

Electronic Supplementary Information for “The impact of G-quadruplex dynamics on inter-tetrad electronic couplings: a hybrid computational study”

Nandi, S.; Coane, C.; Villegas, A.-E.; Ray, A.; Di Felice, R.

The root mean square deviation is defined by:

$$RMSD(t) = \sqrt{\frac{1}{N} \sum_{i=1}^N |\mathbf{r}_i(t) - \mathbf{r}_{ref}|^2}. \quad (1)$$

The index i runs over N atoms in the system, where $N \leq N_{tot}$ and N_{tot} is the total number of atoms that compose the system.

Figure S1 reports the total (black) and partial (blue) RMSD from our trajectories evolved from inter-strand (PDB ID 1K8P, left) and intra-strand (PDB ID 1KF1, right) crystal structures. We applied Equation 1 to one snapshot every 1 ns.

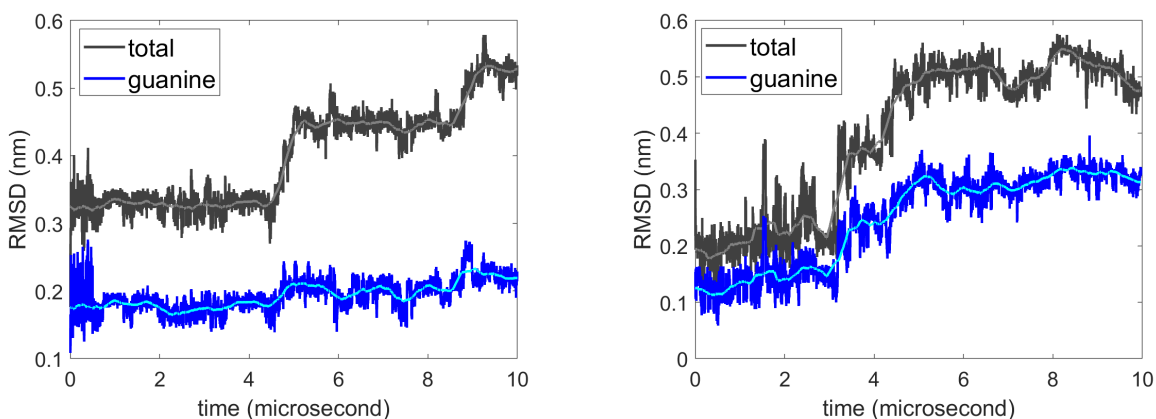


Fig. S1: Left (right): RMSD as a function of time, relative to the equilibrated structure, over the $10\mu s$ trajectory evolved from the crystal structure with PDB ID 1K8P (1KF1). The black trace was obtained by including all the atoms that form the GQ, with backbone, in the summation that define the RMSD (Equation S1). The blue line was obtained by including only the atoms of the guanine bases, with backbone.

