Date: 04-03-22

WEBLEM 5

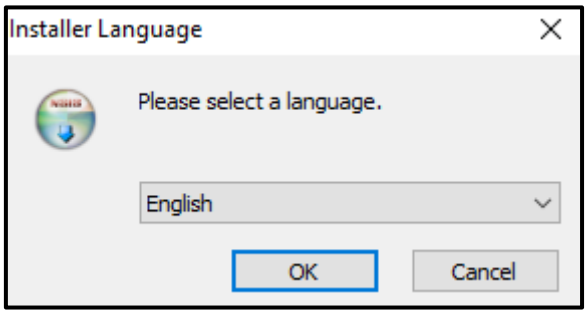
Introduction to Visualization of Tertiary structure using RASMOL & PyMOL

We can obtain all the available information about the 3D structure of this enzyme by browsing through the links or download the PDB file to a local directory in our computer and work with our preferred molecular modelling and visualization package.

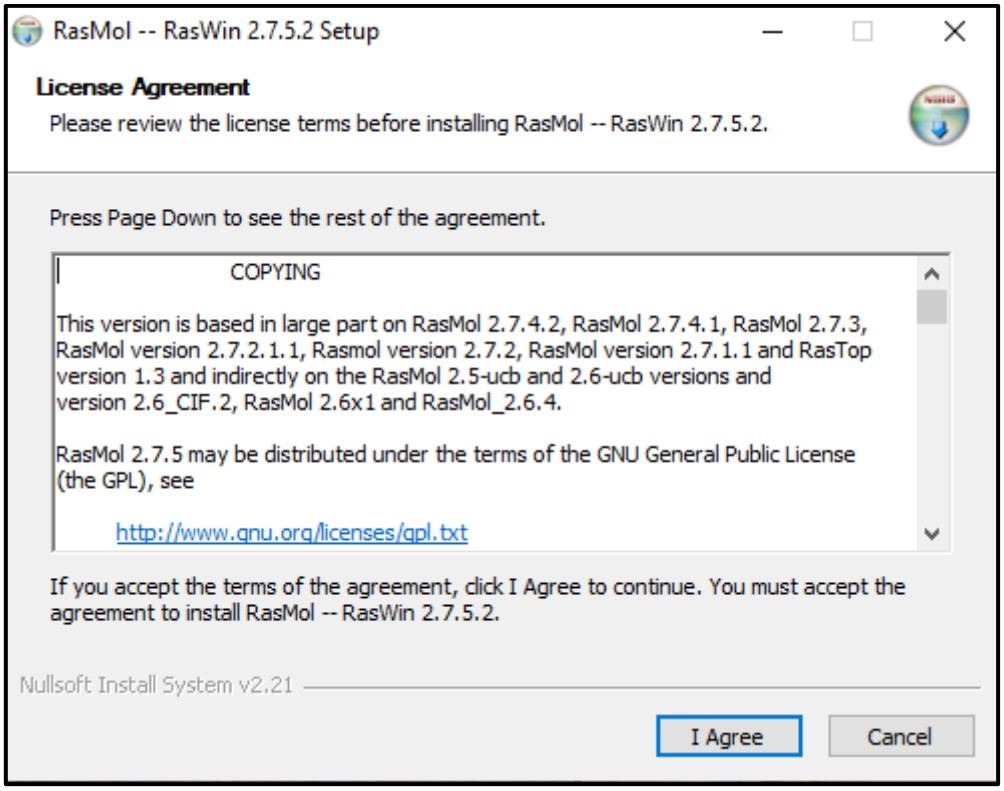
RasMol:

RasMol is a computer program written for molecular graphics visualization intended and used primarily for the depiction and exploration of biological macromolecule structures, such as those found in the Protein Data Bank. It was originally developed by Roger Sayle in the early 90s. Historically, it was an important tool for molecular biologists since the extremely optimized program allowed the software to run on (then) modestly powerful personal computers. Before RasMol, visualization software ran on graphics workstations that, due to their expense, were less accessible to scholars. RasMol has become an important educational tool as well as continuing to be an important tool for research in structural biology.

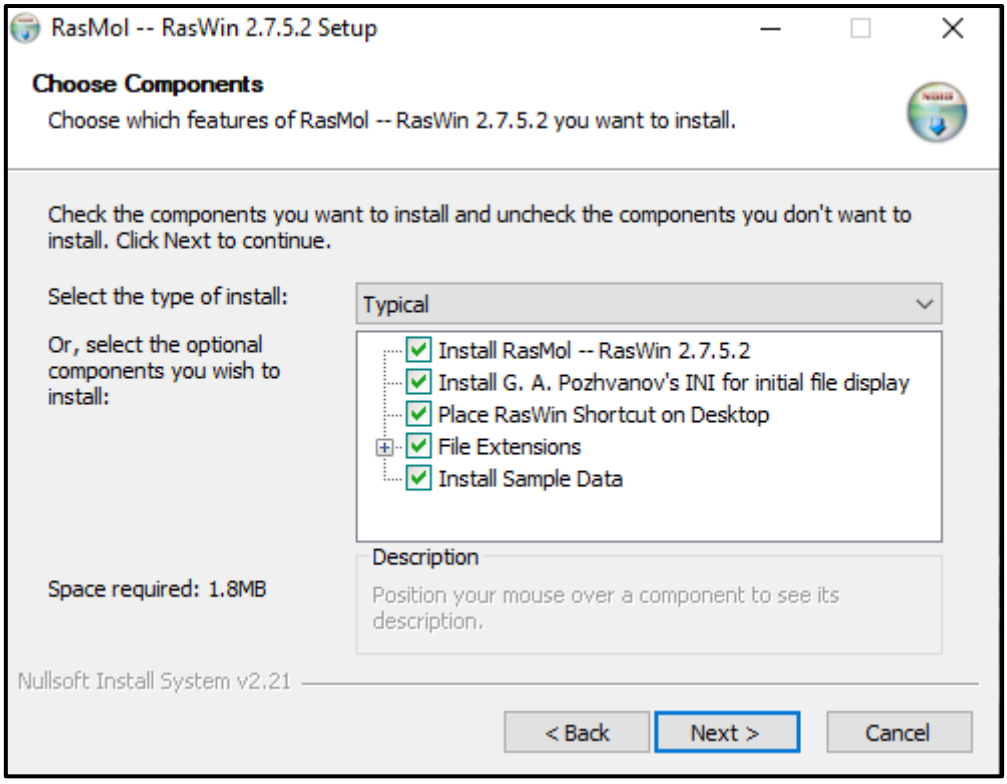
Installation:



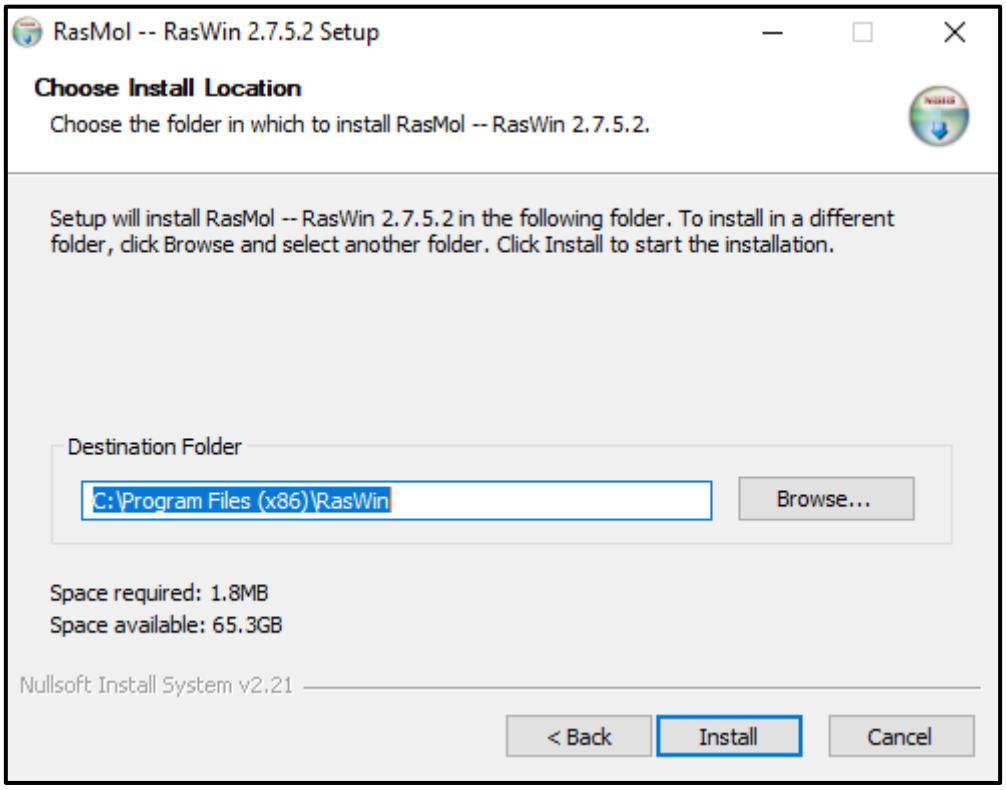
Select language and proceed



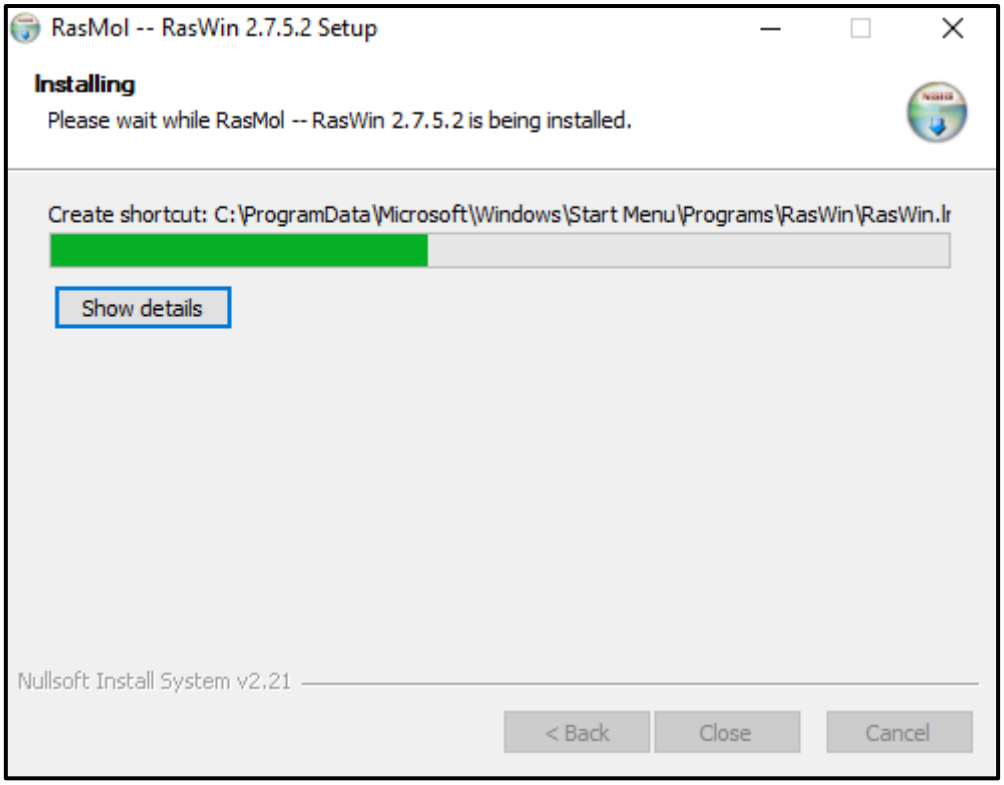
Read the License Agreement and click "I Agree" to proceed



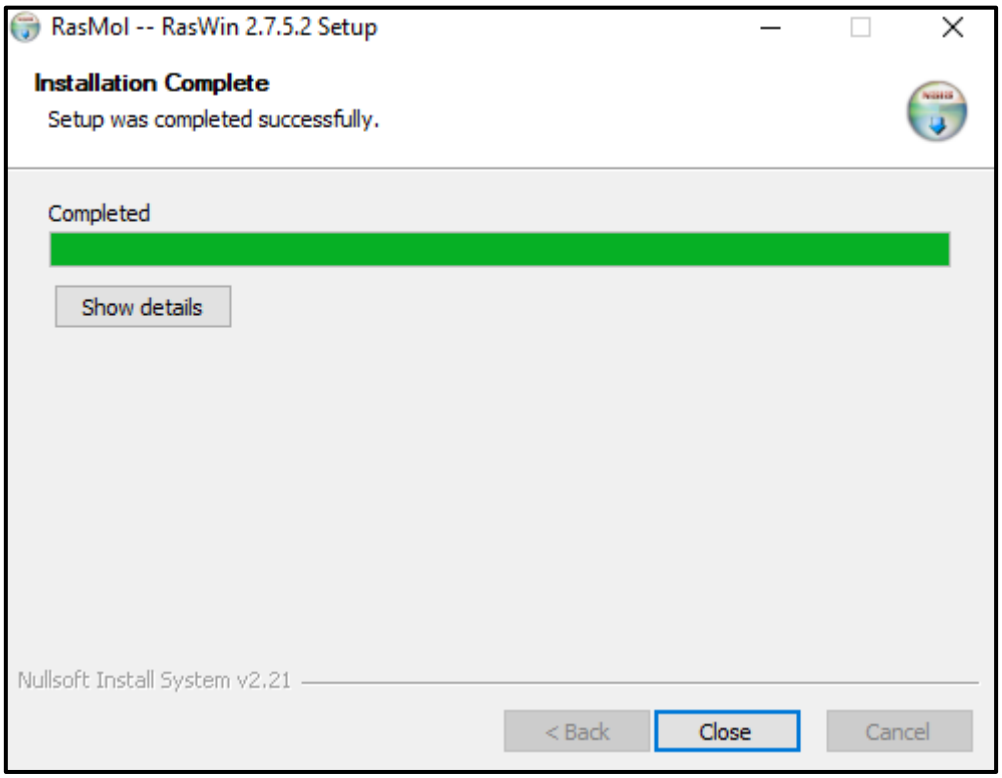
Select the components of RasMol you want to install and click “Next” to proceed



