Supplementary Figures

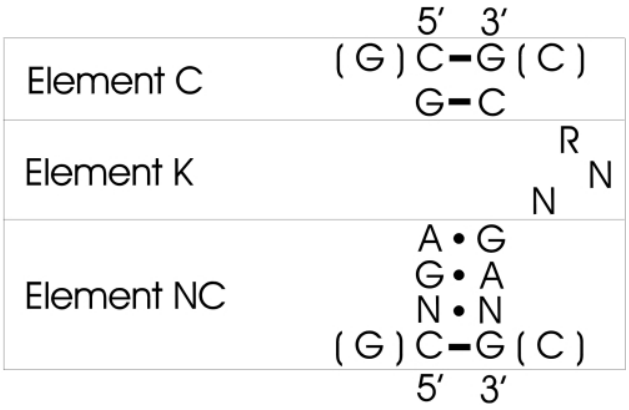

Figure S1. Secondary structure of the consensus Kink turn motif.(Klein et al., 2001) Individual Elements are in the boxes. Lines mark the Watson-Crick base pairs, dots mark the non-Watson-Crick base pairs. Tertiary interaction between **C** and **NC** is mediated by A-minor motif. (Nissen et al., 2001)

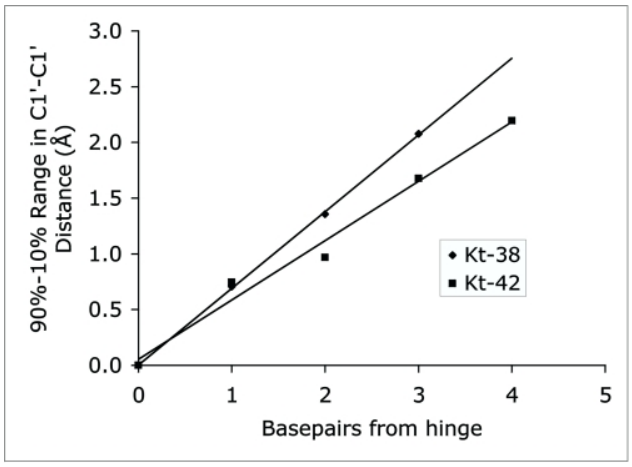

Figure S2. Dependence of the 10% - 90% range of distributions of the C1’-C1’ inter-stem distances as a function of separation (number of nucleotides) from the apical hinge (which is for Kt-38 defined by nucleotides G1027/A939/G1031 and for Kt-42 by C1148/A1215/G1151). The Kt-38 distances (diamonds) are G940-A1032, G941-C1033, and U942-G1034; the Kt-42 distances (squares) are G1216-A1152, G1217-C1153, U1218-A1154 and U1219-G1155.

