# Supplementary material to "Density functional theory including dispersion corrections for intermolecular interactions in a large benchmark set of biologically relevant molecules"

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[1] P. Jurecka, J. Sponer, J. Cerny, and P. Hobza, Phys. Chem. Chem. Phys. **8**, 1985 (2006).

TABLE SI: DFT-D/TZV(2d,2p) intermolecular interaction energies (kcal mol$^{-1}$) for the small dataset.

| No. | Complex (symmetry) | B97-D | | | PBE-D | | B-LYP-D | | $\Delta E^a_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^b$ | CP$^c$ | dev.$^d$ | $\Delta E^b$ | dev.$^d$ | $\Delta E^b$ | dev.$^d$ | |
| Hydrogen bonded complexes (7) | | | | | | | | | |
| 1 | $(NH_3)_2$ ($C_{2h}$) | -3.76 | -0.45 | -0.59 | -4.56 | -1.39 | -4.19 | -1.02 | -3.17 |
| 2 | $(H_2O)_2$ ($C_s$) | -5.16 | -0.69 | -0.14 | -6.41 | -1.39 | -5.89 | -0.87 | -5.02 |
| 3 | Formic acid dimer ($C_{2h}$) | -18.37 | -0.69 | 0.24 | -20.93 | -2.32 | -19.44 | -0.83 | -18.61 |
| 4 | Formamide dimer ($C_{2h}$) | -15.43 | -0.61 | 0.53 | -17.57 | -1.61 | -16.52 | -0.56 | -15.96 |
| 5 | Uracil dimer ($C_{2h}$) | -19.55 | -0.49 | 1.10 | -21.56 | -0.91 | -20.81 | -0.16 | -20.65 |
| 6 | 2-pyridoxine·2-aminopyridine | -17.23 | -0.63 | -0.52 | -19.08 | -2.37 | -18.12 | -1.41 | -16.71 |
| 7 | Adenine·thymine WC | -16.32 | -0.65 | 0.05 | -18.24 | -1.87 | -17.27 | -0.90 | -16.37 |
| Complexes with predominant dispersion contribution (8) | | | | | | | | | |
| 8 | $(CH_4)_2$ ($D_{3d}$) | -0.57 | -0.02 | -0.04 | -0.73 | -0.20 | -0.36 | 0.17 | -0.53 |
| 9 | $(C_2H_4)_2$ ($D_{2d}$) | -1.57 | -0.07 | -0.06 | -2.01 | -0.50 | -1.57 | -0.06 | -1.51 |
| 10 | Benzene·$CH_4$ ($C_3$) | -1.53 | -0.06 | -0.03 | -1.78 | -0.28 | -1.40 | 0.10 | -1.50 |
| 11 | Benzene dimer ($C_{2h}$) | -2.68 | -0.28 | 0.05 | -2.64 | 0.09 | -2.38 | 0.35 | -2.73 |
| 12 | Pyrazine dimer ($C_s$) | -4.08 | -0.28 | 0.34 | -4.17 | 0.25 | -4.08 | 0.34 | -4.42 |
| 13 | Uracil dimer ($C_2$) | -10.12 | -0.70 | 0.00 | -10.23 | -0.11 | -10.62 | -0.50 | -10.12 |
| 14 | Indole·benzene | -4.74 | -0.49 | 0.48 | -4.58 | 0.64 | -4.61 | 0.61 | -5.22 |
| 15 | Adenine·thymine stack | -12.21 | -0.90 | 0.02 | -12.15 | 0.08 | -12.98 | -0.75 | -12.23 |
| Mixed complexes (7) | | | | | | | | | |
| 16 | Ethene·ethine ($C_{2v}$) | -1.77 | -0.08 | -0.24 | -2.06 | -0.53 | -1.66 | -0.13 | -1.53 |
| 17 | Benzene·$H_2O$ ($C_s$) | -4.28 | -0.75 | -1.00 | -4.71 | -1.43 | -4.29 | -1.01 | -3.28 |
| 18 | Benzene·$NH_3$ ($C_s$) | -2.83 | -0.38 | -0.48 | -3.12 | -0.77 | -2.74 | -0.39 | -2.35 |
| 19 | Benzene·HCN ($C_s$) | -5.02 | -0.10 | -0.56 | -5.46 | -1.00 | -4.99 | -0.53 | -4.46 |
| 20 | Benzene dimer ($C_{2v}$) | -3.01 | -0.17 | -0.27 | -3.12 | -0.38 | -2.84 | -0.10 | -2.74 |
| 21 | Indole·benzene T-shape | -6.47 | -0.36 | -0.74 | -6.66 | -0.93 | -6.34 | -0.61 | -5.73 |
| 22 | Phenol dimer | -6.67 | -0.58 | 0.38 | -7.63 | -0.58 | -7.41 | -0.36 | -7.05 |

[a]Estimated CCSD(T)/CBS [1]. [b]No CP correction. [c]Counterpoise correction. [d]$\Delta E - \Delta E_{\rm ref}$.

TABLE SII: DFT/TZV(2df,2pd) intermolecular interaction energies without dispersion correction (kcal mol$^{-1}$) for the small dataset.

| No. | Complex (symmetry) | PBE | | | B-LYP | | | $\Delta E^a_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^b$ | CP$^c$ | dev.$^d$ | $\Delta E^b$ | CP$^c$ | dev.$^d$ | |
| Hydrogen bonded complexes (7) | | | | | | | | |
| 1 | $(NH_3)_2$ ($C_{2h}$) | -3.49 | -0.48 | -0.32 | -2.50 | -0.52 | 0.67 | -3.17 |
| 2 | $(H_2O)_2$ ($C_s$) | -5.73 | -0.75 | -0.71 | -4.87 | -0.81 | 0.15 | -5.02 |
| 3 | Formic acid dimer ($C_{2h}$) | -18.93 | -0.70 | -0.32 | -16.32 | -0.73 | 2.29 | -18.61 |
| 4 | Formamide dimer ($C_{2h}$) | -15.43 | -0.64 | 0.53 | -13.20 | -0.67 | 2.76 | -15.96 |
| 5 | Uracil dimer ($C_{2h}$) | -18.96 | -0.48 | 1.69 | -16.73 | -0.51 | 3.92 | -20.65 |
| 6 | 2-pyridoxine·2-aminopyridine | -16.01 | -0.63 | 0.70 | -13.28 | -0.67 | 3.43 | -16.71 |
| 7 | Adenine·thymine WC | -14.95 | -0.62 | 1.42 | -12.11 | -0.66 | 4.26 | -16.37 |
| Complexes with predominant dispersion contribution (8) | | | | | | | | |
| 8 | $(CH_4)_2$ ($D_{3d}$) | -0.11 | -0.02 | 0.42 | 0.63 | -0.02 | 1.16 | -0.53 |
| 9 | $(C_2H_4)_2$ ($D_{2d}$) | -0.39 | -0.05 | 1.12 | 1.02 | -0.05 | 2.53 | -1.51 |
| 10 | Benzene·$CH_4$ ($C_3$) | -0.12 | -0.05 | 1.38 | 1.25 | -0.06 | 2.75 | -1.50 |
| 11 | Benzene dimer ($C_{2h}$) | 1.65 | -0.25 | 4.38 | 4.51 | -0.28 | 7.24 | -2.73 |
| 12 | Pyrazine dimer ($C_s$) | 0.48 | -0.28 | 4.90 | 3.40 | -0.30 | 7.82 | -4.42 |
| 13 | Uracil dimer ($C_2$) | -3.38 | -0.69 | 6.74 | 0.32 | -0.72 | 10.44 | -10.12 |
| 14 | Indole·benzene | 1.82 | -0.43 | 7.04 | 5.69 | -0.46 | 10.91 | -5.22 |
| 15 | Adenine·thymine stack | -2.17 | -0.88 | 10.06 | 3.01 | -0.92 | 15.24 | -12.23 |
| Mixed complexes (7) | | | | | | | | |
| 16 | Ethene·ethine ($C_{2v}$) | -1.27 | -0.08 | 0.26 | -0.42 | -0.09 | 1.11 | -1.53 |
| 17 | Benzene·$H_2O$ ($C_s$) | -2.82 | -0.79 | 0.46 | -1.36 | -0.83 | 1.92 | -3.28 |
| 18 | Benzene·$NH_3$ ($C_s$) | -1.33 | -0.39 | 1.02 | 0.07 | -0.41 | 2.42 | -2.35 |
| 19 | Benzene·HCN ($C_s$) | -3.00 | -0.10 | 1.46 | -1.15 | -0.11 | 3.31 | -4.46 |
| 20 | Benzene dimer ($C_{2v}$) | -0.31 | -0.15 | 2.43 | 1.62 | -0.16 | 4.36 | -2.74 |
| 21 | Indole·benzene T-shape | -2.48 | -0.35 | 3.25 | 0.21 | -0.36 | 5.94 | -5.73 |
| 22 | Phenol dimer | -4.50 | -0.61 | 2.55 | -2.45 | -0.64 | 4.60 | -7.05 |