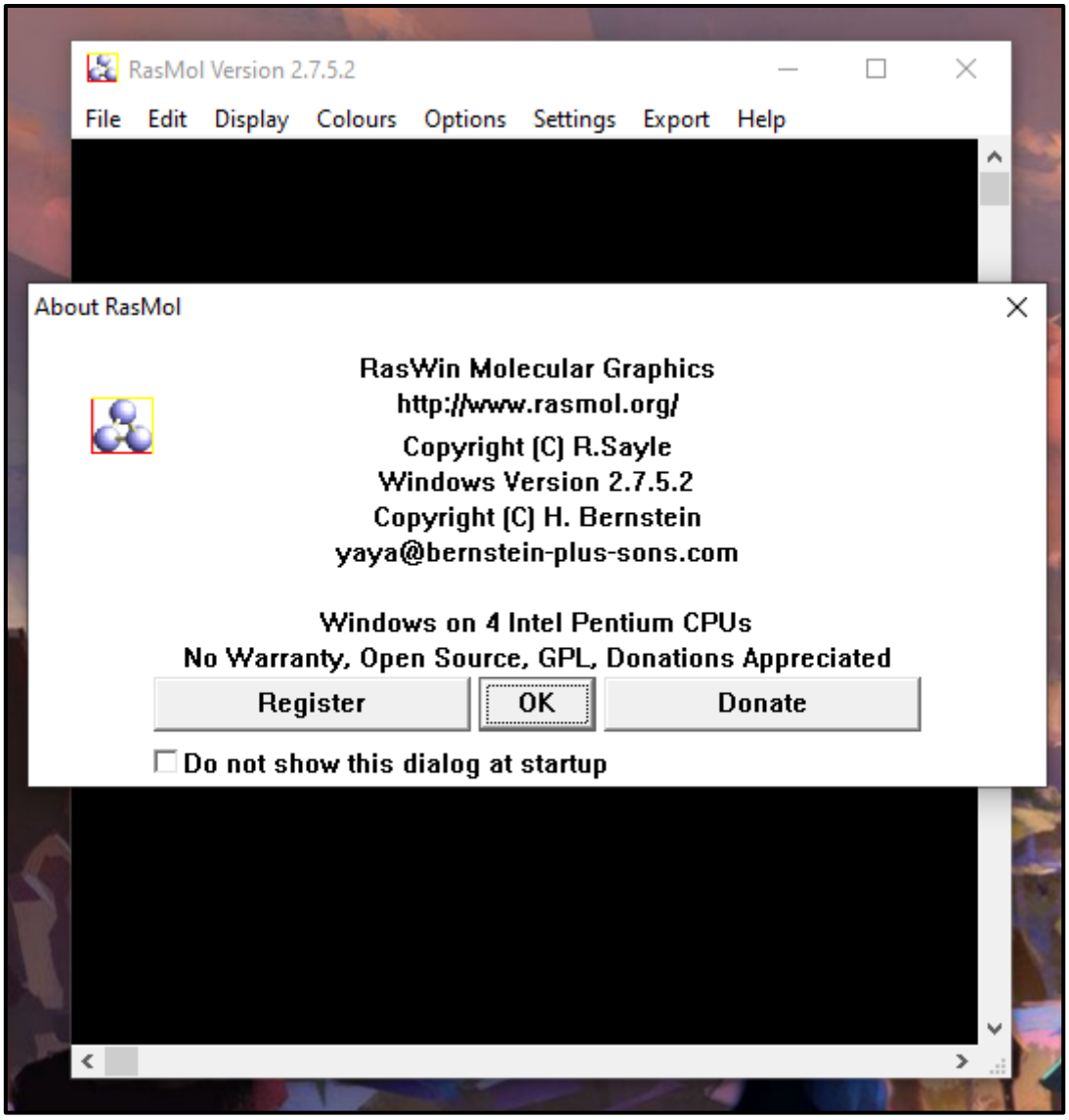
Select the directory in which you want to install RasMol and click “Install” to proceed



The software will now install



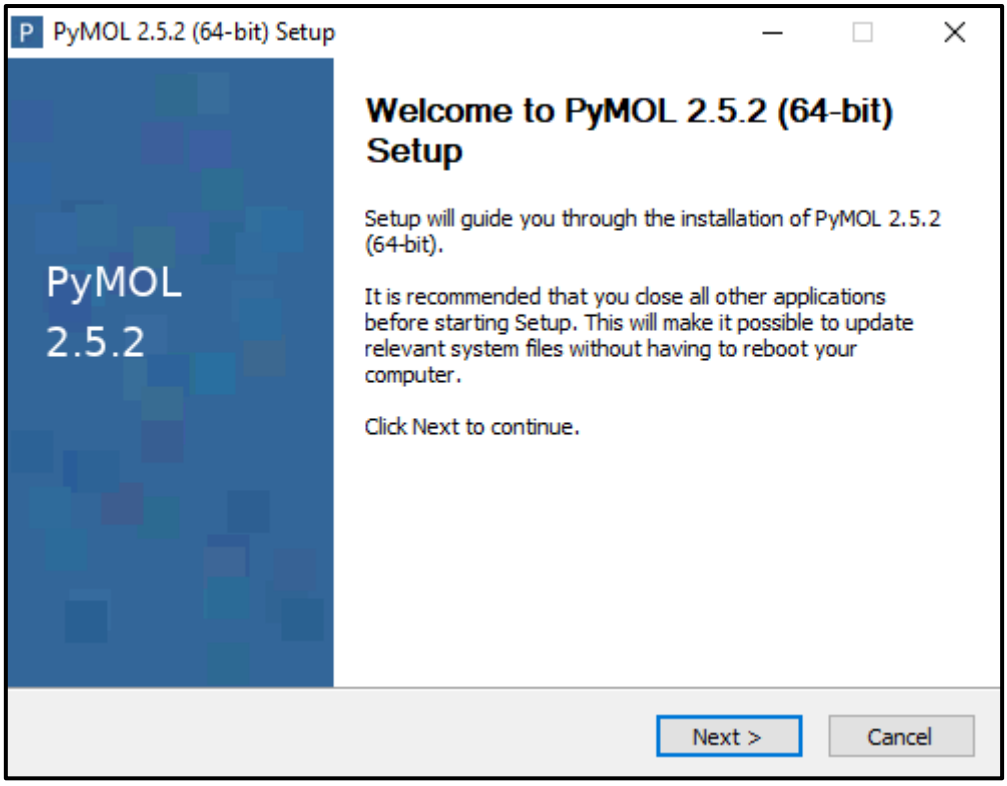
Close the installer after the install is completed



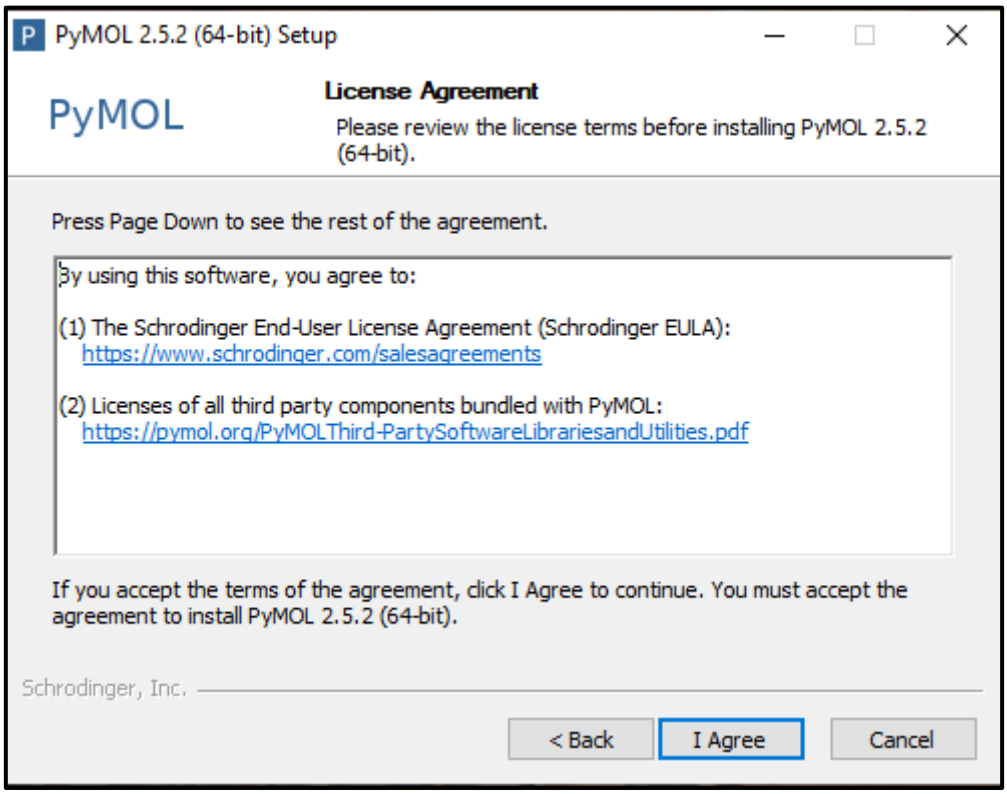
RasMol is now installed

PyMol

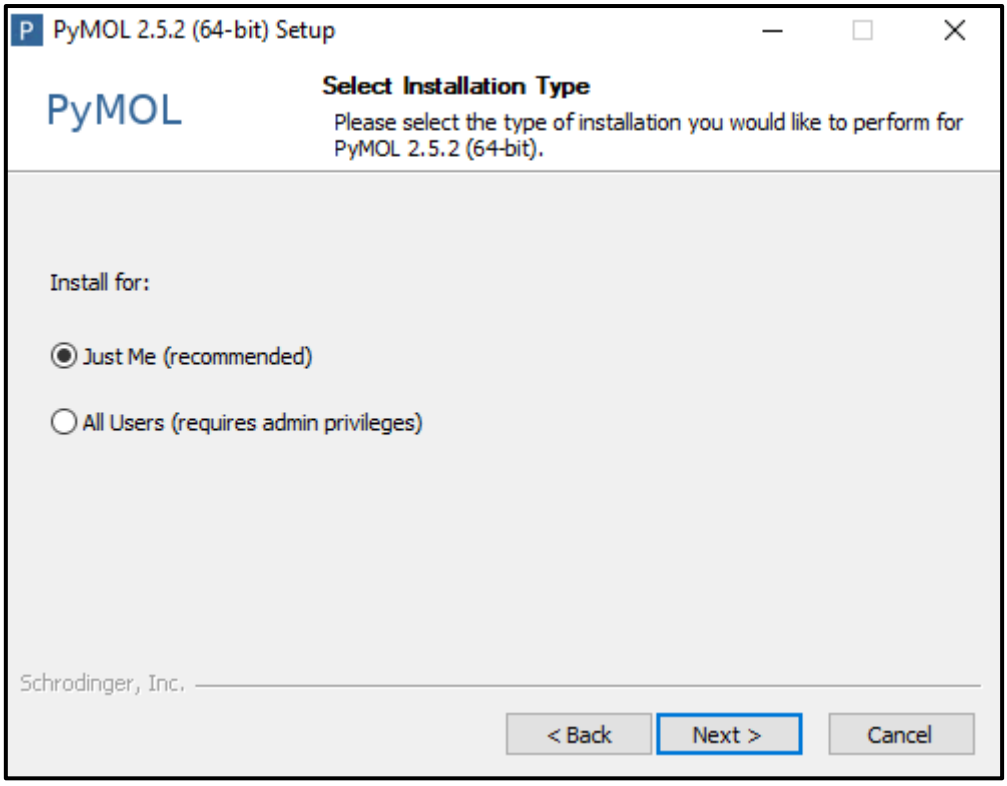
PyMOL, a cross-platform molecular graphics tool, has been widely used for three-dimensional (3D) visualization of proteins, nucleic acids, small molecules, electron densities, surfaces, and trajectories. It is also capable of editing molecules, ray tracing, and making movies. This Python-based software, alongside many Python plugin tools, has been developed to enhance its utilities and facilitate the drug design in PyMOL. To gain an insightful view of useful drug design tools and their functions in PyMOL, we present an extensive discussion on various molecular modeling modules in PyMOL, covering those for visualization and analysis enhancement, protein–ligand modeling, molecular simulations, and drug screening.