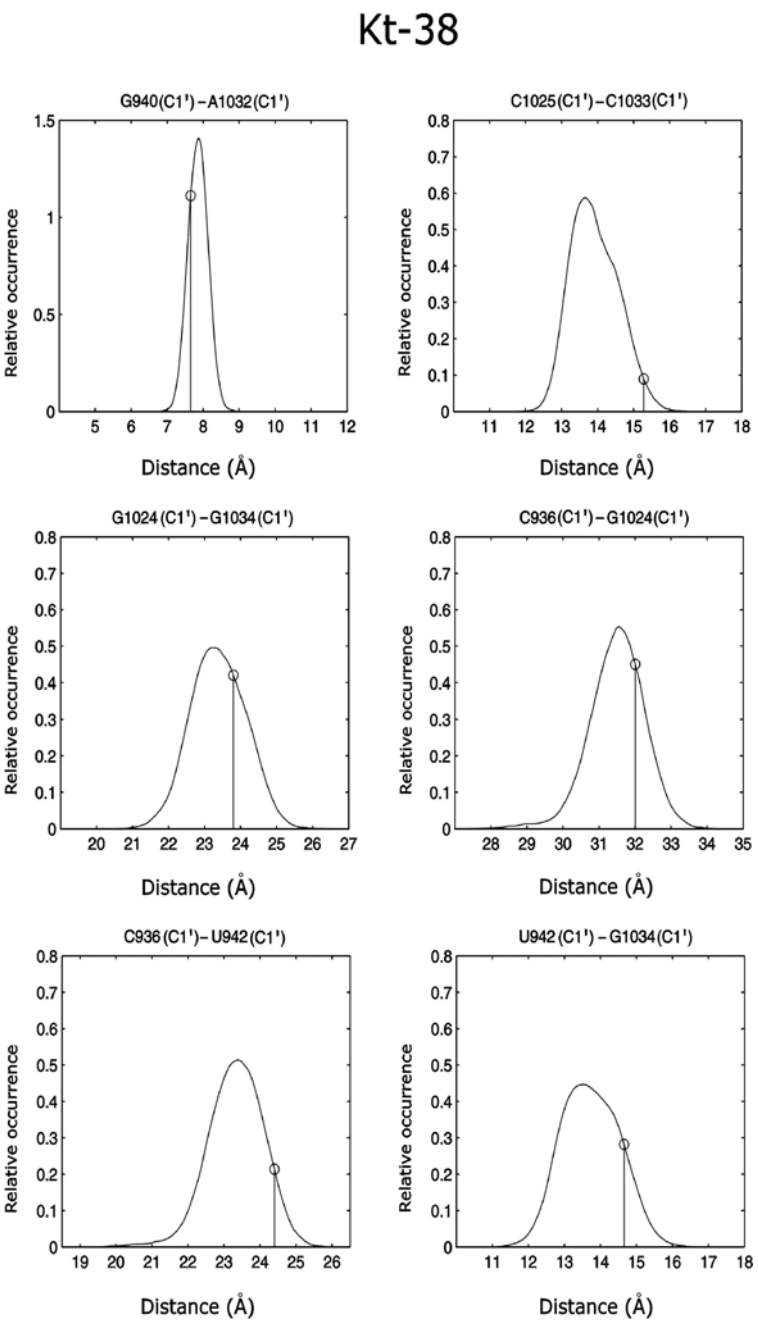

Figure S3. Normalized histograms of selected Kt-38 inter-helical C1'-C1' distances. Corresponding inter-helical distances for Kt-42 are shown in Supplementary Fig. S4. Vertical lines indicate the x-ray values.

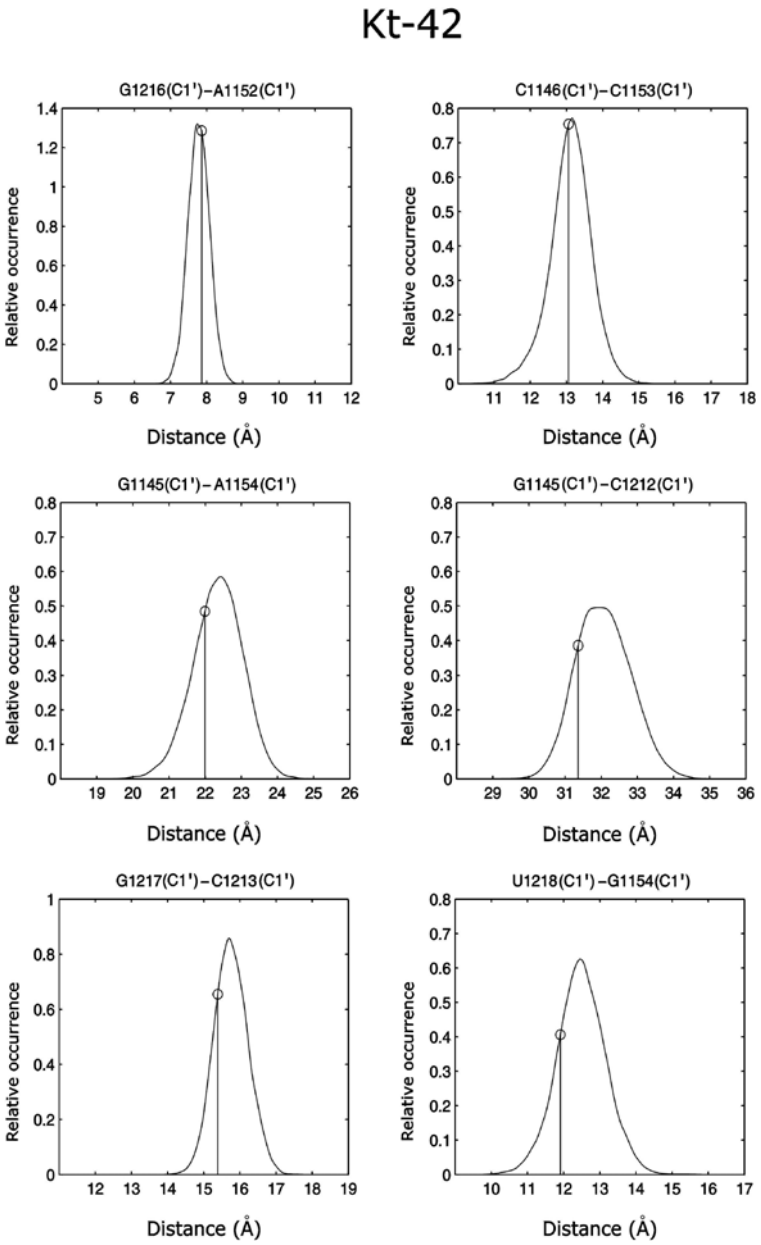

Figure S4: Normalized histograms of selected Kt-42 inter-helical C1'-C1' distances. Corresponding inter-helical distances for Kt-38 are shown in Supplementary Fig. S3. Vertical lines indicate the x-ray values.

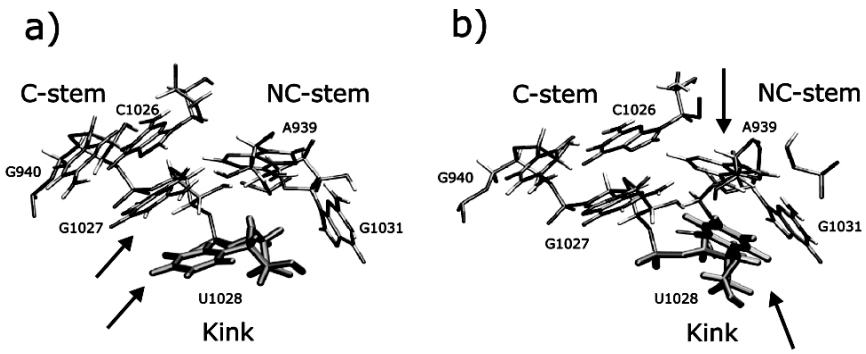

Figure S5: Conformational change of the kink region in simulation of Kt-38 leading to a lateral shift of **C**- and **NC**-stems: initial (a) and final (b) geometry of a core nucleotides localized in the kink region (**K**). Stacked residues are marked by arrows. This observed conformational change did not dramatically influence the global motion of Kt-38, which is driven by the dynamics of A-minor Type I sub-motif (see the text).

