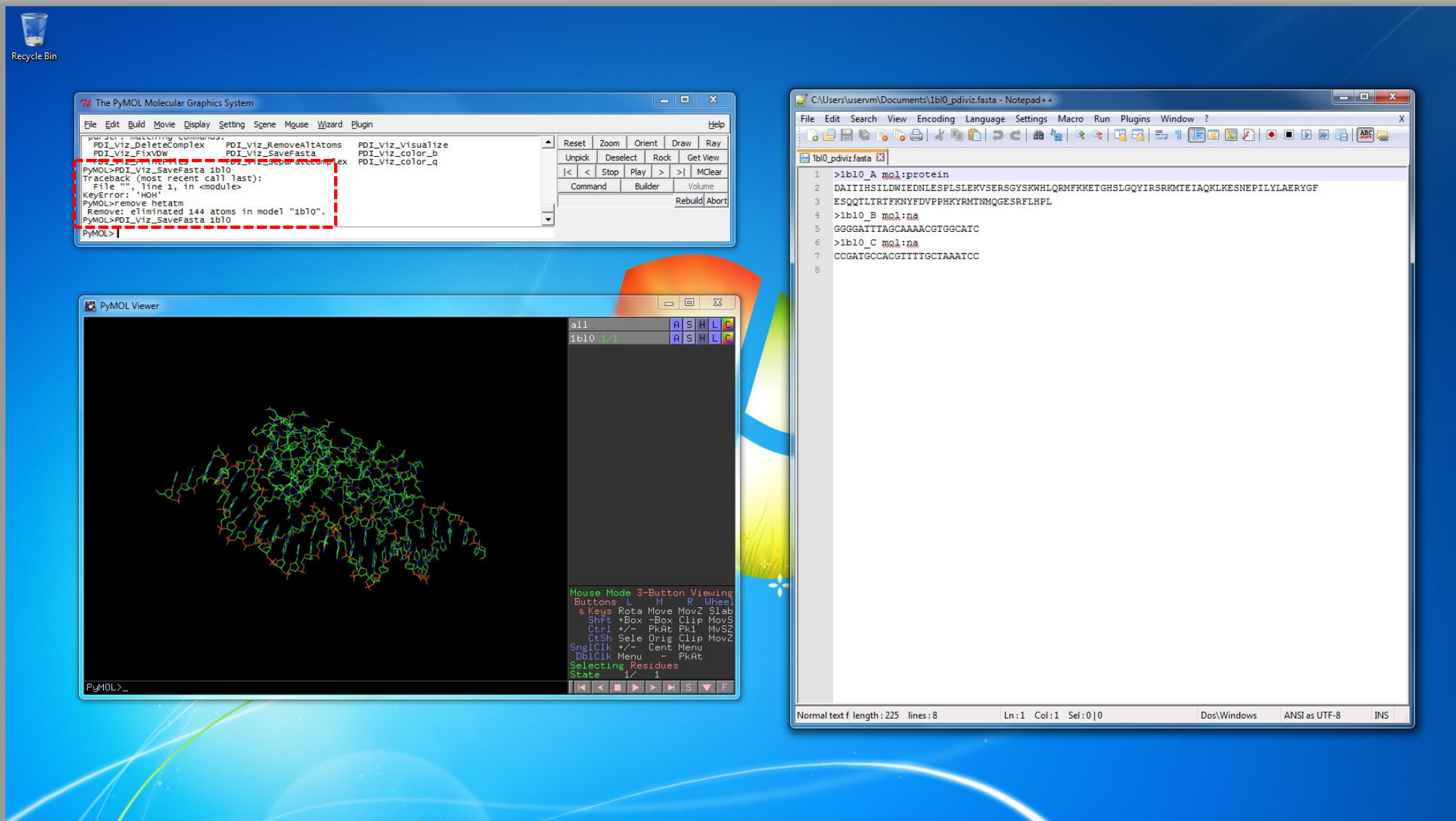
REMARK ID	NAME	RESN	CHAIN	RESI	X	Y	Z	ASA	VDW
1	ATOM	1	N	GLU A 36	-16.270	42.102	35.930	37.676	1.65
2	ATOM	2	CA	GLU A 36	-15.868	41.220	34.796	10.837	1.87
3	ATOM	3	C	GLU A 36	-15.228	39.936	35.322	3.137	1.76
4	ATOM	4	O	GLU A 36	-14.657	39.920	36.427	0.445	1.40
5	ATOM	5	CB	GLU A 36	-14.900	41.960	33.863	13.226	1.87
6	ATOM	6	CG	GLU A 36	-15.593	42.685	32.710	33.554	1.87
7	ATOM	7	CD	GLU A 36	-14.625	43.211	31.656	14.241	1.76
8	ATOM	8	OE1	GLU A 36	-14.814	44.356	31.166	42.386	1.40
9	ATOM	9	OE2	GLU A 36	-13.679	42.475	31.300	35.238	1.40
10	ATOM	10	N	SER A 37	-15.349	38.862	34.538	7.741	1.65
11	ATOM	11	CA	SER A 37	-14.672	37.603	34.829	0.000	1.8
12	ATOM	12	C	SER A 37	-13.327	37.559	34.103	0.423	1.76
13	ATOM	13	O	SER A 37	-13.255	37.697	32.881	15.228	1.40
14	ATOM	14	CB	SER A 37	-15.531	36.397	34.410	31.954	1.87
15	ATOM	15	OG	SER A 37	-14.733	35.227	34.289	4.808	1.40
16	ATOM	16	N	PRO A 38	-12.249	37.334	34.836	0.047	1.65
17	ATOM	17	CA	PRO A 38	-10.944	37.205	34.193	5.047	1.87
18	ATOM	18	C	PRO A 38	-10.665	35.823	33.585	0.000	1.76
19	ATOM	19	O	PRO A 38	-9.573	35.666	33.062	0.000	1.40
20	ATOM	20	CB	PRO A 38	-9.980	37.497	35.336	2.121	1.87
21	ATOM	21	CG	PRO A 38	-10.687	37.042	36.558	0.000	1.87
22	ATOM	22	CD	PRO A 38	-12.155	37.187	36.297	0.000	1.87
23	ATOM	23	N	ALA A 39	-11.596	34.867	33.639	0.000	1.65
24	ATOM	24	CA	ALA A 39	-11.322	33.492	33.176	0.000	1.87
25	ATOM	25	C	ALA A 39	-10.781	33.445	31.745	0.000	1.76
26	ATOM	26	O	ALA A 39	-9.737	32.859	31.497	0.000	1.40
27	ATOM	27	CB	ALA A 39	-12.576	32.619	33.281	2.633	1.87
28	ATOM	28	N	ASP A 40	-11.493	34.077	30.815	0.615	1.65
29	ATOM	29	CA	ASP A 40	-11.093	34.078	29.409	1.236	1.87
30	ATOM	30	C	ASP A 40	-9.746	34.762	29.217	0.570	1.76