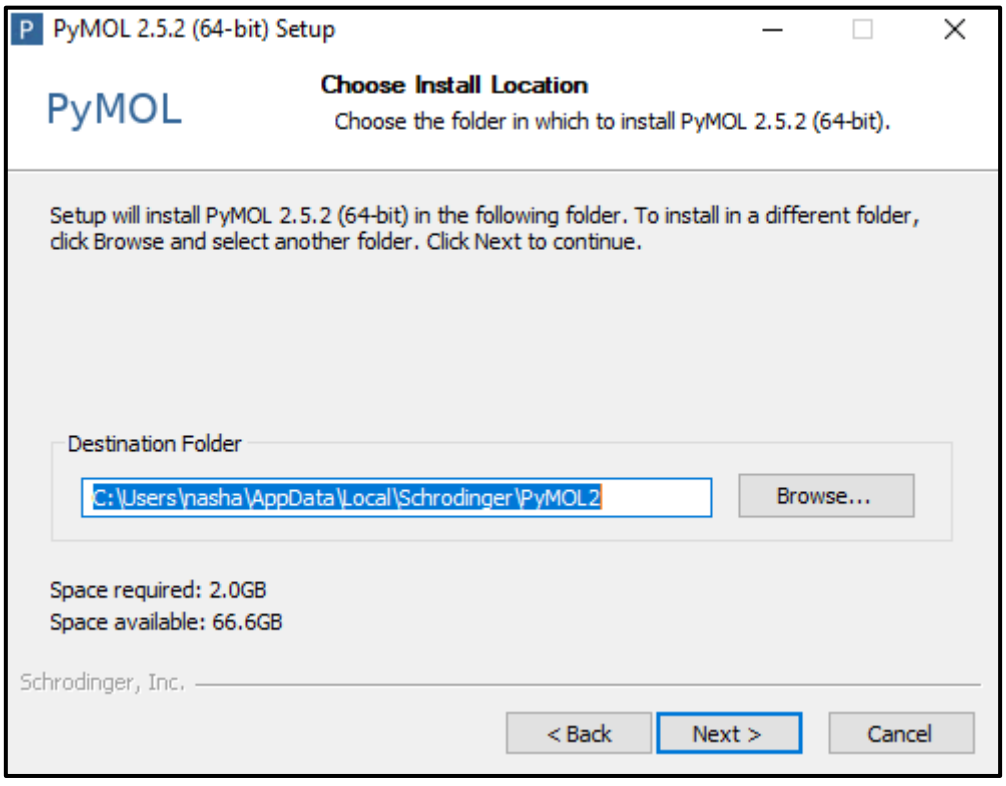
Download and run the installer. Click next to proceed



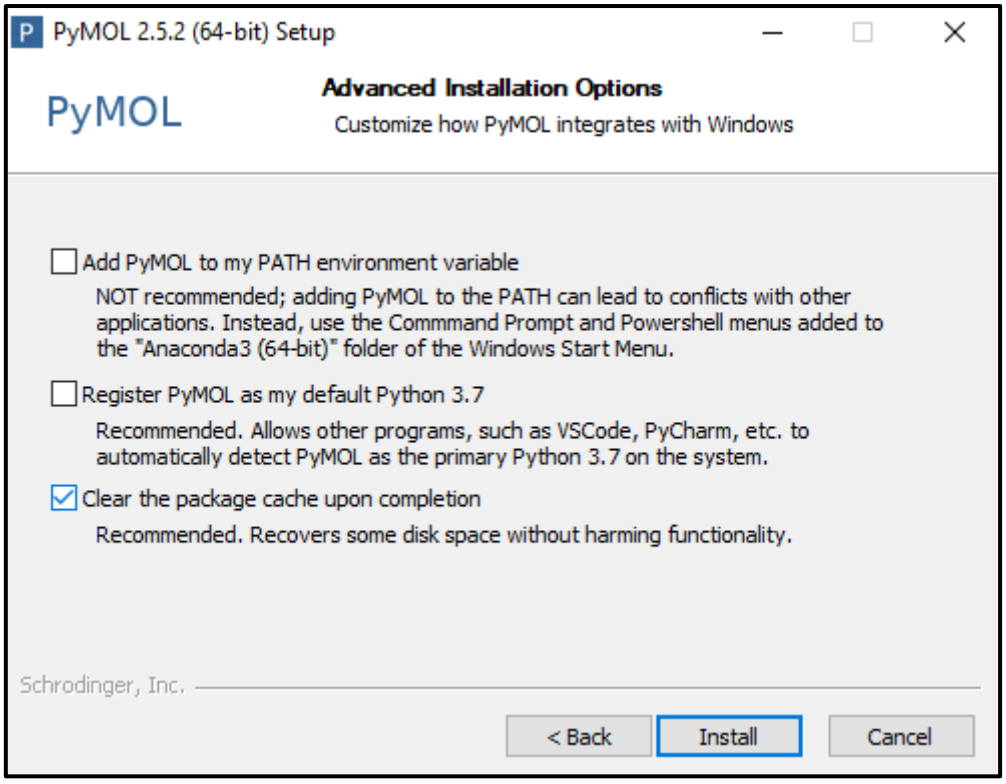
Read the License Agreement and click “I Agree” to proceed



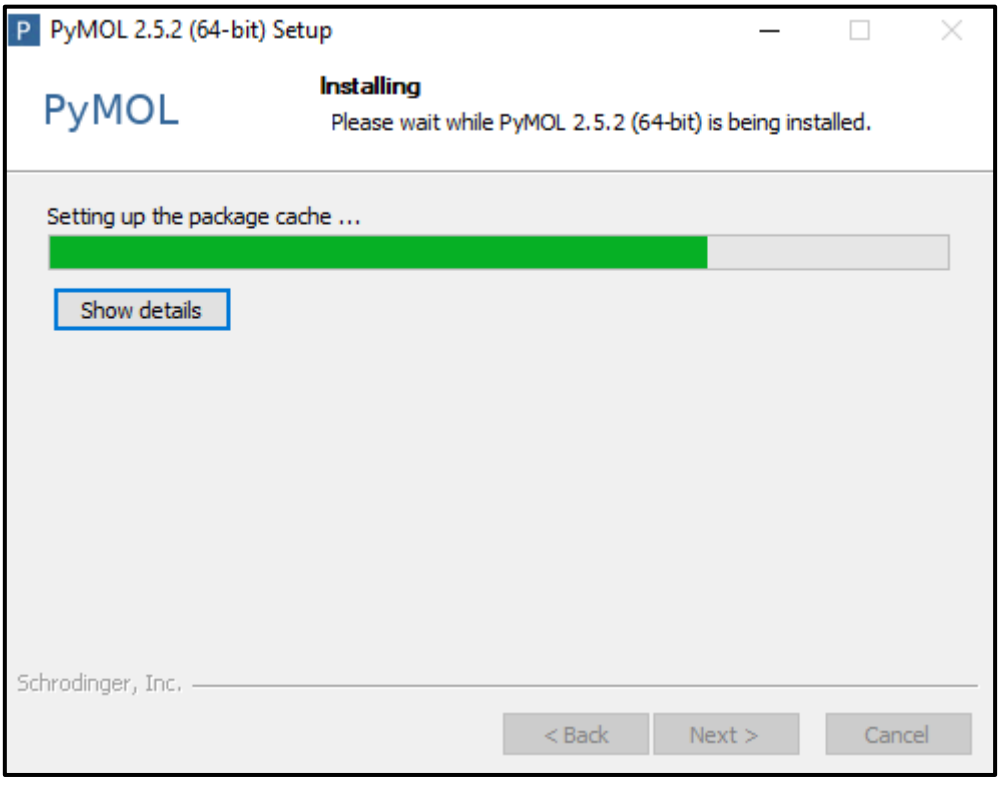
Select the Installation type and click “Next” to proceed



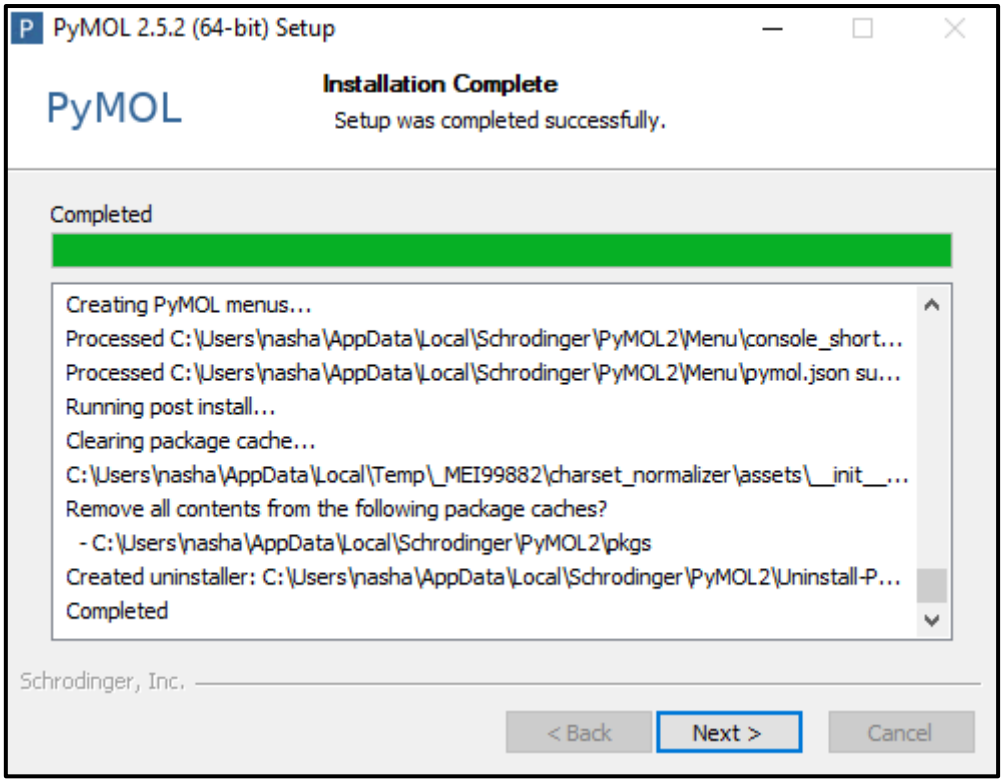
Select the Directory in which you want to install PyMol



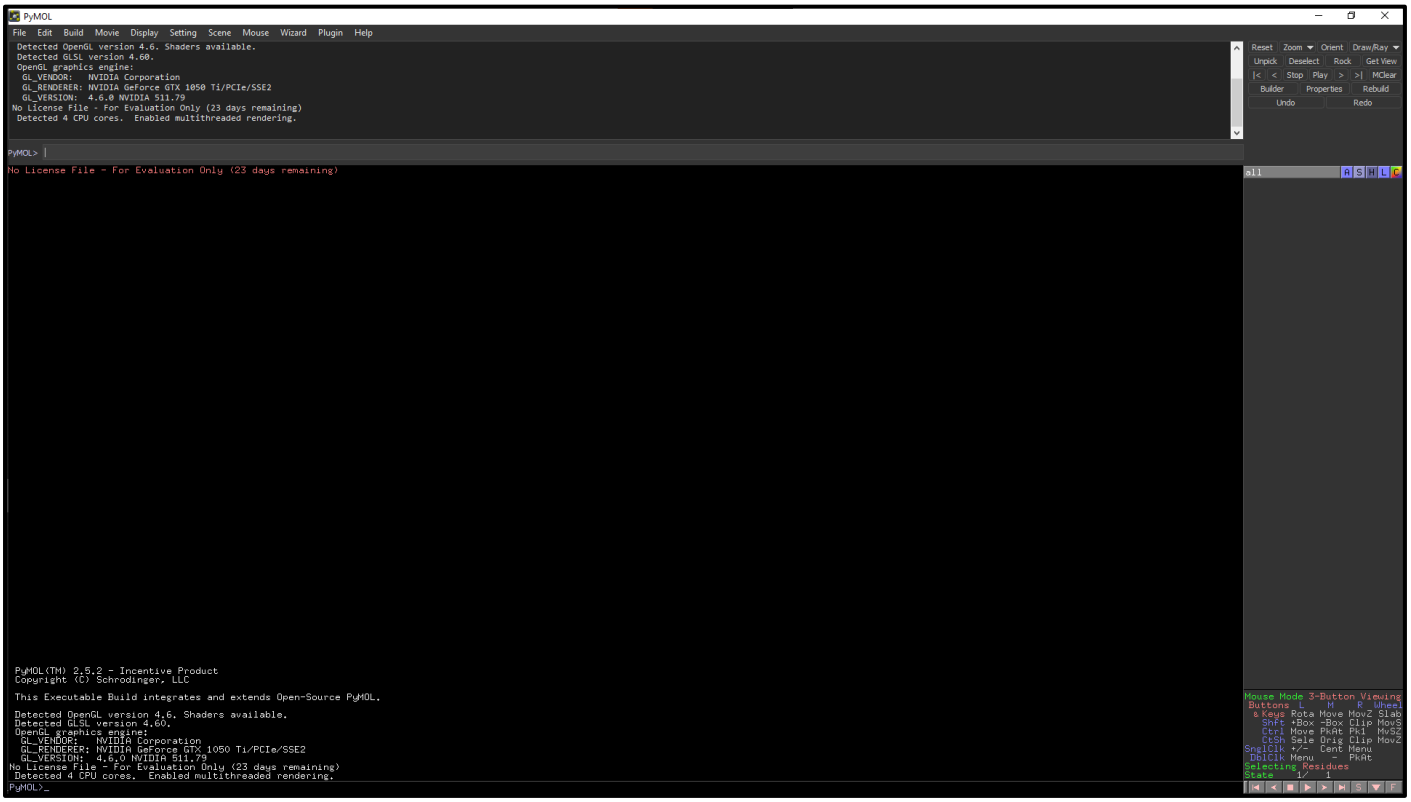
Select the additional options if you want to and click “Install” to start the installation of PyMol



Let the installer install PyMol



After completion click on “Next” to finalize installation



Pymol is now installed

Date: 04-03-22

WEBLEM 6A

To visualize 3D structure of Hemoglobin (1SI4) using RASMOL & PyMOL tool

RASMOL:

