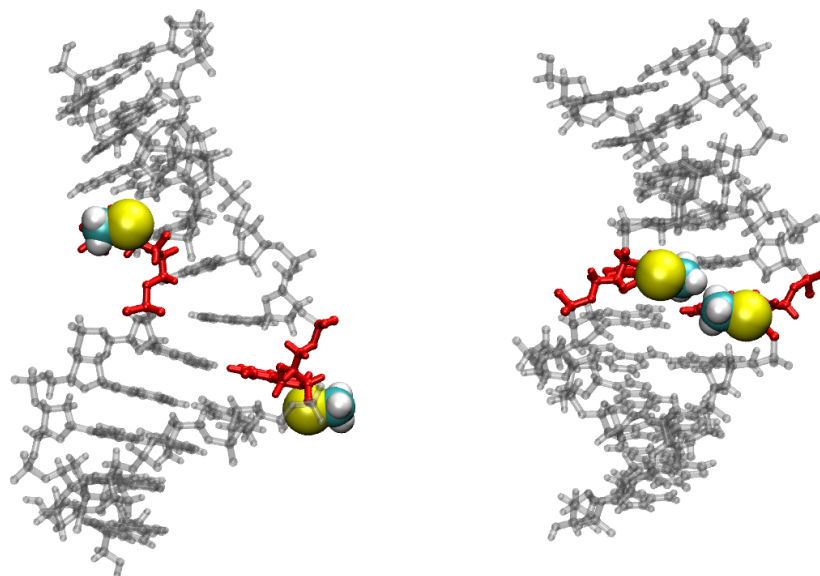


SI Figure 1: Ending MD models for $-SeCH_3$ containing duplexes (sequence **III**). Views into the minor and major grooves (top and bottom panels respectively); $2'$ - $-SeCH_3$ nucleotide built with S sugar (left panels) and N sugar (right panels). For both duplexes, all other nucleotides were built with an S sugar conformation. The sugars, bases, and backbone for the $-SeCH_3$ containing nucleotides are in red; the $SeCH_3$ group (Se=yellow, C=cyan, H=white) are rendered with spheres reflecting their respective van der Waals radius. After simulated melting and annealing, the oligonucleotide built in an overall B-type conformation (left panels) does not properly anneal as exhibited by the extrahelical bases. However, when the same duplex was built with the $-SeCH_3$ nucleotides in an N sugar conformation and all other nucleotides in S sugar conformations, annealing produces a base paired duplex. In these duplexes, the $-SeCH_3$ groups are positioned in the minor groove. (right panels)

Minor groove:



Major groove:

