Supporting information for:

π–π Stacking Tackled with Density Functional Theory

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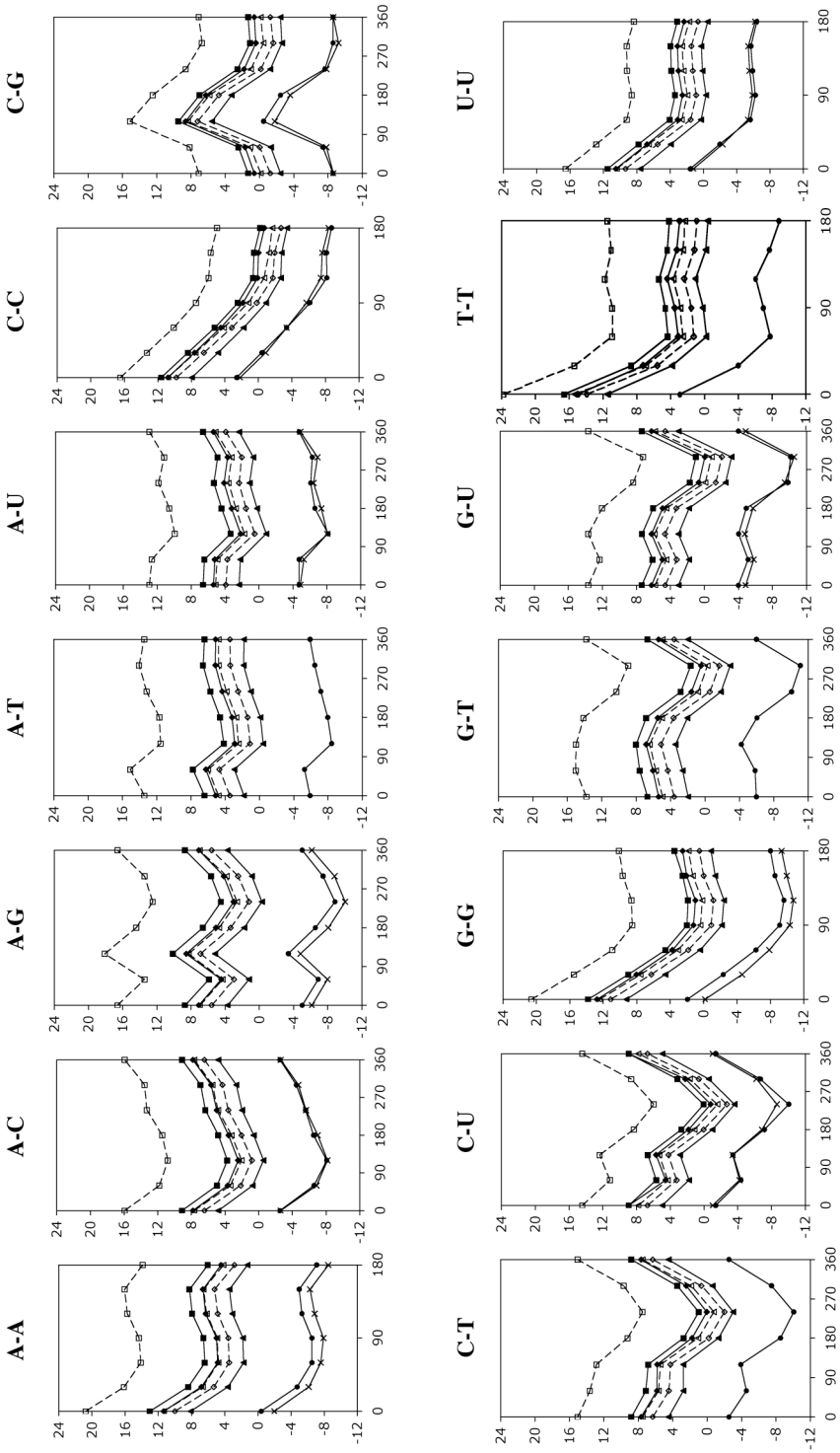

Figure S1. Energy (in kcal/mol) as a function of the twist angle (see Figure 1) for all stacks of DNA bases, computed with standard density functionals. The bold lines with filled circles, triangles, squares and diamonds show the results using LDA, PW91, BLYP and BP86, respectively. The dashed lines with open squares, triangles and diamonds show the results obtained with OLYP, B3LYP and X3LYP, respectively. The bold line with crosses represents results obtained using MP2/6-31G*(0.25).