[a]Estimated CCSD(T)/CBS [1]. [b]No CP correction. [c]Counterpoise correction. [d]$\Delta E - \Delta E_{\rm ref}$.

TABLE SIII: DFT-D/TZV(2df,2pd) intermolecular interaction energies (kcal mol$^{-1}$) for the large dataset.

| No.[a] | Complex | B97-D | | | PBE-D | | B-LYP-D | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | dev.[e] | $\Delta E^c$ | dev.[e] | |
| Hydrogen-bonded DNA base pairs (38) | | | | | | | | | |
| 1 | G···C WC | -30.10 | -0.72 | 1.96 | -32.81 | -0.75 | -31.67 | 0.39 | -32.06 |
| 2 | mG···mC WC | -30.40 | -0.74 | 1.19 | -33.18 | -1.59 | -31.96 | -0.37 | -31.59 |
| 3 | A···T WC | -16.20 | -0.58 | 0.66 | -18.12 | -1.26 | -17.19 | -0.33 | -16.86 |
| 4 | mA···mT H | -17.15 | -0.65 | 1.01 | -19.35 | -1.19 | -18.33 | -0.17 | -18.16 |
| 5 | 8oG···C WC pl | -31.47 | -0.73 | 1.83 | -34.31 | -1.01 | -33.03 | 0.27 | -33.30 |
| 6 | I···C WC pl | -23.65 | -0.61 | 1.25 | -25.80 | -0.90 | -24.71 | 0.19 | -24.90 |
| 7 | G···U wobble | -17.80 | -0.56 | 1.30 | -19.96 | -0.86 | -19.05 | 0.05 | -19.10 |
| 8 | CCH+ | -50.54 | -0.60 | 0.86 | -53.60 | -2.20 | -52.09 | -0.69 | -51.40 |
| 9 | U···U Calcutta pl | -9.23 | -0.47 | 1.07 | -10.91 | -0.61 | -10.28 | 0.02 | -10.30 |
| 10 | U···U pl | -12.44 | -0.49 | 1.26 | -14.52 | -0.82 | -13.72 | -0.02 | -13.70 |
| 11 | 6tG···C WC pl | -28.73 | -0.77 | 0.77 | -31.70 | -2.20 | -29.86 | -0.36 | -29.50 |
| 12 | A···4tU WC | -13.84 | -0.54 | 0.36 | -15.53 | -1.33 | -14.60 | -0.40 | -14.20 |
| 13 | 2-aminoA···T | -19.55 | -0.68 | -0.05 | -22.12 | -2.62 | -21.02 | -1.52 | -19.50 |
| 14 | 2-aminoA···T pl | -19.59 | -0.65 | 0.11 | -22.18 | -2.48 | -21.11 | -1.41 | -19.70 |
| 15 | A···F | -4.84 | -0.43 | 0.36 | -5.83 | -0.63 | -5.53 | -0.33 | -5.20 |
| 16 | G···4tU | -16.22 | -0.56 | 1.58 | -18.28 | -0.48 | -17.50 | 0.30 | -17.80 |
| 17 | G···2tU | -14.92 | -0.57 | 1.68 | -17.18 | -0.58 | -15.67 | 0.93 | -16.60 |
| 18 | A···C pl | -17.94 | -0.55 | -0.34 | -19.72 | -2.12 | -18.70 | -1.10 | -17.60 |
| 19 | G···G pl | -20.52 | -0.63 | 0.78 | -22.39 | -1.09 | -21.70 | -0.40 | -21.30 |
| 20 | G···6tG pl | -20.66 | -0.63 | 1.14 | -22.87 | -1.07 | -21.80 | 0.00 | -21.80 |
| 21 | 6tG···G pl | -21.51 | -0.71 | 1.19 | -23.76 | -1.06 | -22.62 | 0.08 | -22.70 |
| 22 | G···A 1 | -19.71 | -0.70 | -0.31 | -21.70 | -2.30 | -20.76 | -1.36 | -19.40 |
| 23 | G···A 1 pl | -19.32 | -0.57 | -0.42 | -21.28 | -2.38 | -20.53 | -1.63 | -18.90 |
| 24 | G···A 2 | -13.77 | -0.64 | 0.63 | -15.39 | -0.99 | -14.60 | -0.20 | -14.40 |
| 25 | G···A 2 pl | -12.90 | -0.52 | -0.10 | -14.54 | -1.74 | -13.75 | -0.95 | -12.80 |

