Table 54. Potential energy density at the bond critical points (a.u.) for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	-1.309	-1.419	-1.216	-1.523
O2 – C5'	-1.281	-1.408	-1.175	-1.534
N1 – C2	-0.512	-0.603	-0.450	-0.717
N1 – C6	-0.595	-0.668	-0.539	-0.736
N3 – C2	-0.624	-0.707	-0.565	-0.802
N3 – C4	-0.412	-0.488	-0.361	-0.586
C4 – C4'	-0.243	-0.263	-0.226	-0.275
C4 – C5	-0.256	-0.275	-0.239	-0.283
C5 – C6	-0.482	-0.530	-0.446	-0.587
C6 – C6'	-0.270	-0.290	-0.253	-0.302
C5 – C5'	-0.307	-0.321	-0.293	-0.319
C5' – C5"	-0.259	-0.282	-0.240	-0.294
N1 – H1	-0.523	-0.567	-0.490	-0.609
N3 – H3	-0.516	-0.558	-0.484	-0.597
C4 – H4	-0.322	-0.341	-0.308	-0.358
C4' – H41	-0.311	-0.329	-0.298	-0.343
C4' – H42	-0.313	-0.331	-0.300	-0.345
C4' – H43	-0.312	-0.330	-0.300	-0.343
C6' – H61	-0.312	-0.330	-0.300	-0.343
C6' – H62	-0.322	-0.341	-0.308	-0.356
C6' – H63	-0.307	-0.324	-0.295	-0.338
C5" – H51"	-0.314	-0.332	-0.302	-0.344
C5" – H52"	-0.314	-0.332	-0.300	-0.347
C5" – H53"	-0.309	-0.326	-0.296	-0.340