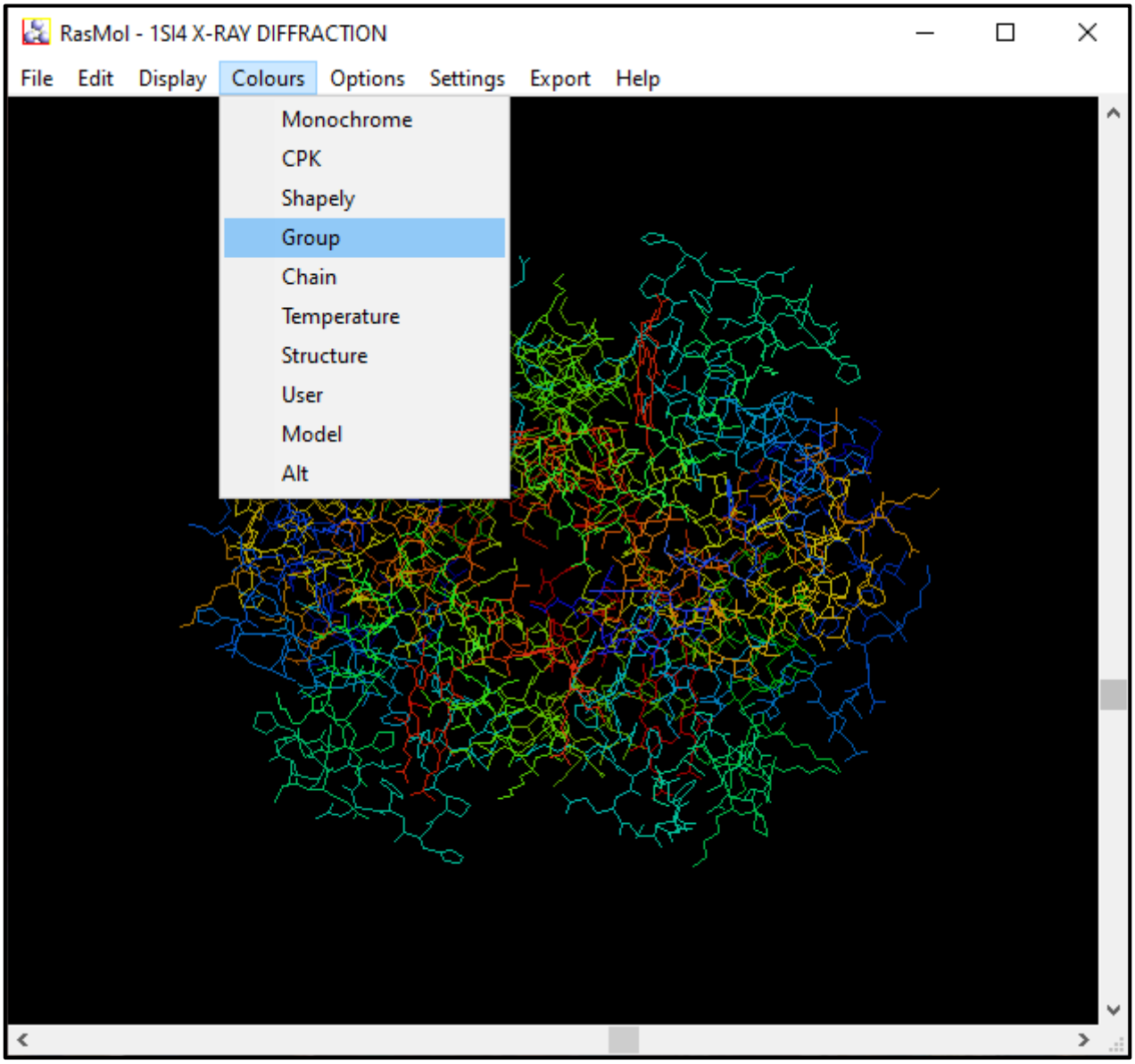


Fig1. PDB Structure of Hemoglobin (1SI4) loaded in RasMol to show it in 3D space with the colour scheme set to Groups

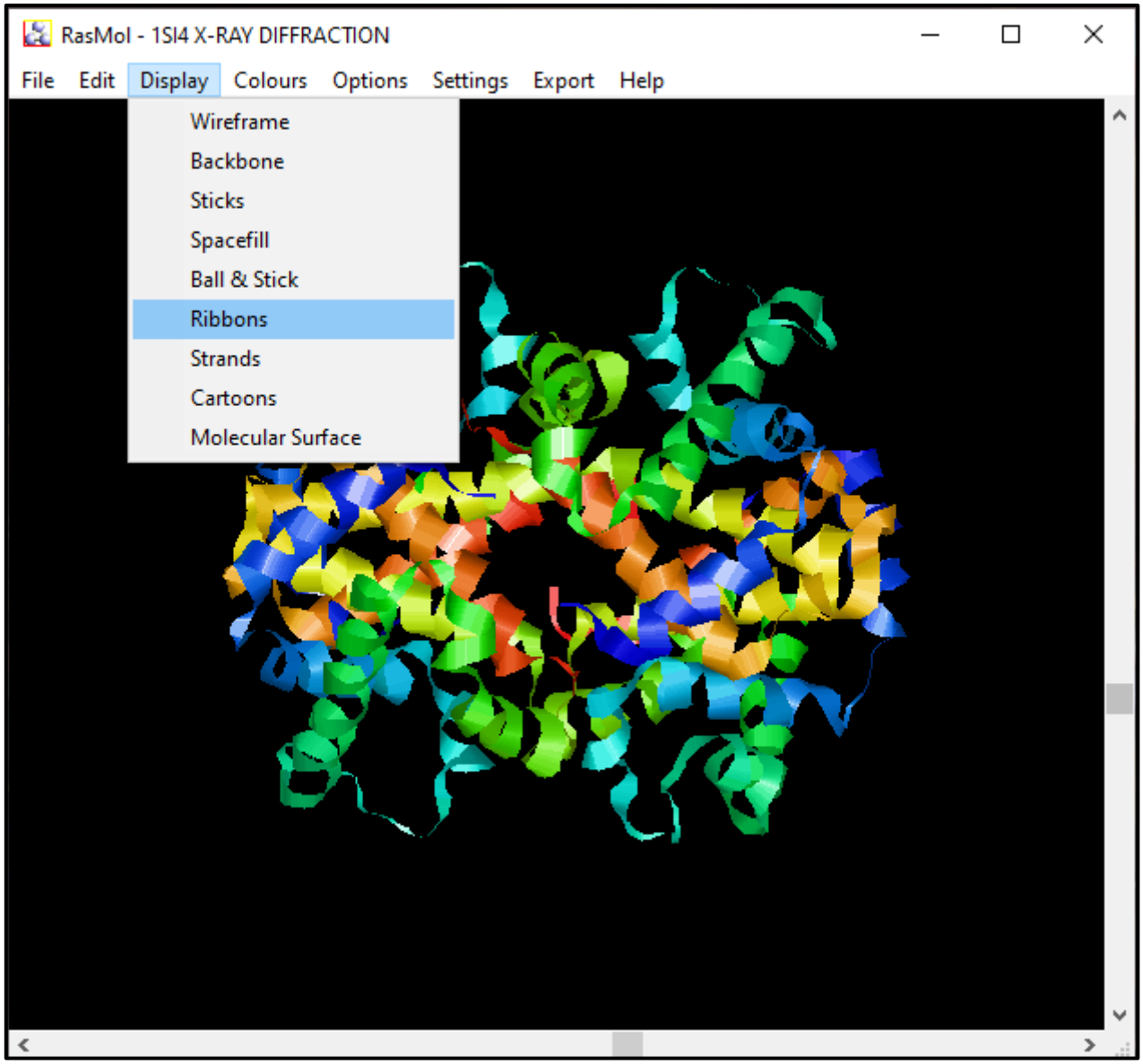


Fig2. PDB structure of Hemoglobin (1SI4) Shown with the display mode set to ribbons

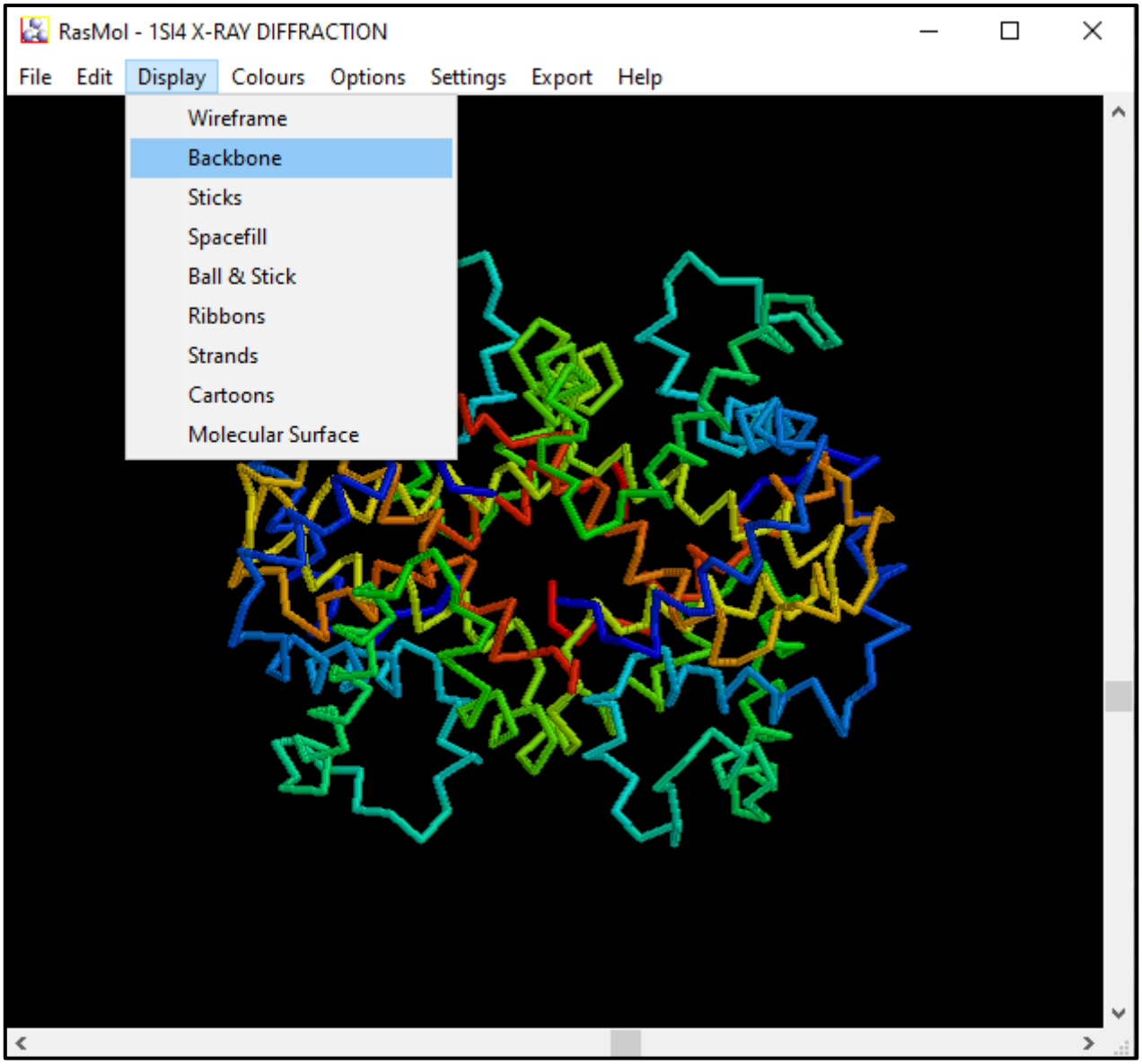


Fig3. PDB structure of Hemoglobin (1SI4) shown with display type set to Backbone

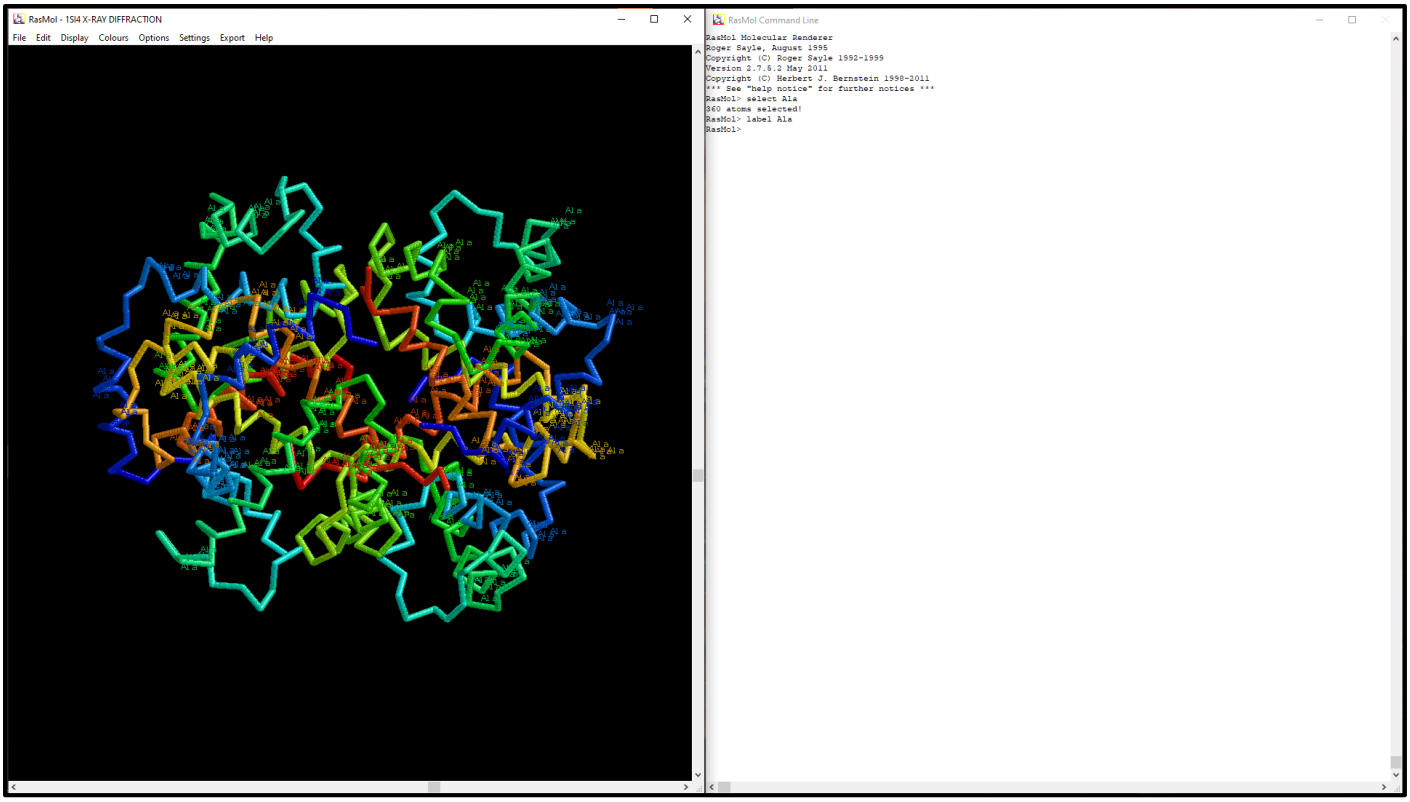


Fig.4 PDB Structure of Hemoglobin (1SI4) visualizing Alanine in the structure.