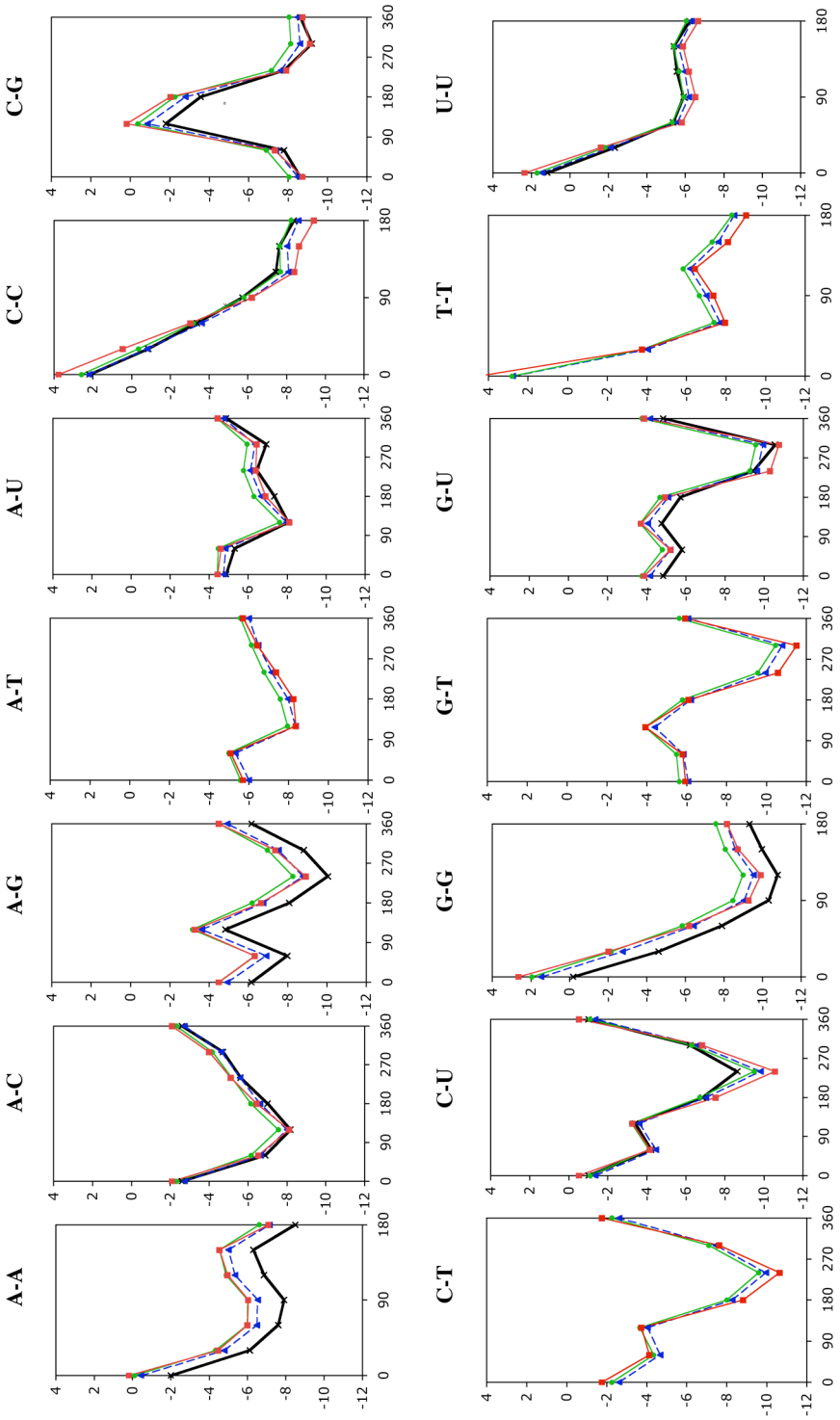

Figure S2. Energy (in kcal/mol) as a function of the twist angle (see Figure 1) for all stacks of DNA bases, computed with the more satisfactorily performing density functionals. The red, blue and green lines show the results obtained with BHandH, KT1 and KT2, respectively. The bold black line with crosses represents results obtained using MP2/6-31G*(0.25).

