

## Temperature Validation using the CSD Python API

The Cambridge Structural Database Python API was used to investigate the variation of atomic displacement parameters (ADPs) with reported data collection temperatures. The distribution of ADPs at a given temperature can be fit to a log-normal distribution. Additional descriptors and parameters including atomic connectivity, R-factor, resolution, and disorder were evaluated. A scoring system was developed to identify datasets with inconsistencies between reported temperature and atomic displacement parameter distributions. To evaluate this tool, a testing data set was created containing random entries with inaccurate data collection temperatures. The scoring system successfully flagged the majority of data sets for which the data collection temperature was altered.

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