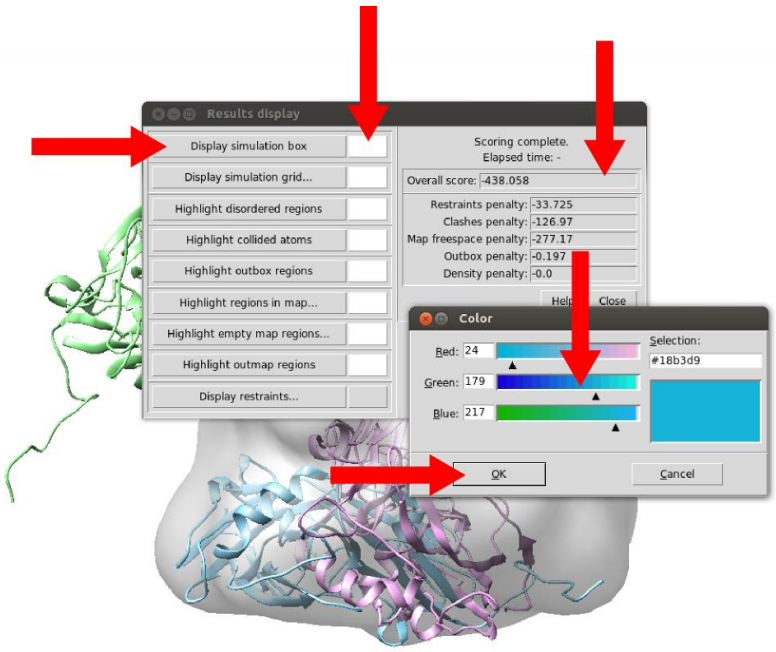
STEP 6 MODEL ANALYSIS

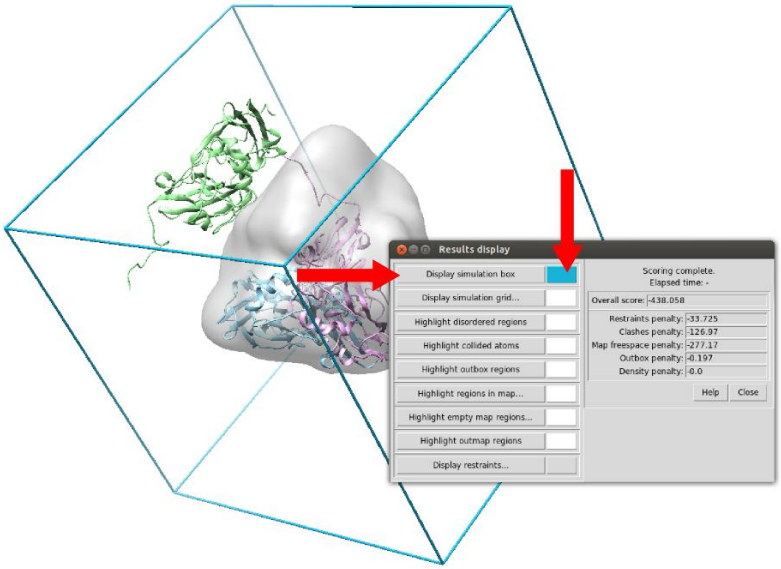
As authors of PyRy3D we wanted to make our software fully transparent for users. This means that we provided some functionalities to show how exactly the program works and how it interprets the structures. For example in the PyRy3D Chimera Extension we implemented **Results Display** tool that enables to visualize scores assigned to structures shown on the screen. Here one can check collided regions of structures, empty fragments of an electron density map or fulfillment of distance restraints.
Thanks to all that features a user does not have to use PyRy3D as a black box, but can do it with full understanding of the scoring process. We hope that such an approach will help to use our program and to create models of better quality.

0. In other words, GUI lets you see **what exactly the particular complex has been punished for, and why.** After performing an evaluation of a complex, a **Results Display window** pops up. In the left panel is a list with complex features to visualize (e.g. **Display simulation box, Display simulation grid..**) with neighboring white boxes to select colors for these objects. In the right panel a program shows detailed punctuation assigned by PyRy3D program for a complex seen in the Chimera window ☺