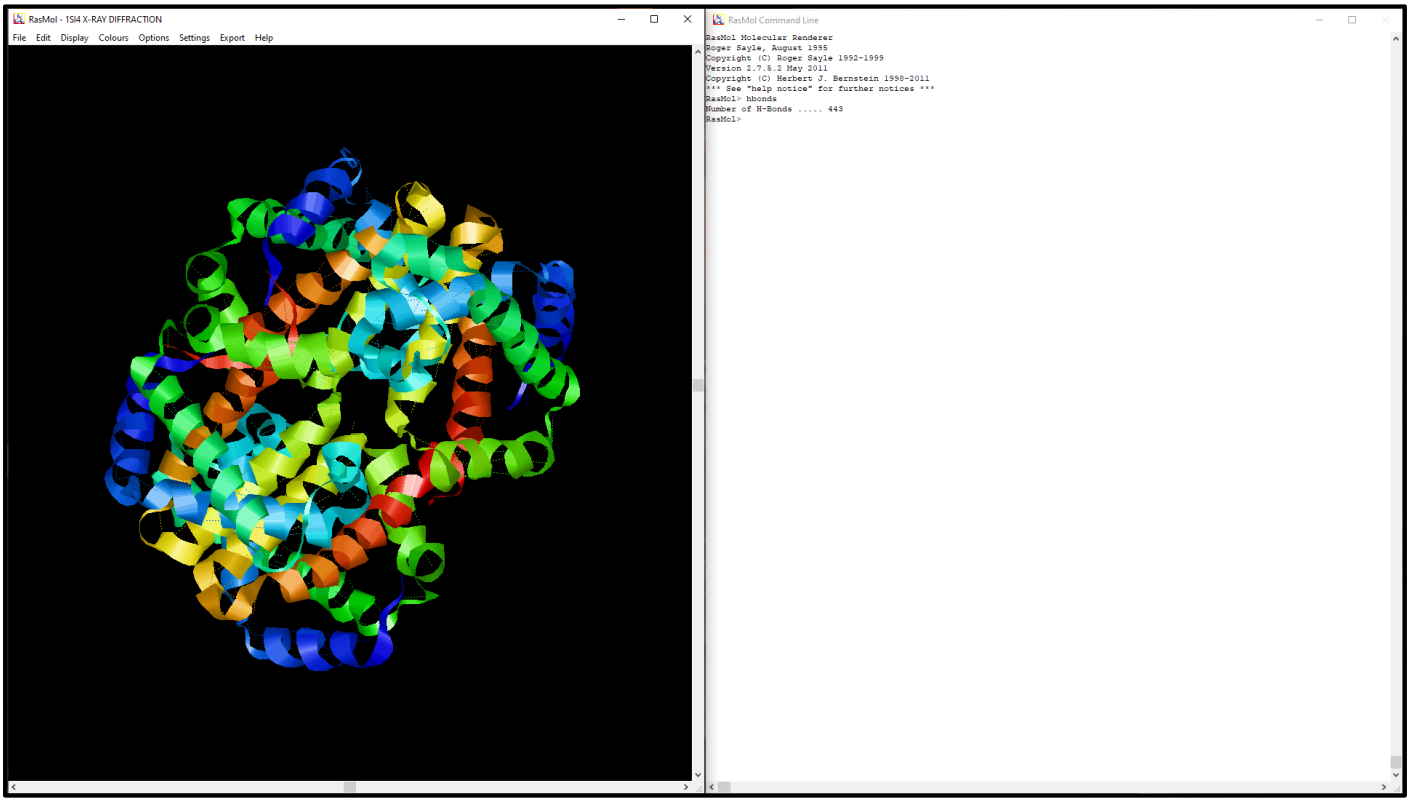


Fig5. PDB structure of Hemoglobin (1SI4) with Hydrogen Bonds visualized

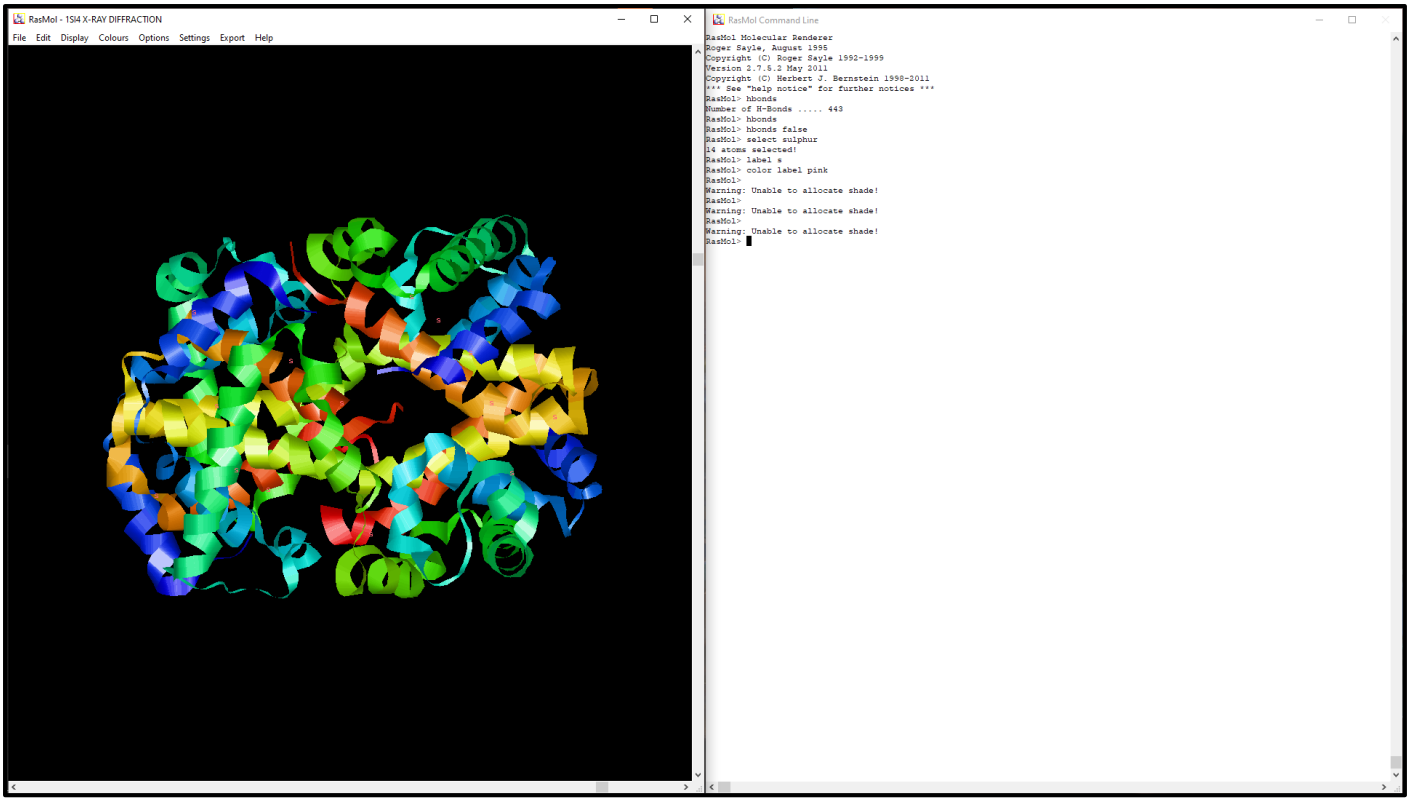


Fig6. PDB structure of Hemoglobin (1SI4) with sulphur atoms visualized with label “s”

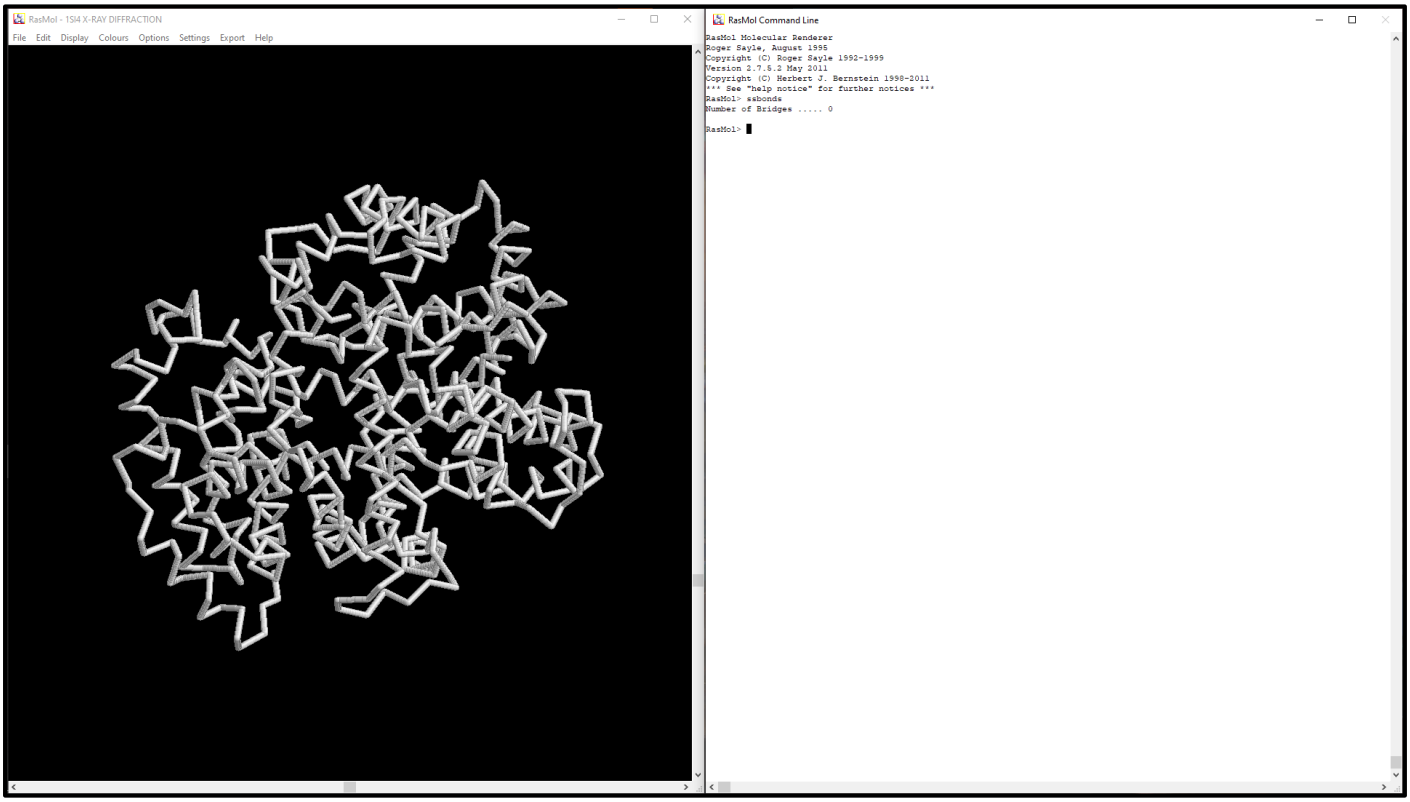


Fig7. PDB structure of Hemoglobin (1SI4) visualizing sulphuer-sulphur bonds (0 in this case)