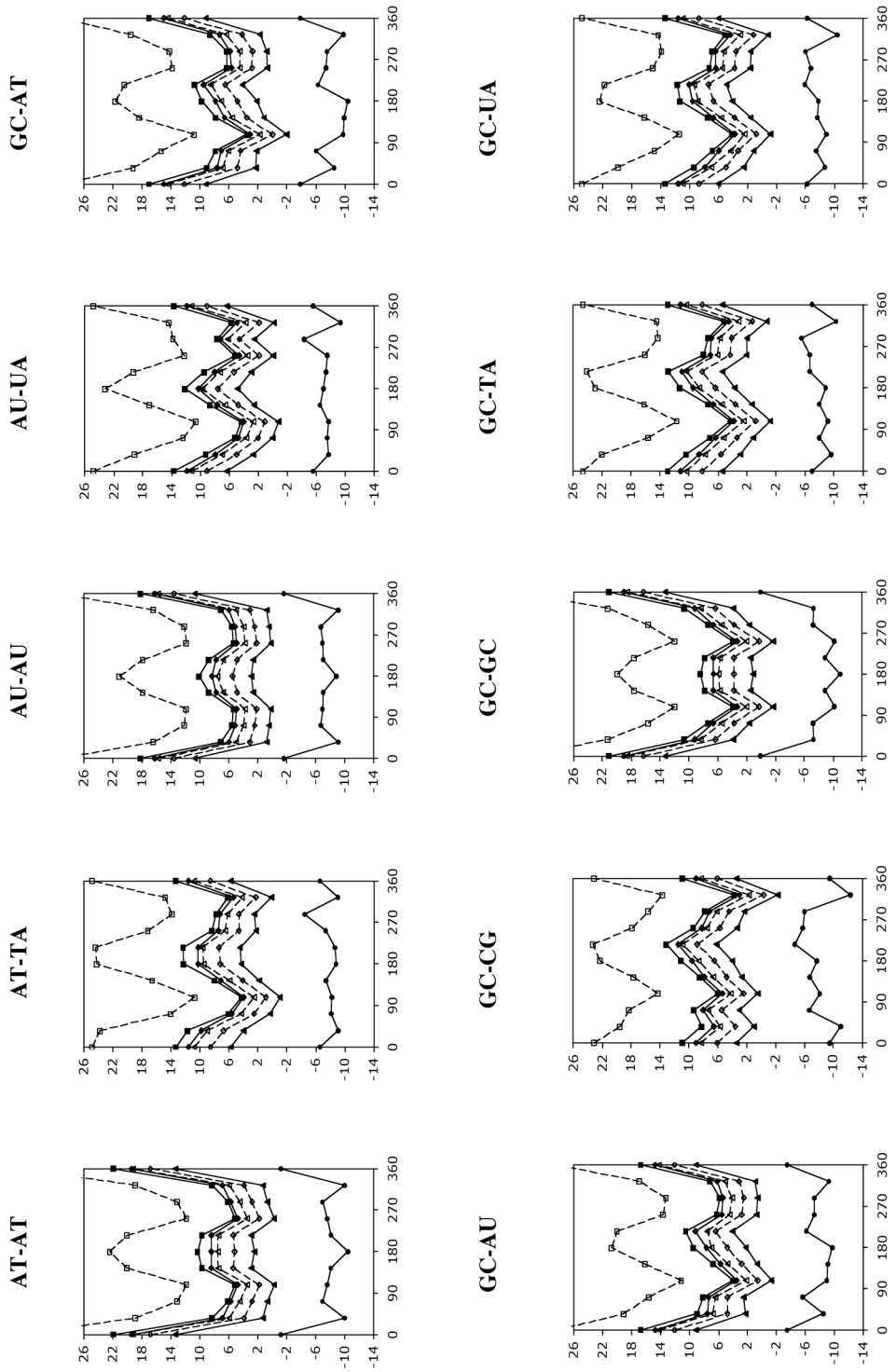

Figure S3. Energy (in kcal/mol) as a function of the twist angle (see Scheme 4) for all stacks of Watson-Crick base pairs, computed with standard density functionals. The bold lines with filled circles, triangles, squares and diamonds show the results obtained using LDA, PW91, BLYP and BP86, respectively. The dashed lines with open squares, triangles and diamonds show the results obtained with OLYP, B3LYP and X3LYP, respectively.