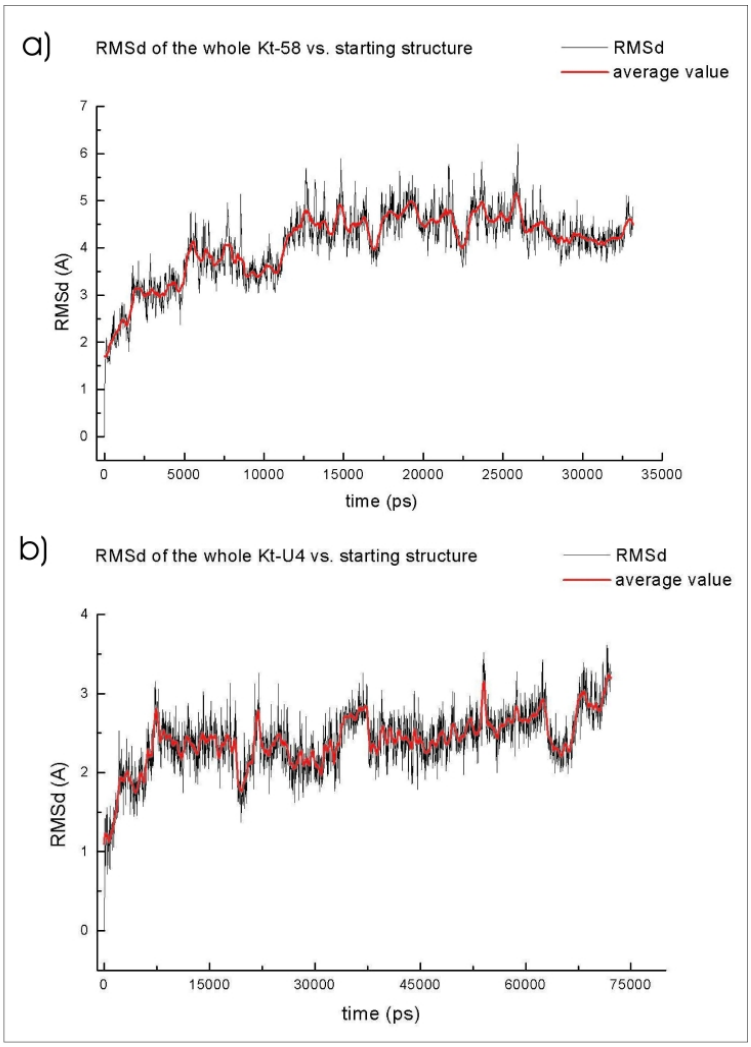

Figure S6: RMSd of coordinate positions of whole RNA Kink-turn motifs. The black lines represent the RMSd values while the red lines show the RMSd adjacent averaging (step 500ps): (a) Kt-58 (b) Kt-U4

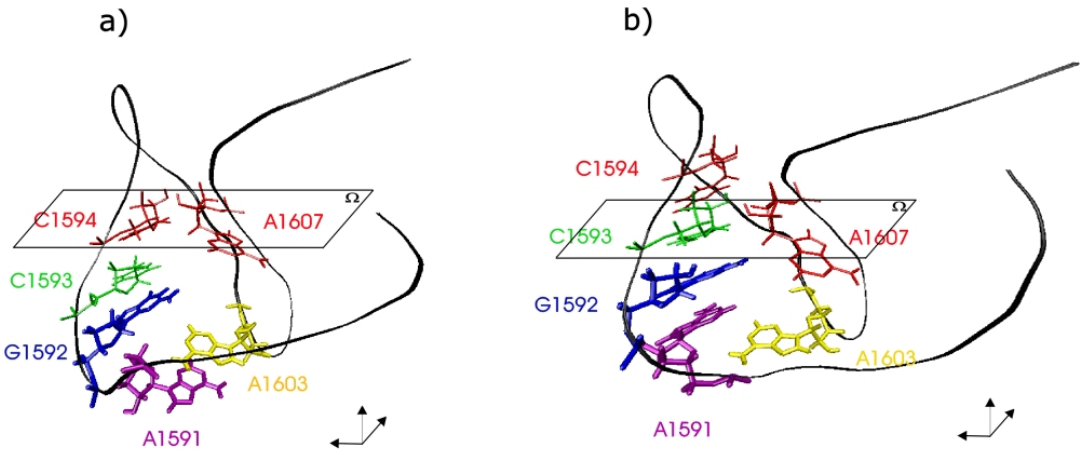

Figure S7: Schematic drawing of the major irreversible conformational change seen in simulation of Kt-58. During the key structural change, the A1591 (purple), initially (a) stacked on A1603 (yellow), rotates with its sugar and finally (b) establishes stacking interaction with G1592 (blue). It results in changes of the phosphodiester torsion angles and opening of the minor groove (black line) together with upward translation of the base pairs by one base step. While C1594 (red) and A1607 (red) were in one plane in the initial (a) structure, after the transition (b) the C1593 (green) ends in the same plane as A1607.

