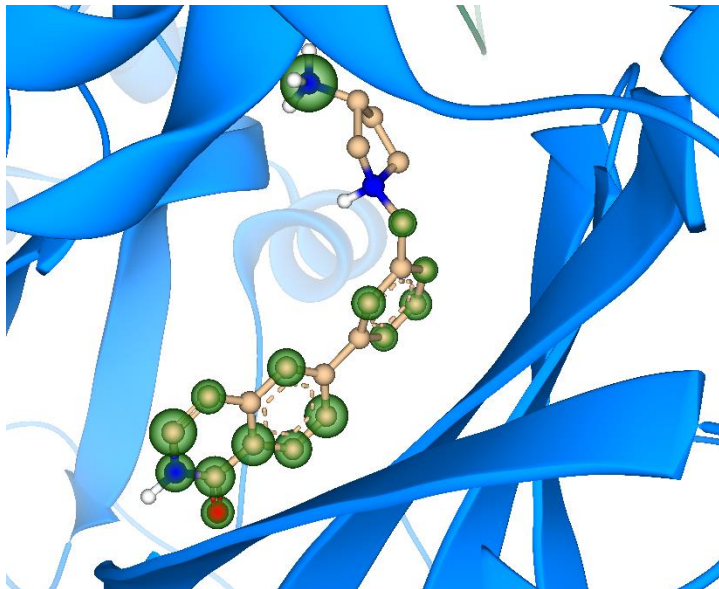# SeeSAR

# BioSolveIT
expect actives!

## Publishing with SeeSAR
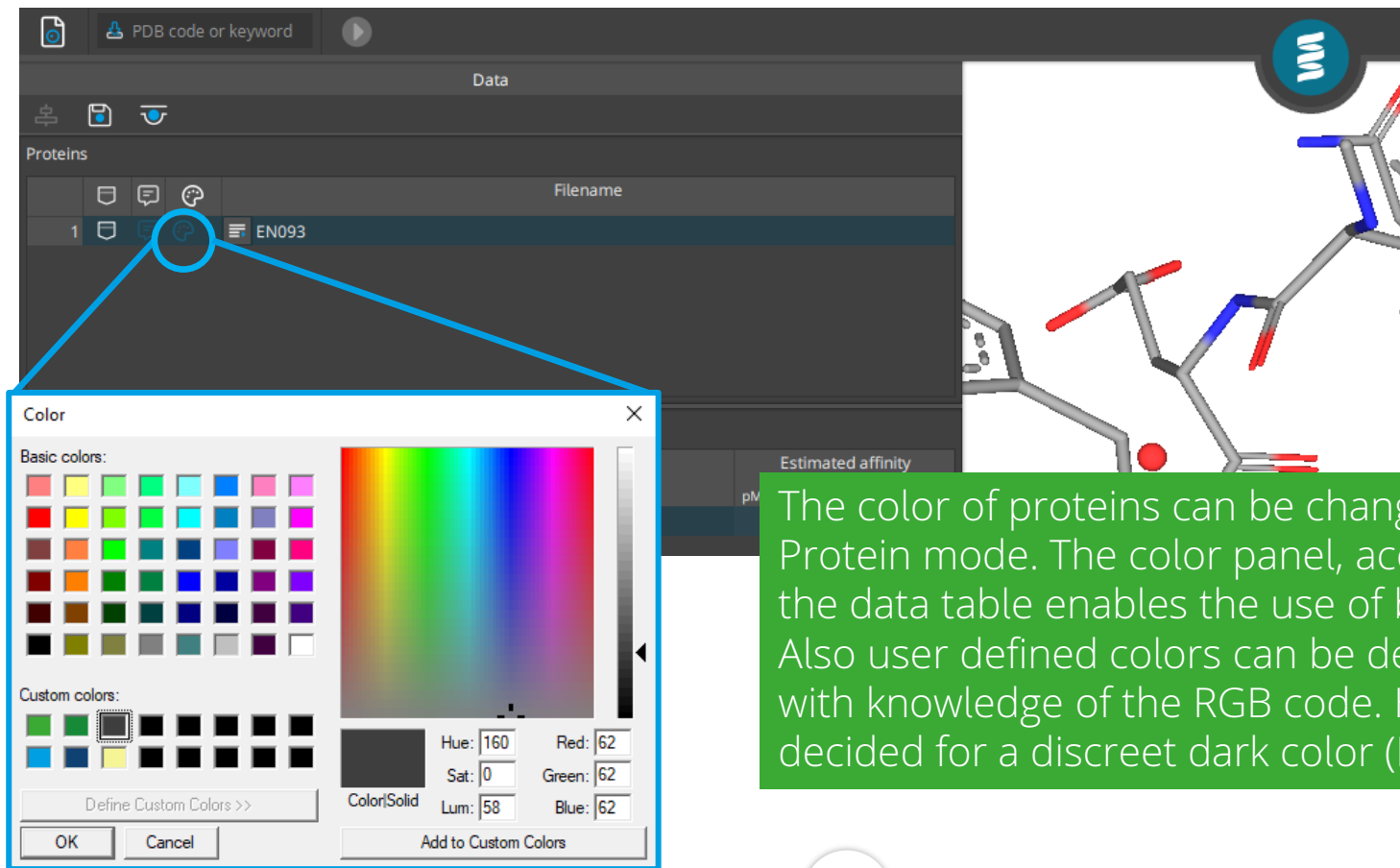How to create high quality images

# Example

For this guide we will use a structure from the publication 'A magnet for the needle in haystacks: "Crystal structure first" fragment hits trigger targeted exploration of the Chemical Space to find novel active matter'.

PDB-ID: 7PIH
Ligand EN093 ($K_i$ = 5.6µM)