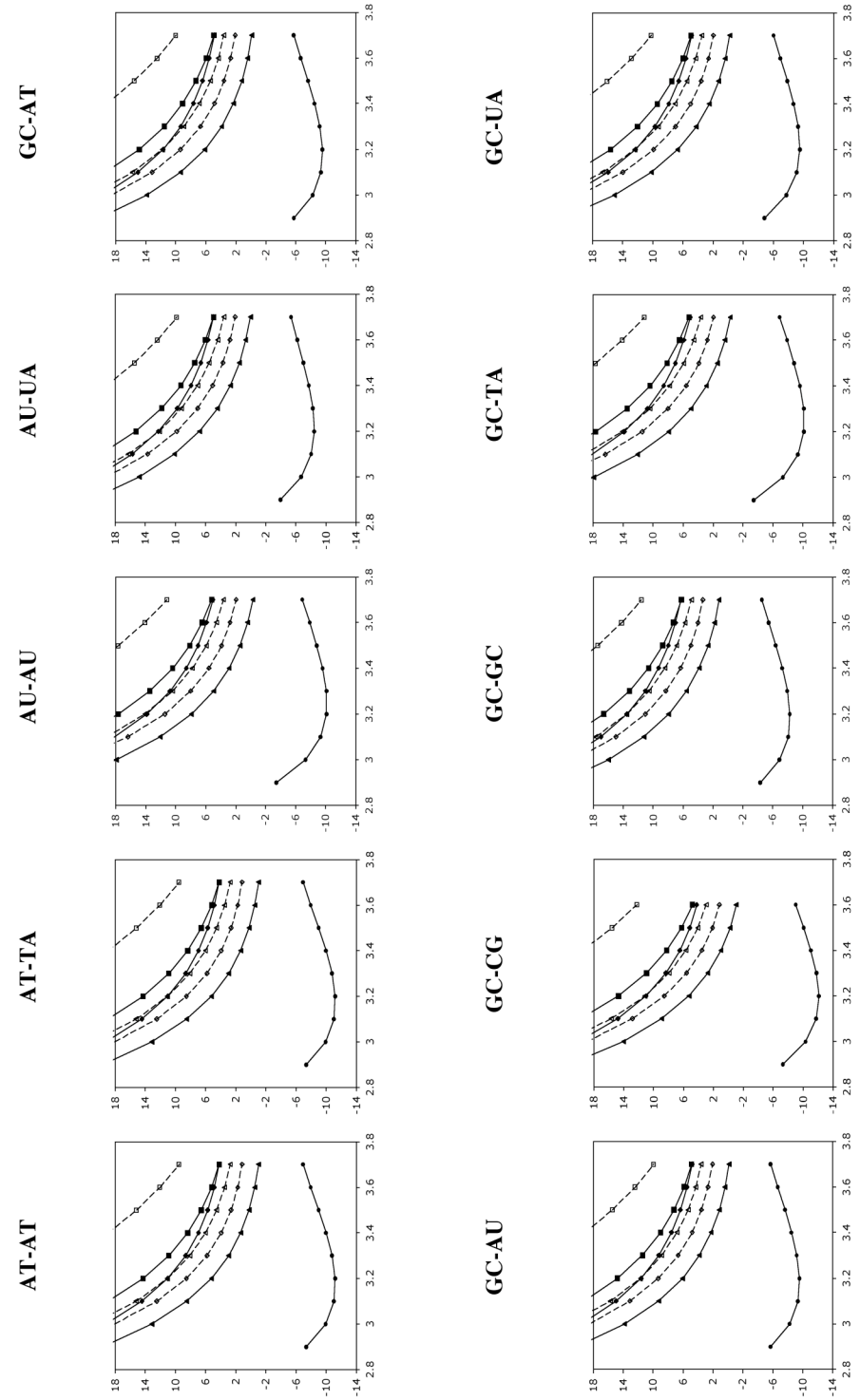

Figure S4. Energy (in kcal/mol) as a function of the vertical separation (in Å) for all stacks of base pairs, computed with various density functionals. The bold lines with filled circles, triangles, squares and diamonds show the results obtained using LDA, PW91, BLYP and BP86, respectively. The dashed lines with open squares, triangles and diamonds show the results obtained with OLYP, B3LYP and X3LYP, respectively.

