Subject: Merge Structure Error
Posted by amorrison on Sun, 14 Mar 2021 07:08:44 GMT
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Hi Thomas,

I was having a play with the merge structure feature (great by the way I didn't know you could do this). When the R-grp decomposition involves breaking a ring and then merging these r-grps the structure is not reproduced as I would have hoped. Is there a way to do this?

Also, when I have multiple different cores I will modify the R-grp labels so that they are consistent across the different cores for SAR analysis. This is straightforward for R-grp labels (i.e. R1, R2, R3 etc) but how would I modify the attachment point label. I can open it in the structure editor but I don't know how to change the attachment point number.

I've uploaded a minimal example of the merge issue.

Finally, thank you for continued development of this excellent tool.

Best,

Angus

File Attachments
1) Merge_Structure_Error.dwar, downloaded 765 times

Subject: Re: Merge Structure Error
Posted by thomas on Sun, 14 Mar 2021 14:56:59 GMT
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Hi Angus,

Thank you for the issue and the prepared file. I thought I have already fixed that, but there was a remaining problem that needed fixing. The current dev version contains the fix for support for reconnecting R-groups.

Attachment points in R-groups are pseudo atoms with atomicNo=0. For them a '?' is used instead of a one/two letter atom symbol. In case of a cyclic backconnection it still is an atomicNo=0, but in addition the atom has a custom label with the nimber of the scaffold's R-group it connects to. In these cases only the label ('1', '2', ...) is displayed instead of an atom symbol. You can modify both in the editor with the '?...' tool. Type in the field for the atom label either ? or 3@?. The '?' sign can also be handled like a normal atom symbol: Type ?, when hovering with the mouse over an atom.

Thomas