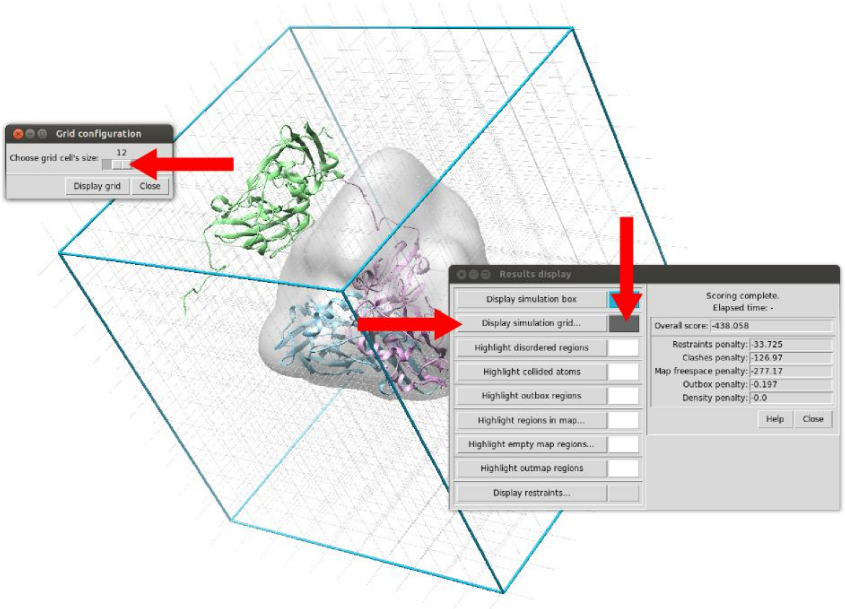


1. **Display simulation box** - displays the simulation box which limits the area of the simulation. Click the square button on the right, **choose light blue color and draw the simulation box**. This is the area where structures can be moved during simulation

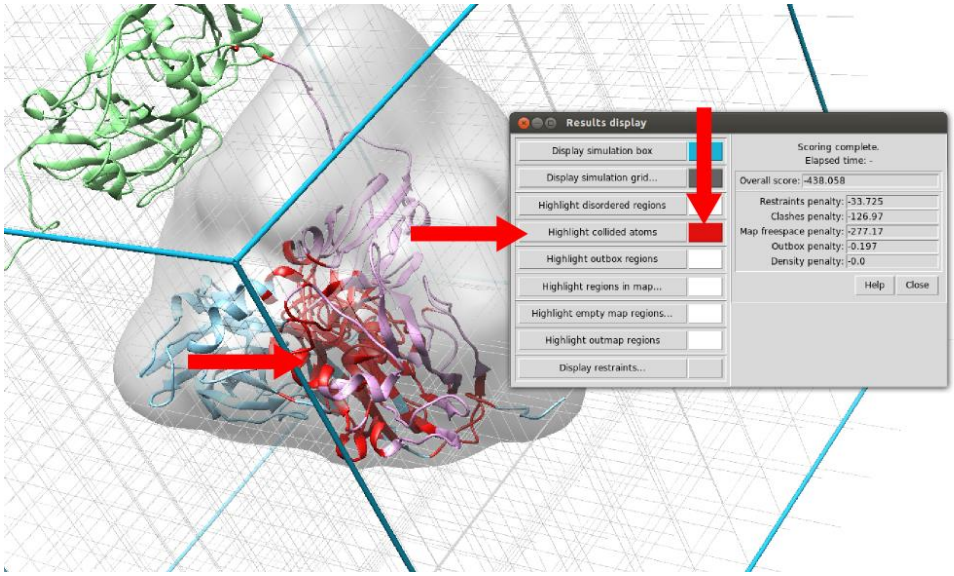
process; all positions outside this box are penalized. The simulation box will appear as a new object in **Model Panel**. You can easily hide it be uncheck **Show**.



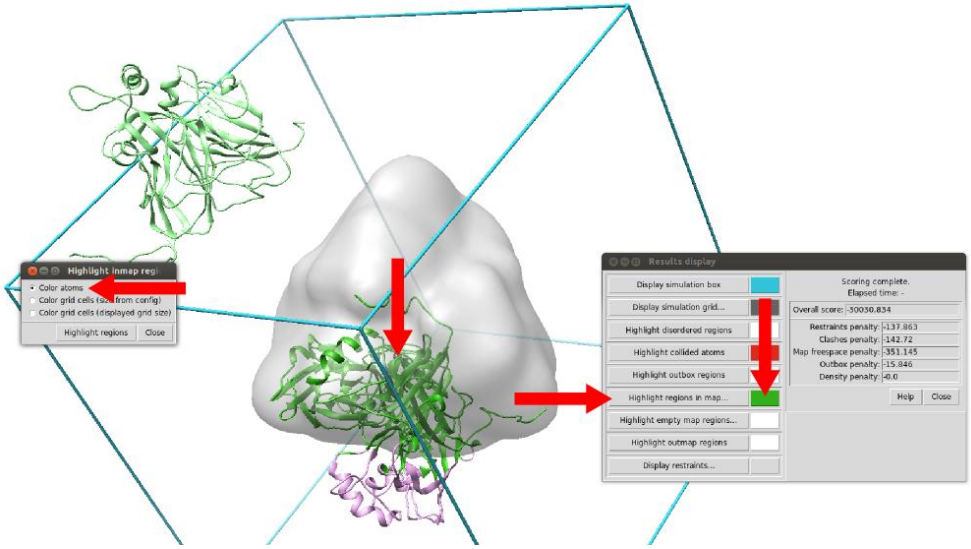
2. **Display simulation grid...** - displays the grid on which the evaluation was based. You can choose the size of the grid's cells. Because of the computational issues, very high-resolution grids cannot be displayed. Display a grey grid with cells' edges **12** Ångstrems long**. Please do not choose to small values (<6 Å) since this process might be very time consuming!**