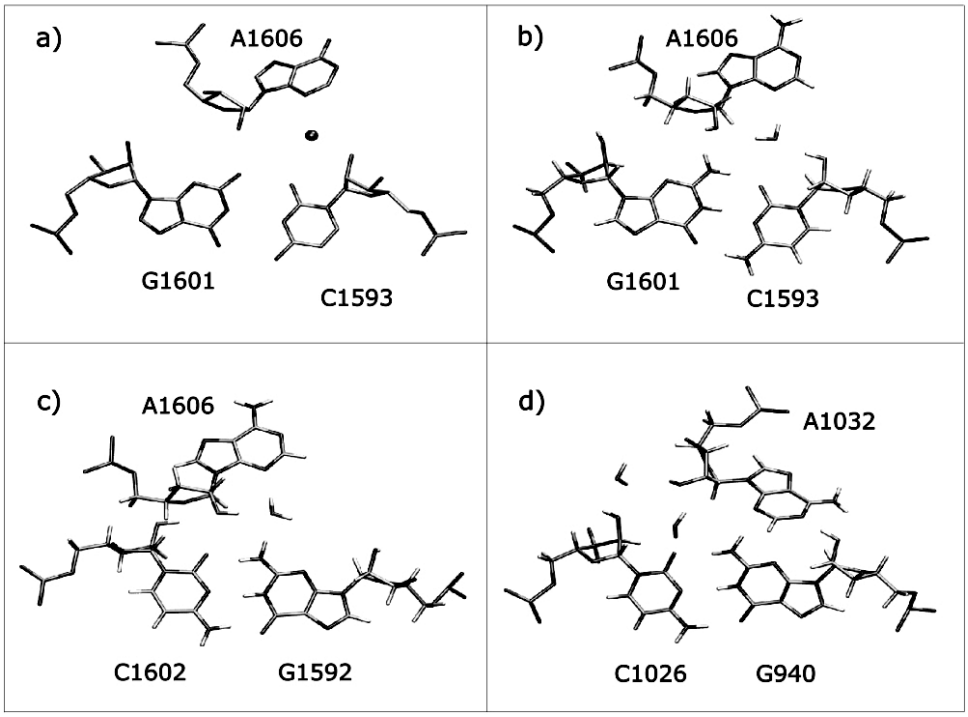

Figure S8: Water mediated second A-minor motifs. (a) x-ray structure of A-minor type 0 interaction in Kt-58 between A1606/G1601=C1593 with water (sphere) inserted between A/C; (b) snapshot, taken from the MD simulation of Kt-58 (initial substate 0-4ns), of A-minor type 0 formed by second adenosine A1606 with long residency hydration site between A/C; (c) snapshot, taken from the MD simulation of Kt-58 (final substate 6-33 ns) showing a new A-minor type I interaction formed by the second adenosine A1606, with water inserted between A/G pair; (d) water inserted A-minor type I from the simulation of Kt-38 (seen also for Kt-42) with insertion of water molecule into the A/C pair.

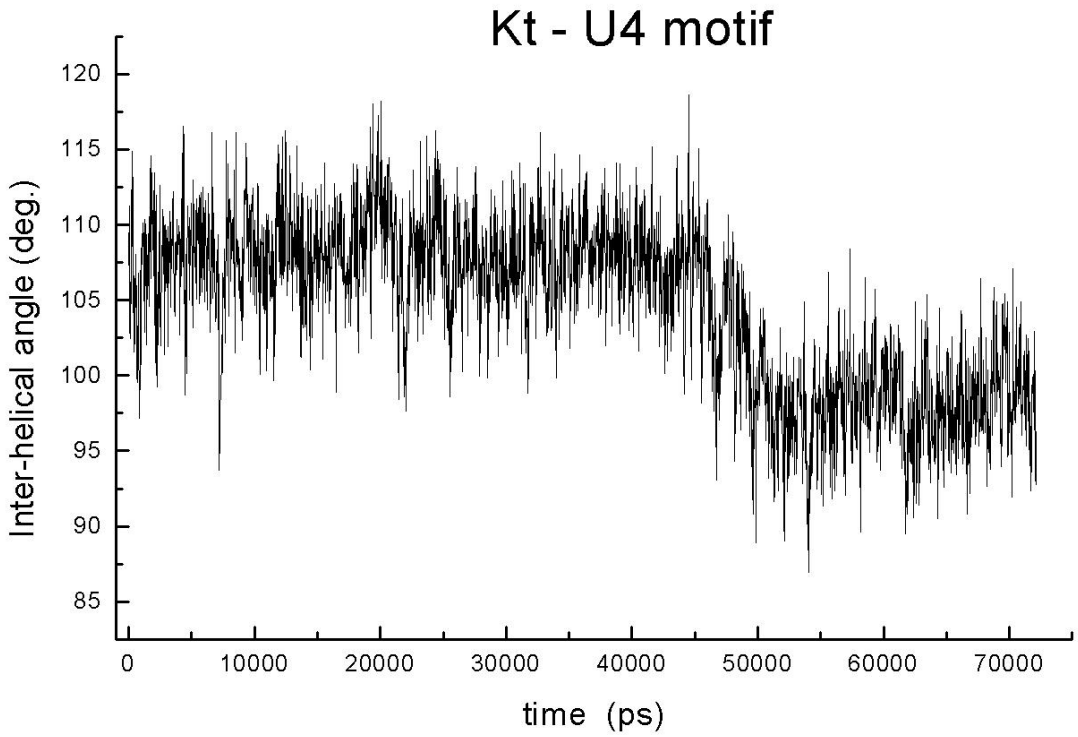

Figure S9: Time dependence of the inter-helical angle from the Kt-U4 simulation. The inter-helical angle was calculated as described in Methods section.

