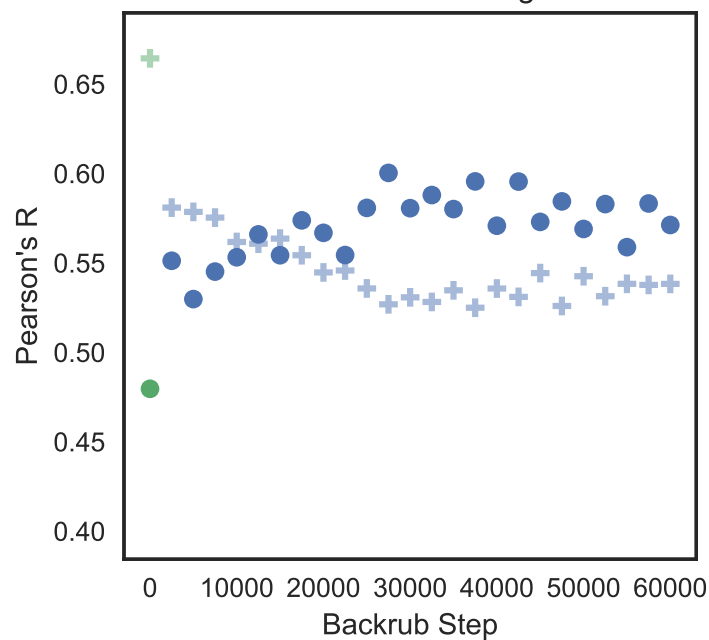
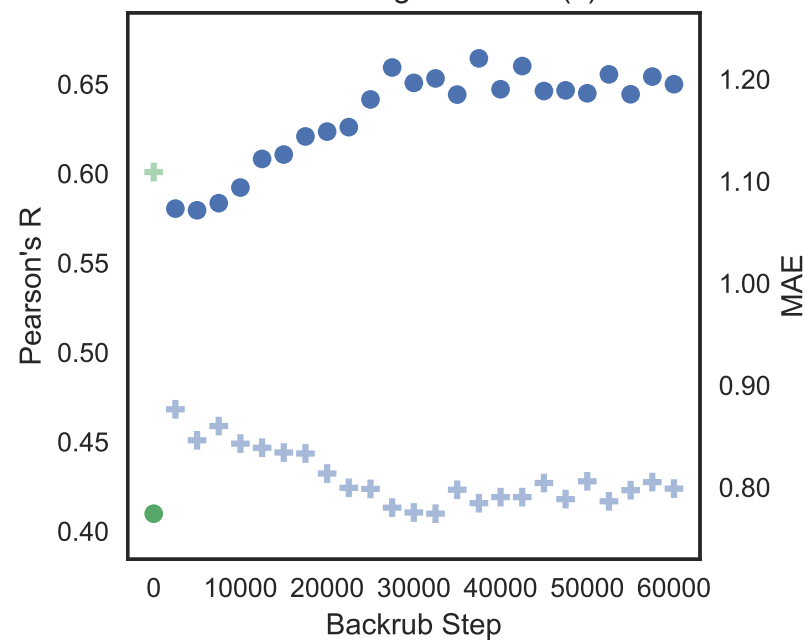


$\Delta\Delta G$ prediction performance vs. number of backrub sampling steps

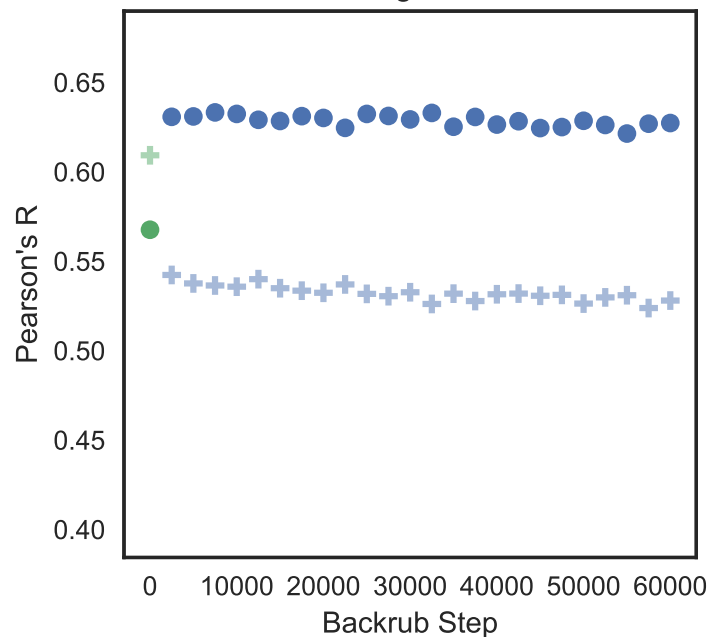
Some small-to-large



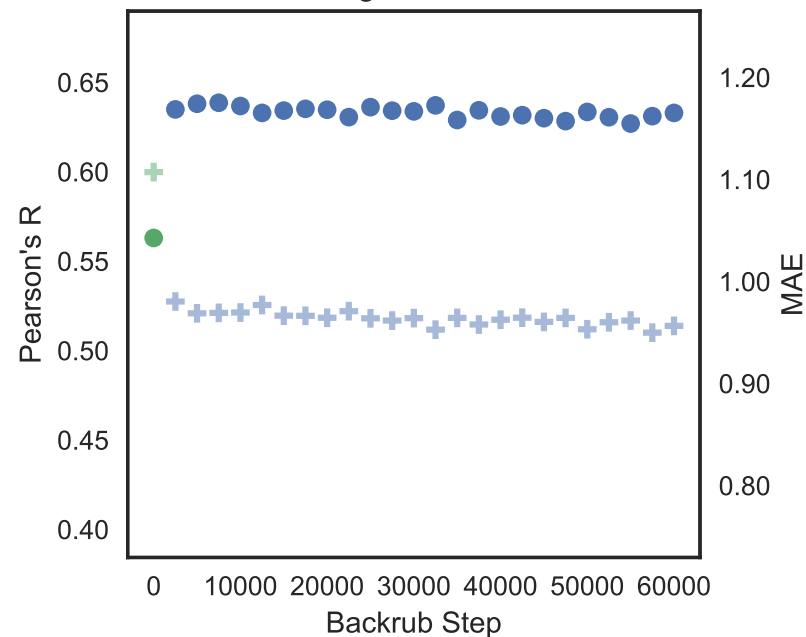
Small-to-large mutation(s)



Some large-to-small



Large-to-small



● R - Flex ddg ● R - No backrub control + MAE - Flex ddg + MAE - No backrub control