The color of proteins can be changed in the Protein mode. The color panel, accessible via the data table enables the use of basic colors. Also user defined colors can be defined, e.g. with knowledge of the RGB code. Here we decided for a discreet dark color (RGB 62-62-62)
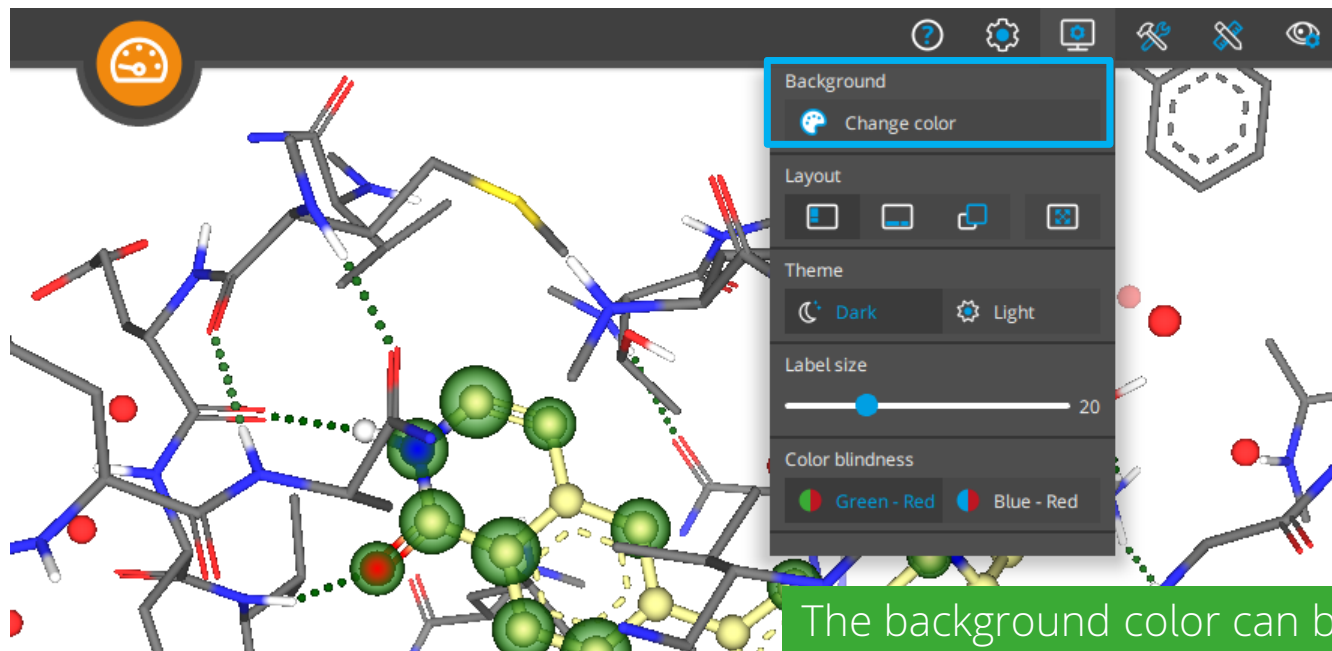
The color of ligands can be changed in other modes including the Analyzer Mode. The color panel equals the panel used to color code the protein. Here we decided for a light color (RGB 245-245-150), that well differentiates from SeeSAR's red/green coloring of HYDE spheres and torsion angles.