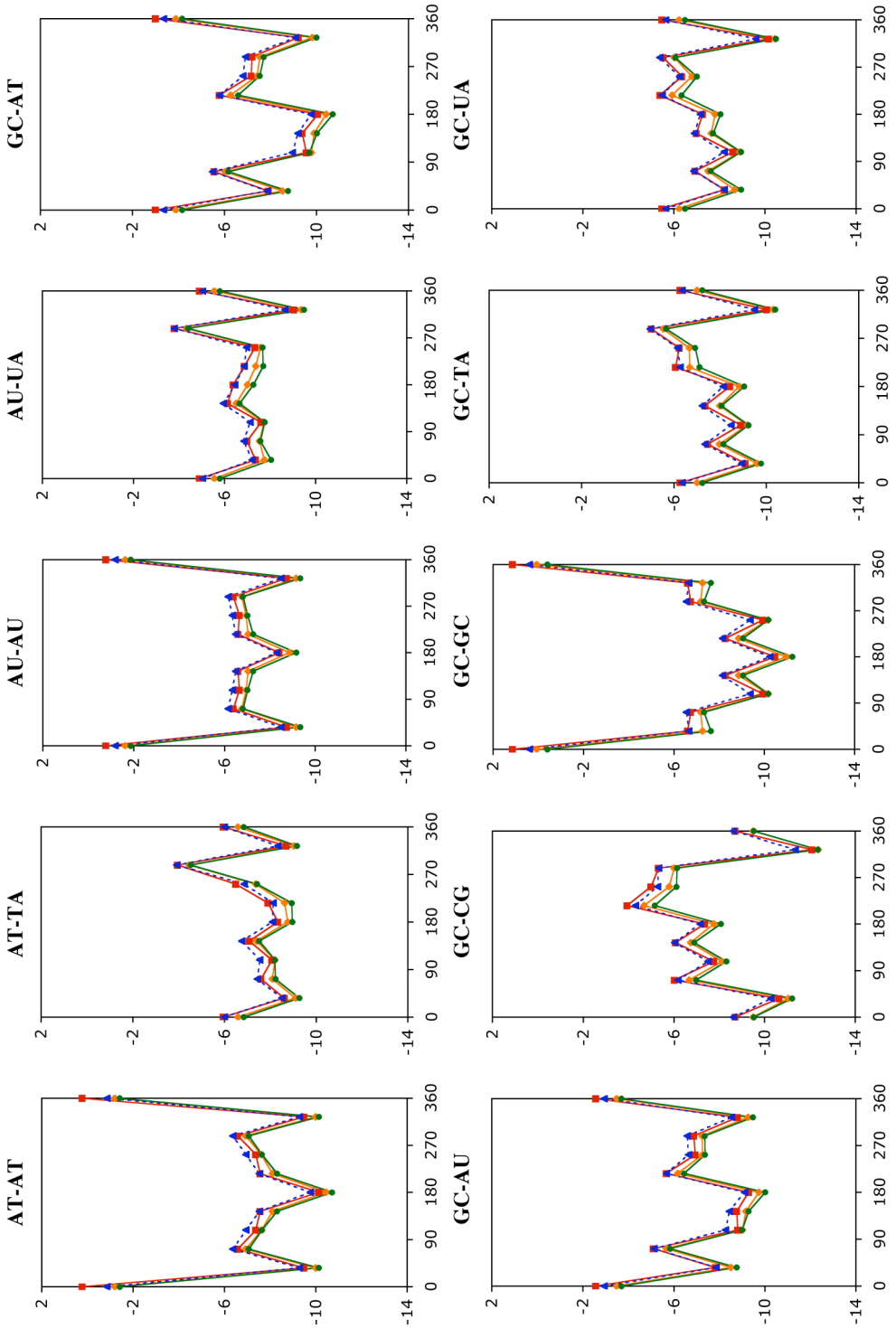

Figure S5. Energy (in kcal/mol) as a function of the twist angle (see Scheme 4) for all stacks of Watson-Crick base pairs, computed with the more satisfactorily performing density functionals LDA (orange diamonds), KT1 (green spheres), KT2 (blue triangles) and BHandH (red squares).