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Protein support in Bioclipse using Jmol and the CDK

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Bioclipse, Jmol, Cdk

Abstract
I have not blogged for about a week now, and been too busy with other things, like finishing my PhD articles/manuscript, my new job at the CUBIC where I continued the work on proper protein support in Bioclipse using the CDK and Jmol:

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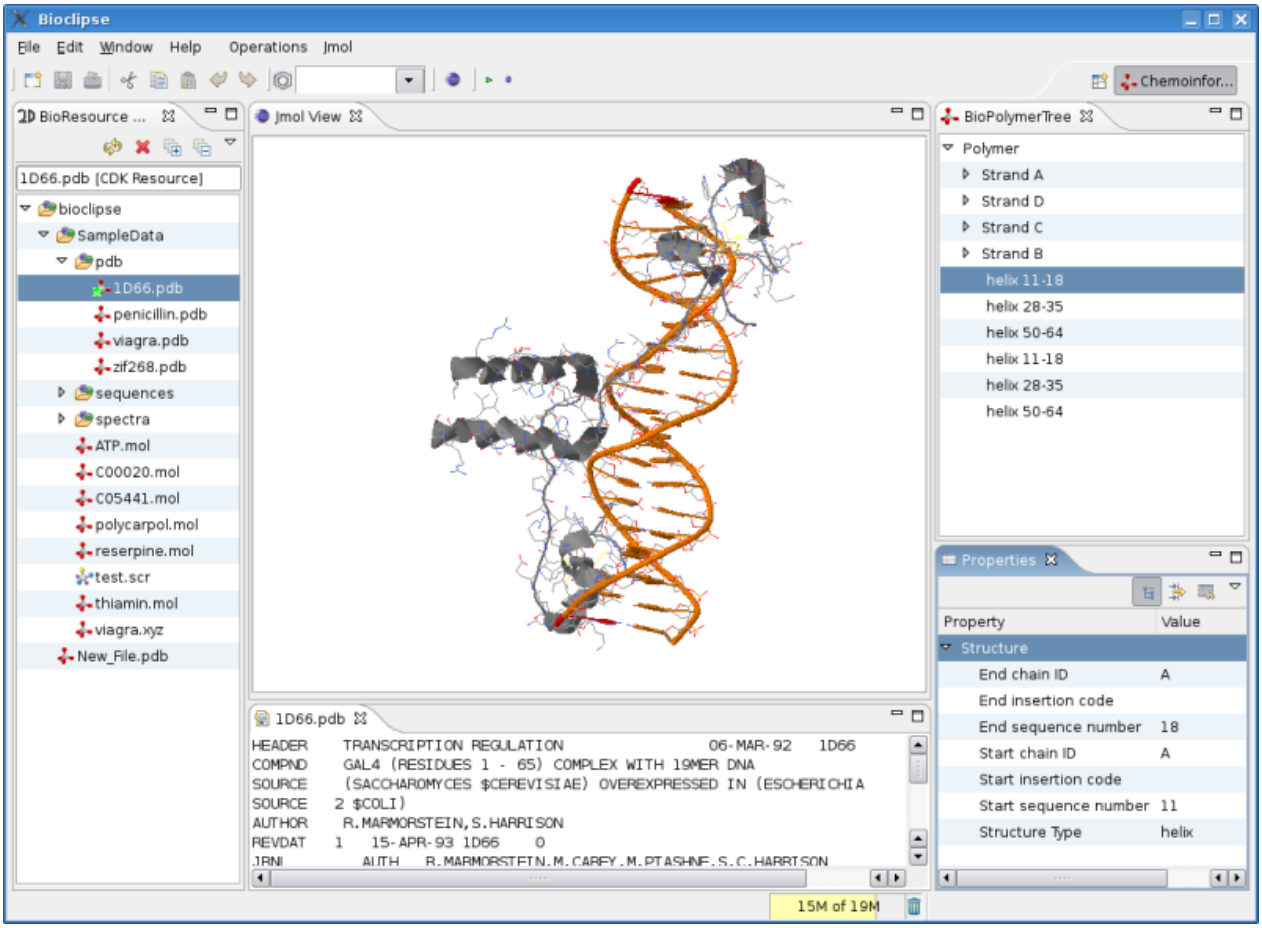

The latter involves getting the CdkJmolAdapter , the interface between the CDK and Jmol, updated for changes since the Jmol as 3D viewer for CDK article in CDK News , the open access journal for CDK related projects.

The screenshot is not showing the actual status: the `CdkJmolAdapter` does not propagate all information to Jmol correctly; as you can see in the screenshot in the `BioPolymerTree` and `Property` views, the CDK now reads the structure information from the PDB file, and I verified that Jmol really extracts this using the `StructureIterator`, but the secundairy structure does not show up yet. I believe the problem is in the `AtomIterator`: issueing the `select protein` script, selects zero atoms.

The above screenshot is using a workaround, and was made by using Jmol's own IO instead of the `CdkJmolAdapter`. But I'm very close and think I will be able to fix this soon.