Subject: Re: 3D structure display is lost after hovering over certain structures
Posted by thomas on Tue, 27 Oct 2020 11:49:07 GMT
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Hello Paul,

thank you for that clear report and the sample file. With that I could quickly find the problem and fix it.
The issue was the following: The 3D-coordinate encoding includes a value for the 'average bond length' to properly scale
a molecule after decoding and assigning relative atom coordinates. In a special case, where hydrogen coordinates
are included in the encoding, the average bond length was still calculated from non-hydrogen atoms only, which failed
in molecules that have no bonds between non-hydrogen as HI. For these molecules H-I distance are still not correct, if
3D-coordinates are not freshly calculated. But they are displayed correctly now and don't crash the 3D-viewer.

The bug is fixed in todays update of DataWarrior's development version.

Thomas