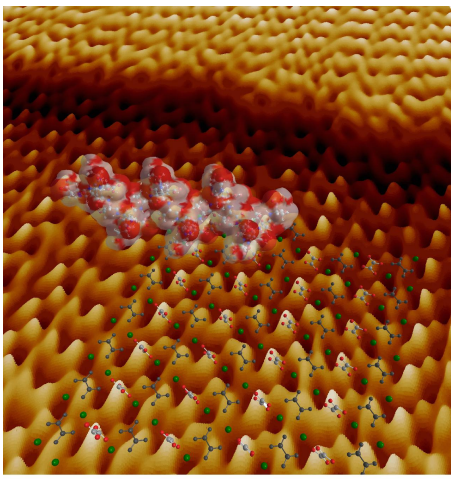
Lawrence Livermore National Laboratory

Autopack

Autopack is an open-source python tool that enables the automatic labeling of packing motifs for large and chemically diverse datasets of molecular crystals.



Category

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Autopack is an open-source python tool that enables the automatic labeling of packing motifs for large and chemically diverse datasets of molecular crystals. Autopack takes advantage of geometric descriptors to find useful cross-sections within the crystal structure to elucidate the associated packing motif. Autopack is capable of processing either crystallographic information files (CIFs) or Cambridge Crystal Structure Database (CCDC) reference codes provided in a CSV file. Internally, Autopack will both validate and filter crystal structures that do not satisfy the packing motif labeling criteria (as explained in the associated publication), limiting the number of manual preprocessing steps. Finally, Autopack also allows for the input of labeled data, providing an opportunity to test the accuracy of Autopack and tune as necessary.

References

1. Donald Loveland, Bhavya Kailkhura, Piyush Karande, Anne M. Hiiszpanski, & T. Yong-Jin Han(November 27, 2020) , https://doi.org/10.1021/acs.jcim.0c01134, Journal of Chemical Information and Modeling, 60(12), 6147-6154