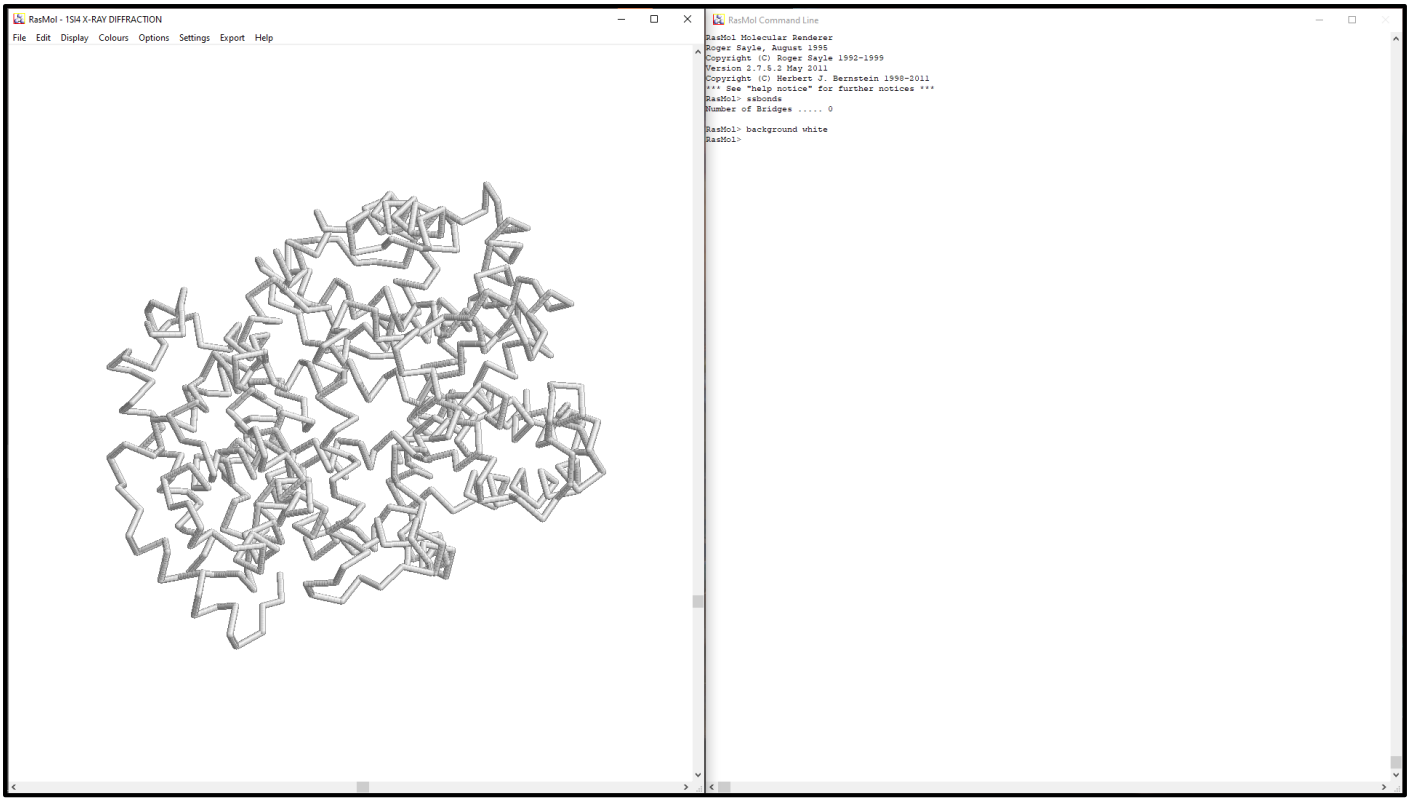


Fig8. PDB structure of Hemoglobin (1SI4) with the background color set to white to clearly see the sulphur-sulphur bonds (0 in this case)

PYMOL:

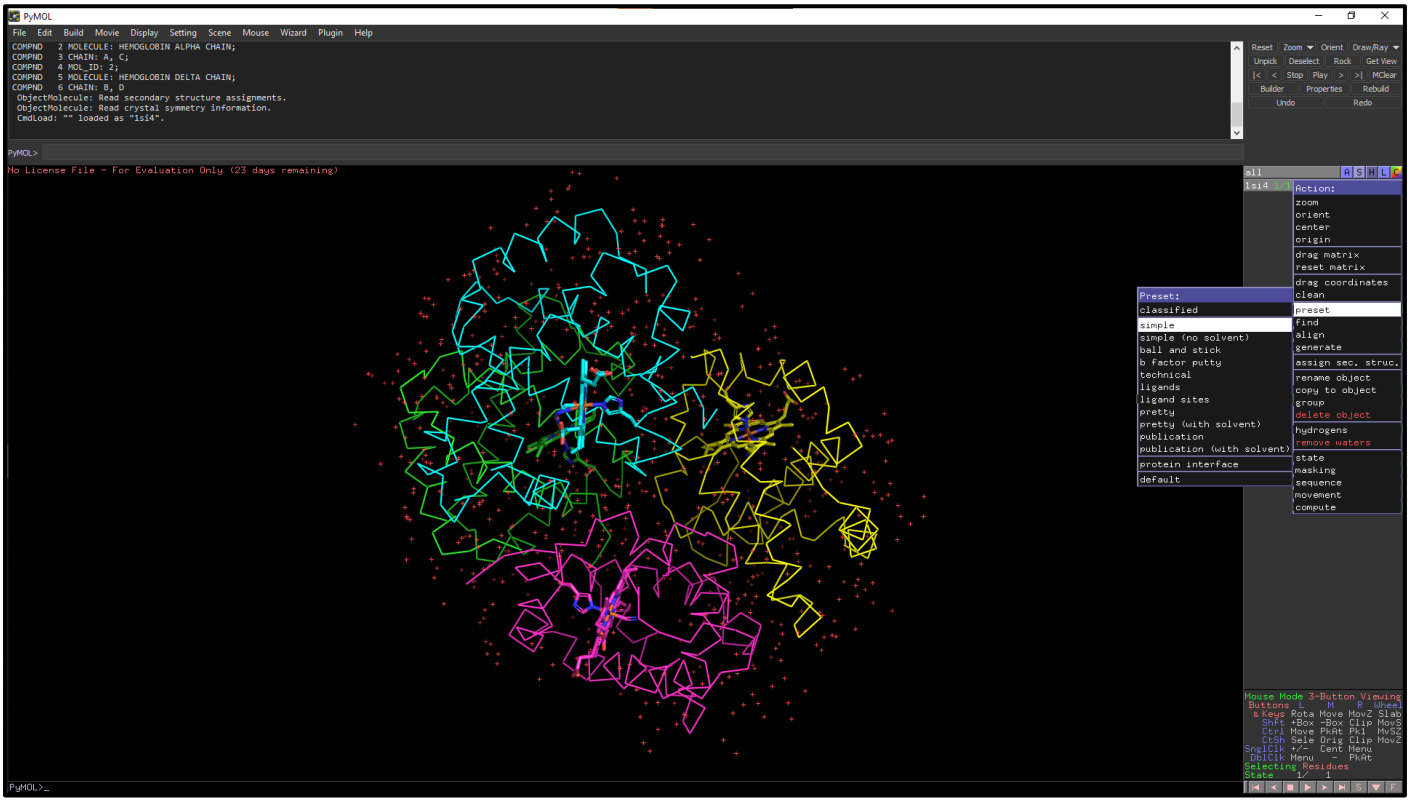


Fig9. PDB structure Hemoglobin (1SI4) loaded in PyMol and set to simple view preset