The background color can be changed in all modes of SeeSAR. Go to the top right toolbar 'Appearance' and open the Background color panel. In publications the background is usually set to white.

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Label Size 12      Label Size 20
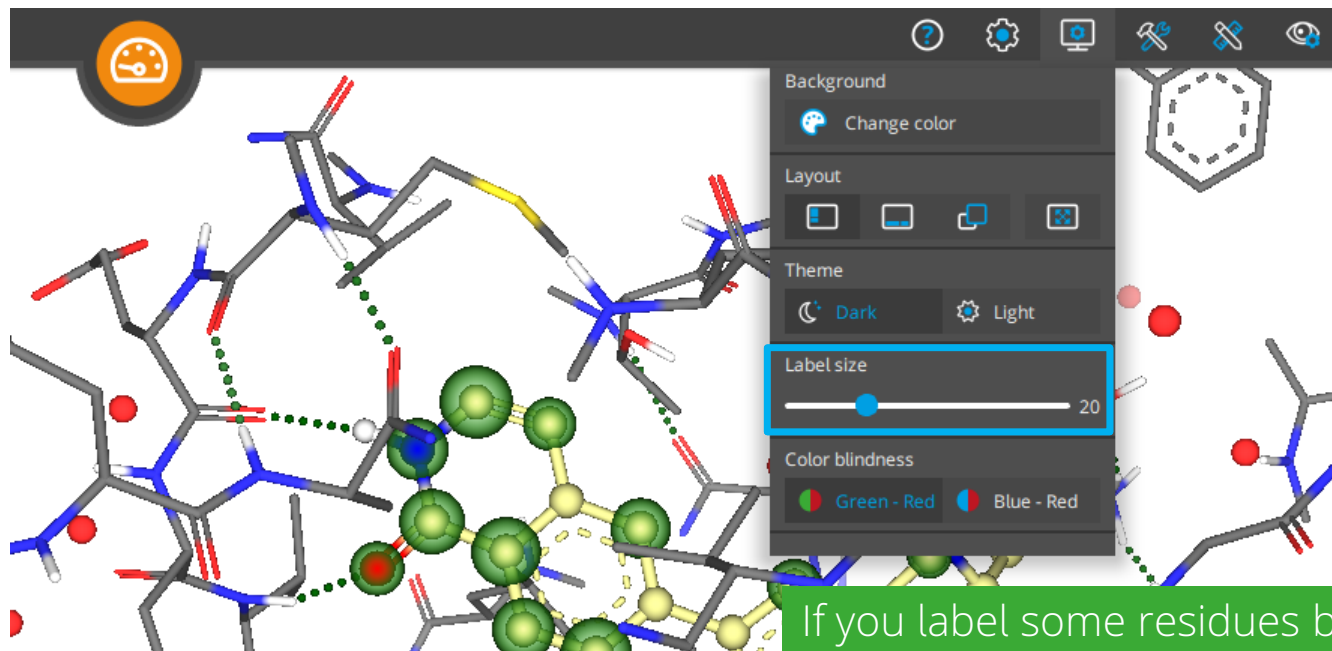
GLU_A_121 ×      GLU_A_121 ×