atpname	resname	chain	resnum	total_ASA	bb_ASA	sc_ASA	majorgroove_ASA	minorgroove_ASA
1	N	GLU A	36	37.676	37.676	0.000	0.000	0.000
2	CA	GLU A	36	10.837	10.837	0.000	0.000	0.000
3	C	GLU A	36	3.137	3.137	0.000	0.000	0.000
4	O	GLU A	36	0.445	0.445	0.000	0.000	0.445
5	CB	GLU A	36	13.226	0.000	13.226	0.000	0.000
6	CG	GLU A	36	33.554	0.000	33.554	0.000	0.000
7	CD	GLU A	36	14.241	0.000	14.241	0.000	0.000
8	OE1	GLU A	36	42.386	0.000	42.386	0.000	0.000
9	OE2	GLU A	36	35.238	0.000	35.238	0.000	0.000
10	N	SER A	37	7.741	7.741	0.000	0.000	7.741
11	CA	SER A	37	0.000	0.000	0.000	0.000	0.000
12	C	SER A	37	0.423	0.423	0.000	0.000	0.000
13	O	SER A	37	15.228	15.228	0.000	0.000	15.228
14	CB	SER A	37	31.954	0.000	31.954	0.000	0.000
15	OG	SER A	37	4.808	0.000	4.808	0.000	0.000
16	N	PRO A	38	0.047	0.047	0.000	0.000	0.047
17	CA	PRO A	38	5.047	5.047	0.000	0.000	0.000
18	C	PRO A	38	0.000	0.000	0.000	0.000	0.000
19	O	PRO A	38	0.000	0.000	0.000	0.000	0.000
20	CB	PRO A	38	2.121	0.000	2.121	0.000	0.000
21	CG	PRO A	38	0.000	0.000	0.000	0.000	0.000
22	CD	PRO A	38	0.000	0.000	0.000	0.000	0.000
23	N	ALA A	39	0.000	0.000	0.000	0.000	0.000
24	CA	ALA A	39	0.000	0.000	0.000	0.000	0.000
25	C	ALA A	39	0.000	0.000	0.000	0.000	0.000
26	O	ALA A	39	0.000	0.000	0.000	0.000	0.000
27	CB	ALA A	39	2.633	0.000	2.633	0.000	0.000
28	N	ASP A	40	0.615	0.615	0.000	0.000	0.615
29	CA	ASP A	40	1.236	1.236	0.000	0.000	0.000
30	C	ASP A	40	0.570	0.570	0.000	0.000	0.000

The PDI_Viz_PrintFiles function saves the BSA calculation data in .asa NACCESS compatible files, and in Excel compatible tab-separated .atmasa format. The red box shows that this function automatically calls FixVDW and RemoveAltAtoms. Its arguments are an object name, a save path (optional, defaults on the current directory) and the visualization mode to save as a PyMOL .pse session file (-1 (disable save session), 0 (all) or 1 to 9, optional). The Blue box highlights the contents of an .asa file and the green box the contents of an .atmasa file.