TABLE SIII: (continued)

| No.[a] | Complex | B97-D | | | PBE-D | | B-LYP-D | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | dev.[e] | $\Delta E^c$ | dev.[e] | |
| 26 | G···A 3 | -18.50 | -0.74 | 0.30 | -20.62 | -1.82 | -19.70 | -0.90 | -18.80 |
| 27 | G···A 4 | -13.84 | -0.55 | -0.34 | -15.46 | -1.96 | -14.61 | -1.11 | -13.50 |
| 28 | A···A 1 pl | -14.95 | -0.52 | -0.45 | -16.69 | -2.19 | -15.73 | -1.23 | -14.50 |
| 29 | A···A 2 pl | -13.86 | -0.55 | -0.16 | -15.66 | -1.96 | -14.73 | -1.03 | -13.70 |
| 30 | A···A 3 pl | -12.11 | -0.59 | 0.09 | -13.85 | -1.65 | -13.02 | -0.82 | -12.20 |
| 31 | 8oG···G | -21.28 | -0.63 | 1.52 | -23.69 | -0.89 | -22.60 | 0.20 | -22.80 |
| 32 | 2tU···.2tU pl | -10.70 | -0.54 | 1.90 | -12.91 | -0.31 | -11.51 | 1.09 | -12.60 |
| 33 | mA···mT WC[f] | -16.44 | -0.60 | -0.04 | -18.31 | -1.91 | -17.39 | -0.99 | -16.40 |
| 34 | mG···mC WC*[f,g] | -33.39 | -0.79 | 2.41 | -36.15 | -0.35 | -34.93 | 0.87 | -35.80 |
| 35 | mA···mT WC[f] | -18.24 | -0.63 | 0.16 | -19.99 | -1.59 | -19.10 | -0.70 | -18.40 |
| 36 | G···A HB | -13.80 | -0.70 | -2.50 | -15.59 | -4.29 | -14.64 | -3.34 | -11.30 |
| 37 | C···G WC | -30.89 | -0.75 | -0.19 | -33.91 | -3.21 | -32.55 | -1.85 | -30.70 |
| 38 | G···C WC | -30.55 | -0.74 | 0.85 | -33.60 | -2.20 | -32.25 | -0.85 | -31.40 |
| Interstrand base pairs (32) | | | | | | | | | |
| 39 | GG0/3.36 CGis036 | -4.21 | -0.45 | -0.53 | -4.07 | -0.39 | -3.89 | -0.21 | -3.68 |
| 40 | GG0/3.36 GCis036 | -4.03 | -0.91 | 0.79 | -3.48 | 1.34 | -4.18 | 0.64 | -4.82 |
| 41 | AA20/3.05 TAis2005[h] | -2.56 | -0.34 | -0.40 | -2.79 | -0.63 | -2.60 | -0.44 | -2.16 |
| 42 | AA20/3.05 ATis2005[h] | -4.66 | -0.55 | -2.32 | -4.48 | -2.14 | -4.83 | -2.49 | -2.34 |
| 43 | GC0/3.25 C//Cis | 2.80 | -0.13 | -0.29 | 2.90 | -0.19 | 2.94 | -0.15 | 3.09 |
| 44 | GC0/3.25 G//Gis | 1.46 | -0.57 | -0.47 | 1.51 | -0.42 | 1.81 | -0.12 | 1.93 |
| 45 | CG0/3.19 C//Cis[i] | 0.82 | -0.18 | -0.42 | 0.88 | -0.36 | 1.05 | -0.19 | 1.24 |
| 46 | CG0/3.19 G//Gis[i] | -5.00 | -0.81 | -1.09 | -4.84 | -0.93 | -4.79 | -0.88 | -3.91 |
| 47 | GA10/3.15 A//Cis | -0.26 | -0.32 | 0.05 | -0.22 | 0.09 | 0.01 | 0.32 | -0.31 |
| 48 | GA10/3.15 T//Gis | 0.51 | -0.24 | -0.07 | 0.53 | -0.05 | 0.75 | 0.17 | 0.58 |
| 49 | AG08/3.19 T//Gis | -0.89 | -0.46 | -0.42 | -1.02 | -0.55 | -0.81 | -0.34 | -0.47 |
| 50 | AG08/3.19 A//Cis | -0.60 | -0.33 | -0.42 | -0.58 | -0.40 | -0.37 | -0.19 | -0.18 |
| 51 | TG03.19 A//Gis | -4.83 | -0.59 | -0.61 | -4.65 | -0.43 | -4.63 | -0.41 | -4.22 |

TABLE SIII: (continued)

| No.[a] | Complex | B97-D | | | PBE-D | | B-LYP-D | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | dev.[e] | $\Delta E^c$ | dev.[e] | |
| 52 | TG03.19 T//Cis | -1.45 | -0.15 | -0.30 | -1.34 | -0.19 | -1.25 | -0.10 | -1.15 |
| 53 | GT10/3.15 T//Cis | 0.02 | -0.14 | -0.28 | 0.12 | -0.18 | 0.21 | -0.09 | 0.30 |
| 54 | GT10/3.15 A//Gis | -4.48 | -0.49 | -0.42 | -4.59 | -0.53 | -4.42 | -0.36 | -4.06 |
| 55 | AT10/3.26 T//Tis | 0.54 | -0.17 | -0.34 | 0.64 | -0.24 | 0.82 | -0.06 | 0.88 |
| 56 | AT10/3.26 A//Ais | -1.42 | -0.45 | -0.50 | -1.40 | -0.48 | -1.21 | -0.29 | -0.92 |
| 57 | TA08/3.16 A//Ais | -1.53 | -0.39 | 0.02 | -1.55 | -0.00 | -1.58 | -0.03 | -1.55 |
| 58 | TA08/3.16 T//Tis | 0.54 | -0.14 | -0.16 | 0.62 | -0.08 | 0.72 | 0.02 | 0.70 |
| 59 | AA0/3.24 A//Tis | -2.06 | -0.22 | -0.35 | -1.87 | -0.16 | -1.70 | 0.01 | -1.71 |
| 60 | AA0/3.24 T//Ais | -1.79 | -0.26 | -0.49 | -1.67 | -0.37 | -1.48 | -0.18 | -1.30 |
| 61 | mA···mA IS[f] | -1.12 | -0.52 | -0.42 | -1.20 | -0.50 | -1.01 | -0.31 | -0.70 |
| 62 | mT···mT IS[f] | 0.63 | -0.20 | -0.37 | 0.72 | -0.28 | 0.90 | -0.10 | 1.00 |
| 63 | mG···mG IS[f] | -5.47 | -0.82 | -0.97 | -5.04 | -0.54 | -5.14 | -0.64 | -4.50 |
| 64 | mC···mC IS[f] | 0.89 | -0.26 | -0.51 | 0.83 | -0.57 | 0.99 | -0.41 | 1.40 |
| 65 | mA···mG IS[f] | -5.23 | -0.50 | -0.43 | -5.26 | -0.46 | -4.98 | -0.18 | -4.80 |
| 66 | mT···mC IS[f] | -0.43 | -0.18 | -0.33 | -0.30 | -0.20 | -0.21 | -0.11 | -0.10 |
| 67 | C···A IS | -2.58 | -0.45 | 0.42 | -2.96 | 0.04 | -2.74 | 0.26 | -3.00 |
| 68 | G···G IS | -5.78 | -0.38 | -0.58 | -5.77 | -0.57 | -5.61 | -0.41 | -5.20 |
| 69 | G···G IS | 0.30 | -0.72 | -0.50 | 0.05 | -0.75 | 0.41 | -0.39 | 0.80 |
| 70 | C···C IS | 2.79 | -0.11 | -0.31 | 2.89 | -0.21 | 2.91 | -0.19 | 3.10 |
| Stacked base pairs (54) | | | | | | | | | |
| 71 | G···C S | -18.57 | -0.98 | 0.45 | -19.20 | -0.18 | -19.78 | -0.76 | -19.02 |
| 72 | mG···mC S | -19.08 | -1.09 | 1.27 | -19.67 | 0.68 | -20.59 | -0.24 | -20.35 |
| 73 | A···T S | -12.11 | -0.80 | 0.19 | -12.08 | 0.22 | -12.85 | -0.55 | -12.30 |
| 74 | mA···mT S | -14.55 | -0.95 | 0.02 | -14.80 | -0.23 | -16.01 | -1.44 | -14.57 |
| 75 | CC1 | 2.09 | -0.66 | -0.36 | 2.09 | -0.36 | 2.12 | -0.33 | 2.45 |
| 76 | CC2 | -3.85 | -0.71 | -0.00 | -3.81 | 0.04 | -3.97 | -0.12 | -3.85 |
| 77 | CC3 | -8.39 | -0.77 | 0.49 | -8.46 | 0.42 | -8.71 | 0.17 | -8.88 |

