Subject: Re: Converting COD2020 to SDF
Posted by ghutchis on Thu, 28 Jan 2021 16:00:08 GMT
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On my laptop at home, I had the most recent version - but I replaced the JAR and everything seems to be running smoothly.

I'm aware of the codcif2sdf tools - I'm the maintainer of Open Babel.. I also remember that Thomas mentioned to me that he has done some additional sanity checks in hiss version.

Perhaps it's a separate question - how is the DWAR compiled from COD? Do you take the codcif2sdf SDF and pull them together into the DWAR or something else?

(Prompted by a few people, I'm working to put up a resource that rsync's from COD and provides the SDF.