Subject: Re: Bug in how stereochemistry is reported
Posted by richards99 on Thu, 04 Mar 2021 08:44:58 GMT
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Thanks Thomas,
Looking into it, it does appear to be related as to whether the structure is specified as chiral or not.

The problem is various tools I am using are not compatible with V3000 flags, and simply writes out structures SDF format with the appropriate R or S stereochemistry and nothing else, so no '1' as the fifth entry for instance.
Then when I read into DataWarrior, and then save back out to an SDF, the stereochemistry can often be flipped to what it was originally. Presumably because DW doesn't care which isomer it shows as it thinks there is a mixture anyway.
Even if DW believes the stereo centre is a mixture, it would still be useful if it did not alter the provided stereochemistry it was given.

Simon.