If you label some residues before exporting the pose image the label size should be adjusted. This can be done in the same 'Appearance' setting as used to set the background color.
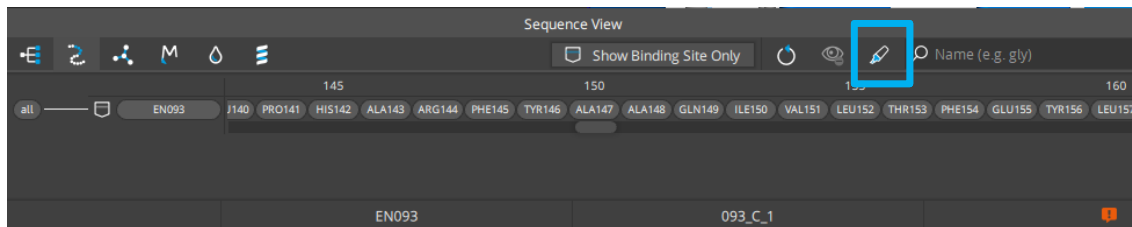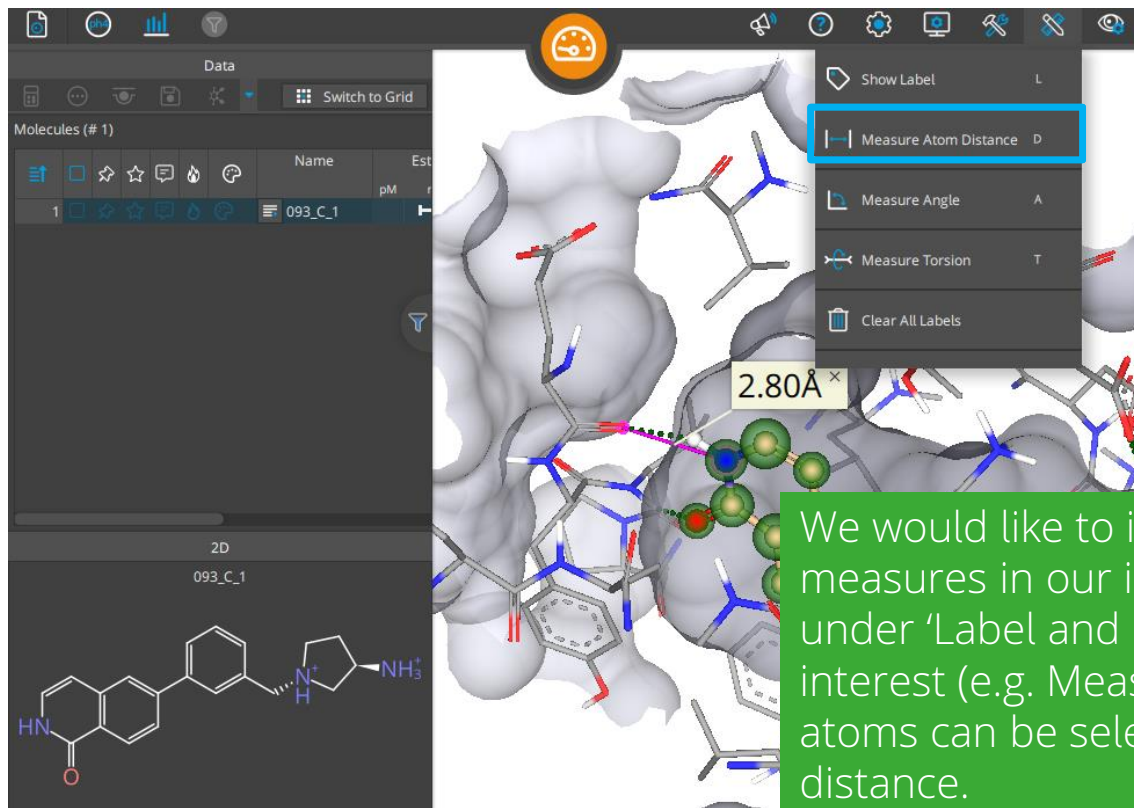
# Define a Scene



In our image, we would like to focus on hydrogen bond interactions:
In the Sequence View under the 'Show/hide residues' tab we toggle off all residues.
Next we like to show only those that are part of a protein-ligand hydrogen bond 'Show all interacting components'.
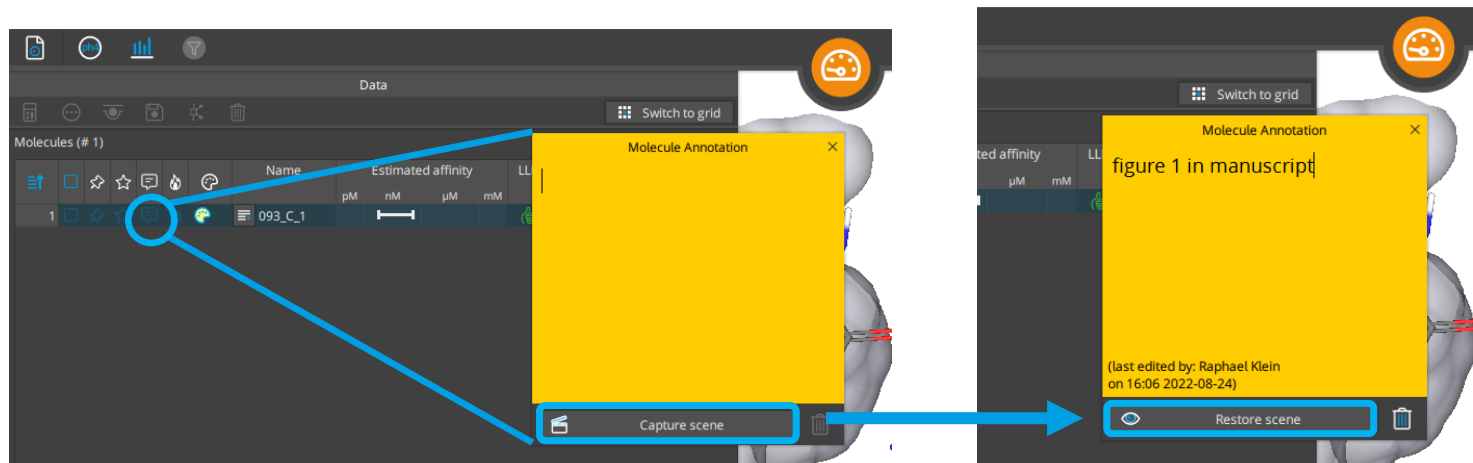
We would like to include some labels or measures in our image. Therefore we enable under 'Label and measure' the functionality of interest (e.g. Measure Atom Distance). In 3d two atoms can be selected to measure their distance.