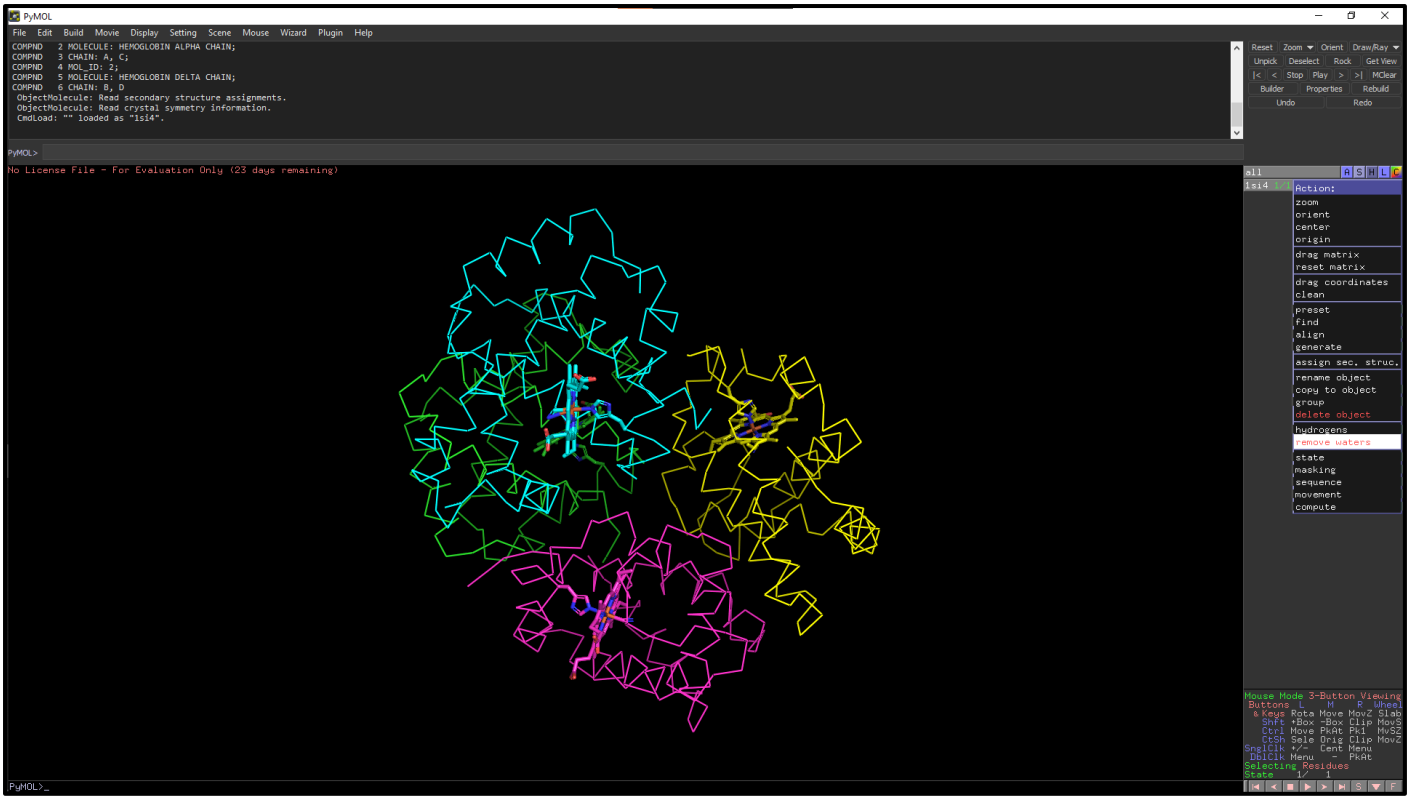


Fig10. PDB structure of Hemoglobin (1SI4) with waters removed

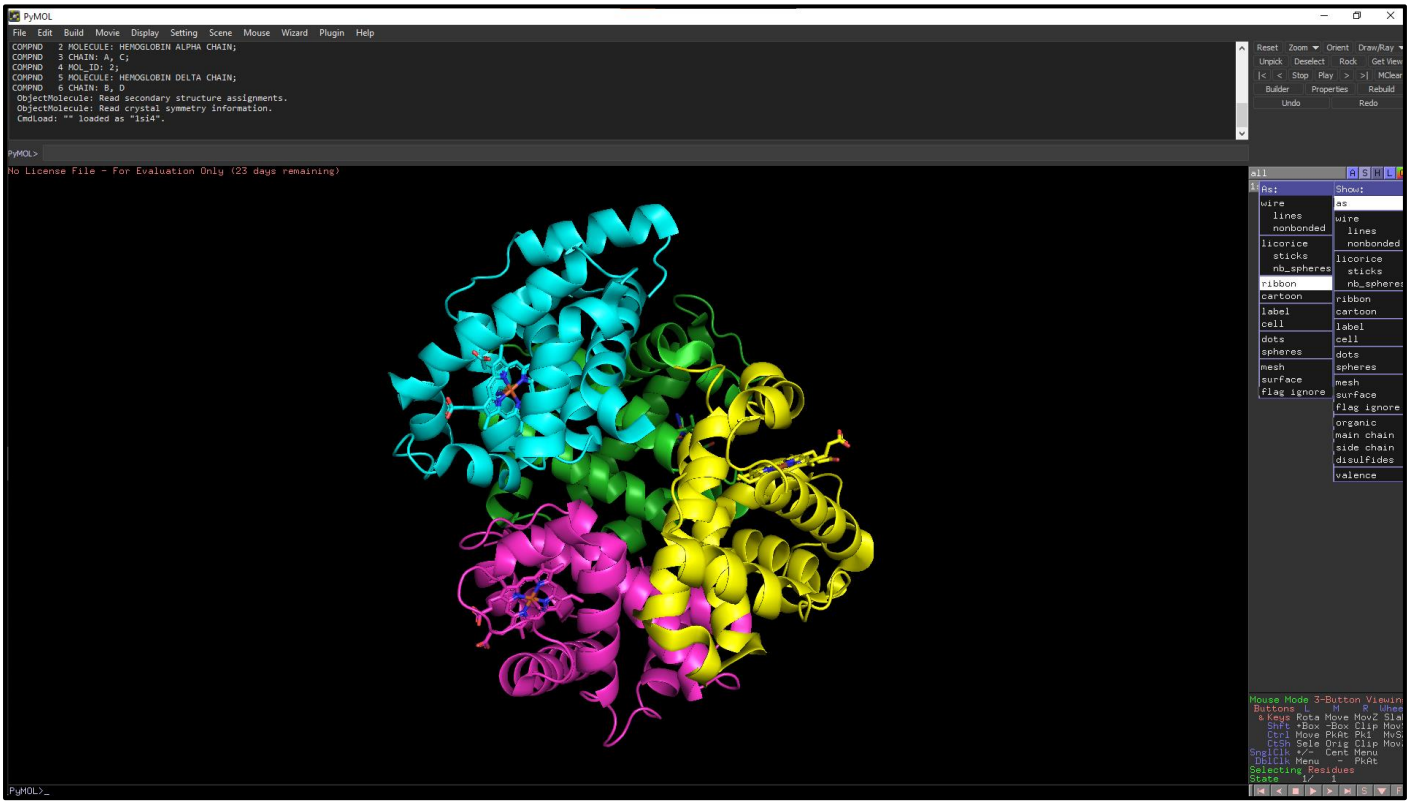


Fig11. PDB structure of Hemoglobin (1SI4) with visual style set to ribbon

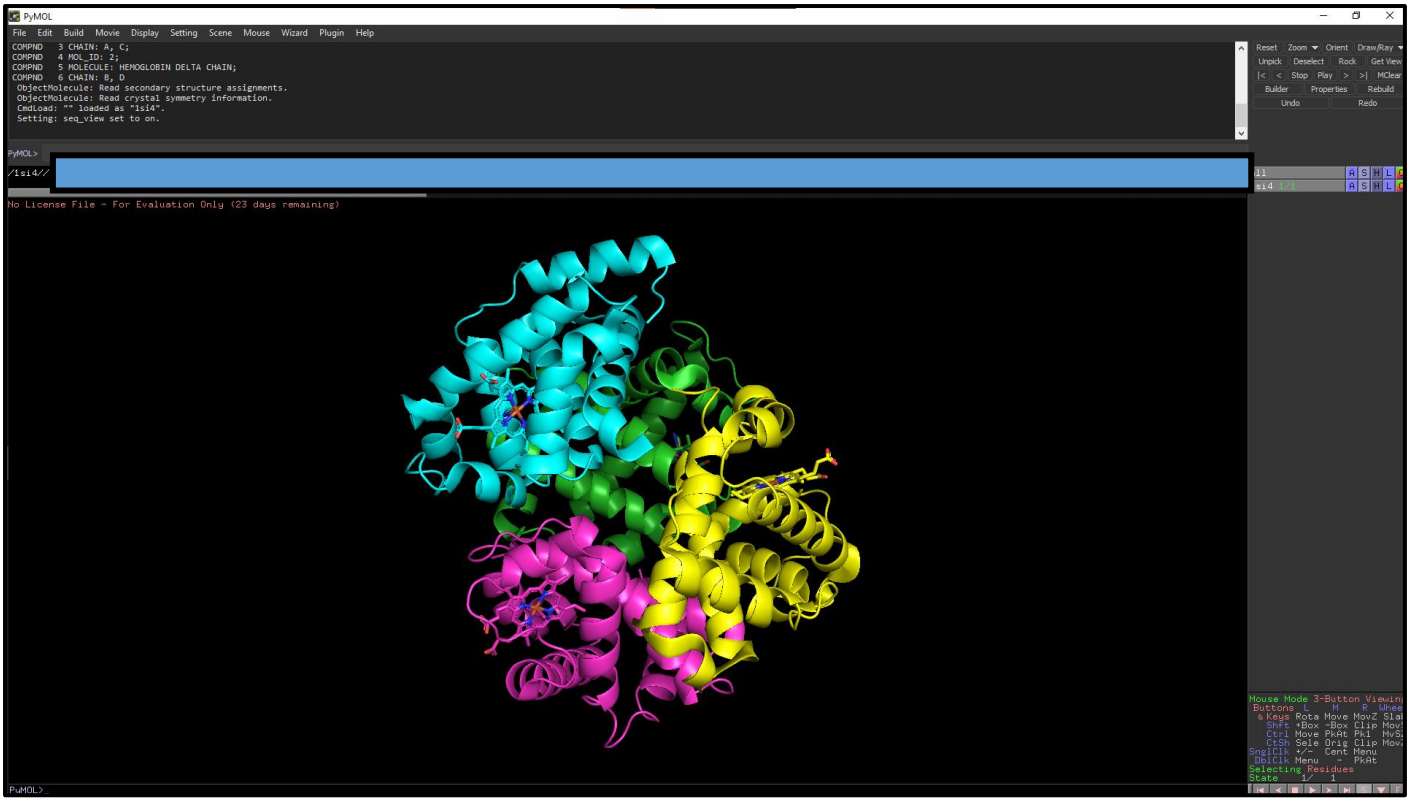


Fig12. PDB structure of Hemoglobin (1SI4) with the sequence displayed

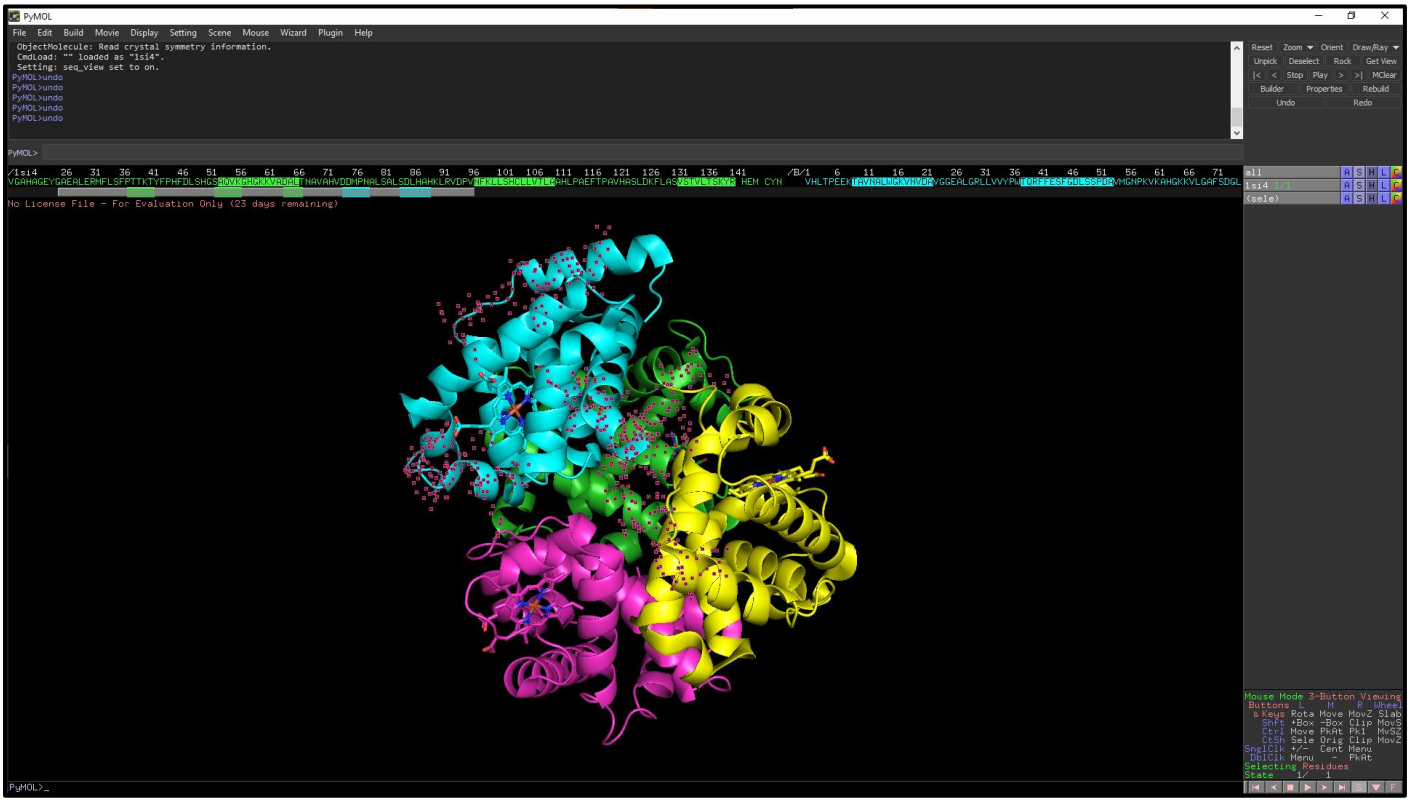


Fig13. PDB structure of Hemoglobin (1SI4) with random segments from sequence selected and visualized

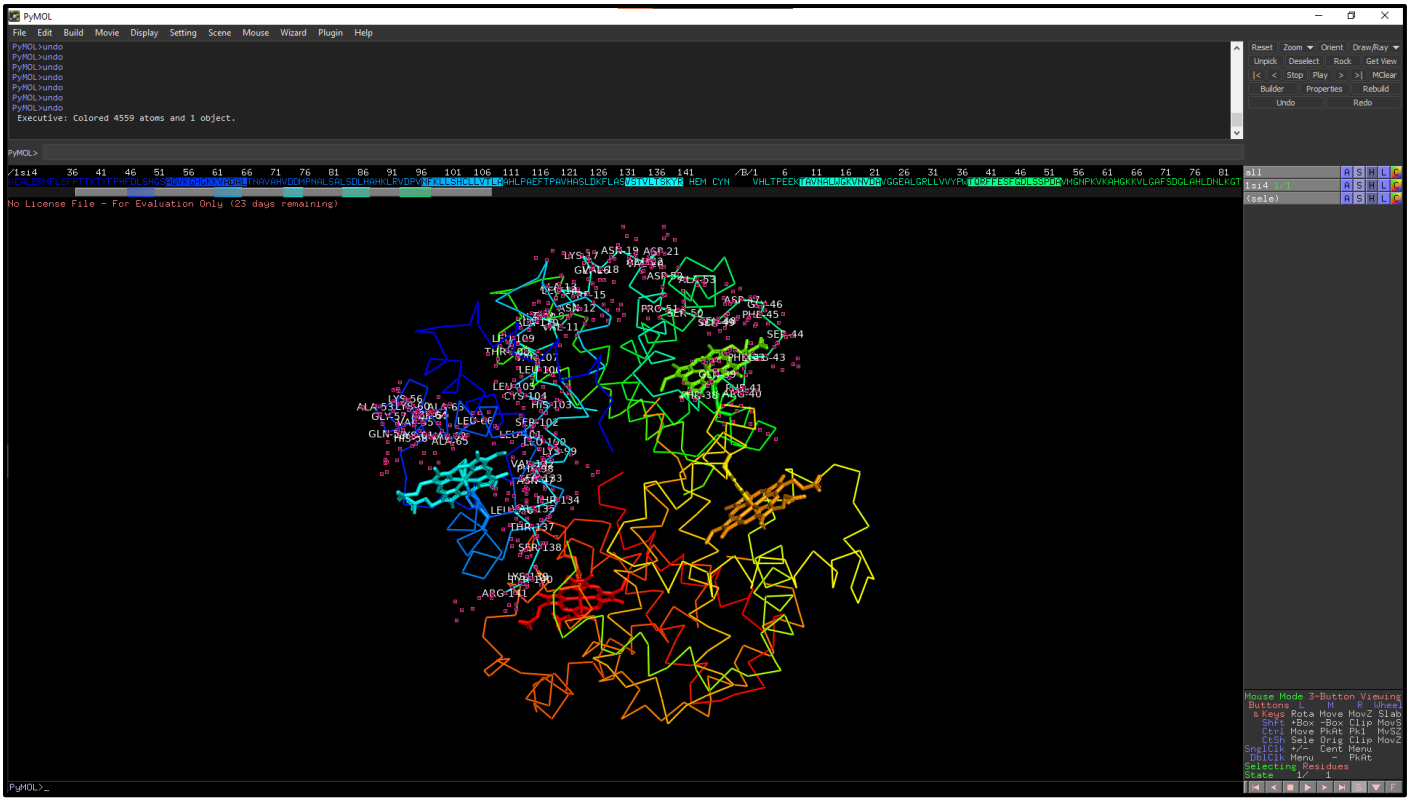


Fig14. PDB structure of Hemoglobin (1SI4) with the residues of the randomly selected segments from sequence visualized

