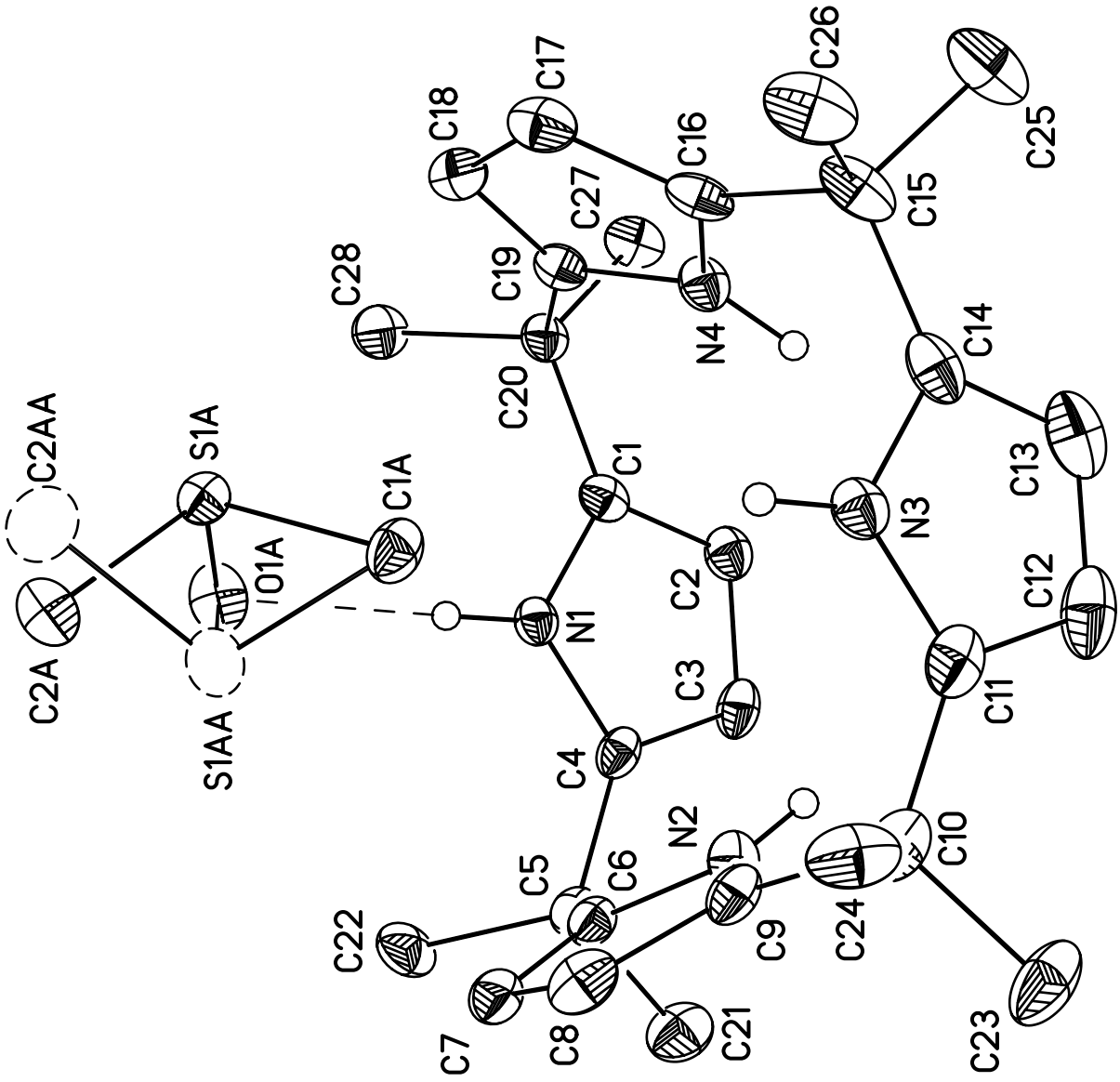
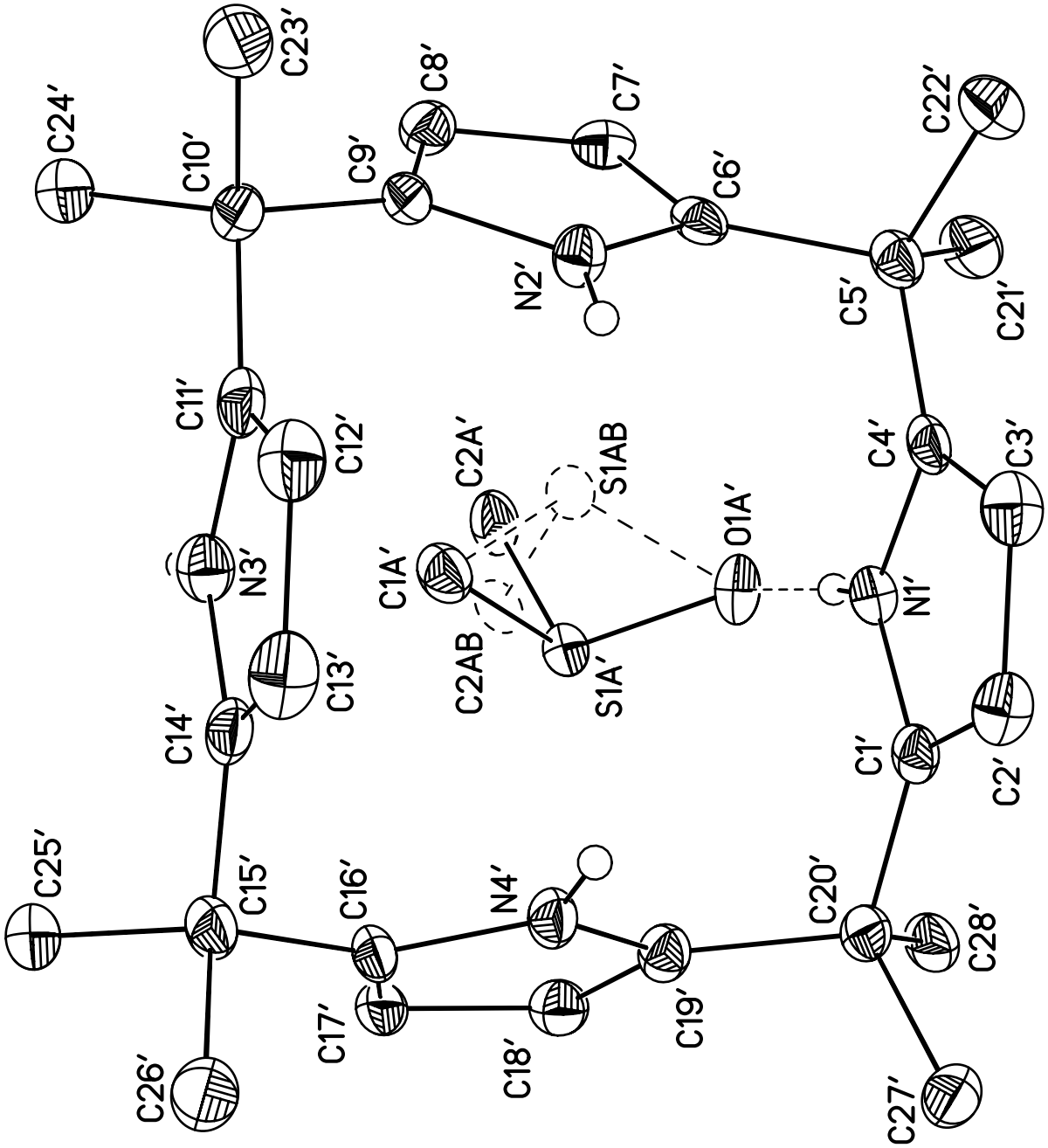
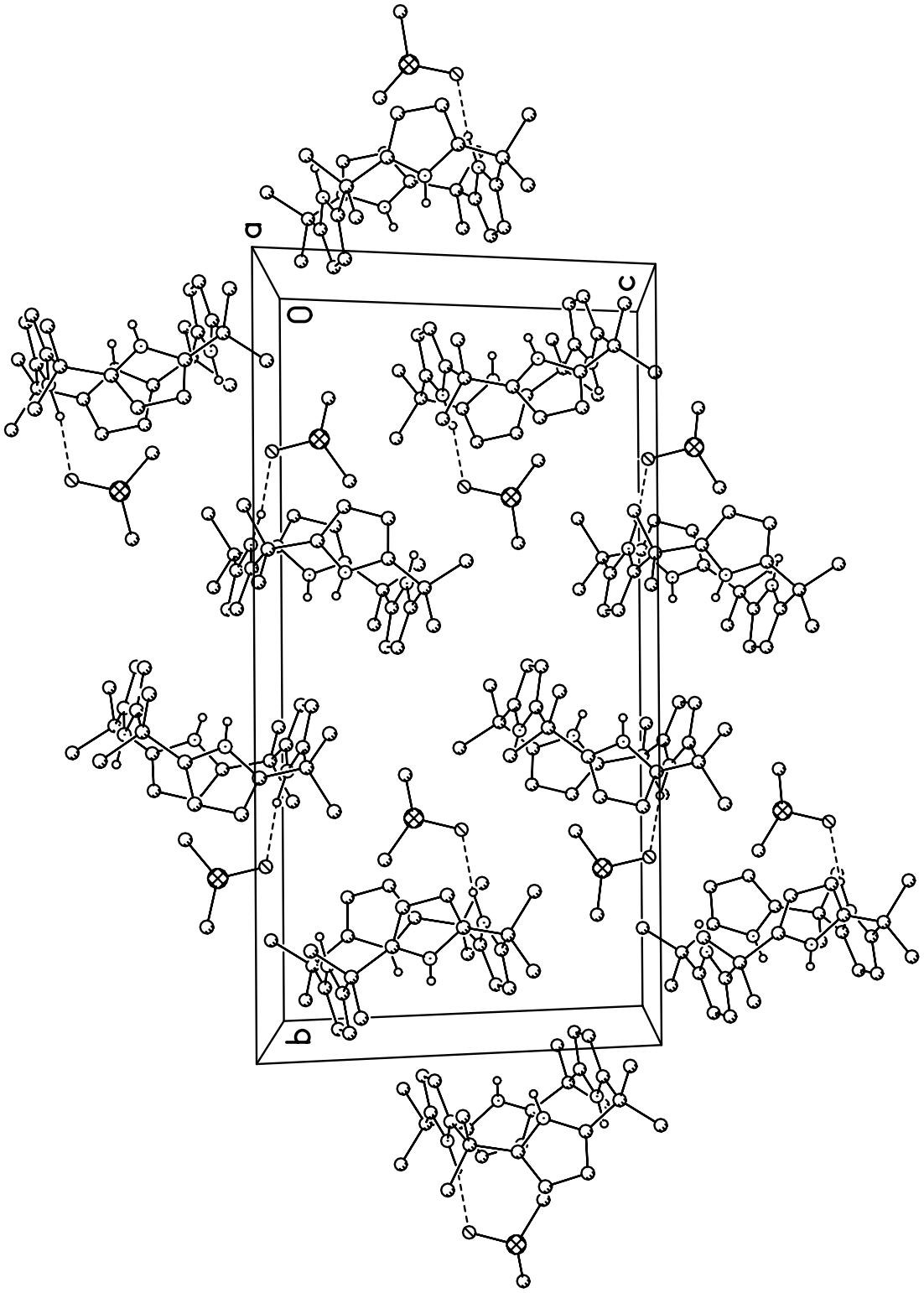


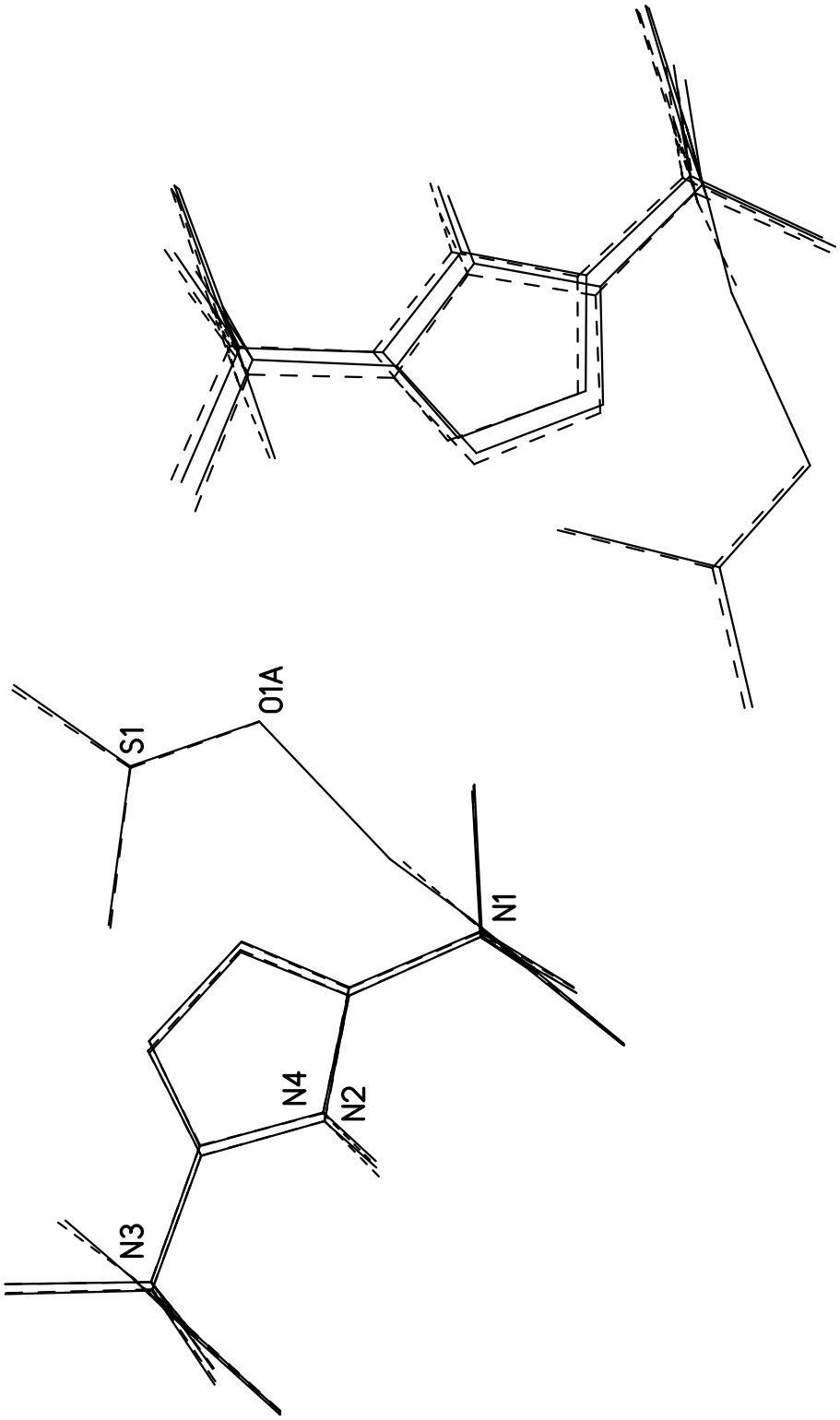
Supplementary Figure 1. View of molecule 1 of the low-temperature phase showing the atom-labeling scheme. Displacement ellipsoids are drawn to the 30% probability level. The labeling scheme is consistent with that used for the room-temperature phase.



Supplementary Figure 2. View of molecule 2 of the low-temperature phase showing the atom-labeling scheme. Displacement ellipsoids are drawn to the 30% probability level.



Supplementary Figure 3. Unit-cell packing diagram for the room-temperature phase of the meso-octamethylcalix[4]pyrrole-DMSO complex. The orientation used is identical to that of the low-temperature triclinic phase.



Supplementary Figure 4. Fit by least-squares of atoms from molecule 1 (dashed lines) of the low-temperature phase to the equivalent atoms (solid lines) of the room temperature phase (matched pair on left). All non-H atoms were included in the fit. The pair on the right is the symmetry generated molecule of the room temperature phase and molecule 2 of the low-temperature phase. The distance between the centers of these two molecules is 0.12 Angstroms