TABLE SIII: (continued)

| No.[a] | Complex | B97-D | | | PBE-D | | B-LYP-D | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | dev.[e] | $\Delta E^c$ | dev.[e] | |
| 78 | CC4 | -9.17 | -0.79 | 0.75 | -9.08 | 0.84 | -9.42 | 0.50 | -9.92 |
| 79 | CC5 | 0.27 | -0.75 | -0.05 | 0.15 | -0.17 | 0.14 | -0.18 | 0.32 |
| 80 | CC6 | 0.50 | -0.78 | -0.14 | 0.36 | -0.28 | 0.40 | -0.24 | 0.64 |
| 81 | CC7 | -1.18 | -0.61 | -0.20 | -1.24 | -0.26 | -1.12 | -0.14 | -0.98 |
| 82 | CC8 | -8.14 | -0.77 | 0.96 | -8.13 | 0.97 | -8.43 | 0.67 | -9.10 |
| 83 | CC9 | -8.67 | -0.73 | 0.44 | -8.50 | 0.61 | -8.76 | 0.35 | -9.11 |
| 84 | CC10 | -7.98 | -0.82 | 0.29 | -7.82 | 0.45 | -8.11 | 0.16 | -8.27 |
| 85 | CC11 | -8.68 | -0.69 | 0.75 | -8.57 | 0.86 | -8.89 | 0.54 | -9.43 |
| 86 | CC12 | -6.62 | -0.62 | 0.81 | -6.63 | 0.80 | -6.84 | 0.59 | -7.43 |
| 87 | CC13 | -8.39 | -0.76 | 0.41 | -8.33 | 0.47 | -8.43 | 0.37 | -8.80 |
| 88 | CC14 | -8.45 | -0.76 | 0.66 | -8.42 | 0.69 | -8.80 | 0.31 | -9.11 |
| 89 | AAst | -8.55 | -0.77 | 0.03 | -8.11 | 0.47 | -8.62 | -0.04 | -8.58 |
| 90 | GGst | -12.55 | -0.91 | 0.12 | -12.04 | 0.63 | -12.77 | -0.10 | -12.67 |
| 91 | ACst | -9.80 | -0.71 | 0.42 | -9.53 | 0.69 | -9.86 | 0.36 | -10.22 |
| 92 | GAst | -11.06 | -0.79 | 0.32 | -10.56 | 0.82 | -11.19 | 0.19 | -11.38 |
| 93 | CCst | -9.43 | -0.68 | 0.59 | -9.28 | 0.74 | -9.54 | 0.48 | -10.02 |
| 94 | AUst | -9.63 | -0.67 | 0.16 | -9.45 | 0.34 | -9.76 | 0.03 | -9.79 |
| 95 | GCst | -10.82 | -0.82 | -0.22 | -10.60 | 0.00 | -10.84 | -0.24 | -10.60 |
| 96 | CUst | -9.85 | -0.63 | 0.57 | -9.91 | 0.51 | -10.12 | 0.30 | -10.42 |
| 97 | UUst | -7.53 | -0.50 | -0.07 | -7.46 | -0.00 | -7.51 | -0.05 | -7.46 |
| 98 | GUst | -11.85 | -0.74 | 0.24 | -11.66 | 0.43 | -12.10 | -0.01 | -12.09 |
| 99 | GG0/3.36 CCs036[j] | -1.93 | -0.67 | -0.31 | -1.90 | -0.28 | -1.96 | -0.34 | -1.62 |
| 100 | GG0/3.36 GGs036[j] | -5.09 | -0.23 | -1.55 | -4.91 | -1.37 | -4.79 | -1.25 | -3.54 |
| 101 | AA20/3.05 AAs2005 | -6.22 | -0.78 | -0.16 | -5.77 | 0.29 | -6.47 | -0.41 | -6.06 |
| 102 | AA20/3.05 TTs2005 | -2.28 | -0.28 | 1.90 | -2.53 | 1.65 | -2.34 | 1.84 | -4.18 |
| 103 | GC0/3.25 G//Cs | -11.11 | -0.86 | -0.31 | -10.85 | -0.05 | -11.46 | -0.66 | -10.80 |

TABLE SIII: (continued)

| No.[a] | Complex | B97-D | | | PBE-D | | B-LYP-D | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | dev.[e] | $\Delta E^c$ | dev.[e] | |
| 104 | CG0/3.19 G//Cs | -7.25 | -0.68 | 0.63 | -7.22 | 0.66 | -7.78 | 0.10 | -7.88 |
| 105 | GA10/3.15 A//Gs | -9.86 | -0.99 | -0.72 | -9.38 | -0.24 | -10.19 | -1.05 | -9.14 |
| 106 | GA10/3.15 T//Cs | -5.18 | -0.65 | -0.49 | -5.08 | -0.39 | -5.21 | -0.52 | -4.69 |
| 107 | AG08/3.19 A//Gs | -7.77 | -0.67 | -0.19 | -7.23 | 0.35 | -7.89 | -0.31 | -7.58 |
| 108 | AG08/3.19 T//Cs | -6.38 | -0.56 | -0.31 | -6.23 | -0.16 | -6.50 | -0.43 | -6.07 |
| 109 | TG03.19 T//Gs | -5.47 | -0.59 | 0.20 | -5.40 | 0.27 | -5.84 | -0.17 | -5.67 |
| 110 | TG03.19 A//Cs | -4.83 | -0.78 | 0.13 | -4.82 | 0.14 | -5.29 | -0.33 | -4.96 |
| 111 | GT10/3.15 T//Gs | -5.49 | -0.70 | -0.53 | -5.22 | -0.26 | -5.84 | -0.88 | -4.96 |
| 112 | GT10/3.15 A//Cs | -5.52 | -0.71 | -0.08 | -5.20 | 0.24 | -5.62 | -0.18 | -5.44 |
| 113 | AT10/3.26 A//Ts | -7.14 | -0.55 | -0.50 | -6.71 | -0.07 | -7.21 | -0.57 | -6.64 |
| 114 | TA08/3.16 A//Ts | -5.10 | -0.74 | 0.97 | -4.93 | 1.14 | -5.78 | 0.29 | -6.07 |
| 115 | AA0/3.24 A//As | -6.40 | -0.75 | -0.15 | -5.96 | 0.29 | -6.64 | -0.39 | -6.25 |
| 116 | AA0/3.24 T//Ts | -4.36 | -0.55 | -0.50 | -4.37 | -0.51 | -4.80 | -0.94 | -3.86 |
| 117 | mA$\cdots$mT S[f] | -8.54 | -0.63 | -0.44 | -7.94 | 0.16 | -8.51 | -0.41 | -8.10 |
| 118 | mG$\cdots$mC S[f] | -7.76 | -0.61 | 0.14 | -7.30 | 0.60 | -7.67 | 0.23 | -7.90 |
| 119 | mA$\cdots$mC S[f] | -6.57 | -0.79 | 0.13 | -6.11 | 0.59 | -6.51 | 0.19 | -6.70 |
| 120 | mT$\cdots$mG S[f] | -7.04 | -0.69 | -0.84 | -6.32 | -0.12 | -6.80 | -0.60 | -6.20 |
| 121 | G$\cdots$C S | -7.79 | -0.81 | -0.09 | -7.42 | 0.28 | -7.86 | -0.16 | -7.70 |
| 122 | A$\cdots$G S | -7.09 | -0.90 | -0.59 | -6.69 | -0.19 | -7.40 | -0.90 | -6.50 |
| 123 | C$\cdots$G S | -10.92 | -0.80 | 1.48 | -10.68 | 1.72 | -11.11 | 1.29 | -12.40 |
| 124 | G$\cdots$C S | -11.14 | -0.81 | 0.46 | -10.90 | 0.70 | -11.25 | 0.35 | -11.60 |
| Amino acid pairs (19) | | | | | | | | | |
| 125 | F30-K46 | -3.63 | -0.25 | -0.53 | -3.47 | -0.37 | -3.24 | -0.14 | -3.10 |
| 126 | F30-L33 | -5.53 | -0.60 | -0.53 | -5.97 | -0.97 | -6.03 | -1.03 | -5.00 |
| 127 | F30-Y13 | -4.66 | -0.31 | -0.76 | -4.49 | -0.59 | -4.39 | -0.49 | -3.90 |
| 128 | F30-F49 | -3.17 | -0.11 | 0.13 | -2.94 | 0.36 | -2.88 | 0.42 | -3.30 |
| 129 | F30-Y4 | -5.81 | -0.29 | 1.19 | -5.04 | 1.96 | -5.38 | 1.62 | -7.00 |