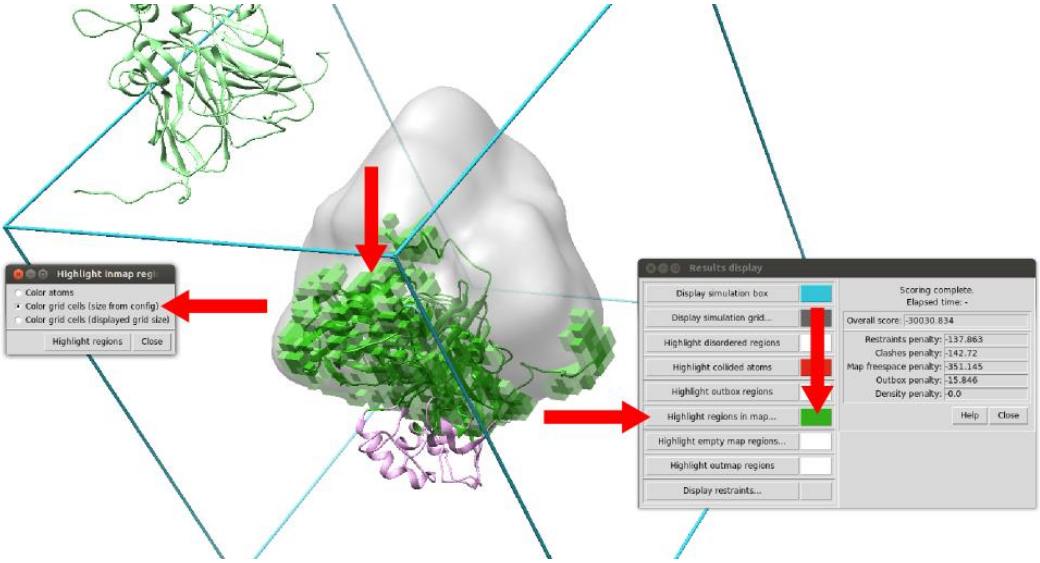
3. **Highlight collided atoms** - colors regions (atoms) where collisions between complexes' components occur. **Color them red**. This operation might be time consuming.



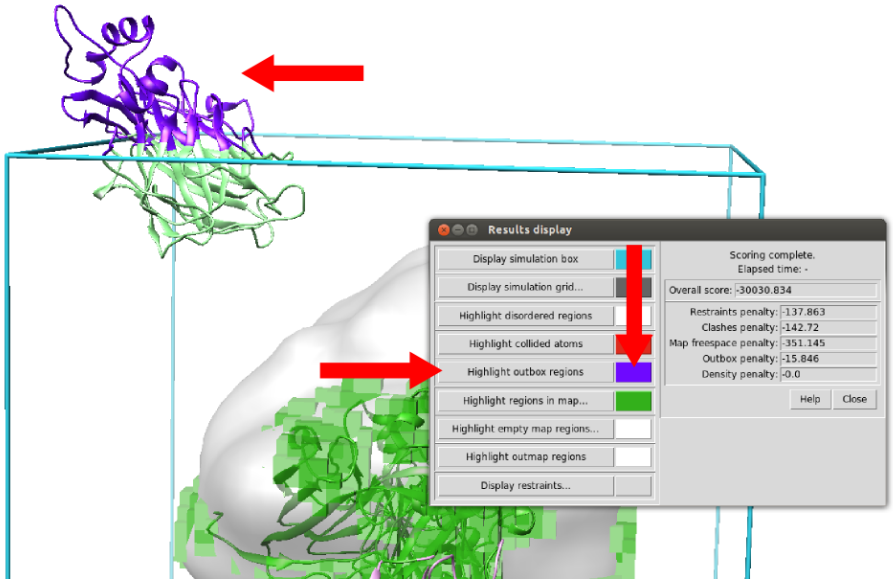
4. **Highlight regions in map** - colors regions (atoms or simulation grid cells) that correspond to atoms fitted inside the electron density map. **Color atoms green**. Coloring atoms might take some time.



