Abstract

Nucleic acids (NA) are biochemical macromolecular substances essential for all living organisms - their function is to store genetic information and control the process of protein biosynthesis. Nucleic acids are composed of polynucleotide chains. According to the composition of these, we distinguish two basic types of nucleic acids: DNA (Deoxyribonucleic Acid) and RNA (Ribonucleic Acid). Based on the internal nucleotide sequence and external interactions, these chains are formed into different spatial conformations. At the dinucleotide level, these conformations are described and classified by so-called classes of dinucleotide conformers - NtC.

The X-ray crystallography method has been used for over 50 years to reveal the three-dimensional structures of biological macromolecules. The principle of this is the interaction of X-rays with the electron cloud of atoms in the crystal. Atomic positions are then determined based on the calculated electron density. However, with the resolution available for most macromolecular crystals, these crystallographic data are not sufficient to derive a chemically acceptable structure, so stereochemical restraints apply.

Stereochemical restraints are dictionaries describing specific bond lengths, bond angles, torsion angles, planes, and chirality. Using these values, structural macromolecular models are modified and improved. Based on data obtained from structural databases, we studied the latest version of these stereochemical restraints.

Key Words: NA structure, NA conformation, stereochemical restraints, refinement, structure database, CSD, PDB