TABLE SIII: (continued)

| No.[a] | Complex | B97-D | | | PBE-D | | B-LYP-D | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | dev.[e] | $\Delta E^c$ | dev.[e] | |
| 130 | F49-C39 | -2.50 | -0.16 | -0.40 | -2.60 | -0.50 | -2.59 | -0.49 | -2.10 |
| 131 | F49-C6 | -4.88 | -0.41 | 0.12 | -4.55 | 0.45 | -4.43 | 0.57 | -5.00 |
| 132 | F49-K46 | -4.72 | -0.56 | 0.08 | -5.23 | -0.43 | -5.17 | -0.37 | -4.80 |
| 133 | F49-V5 | -6.25 | -0.61 | 0.45 | -7.00 | -0.30 | -6.94 | -0.24 | -6.70 |
| 134 | F49-W37[k] | -2.19 | -0.09 | 0.31 | -2.16 | 0.34 | -1.97 | 0.53 | -2.50 |
| 135 | F49-Y4 | -4.03 | -0.25 | -0.93 | -3.85 | -0.75 | -3.81 | -0.71 | -3.10 |
| 136 | F49-PB (Y4-V5) | -3.62 | -0.33 | -0.82 | -3.31 | -0.51 | -3.14 | -0.34 | -2.80 |
| 137 | F49-PB (V5-C6) | -7.62 | -0.63 | 0.58 | -8.06 | 0.14 | -8.12 | 0.08 | -8.20 |
| 138 | E47-K6 (1IU5) | -78.77 | -1.02 | 1.96 | -80.21 | 0.52 | -80.03 | 0.70 | -80.73 |
| 139 | E49-K6 (1BQ9) | -110.34 | -1.11 | 3.01 | -111.19 | 2.16 | -110.86 | 2.49 | -113.35 |
| 140 | E54-K2 (1SMM) | -93.45 | -0.83 | -5.16 | -93.80 | -5.51 | -93.87 | -5.58 | -88.29 |
| 141 | E50-K30 (1BRF) | -61.26 | -0.35 | -0.90 | -61.57 | -1.21 | -62.00 | -1.64 | -60.36 |
| 142 | E50-K52 (1BRF) | -94.36 | -1.43 | 2.78 | -95.52 | 1.62 | -95.42 | 1.72 | -97.14 |
| 143 | E49-K6 (1BRF) | -71.00 | -0.95 | 3.24 | -72.17 | 2.07 | -71.76 | 2.48 | -74.24 |

[a]The calculated $\Delta E$ values are in the same sequence as the structures in the database. [b]Estimated CCSD(T)/CBS. The reference $\Delta E$ values of No. 41 and 42, No. 45 and 46, as well as No. 100 and 102 from Table 1 of Ref. [1] are interchanged. This is justified by a RI-MP2/aug-cc-pVDZ calculation and a comparison of the resulting $\Delta E$ values with the first column of Table 1 in Ref. [1]. In the discussion and the statistical analysis, the results for complexes No. 40, 42, 100, and 102 (after the interchange described above) are omitted, because the structures in the database disagree with their description given in Table 1 of Ref. [1]. Under the assumption, that the last pair of capital letters in the name describes the complex, No. 40 should be GC, but the 40th complex of the database is GG. Similarly, No. 42 (after interchange) has the name AT, while the 42nd coordinates in the database are TT, No. 100 (after interchange) is named GG, whereas the 100th complex in the database is CG, and the name of No. 102 is TT, but the 102nd coordinates in the database are AT. [c]No CP correction. [d]Counterpoise correction. [e]$\Delta E - \Delta E_{\rm ref}$. [f]Base pair methylated. [g]The * is missing in the database. [h]Rows 41 and 42 of

Table 1 in Ref. [1] are interchanged. [i]Rows 45 and 46 of Table 1 in Ref. [1] are interchanged. [j]Rows 99 and 100 of Table 1 in Ref. [1] are interchanged. [k]Residue 37 of 1RB9 is tryptophan (W), not tyrosine (Y).

TABLE SIV: DFT/TZV(2df,2pd) intermolecular interaction energies without dispersion correction (kcal mol$^{-1}$) for the large dataset.