Command Line Functions

PDI_Viz_SaveFasta



The PDI_Viz_SaveFasta function saves the selected model protein and DNA sequences in a standard FASTA file. Currently it does not support non standard residues or atoms, so they must be removed as shown in the red box. It's only argument is the object name of the protein-DNA complex. The file is saved in the current working directory.

Batch mode

```
batch_test : bash - Konsole
batch_test : bash
jr1 ~/Dropbox/Software/dna_viz $ cd batch_test/
jr1 ~/Dropbox/Software/dna_viz/batch_test $ pymol.bin -c -r ../PDIviz1.py -d "fetch 1bl0, async=0; fetch 1p3i, async=0; PDI_Viz_PrintFiles 1bl0; PDI_Viz_PrintFiles 1p3i;"
PyMOL(TM) 1.7.4.1 - Incentive Product
Copyright (C) Schrodinger, LLC

This PyMOL Executable Build is available only to PyMOL Power, Casual, and
Developer Users who have a valid license to use this software product. Any
other usage is specifically prohibited and may constitute a violation of
United States and international copyright laws.

This Executable Build integrates and extends Open-Source PyMOL.
Command mode. No graphics front end.
Detected 8 CPU cores. Enabled multithreaded rendering.
PyMOL>run ../PDIviz1.py, main
PyMOL>fetch 1bl0, async=0; fetch 1p3i, async=0; PDI_Viz_PrintFiles 1bl0; PDI_Viz_PrintFiles 1p3i;
HEADER      TRANSCRIPTION/DNA                      22-JUL-98   1BL0
TITLE       MULTIPLE ANTIBIOTIC RESISTANCE PROTEIN (MARA)/DNA COMPLEX
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: DNA (5'-
COMPND      3 D(*GP*GP*GP*GP*AP*TP*TP*TP*AP*GP*CP*AP*AP*AP*AP*CP*GP*TP*GP
COMPND      4 *GP*CP*AP* TP*C)-3');
COMPND      5 CHAIN: B;
COMPND      6 ENGINEERED: YES;
COMPND      7 MOL_ID: 2;
COMPND      8 MOLECULE: DNA (5'-
COMPND      9 D(*CP*CP*GP*AP*TP*GP*CP*CP*AP*CP*GP*TP*TP*TP*TP*GP*CP*TP*AP
COMPND     10 *AP*AP*TP* CP*C)-3');
COMPND     11 CHAIN: C;
COMPND     12 SYNONYM: MARA;
COMPND     13 ENGINEERED: YES;
COMPND     14 MOL_ID: 3;
COMPND     15 MOLECULE: PROTEIN (MULTIPLE ANTIBIOTIC RESISTANCE PROTEIN);
COMPND     16 CHAIN: A;
COMPND     17 ENGINEERED: YES
ObjectMolecule: Read secondary structure assignments.
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 8 symmetry operators.
CmdLoad: "../1bl0.pdb" loaded as "1bl0".
HEADER      STRUCTURAL PROTEIN/DNA                  17-APR-03   1P3I
TITLE       CRYSTALLOGRAPHIC STUDIES OF NUCLEOSOME CORE PARTICLES
TITLE       2 CONTAINING HISTONE 'SIN' MUTANTS
COMPND      MOL_ID: 1;
COMPND      2 MOLECULE: PALINDROMIC 146BP HUMAN ALPHA-SATELLITE DNA
COMPND      3 FRAGMENT;
COMPND      4 CHAIN: I, J;
COMPND      5 ENGINEERED: YES;
COMPND      6 MOL_ID: 2;
COMPND      7 MOLECULE: HISTONE H3;
COMPND      8 CHAIN: A, E;
COMPND      9 ENGINEERED: YES;
COMPND     10 MOL_ID: 3;
COMPND     11 MOLECULE: HISTONE H4;
```

