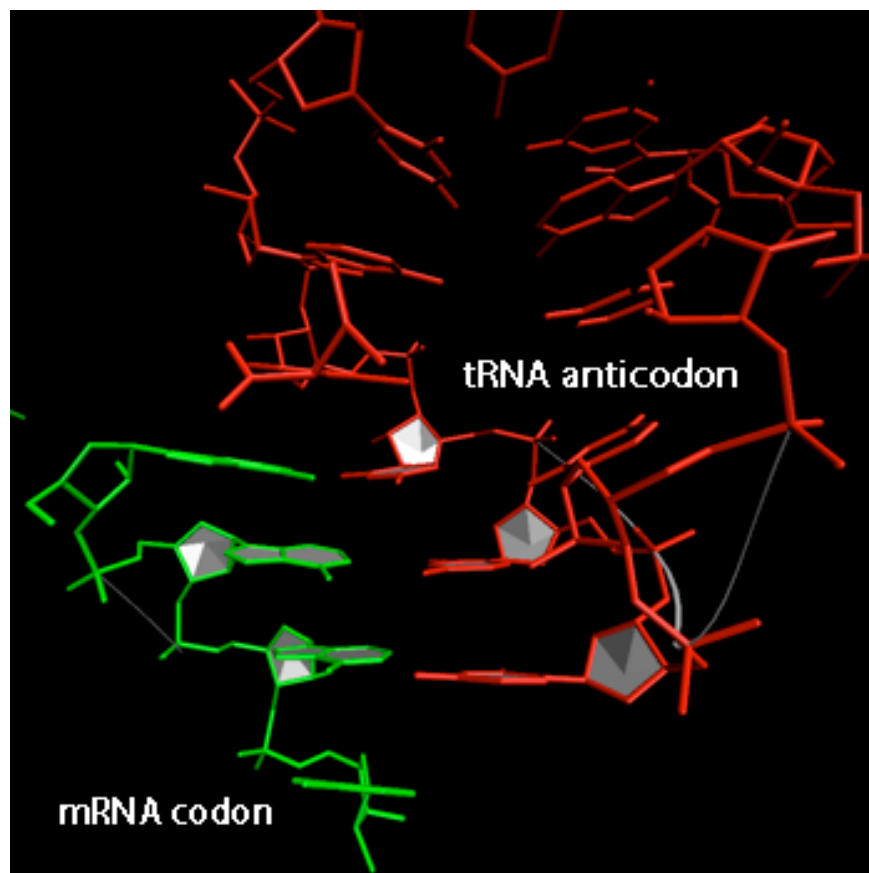


Molecular Orbital Interactions in the Anticodon of Transfer RNA
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Accurate recognition of messenger ribonucleic acid (mRNA) by various transfer RNA (tRNA) molecules is essential to protein synthesis. Stair-stepped base stacking in the anticodon is required for correct cognate codon recognition and proper amino acid placement in the polypeptide chain. The interactions stabilizing the stair-stepped conformation are unknown. Anticodon base structures were obtained from experimentally determined tRNA crystal structures and hydrogen atoms were geometrically optimized. Density functional calculations and natural bond orbital analysis were performed on the anticodon structures at the M05-2X/6-31+G(d,p) level of theory. Significant molecular orbital interactions were identified and trends noted. Patterns of stabilizing interactions were compared with those from A'-standard RNA to establish the interactions vital to the stair-stepped conformation of the tRNA anticodon. Interactions noted from the crystal structures indicate multiple conformation-stabilizing interactions present in the majority of stair-stepped anticodon structures.



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