| No.[a] | Complex | PBE | | | B-LYP | | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | CP[d] | dev.[e] | |
| Hydrogen-bonded DNA base pairs (38) | | | | | | | | |
| 1 | G···C WC | -29.00 | -0.76 | 3.06 | -25.57 | -0.81 | 6.49 | -32.06 |
| 2 | mG···mC WC | -29.16 | -0.79 | 2.43 | -25.52 | -0.84 | 6.07 | -31.59 |
| 3 | A···T WC | -14.95 | -0.62 | 1.91 | -12.11 | -0.66 | 4.75 | -16.86 |
| 4 | mA···mT H | -16.07 | -0.70 | 2.09 | -13.08 | -0.75 | 5.08 | -18.16 |
| 5 | 8oG···C WC pl | -30.33 | -0.78 | 2.97 | -26.66 | -0.83 | 6.64 | -33.30 |
| 6 | I···C WC pl | -22.36 | -0.66 | 2.54 | -19.20 | -0.70 | 5.70 | -24.90 |
| 7 | G···U wobble | -16.95 | -0.60 | 2.15 | -14.22 | -0.64 | 4.88 | -19.10 |
| 8 | CCH+ | -49.46 | -0.64 | 1.94 | -45.46 | -0.68 | 5.94 | -51.40 |
| 9 | U···U Calcutta pl | -8.93 | -0.51 | 1.37 | -7.11 | -0.54 | 3.19 | -10.30 |
| 10 | U···U pl | -12.17 | -0.52 | 1.53 | -9.97 | -0.56 | 3.73 | -13.70 |
| 11 | 6tG···C WC pl | -28.16 | -0.83 | 1.34 | -24.19 | -0.91 | 5.31 | -29.50 |
| 12 | A···4tU WC | -12.59 | -0.58 | 1.61 | -9.91 | -0.63 | 4.29 | -14.20 |
| 13 | 2-aminoA···T | -17.91 | -0.73 | 1.59 | -14.29 | -0.77 | 5.21 | -19.50 |
| 14 | 2-aminoA···T pl | -18.21 | -0.69 | 1.49 | -14.76 | -0.73 | 4.94 | -19.70 |
| 15 | A···F | -3.75 | -0.46 | 1.45 | -2.20 | -0.49 | 3.00 | -5.20 |
| 16 | G···4tU | -15.45 | -0.60 | 2.35 | -12.98 | -0.65 | 4.82 | -17.80 |
| 17 | G···2tU | -14.32 | -0.61 | 2.28 | -11.09 | -0.67 | 5.51 | -16.60 |
| 18 | A···C pl | -16.53 | -0.59 | 1.07 | -13.59 | -0.63 | 4.01 | -17.60 |
| 19 | G···G pl | -19.21 | -0.68 | 2.09 | -16.61 | -0.72 | 4.69 | -21.30 |
| 20 | G···6tG pl | -19.48 | -0.67 | 2.32 | -16.38 | -0.72 | 5.42 | -21.80 |
| 21 | 6tG···G pl | -20.20 | -0.77 | 2.50 | -16.91 | -0.83 | 5.79 | -22.70 |
| 22 | G···A 1 | -17.71 | -0.75 | 1.69 | -14.38 | -0.80 | 5.02 | -19.40 |
| 23 | G···A 1 pl | -17.53 | -0.61 | 1.37 | -14.54 | -0.65 | 4.36 | -18.90 |
| 24 | G···A 2 | -12.37 | -0.69 | 2.03 | -9.78 | -0.74 | 4.62 | -14.40 |
| 25 | G···A 2 pl | -11.50 | -0.57 | 1.30 | -8.89 | -0.60 | 3.91 | -12.80 |

TABLE SIV: (continued)

| No.[a] | Complex | PBE | | | B-LYP | | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | CP[d] | dev.[e] | |
| 26 | G···A 3 | -16.89 | -0.80 | 1.91 | -13.72 | -0.85 | 5.08 | -18.80 |
| 27 | G···A 4 | -12.28 | -0.59 | 1.22 | -9.54 | -0.63 | 3.96 | -13.50 |
| 28 | A···A 1 pl | -13.70 | -0.56 | 0.80 | -10.95 | -0.60 | 3.55 | -14.50 |
| 29 | A···A 2 pl | -12.74 | -0.60 | 0.96 | -10.06 | -0.64 | 3.64 | -13.70 |
| 30 | A···A 3 pl | -10.97 | -0.63 | 1.23 | -8.41 | -0.67 | 3.79 | -12.20 |
| 31 | 8oG···G | -20.41 | -0.68 | 2.39 | -17.36 | -0.72 | 5.44 | -22.80 |
| 32 | 2tU···.2tU pl | -10.44 | -0.58 | 2.16 | -7.55 | -0.63 | 5.05 | -12.60 |
| 33 | mA···mT WC[f] | -14.97 | -0.64 | 1.43 | -12.04 | -0.68 | 4.36 | -16.40 |
| 34 | mG···mC WC*[f,g] | -32.00 | -0.84 | 3.80 | -28.29 | -0.90 | 7.51 | -35.80 |
| 35 | mA···mT WC[f] | -16.60 | -0.67 | 1.80 | -13.67 | -0.72 | 4.73 | -18.40 |
| 36 | G···A HB | -11.93 | -0.75 | -0.63 | -8.77 | -0.79 | 2.53 | -11.30 |
| 37 | C···G WC | -29.83 | -0.81 | 0.87 | -26.02 | -0.86 | 4.68 | -30.70 |
| 38 | G···C WC | -29.62 | -0.79 | 1.78 | -25.87 | -0.85 | 5.53 | -31.40 |
| Interstrand base pairs (32) | | | | | | | | |
| 39 | GG0/3.36 CGis036 | -2.89 | -0.48 | 0.79 | -1.98 | -0.51 | 1.70 | -3.68 |
| 40 | GG0/3.36 GCis036 | 3.57 | -0.98 | 8.39 | 7.10 | -1.03 | 11.92 | -4.82 |
| 41 | AA20/3.05 TAis2005[h] | -1.54 | -0.36 | 0.62 | -0.61 | -0.39 | 1.55 | -2.16 |
| 42 | AA20/3.05 ATis2005[h] | 1.87 | -0.60 | 4.21 | 5.32 | -0.63 | 7.66 | -2.34 |
| 43 | GC0/3.25 C//Cis | 3.14 | -0.13 | 0.05 | 3.33 | -0.15 | 0.24 | 3.09 |
| 44 | GC0/3.25 G//Gis | 3.26 | -0.60 | 1.33 | 4.60 | -0.64 | 2.67 | 1.93 |
| 45 | CG0/3.19 C//Cis[i] | 1.38 | -0.19 | 0.14 | 1.85 | -0.21 | 0.61 | 1.24 |
| 46 | CG0/3.19 G//Gis[i] | -0.01 | -0.89 | 3.90 | 2.95 | -0.92 | 6.86 | -3.91 |
| 47 | GA10/3.15 A//Cis | 0.79 | -0.33 | 1.10 | 1.63 | -0.36 | 1.94 | -0.31 |
| 48 | GA10/3.15 T//Gis | 1.18 | -0.25 | 0.60 | 1.79 | -0.27 | 1.21 | 0.58 |
| 49 | AG08/3.19 T//Gis | 0.77 | -0.49 | 1.24 | 2.06 | -0.52 | 2.53 | -0.47 |
| 50 | AG08/3.19 A//Cis | 0.43 | -0.35 | 0.61 | 1.23 | -0.38 | 1.41 | -0.18 |
| 51 | TG03.19 A//Gis | -0.90 | -0.64 | 3.32 | 1.37 | -0.67 | 5.59 | -4.22 |