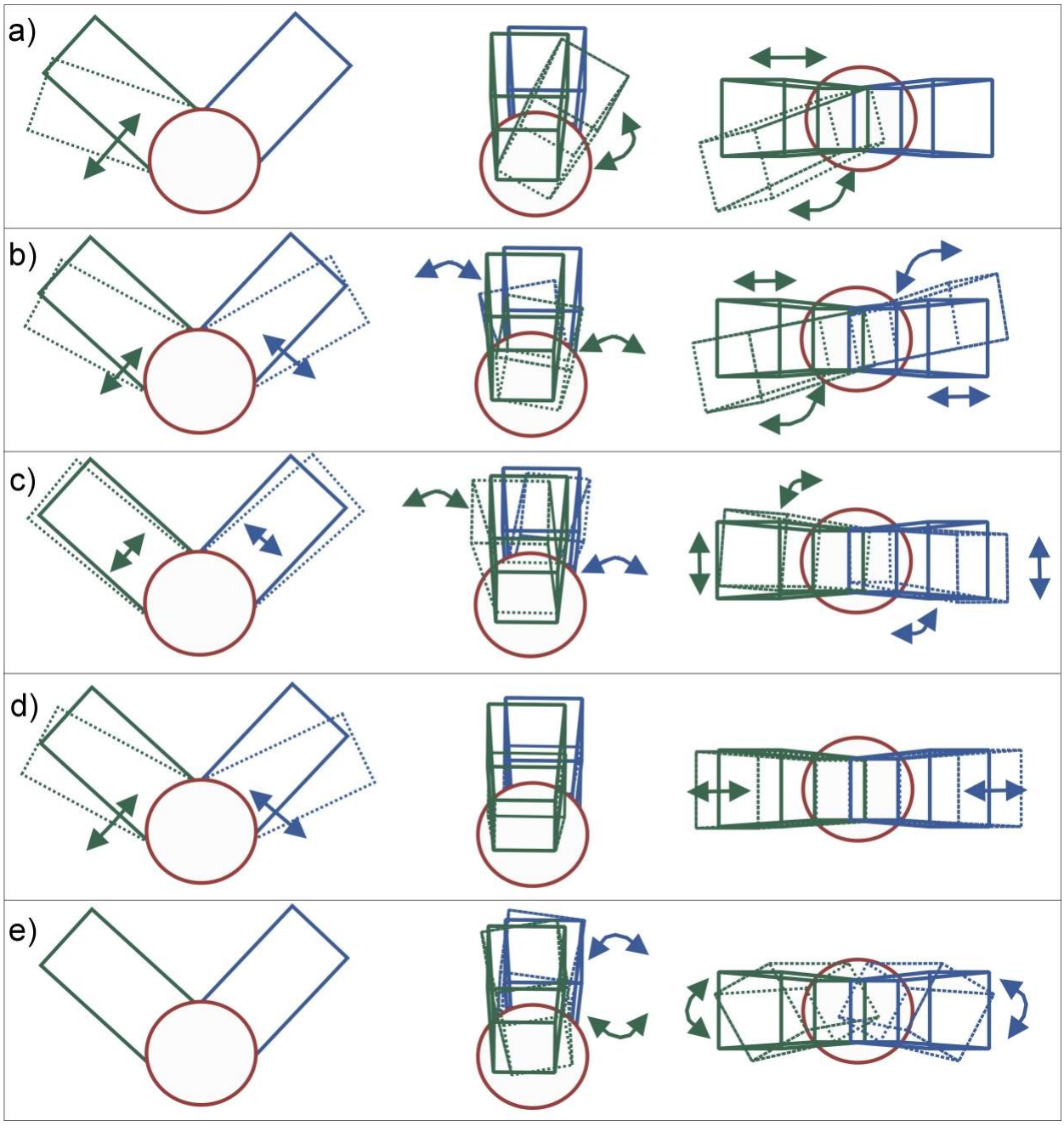

Figure S10: Essential Dynamics Analysis for Kt-42 simulation. The schematic representation of the five largest modes of the Kt-42 motion. The green color represents the **NC**-stem, red color represents the element **K**, blue color represents the **C**-stem and the arrows symbolize the oscillatory character. Individual modes 0-4 are shown in the parts a-e, in three different view angles.

