
Subject: Viewing 3D confs with protein

Posted by [chemtv](#) on Mon, 09 Mar 2026 16:54:46 GMT

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Thanks for all the new capabilities. After an external docking... I have figured out how to "Append" a reference xray ligand and a very small active site selection (as SDFs). My question is: After I set the active site to be shown with another structure that works fine... but if I choose a molecule in the middle of the table, I can't get to the graphics window to rotate the view without it changing the ligand I'm trying to examine. Is there a special key to press to prevent the cursor from selecting neighboring molecules? If not I suppose I can set the "Horizontal Structure Count" to 1? Is that the only solution? Maybe I am just trying to look at too many structures anyway :roll:

Thanks,
Greg

Subject: Re: Viewing 3D confs with protein

Posted by [thomas](#) on Sat, 21 Mar 2026 17:16:22 GMT

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Sorry for the late reply. Do I understand correctly: You have a docking poses in the detail view and navigate the mouse over the structure view. When moving the mouse pointer from one structure to the next, the detail view changes to display the pose of that other structure. When the mouse pointer is in the middle of the structure view, there is no way to move the mouse to the detail view to change view properties like rotation and zoom state.

Yes, this is true. A workaround may be to scroll the structure view to a position that the structure of interest is at the upper or lower edge. Then your mouse doesn't need to traverse other structure on its way to the detail view. The idea to prevent detail view updates when pressing a key during mouse movement is interesting. I have added that feature with the ALT-key. It will be part of the next update.