TABLE SIV: (continued)

| No.[a] | Complex | PBE | | | B-LYP | | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | CP[d] | dev.[e] | |
| 52 | TG03.19 T//Cis | -0.99 | -0.15 | 0.16 | -0.69 | -0.17 | 0.46 | -1.15 |
| 53 | GT10/3.15 T//Cis | 0.38 | -0.14 | 0.08 | 0.62 | -0.16 | 0.32 | 0.30 |
| 54 | GT10/3.15 A//Gis | -2.61 | -0.52 | 1.45 | -1.26 | -0.55 | 2.80 | -4.06 |
| 55 | AT10/3.26 T//Tis | 1.10 | -0.17 | 0.22 | 1.55 | -0.19 | 0.67 | 0.88 |
| 56 | AT10/3.26 A//Ais | 0.02 | -0.48 | 0.94 | 1.06 | -0.51 | 1.98 | -0.92 |
| 57 | TA08/3.16 A//Ais | 1.84 | -0.41 | 3.39 | 3.86 | -0.44 | 5.41 | -1.55 |
| 58 | TA08/3.16 T//Tis | 0.90 | -0.15 | 0.20 | 1.18 | -0.17 | 0.48 | 0.70 |
| 59 | AA0/3.24 A//Tis | -1.03 | -0.23 | 0.68 | -0.35 | -0.25 | 1.36 | -1.71 |
| 60 | AA0/3.24 T//Ais | -0.92 | -0.27 | 0.38 | -0.29 | -0.29 | 1.01 | -1.30 |
| 61 | mA$\cdots$mA IS[f] | 0.59 | -0.55 | 1.29 | 1.86 | -0.59 | 2.56 | -0.70 |
| 62 | mT$\cdots$mT IS[f] | 1.22 | -0.21 | 0.22 | 1.70 | -0.23 | 0.70 | 1.00 |
| 63 | mG$\cdots$mG IS[f] | 0.04 | -0.89 | 4.54 | 2.98 | -0.93 | 7.48 | -4.50 |
| 64 | mC$\cdots$mC IS[f] | 1.72 | -0.28 | 0.32 | 2.40 | -0.30 | 1.00 | 1.40 |
| 65 | mA$\cdots$mG IS[f] | -3.47 | -0.53 | 1.33 | -2.11 | -0.56 | 2.69 | -4.80 |
| 66 | mT$\cdots$mC IS[f] | 0.02 | -0.19 | 0.12 | 0.30 | -0.21 | 0.40 | -0.10 |
| 67 | C$\cdots$A IS | -1.22 | -0.48 | 1.78 | 0.05 | -0.51 | 3.05 | -3.00 |
| 68 | G$\cdots$G IS | -4.52 | -0.40 | 0.68 | -3.61 | -0.43 | 1.59 | -5.20 |
| 69 | G$\cdots$G IS | 2.77 | -0.78 | 1.97 | 4.75 | -0.81 | 3.95 | 0.80 |
| 70 | C$\cdots$C IS | 3.12 | -0.11 | 0.02 | 3.29 | -0.13 | 0.19 | 3.10 |
| Stacked base pairs (54) | | | | | | | | |
| 71 | G$\cdots$C S | -10.04 | -1.07 | 8.98 | -5.13 | -1.13 | 13.89 | -19.02 |
| 72 | mG$\cdots$mC S | -7.24 | -1.21 | 13.11 | -0.69 | -1.27 | 19.66 | -20.35 |
| 73 | A$\cdots$T S | -2.17 | -0.88 | 10.13 | 3.01 | -0.92 | 15.31 | -12.30 |
| 74 | mA$\cdots$mT S | -1.10 | -1.06 | 13.47 | 5.91 | -1.11 | 20.48 | -14.57 |
| 75 | CC1 | 7.72 | -0.72 | 5.27 | 11.12 | -0.77 | 8.67 | 2.45 |
| 76 | CC2 | 2.40 | -0.78 | 6.25 | 5.96 | -0.83 | 9.81 | -3.85 |
| 77 | CC3 | -2.23 | -0.84 | 6.65 | 1.26 | -0.89 | 10.14 | -8.88 |

TABLE SIV: (continued)

| No.[a] | Complex | PBE | | | B-LYP | | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | CP[d] | dev.[e] | |
| 78 | CC4 | -2.93 | -0.86 | 6.99 | 0.42 | -0.91 | 10.34 | -9.92 |
| 79 | CC5 | 6.07 | -0.81 | 5.75 | 9.61 | -0.86 | 9.29 | 0.32 |
| 80 | CC6 | 6.41 | -0.86 | 5.77 | 10.09 | -0.90 | 9.45 | 0.64 |
| 81 | CC7 | 2.49 | -0.66 | 3.47 | 4.84 | -0.70 | 5.82 | -0.98 |
| 82 | CC8 | -2.92 | -0.83 | 6.18 | -0.10 | -0.87 | 9.00 | -9.10 |
| 83 | CC9 | -2.30 | -0.79 | 6.81 | 1.16 | -0.84 | 10.27 | -9.11 |
| 84 | CC10 | -1.90 | -0.90 | 6.37 | 1.35 | -0.95 | 9.62 | -8.27 |
| 85 | CC11 | -2.83 | -0.76 | 6.60 | 0.30 | -0.79 | 9.73 | -9.43 |
| 86 | CC12 | -3.50 | -0.66 | 3.93 | -1.82 | -0.69 | 5.61 | -7.43 |
| 87 | CC13 | -3.20 | -0.83 | 5.60 | -0.22 | -0.87 | 8.58 | -8.80 |
| 88 | CC14 | -2.15 | -0.82 | 6.96 | 1.23 | -0.88 | 10.34 | -9.11 |
| 89 | AAst | -0.77 | -0.83 | 7.81 | 3.12 | -0.88 | 11.70 | -8.58 |
| 90 | GGst | -3.86 | -0.98 | 8.81 | 0.31 | -1.02 | 12.98 | -12.67 |
| 91 | ACst | -2.75 | -0.78 | 7.47 | 0.98 | -0.82 | 11.20 | -10.22 |
| 92 | GAst | -2.77 | -0.85 | 8.61 | 1.28 | -0.90 | 12.66 | -11.38 |
| 93 | CCst | -3.30 | -0.75 | 6.72 | 0.02 | -0.79 | 10.04 | -10.02 |
| 94 | AUst | -2.49 | -0.74 | 7.30 | 1.37 | -0.77 | 11.16 | -9.79 |
| 95 | GCst | -4.03 | -0.89 | 6.57 | -0.33 | -0.93 | 10.27 | -10.60 |
| 96 | CUst | -4.06 | -0.69 | 6.36 | -0.76 | -0.73 | 9.66 | -10.42 |
| 97 | UUst | -2.14 | -0.55 | 5.32 | 1.01 | -0.58 | 8.47 | -7.46 |
| 98 | GUst | -4.57 | -0.81 | 7.52 | -0.76 | -0.84 | 11.33 | -12.09 |
| 99 | GG0/3.36 CCs036[j] | 2.63 | -0.73 | 4.25 | 5.29 | -0.77 | 6.91 | -1.62 |
| 100 | GG0/3.36 GGs036[j] | -4.30 | -0.24 | -0.76 | -3.81 | -0.26 | -0.27 | -3.54 |
| 101 | AA20/3.05 AAs2005 | 2.01 | -0.85 | 8.07 | 5.98 | -0.90 | 12.04 | -6.06 |
| 102 | AA20/3.05 TTs2005 | -0.98 | -0.30 | 3.20 | 0.14 | -0.32 | 4.32 | -4.18 |
| 103 | GC0/3.25 G//Cs | -3.16 | -0.93 | 7.64 | 0.85 | -0.99 | 11.65 | -10.80 |

