SUPPLEMENTAL FIGURE 2. Total charge density on guanosine analogs.
Calculated total charge density, corresponding to the HOMO molecular orbital, with positive density in red and negative density in blue, for 9-methylguanine and its analogs. 9-Methylguanine, which is identical to guanosine except for the methyl group that replaces the ribose ring, was used to simplify the calculations.
SUPPLEMENTAL FIGURE 3. Total charge density on inosine analogs. Calculated total charge density, corresponding to the HOMO molecular orbital, with positive density in red and negative density in blue, for 9-methylhypoxanthine and its analogs. 9-Methylhypoxanthine, which is identical to inosine except for the methyl group that replaces the ribose ring, was used to simplify the calculations.