# Capture a Scene



Within SeeSAR a specific Scene can be arranged and captured within the 'Molecule Annotation' box. A scene is defined as the 3d view of the protein-ligand complex with all settings like colors, view of specific residues or cartoon toggled on/off, clipped binding site surface, etc. Later on exactly the same view and settings can be restored.

# Export a Scene
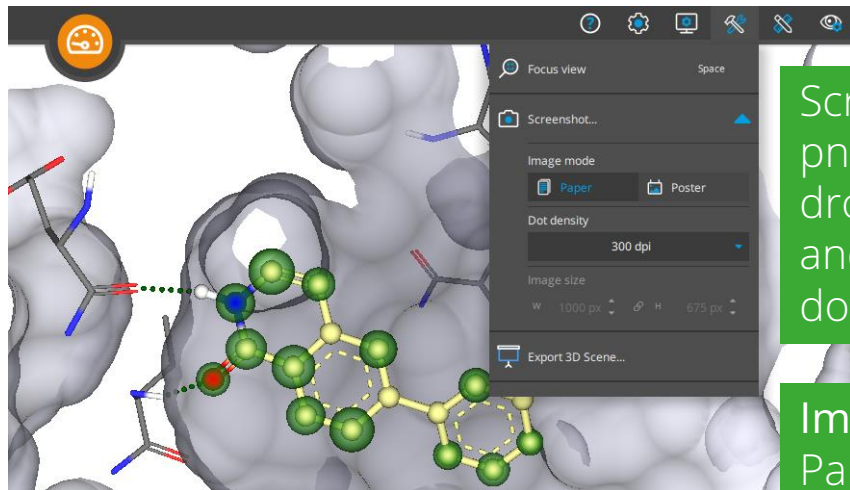


Screenshots of the Scene can be exported as png image file. Go to 'Utilities' and use the dropdown of Screenshots to adjust dot density and resolution. Most journals require a minimum dot density of 300 dpi.