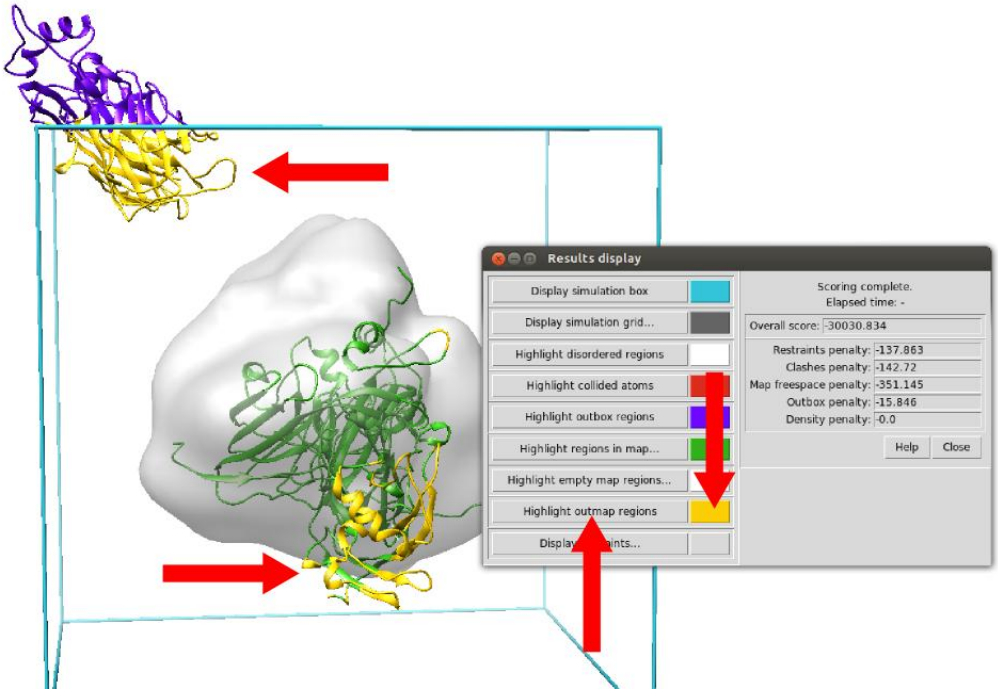
Color grid cells green:



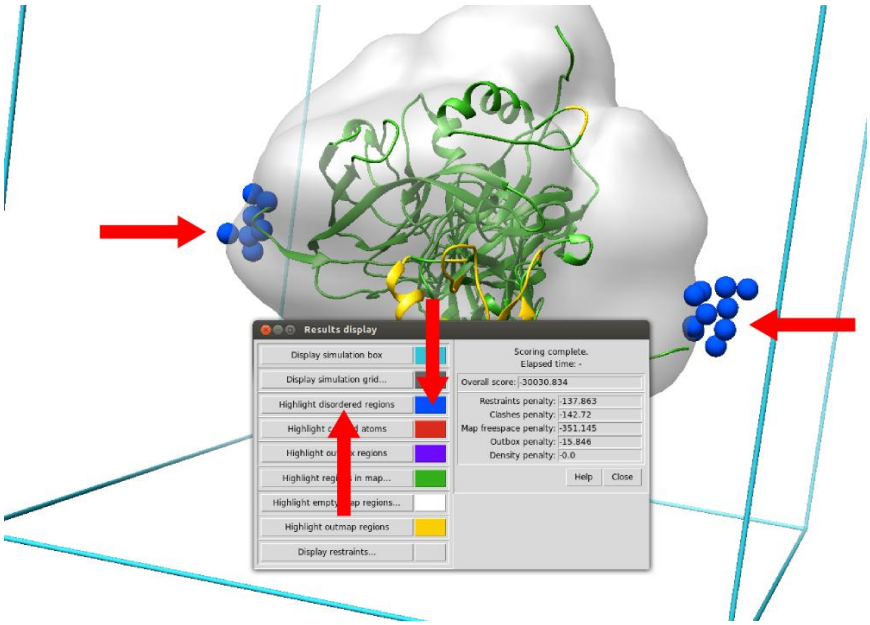
5. **Highlight outbox regions** - colors heavily punished atoms which are situated outside of the simulation box. **Color them** purple. This operation might be time consuming.



6. **Highlight outmap regions** - colors regions (atoms) that are situated outside the electron density map. **Color them** yellow. To create the following image the structures in Chimera where rotated to show corresponding regions.



7. **Highlight disordered regions** - if there's a disordered region in the structure that's being evaluated, pseudoresidues are generated to fill the region without structural coordinates. The feature allows for visualizing the pseudoresidues as colored spheres. **Display the pseudoresidues colored blue**.



8. **Display restraints** - if you're using spatial restraints, you can see their complete list with differences between user defined values (as in **1nic.restr.txt** file) and values occurring in the evaluated complex. Select a restraint of interest in **Restraints** field and choose a **color** -> program will draw a line between mentioned atoms. To prepare the following image we hidden a density map, simulation map object and reoriented a complex to make the interpretation easier.