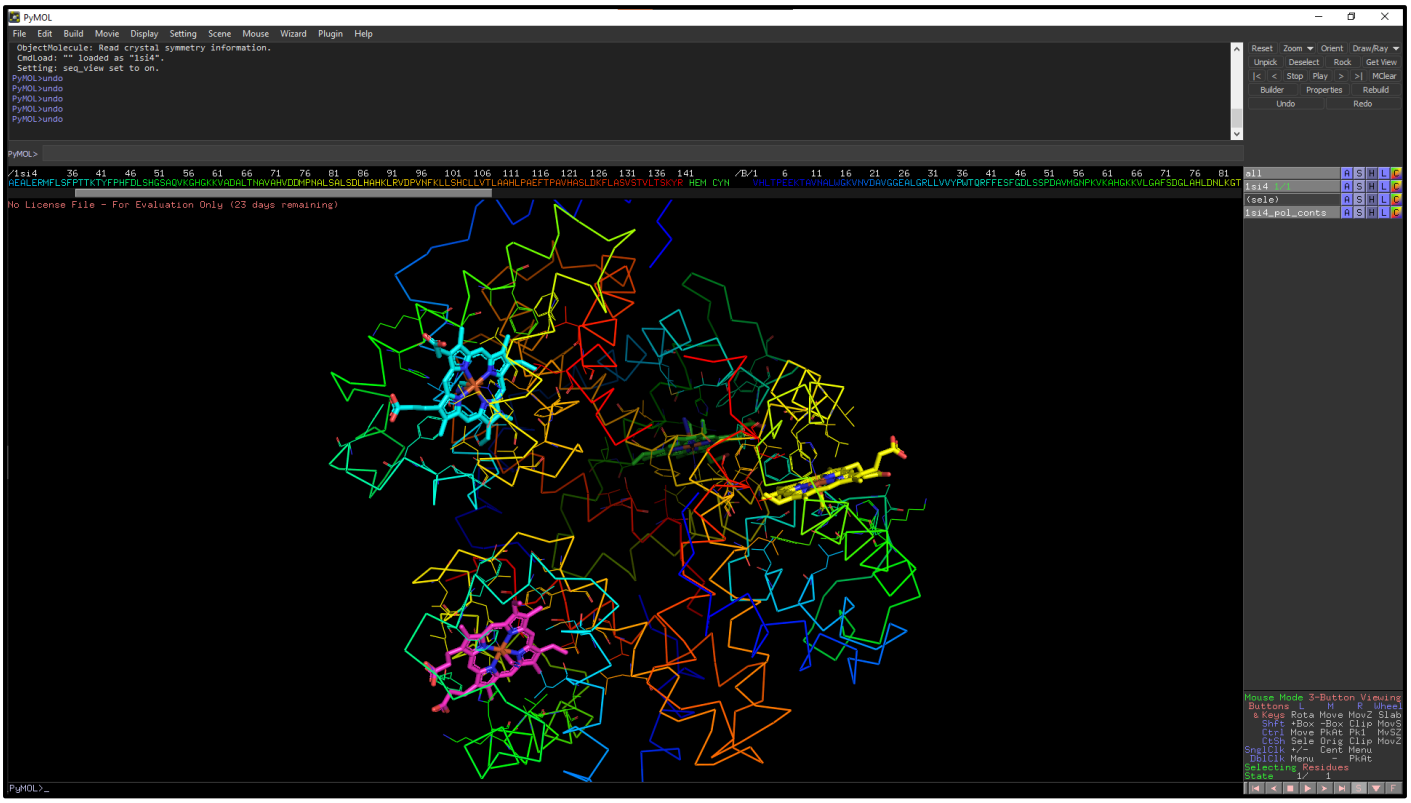


Fig15. PDB structure of Hemoglobin (1SI4) with it set to preset ligand view

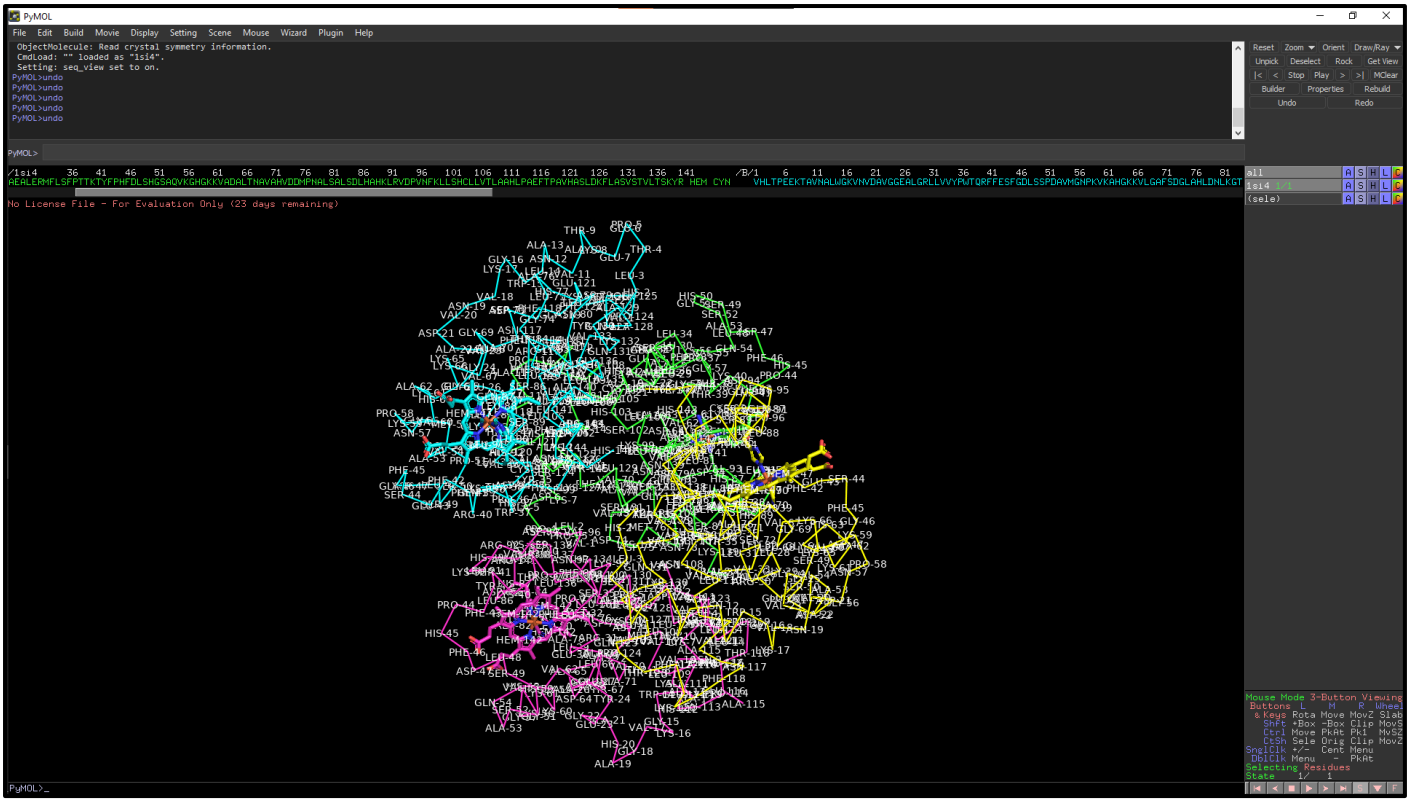


Fig16. PDB structure of Hemoglobin (1SI4) with all its residues labelled

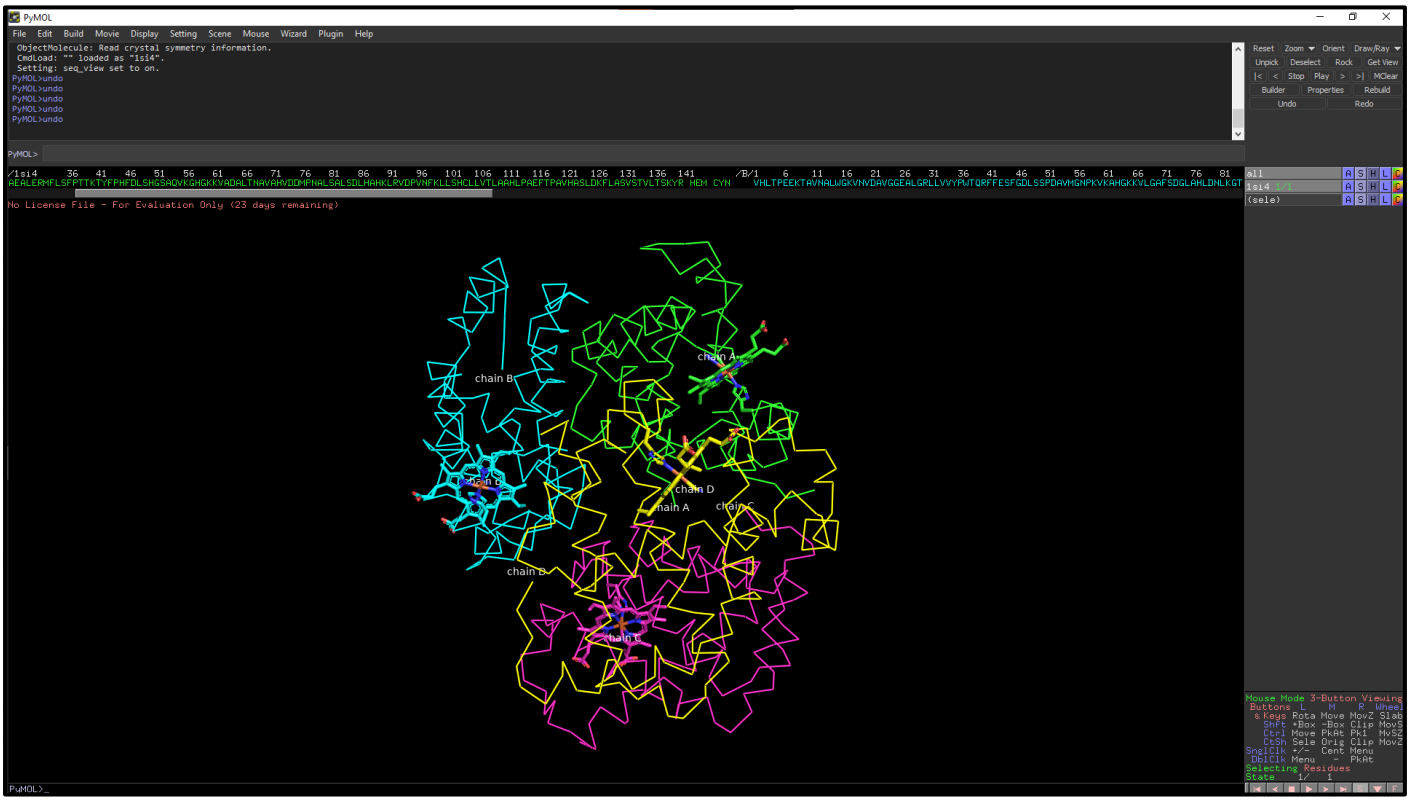


Fig17. PDB structure of Hemoglobin (1SI4) with all its chains labelled

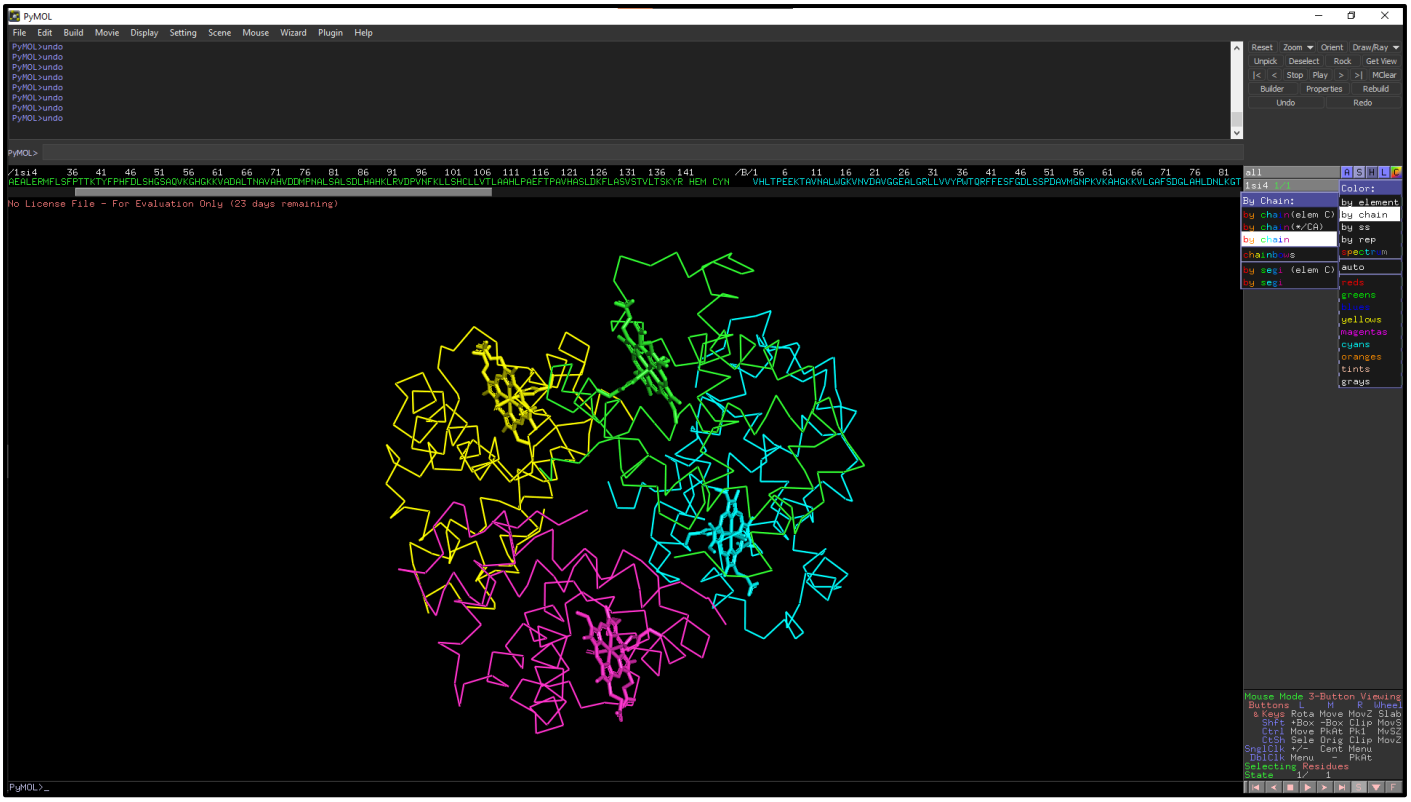


Fig18. PDB structure of Hemoglobin (1SI4) visualized with the chain color scheme set to rainbow