TABLE SIV: (continued)

| No.[a] | Complex | PBE | | | B-LYP | | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | CP[d] | dev.[e] | |
| 104 | CG0/3.19 G//Cs | -2.54 | -0.72 | 5.34 | -0.30 | -0.77 | 7.58 | -7.88 |
| 105 | GA10/3.15 A//Gs | -0.68 | -1.07 | 8.46 | 3.73 | -1.12 | 12.87 | -9.14 |
| 106 | GA10/3.15 T//Cs | 0.18 | -0.71 | 4.87 | 3.21 | -0.75 | 7.90 | -4.69 |
| 107 | AG08/3.19 A//Gs | -0.98 | -0.71 | 6.60 | 2.11 | -0.76 | 9.69 | -7.58 |
| 108 | AG08/3.19 T//Cs | -1.28 | -0.60 | 4.79 | 1.43 | -0.64 | 7.50 | -6.07 |
| 109 | TG03.19 T//Gs | -0.57 | -0.63 | 5.10 | 1.88 | -0.66 | 7.55 | -5.67 |
| 110 | TG03.19 A//Cs | 0.65 | -0.84 | 5.61 | 3.45 | -0.89 | 8.41 | -4.96 |
| 111 | GT10/3.15 T//Gs | 2.63 | -0.76 | 7.59 | 6.72 | -0.80 | 11.68 | -4.96 |
| 112 | GT10/3.15 A//Cs | 1.34 | -0.77 | 6.78 | 4.83 | -0.82 | 10.27 | -5.44 |
| 113 | AT10/3.26 A//Ts | 0.09 | -0.59 | 6.73 | 3.68 | -0.63 | 10.32 | -6.64 |
| 114 | TA08/3.16 A//Ts | 4.80 | -0.82 | 10.87 | 9.79 | -0.85 | 15.86 | -6.07 |
| 115 | AA0/3.24 A//As | 1.40 | -0.81 | 7.65 | 5.15 | -0.86 | 11.40 | -6.25 |
| 116 | AA0/3.24 T//Ts | 2.33 | -0.60 | 6.19 | 5.92 | -0.63 | 9.78 | -3.86 |
| 117 | mA$\cdots$mT S[f] | 0.09 | -0.69 | 8.19 | 4.34 | -0.73 | 12.44 | -8.10 |
| 118 | mG$\cdots$mC S[f] | -3.70 | -0.65 | 4.20 | -1.91 | -0.70 | 5.99 | -7.90 |
| 119 | mA$\cdots$mC S[f] | 0.73 | -0.85 | 7.43 | 4.42 | -0.91 | 11.12 | -6.70 |
| 120 | mT$\cdots$mG S[f] | 0.80 | -0.76 | 7.00 | 4.59 | -0.80 | 10.79 | -6.20 |
| 121 | G$\cdots$C S | -0.81 | -0.89 | 6.89 | 2.71 | -0.93 | 10.41 | -7.70 |
| 122 | A$\cdots$G S | 1.11 | -0.99 | 7.61 | 5.08 | -1.03 | 11.58 | -6.50 |
| 123 | C$\cdots$G S | -4.09 | -0.86 | 8.31 | -0.57 | -0.91 | 11.83 | -12.40 |
| 124 | G$\cdots$C S | -4.57 | -0.87 | 7.03 | -1.13 | -0.92 | 10.47 | -11.60 |
| Amino acid pairs (19) | | | | | | | | |
| 125 | F30-K46 | -1.28 | -0.28 | 1.82 | 0.26 | -0.29 | 3.36 | -3.10 |
| 126 | F30-L33 | -0.88 | -0.66 | 4.12 | 2.12 | -0.70 | 7.12 | -5.00 |
| 127 | F30-Y13 | -1.30 | -0.34 | 2.60 | 0.71 | -0.36 | 4.61 | -3.90 |
| 128 | F30-F49 | -0.34 | -0.13 | 2.96 | 1.26 | [k] | 4.56 | -3.30 |
| 129 | F30-Y4 | 0.57 | -0.33 | 7.57 | 3.60 | -0.35 | 10.60 | -7.00 |

TABLE SIV: (continued)

| No.[a] | Complex | PBE | | | B-LYP | | | $\Delta E^b_{\rm ref}$ |
|---|---|---|---|---|---|---|---|---|
| | | $\Delta E^c$ | CP[d] | dev.[e] | $\Delta E^c$ | CP[d] | dev.[e] | |
| 130 | F49-C39 | 0.13 | -0.18 | 2.23 | 1.78 | -0.18 | 3.88 | -2.10 |
| 131 | F49-C6 | 0.26 | -0.45 | 5.26 | 3.27 | -0.49 | 8.27 | -5.00 |
| 132 | F49-K46 | -1.58 | -0.61 | 3.22 | 0.66 | -0.63 | 5.46 | -4.80 |
| 133 | F49-V5 | -1.08 | -0.66 | 5.62 | 2.55 | -0.70 | 9.25 | -6.70 |
| 134 | F49-W37[l] | -0.28 | -0.10 | 2.22 | 1.05 | [k] | 3.55 | -2.50 |
| 135 | F49-Y4 | 0.80 | -0.29 | 3.90 | 3.62 | -0.29 | 6.72 | -3.10 |
| 136 | F49-PB (Y4-V5) | -0.94 | -0.37 | 1.86 | 0.66 | -0.38 | 3.46 | -2.80 |
| 137 | F49-PB (V5-C6) | -2.73 | -0.69 | 5.47 | 0.41 | -0.73 | 8.61 | -8.20 |
| 138 | E47-K6 (1IU5) | -75.95 | -1.11 | 4.78 | -73.22 | -1.17 | 7.51 | -80.73 |
| 139 | E49-K6 (1BQ9) | -107.19 | -1.19 | 6.16 | -104.44 | -1.26 | 8.91 | -113.35 |
| 140 | E54-K2 (1SMM) | -92.29 | -0.88 | -4.00 | -91.45 | -0.94 | -3.16 | -88.29 |
| 141 | E50-K30 (1BRF) | -61.37 | -0.37 | -1.01 | -61.69 | -0.41 | -1.33 | -60.36 |
| 142 | E50-K52 (1BRF) | -91.10 | -1.53 | 6.04 | -88.35 | -1.63 | 8.79 | -97.14 |
| 143 | E49-K6 (1BRF) | -67.96 | -1.04 | 6.28 | -65.02 | -1.08 | 9.22 | -74.24 |

[a]The calculated $\Delta E$ values are in the same sequence as the structures in the database. [b]Estimated CCSD(T)/CBS. The reference $\Delta E$ values of No. 41 and 42, No. 45 and 46, as well as No. 100 and 102 from Table 1 of Ref. [1] are interchanged. This is justified by a RI-MP2/aug-cc-pVDZ calculation and a comparison of the resulting $\Delta E$ values with the first column of Table 1 in Ref. [1]. [c]No CP correction. [d]Counterpoise correction. [e]$\Delta E - \Delta E_{\rm ref}$. [f]Base pair methylated. [g]The * is missing in the database. [h]Rows 41 and 42 of Table 1 in Ref. [1] are interchanged. [i]Rows 45 and 46 of Table 1 in Ref. [1] are interchanged. [j]Rows 99 and 100 of Table 1 in Ref. [1] are interchanged. [k]Calculation of a fragment with the full basis set of the complex did not converge to an energy below the fragment energy obtained with the fragment basis alone. [l]Residue 37 of 1RB9 is tryptophan (W), not tyrosine (Y).