This example will execute the plugin in batch mode from a Unix terminal. We will print the SASA data of two complexes, 1bl0 and 1p3i. In the green box you can see that the plugin should be executed with the -r switch, so PyMOL loads the plugin prior to executing any user commands. The -c switch tells PyMOL to start in command line mode, without GUI; and the -d option tells PyMOL to execute user provided commands. After loading both structures using fetch, we call PDI_Viz_PrintFiles with the object name as the single argument.

```
batch_test : bash - Konsole
batch_test : bash
ObjectMolecule: Read crystal symmetry information.
Symmetry: Found 4 symmetry operators.
Cmdload: "../1p3i.pdb" loaded as "1p3i".
Saving data for 1bl0
Saving data for 1p3i
Begin file output for 1p3i
0 alternate atoms removed
Atom radii fixed.
Complex SASA:      74029.0
Free protein SASA:  35292.9
Free DNA SASA:      51879.2
Protein backbone SASA: 6437.1
Protein side chain SASA: 28855.8
DNA backbone SASA:  39865.5
DNA bases SASA:     12013.6
Buried protein surface: 6176.1
Buried protein backbone surface: 974.6
Buried protein side chain surface: 5201.5
Buried DNA surface: 6966.9
Buried DNA backbone surface: 6698.0
Buried DNA bases surface: 268.9
DNA major groove surface: 9490.7
DNA minor groove surface: 2520.1
Buried DNA major groove surface: 76.2
Buried DNA minor groove surface: 192.7
Interface Area: 6571.5
1p3i done.
DATA SAVED!
Begin file output for 1bl0
0 alternate atoms removed
Atom radii fixed.
Complex SASA:      13133.8
Free protein SASA:  6807.4
Free DNA SASA:      8726.4
Protein backbone SASA: 1075.3
Protein side chain SASA: 5732.1
DNA backbone SASA:  6586.4
DNA bases SASA:     2139.9
Buried protein surface: 1203.4
Buried protein backbone surface: 66.7
Buried protein side chain surface: 1136.7
Buried DNA surface: 1196.5
Buried DNA backbone surface: 804.2
Buried DNA bases surface: 392.4
DNA major groove surface: 1625.8
DNA minor groove surface: 466.7
Buried DNA major groove surface: 392.4
Buried DNA minor groove surface: 0.0
Interface Area: 1200.0
1bl0 done.
DATA SAVED!
PyMOL: normal program termination.
```

Here we show the console output of the command. Both 1p3i (green box) and 1bl0 (red box) completed without errors.

```
batch_test : bash - Konsole
batch_test : bash
jri ~/Dropbox/Software/dna_viz/batch_test $ ls
1b10.pdb          1b10_pdiviz_dna_bb.atmasa      1p3i.pdb          1p3i_pdiviz_dna_bb.atmasa
1b10_pdiviz.asa   1b10_pdiviz_dna_bb_protein.asa 1p3i_pdiviz.asa   1p3i_pdiviz_dna_bb_protein.asa
1b10_pdiviz.atmasa 1b10_pdiviz_dna_bb_protein.atmasa 1p3i_pdiviz.atmasa 1p3i_pdiviz_dna_bb_protein.atmasa
1b10_pdiviz_dna.asa 1b10_pdiviz_dna_wo_major_groove_protein.asa 1p3i_pdiviz_dna.asa 1p3i_pdiviz_dna_wo_major_groove_protein.asa
1b10_pdiviz_dna.atmasa 1b10_pdiviz_dna_wo_major_groove_protein.atmasa 1p3i_pdiviz_dna.atmasa 1p3i_pdiviz_dna_wo_major_groove_protein.atmasa
1b10_pdiviz_dna_base.asa 1b10_pdiviz_dna_wo_minor_groove_protein.asa 1p3i_pdiviz_dna_base.asa 1p3i_pdiviz_dna_wo_minor_groove_protein.asa
1b10_pdiviz_dna_base.atmasa 1b10_pdiviz_dna_wo_minor_groove_protein.atmasa 1p3i_pdiviz_dna_base.atmasa 1p3i_pdiviz_dna_wo_minor_groove_protein.atmasa
1b10_pdiviz_dna_base_protein.asa 1b10_pdiviz_protein.asa 1p3i_pdiviz_dna_base_protein.asa 1p3i_pdiviz_protein.asa
1b10_pdiviz_dna_base_protein.atmasa 1b10_pdiviz_protein.atmasa 1p3i_pdiviz_dna_base_protein.atmasa 1p3i_pdiviz_protein.atmasa
1b10_pdiviz_dna_bb.asa 1b10_pdiviz_stats.csv 1p3i_pdiviz_dna_bb.asa 1p3i_pdiviz_stats.csv
jri ~/Dropbox/Software/dna_viz/batch_test $
```

As a result, a number of output files are generated for 1b10 (green) and 1p3i (red)

Sample shell script

This following shell script will run PDIviz in batch mode and generate ASA files and PyMOL sessions for all *.pdb files in the current directory.

```
for PDB in *.pdb
do
    BNAME=$(basename "$PDB")
    PDBID="${BNAME%.*}"
    pymol -c -r PDIviz1.py -d "load $PDB; PDI_Viz_PrintFiles $PDBID,savesession=0"
done
```