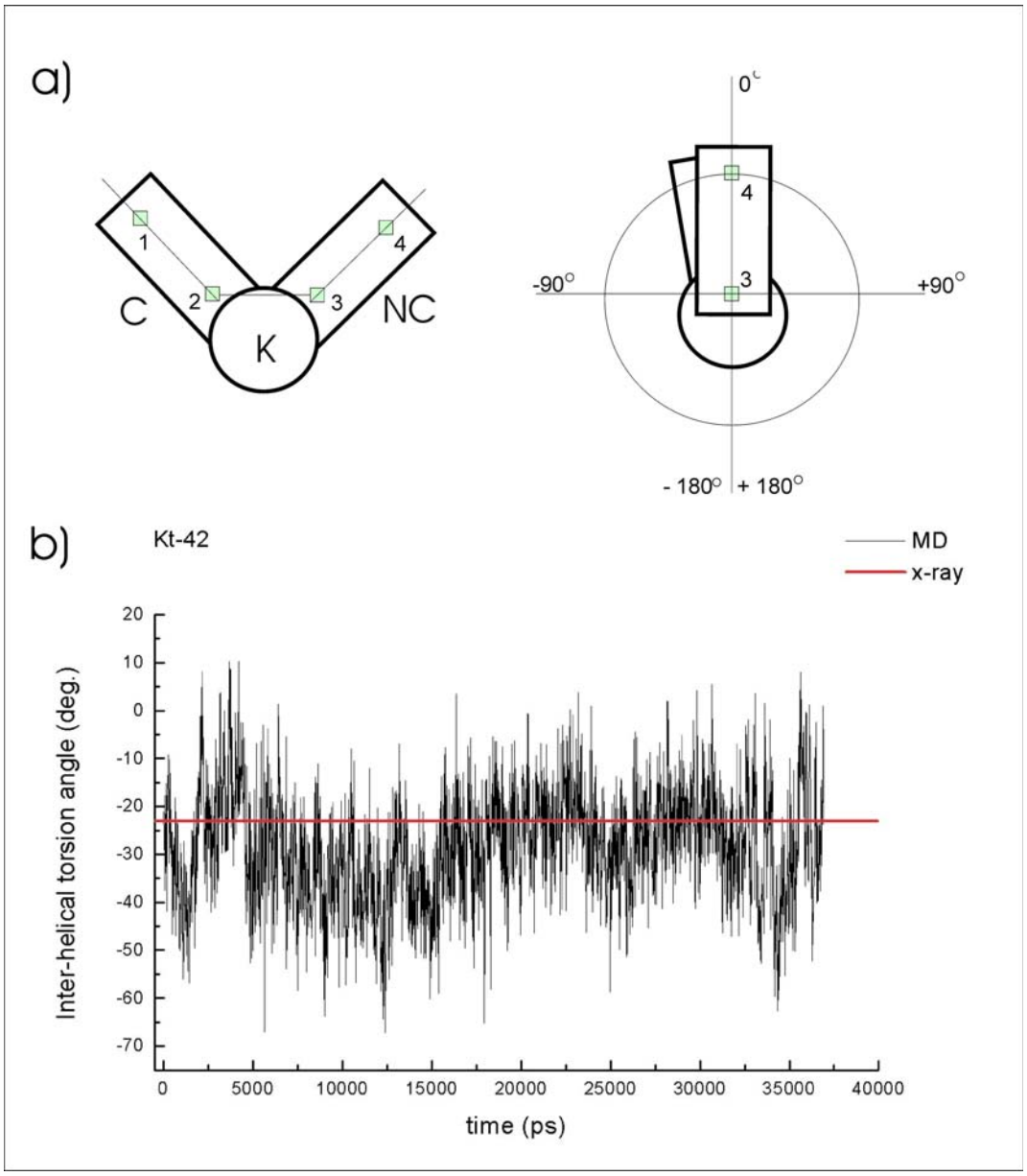

Figure S11: Inter-helical torsion angle represents the direction of the second helix axis with respect to the first stem axis. (a) schematic representation of inter-helical twisting revealed by EDA applied on Kt-42. Numbered squares represent the centers of mass of particular parts of C- and NC-stem (see definition in Methods section) (b) time dependence of inter-helical torsion angle. Black line represents the data from MD simulation while red line represents the x-ray value.

