flexible and tolerant of the conformational changes important for molecular recognition.

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CONFORMATIONAL VARIABILITY OF RNA BACKBONE

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As shown by ribozyme and especially ribosome structures solved in last few years, molecules of RNA form complicated 3D folds which have no match among known DNA structures but their complexity is quite comparable to that of protein folds. Complicated RNA folds are enabled by a high flexibility of the nucleotide backbone but little is known about its conformational behavior. A well refined structure of the large ribosome subunit 50S at 2.4A, NDB structure RR0033 (PDB ID 1JJ2), Ban *et al.* Science **289**, 905 (2000), provides a database of over 2700 nucleotides. This work analyzes conformations of these nucleotides by a combination of Fourier averaging and clustering techniques.

Majority of all nucleotides of RR0033, about 70%, are in the A-type conformation, this main conformational type can be further classified into three subclasses. The remaining 30% of nucleotides with other than A-type conformations were analyzed in a greater detail. The backbone torsion angles for each nucleotide were grouped into eight sets of three angles with the main emphasis on the torsions around the two phosphodiester bonds, O3*-P (torsion zeta) and P-O5* (alpha). Each set of three torsions results in a 3D distribution of points in a parametric torsional space and this distributions was Fourier transformed into densities of nucleotide conformations. Peak positions (maxima) of these maps confine the most probable (di)nucleotide conformations.

Nucleotides belonging to the same peaks in several torsional 3D maps have similar geometry. Such nucleotides were grouped and compared in Cartesian (real) 3D space. In such a way, twelwe types of highly untypical (non-A) nucleotide conformations were identified and their Cartesian coordinates determined. These untypical nucleotide conformations can be useful in e.g.refinement process and are available upon request.

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STRUCTURE AND DYNAMICS OF RIBOSOMAL 5S RNA AND ITS COMPLEX WITH RIBOSOMAL PROTEIN L25

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Ribosomal 5S RNA (5S rRNA) is an integral component of the large ribosomal subunit in all known organisms with the exception of the small ribosomes of fungal and animal mitochondria. The 5S rRNA of *Escherichia coli* (*E. coli*) interacts with ribosomal proteins L5, L18 and L25 and enhances protein synthesis by stabilization of the ribosome structure but its exact role in protein synthesis is still not known. 5S rRNA contains internal loop - **Loop E**. The Loop E is a salient example of a uniquely structured non-Watson-Crick motif, as it contains seven consecutive non-Watson-Crick base pairs, including wobble G.U base pair and substantial cross-strand purine stacking. This unique duplex architecture together with adjacent sequence helix IV form binding site for ribosomal protein L25.

To understand the structure and function of internal Loop E and interaction between 5S rRNA Loop E and ribosomal protein L25, we have carried out set of molecular dynamics simulations.

Initial structures were directly taken from x-ray crystallography - crystal structure of 5S rRNA Loop E (*E. coli*) [1] and crystal structure of ribosomal protein L25 complexed with the 5S rRNA fragment [2]. Another studied structure was chloroplast Loop E for which there is no atomic resolution structure yet available and which is sufficiently different from bacterial Loop E motifs in sequence, but evolutionarily related to it. Model of chloroplast Loop E was proposed based on homology modeling [3], initial structure for this model was bacterial Loop E, mutation of three base pairs was performed based on the isosteric mutation.

Main focus of our investigation was to study of the structure, dynamics, hydration and cation binding of non-Watson-Crick base pairs and interaction between ribosomal protein L25 and 5S rRNA Loop E. Another aim of this study was to test the usefulness of the MD technique in