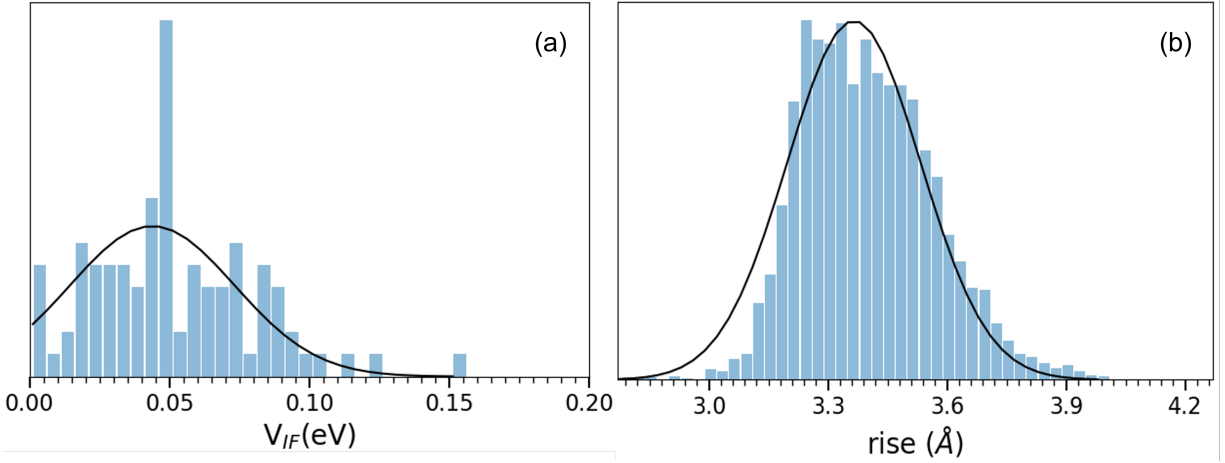
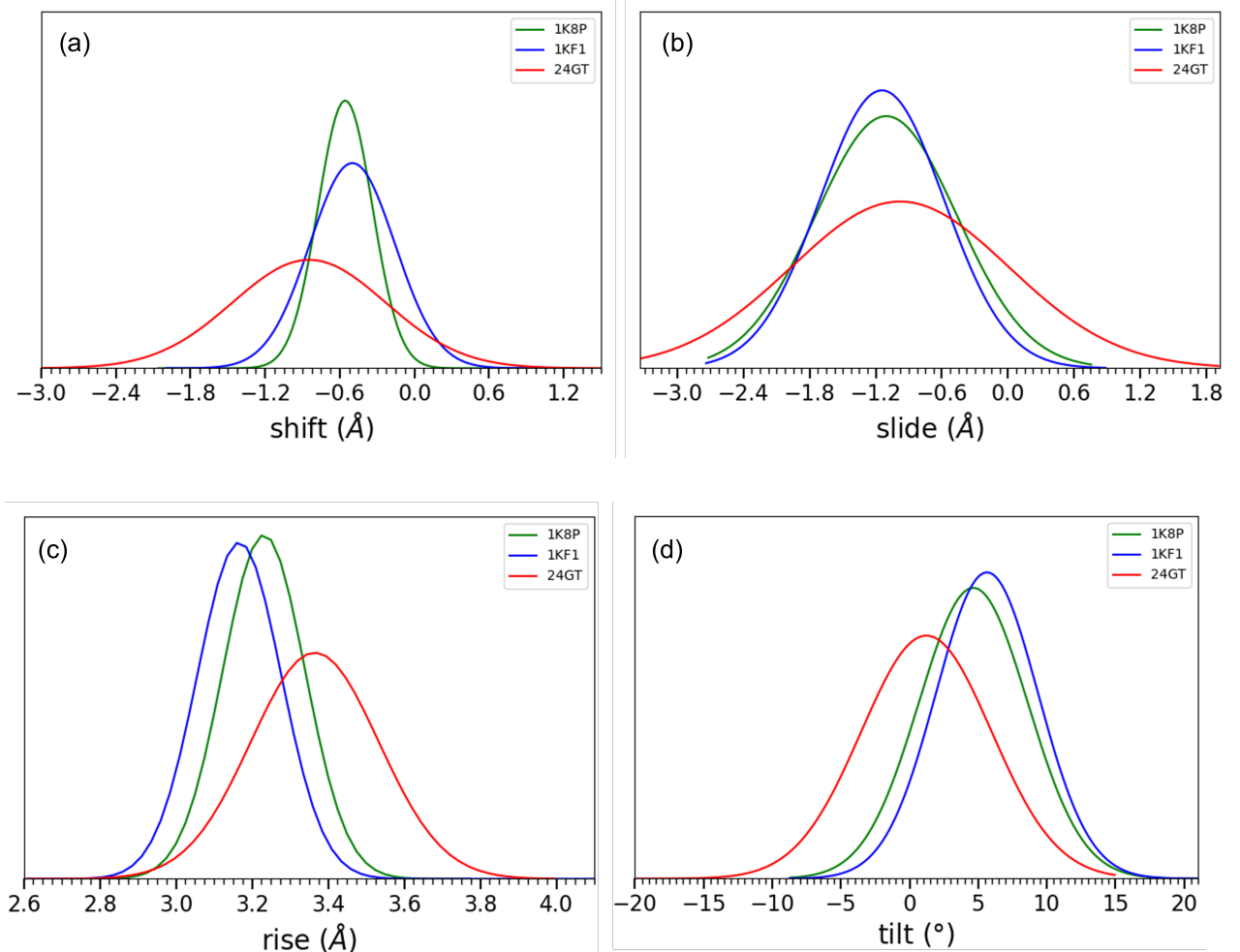


Fig. S2: Histogram plots of the transfer integral (a) and the rise (b) from the room-temperature MD trajectory of 24GT. The statistics for V_{IF} were obtained over 96 G-G stacks that were subjected to CDFT-CI calculations. The statistics for the rise were collected over 4800 G-G stacks. Details of the structure selection are explained in Materials and Methods in the main text. The black curve in each panel is the Gaussian fit of the distribution: the R^2 is 0.6 in (a), 0.97 in (b).