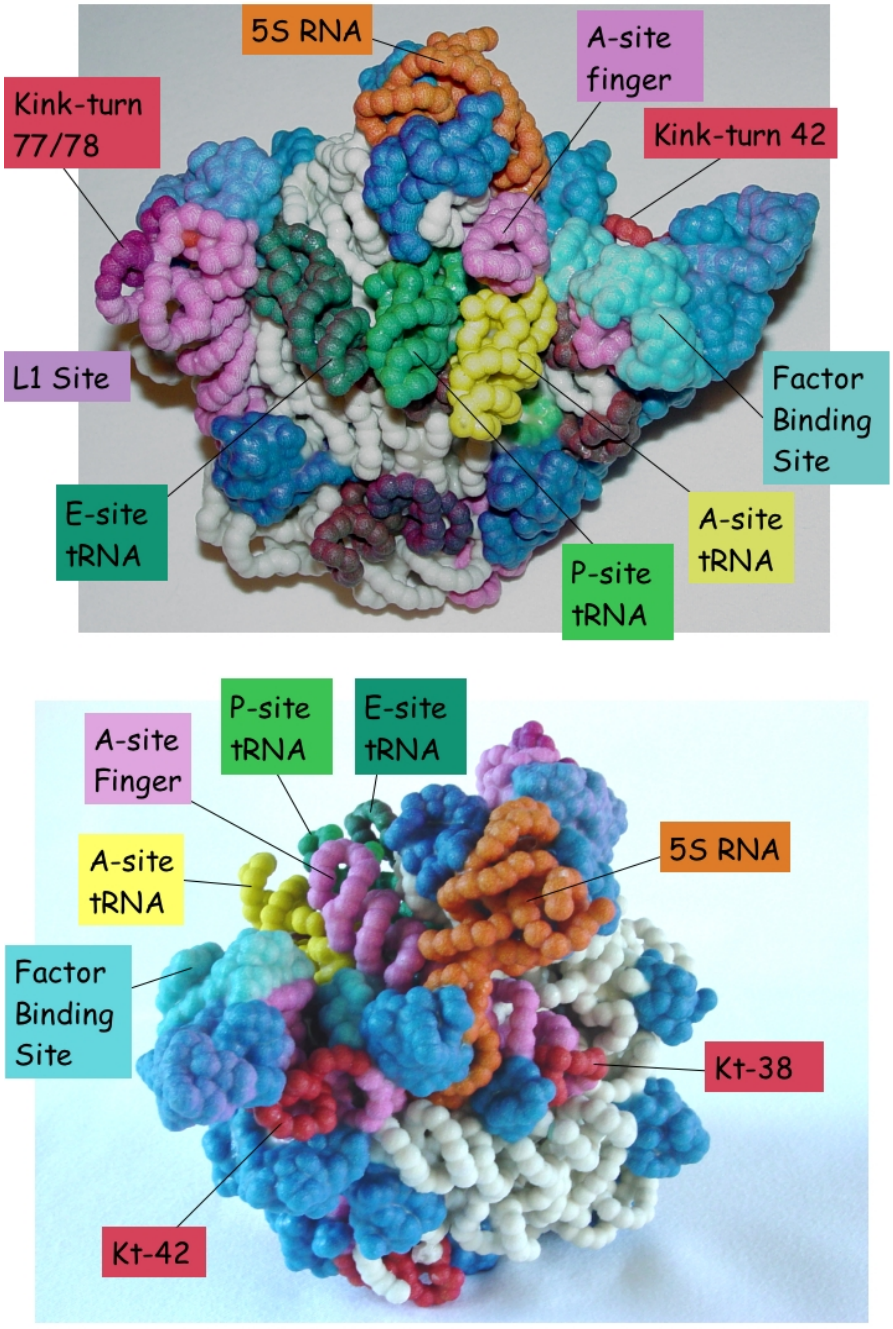

Figure S12: Model of the 50S ribosomal subunit of *T. thermophilus* showing positions of K-turns relative to other functional elements of the ribosome. Ribosomal proteins are shown in blue. 5S rRNA is shown in orange and 23S rRNA in white, except for RNA protuberances that are connected to the rest of the 50S subunit by Kink-turns. The K-turns are shown in red and the associated protuberances in pink. The coordinates used in building the model are from the 5.5 Å structure of the 70S subunit.(Yusupov et al., 2001)