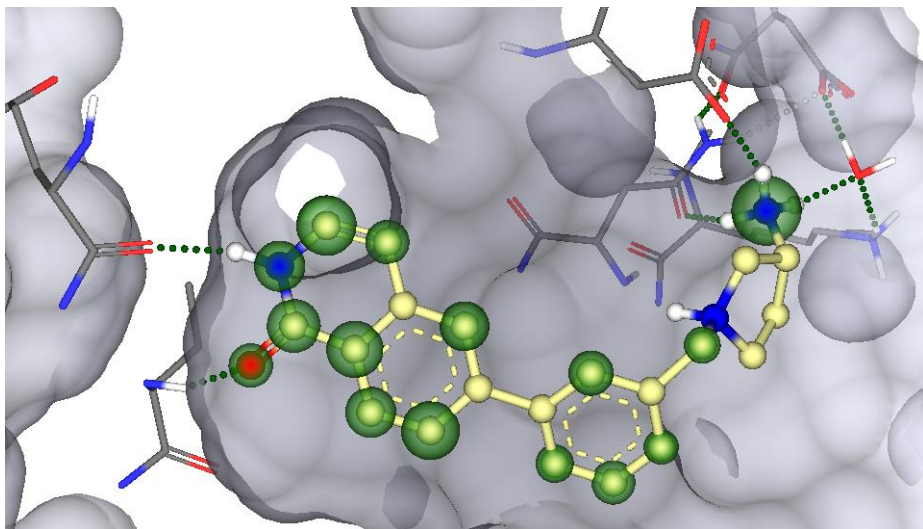
Image mode
Paper: Use current resolution and capture labels
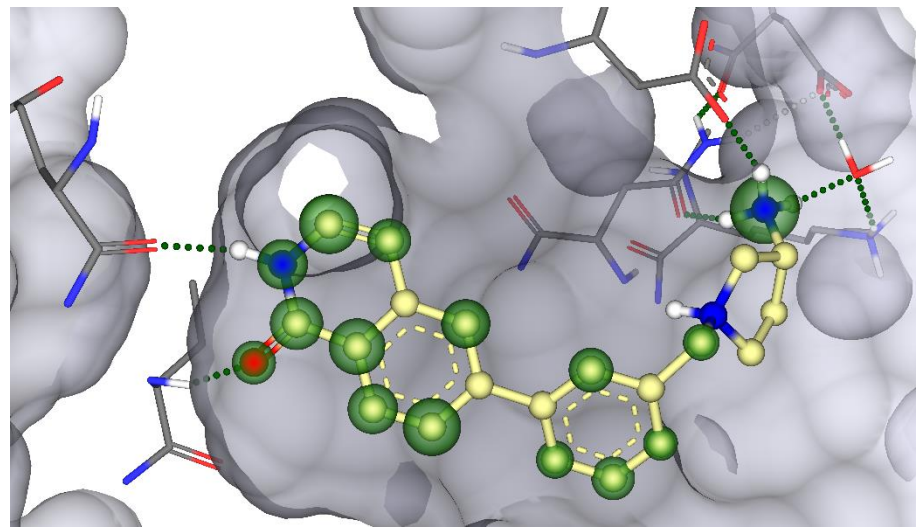Poster: Use custom resolution and don't capture labels.
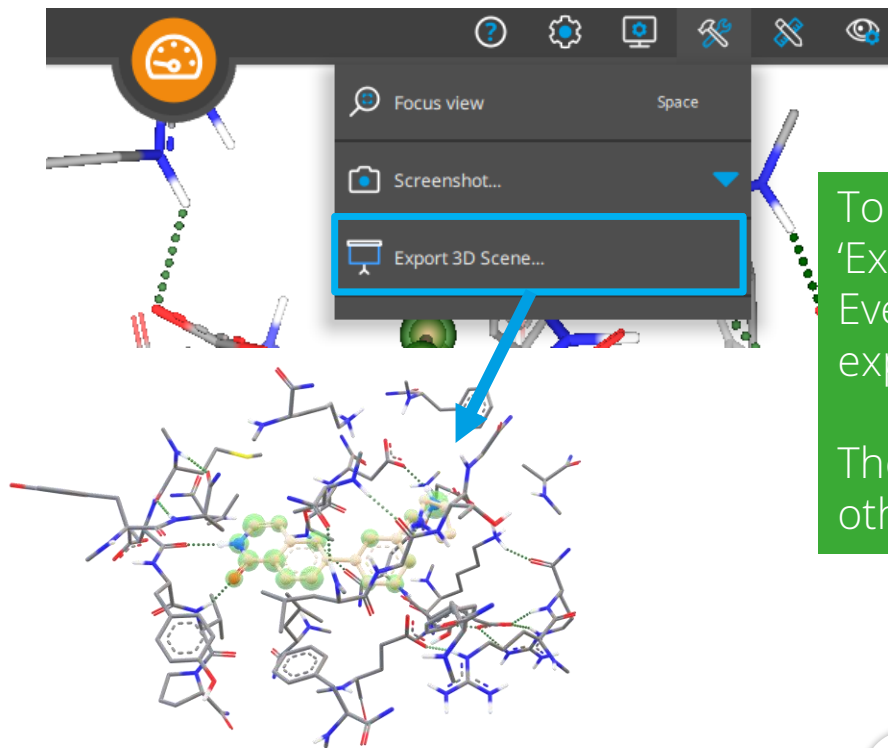Image size (check journal guidelines):
px x dpi = mm

300 dpi
1241px · 787px

300 dpi
8000px · 5073px

# 3D Export

To create a 3D model of your complex select 'Export 3D Scene' in the Utilities menu. Everything visible in the 3D window will be exported to the 3D Model.

The glb file can be used in presentations and other interfaces that support the format.