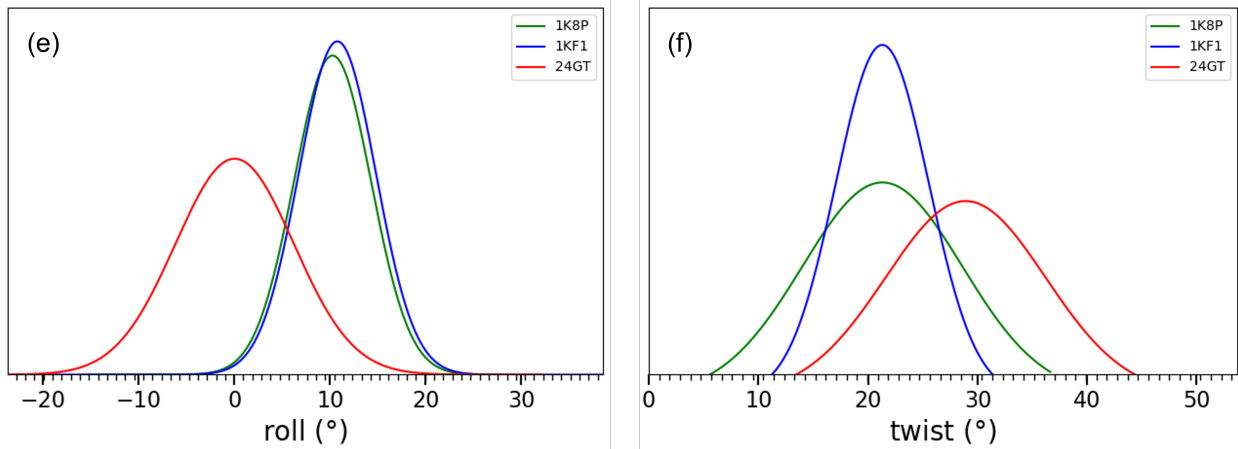


Fig. S3: Distribution curves of the six intra-strand inter-base-pair helix shape parameters, i.e shift (a), slide (b), rise (c), tilt (d), roll (e), twist (f). Green, blue and red lines refer to 1K8P, 1KF1 and 24GT. Each curve is normalized i.e. the area under the curve is equal to 1 in all the six panels.

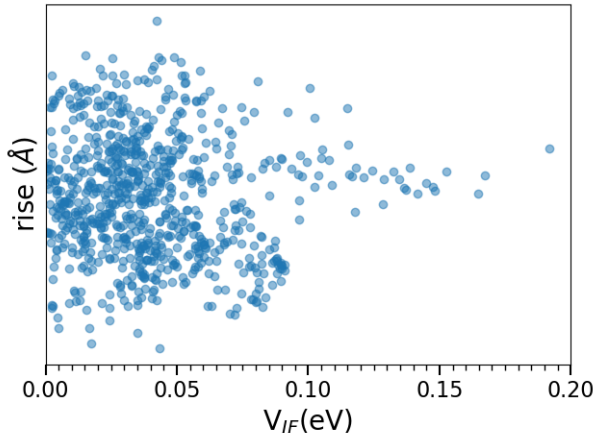


Fig. S4: Scatter plot between transfer integral and rise for the trajectory evolved from the crystal structure with PDB ID 1K8P, which reveals negligible linear correlation directly between these two quantities. The corresponding Pearson’s correlation coefficients is $P(V_{IF}\text{-rise}) = 0.03$.

Table S1: Pearson’s correlation coefficients between V_{IF} and individual shape parameters in the three trajectories of this study. These values reveal negligible, or in few cases little, linear correlations between the transfer integral and individual shape parameters, for three different GQ topologies explored in this study.

	$P(V_{IF}\text{-shift})$	$P(V_{IF}\text{-slide})$	$P(V_{IF}\text{-rise})$	$P(V_{IF}\text{-tilt})$	$P(V_{IF}\text{-roll})$	$P(V_{IF}\text{-twist})$
1K8P	0.01	0.49	0.03	-0.06	-0.22	0.0
1KF1	-0.15	0.29	-0.06	-0.06	-0.09	-0.02
24GT	0.06	-0.26	-0.17	0.06	0.21	-0.12