Table 55. Electronic energy density $h(\mathbf{r})$ 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	-0.707	-0.748	-0.671	-0.777
O2 – C5'	-0.669	-0.708	-0.632	-0.736
N1 – C2	-0.362	-0.419	-0.318	-0.470
N1 – C6	-0.400	-0.436	-0.367	-0.454
N3 – C2	-0.437	-0.488	-0.396	-0.532
N3 – C4	-0.285	-0.328	-0.251	-0.359
C4 – C4'	-0.189	-0.208	-0.172	-0.224
C4 – C5	-0.199	-0.218	-0.183	-0.230
C5 – C6	-0.354	-0.391	-0.326	-0.432
C6 – C6'	-0.210	-0.230	-0.194	-0.245
C5 – C5'	-0.236	-0.252	-0.221	-0.259
C5' – C5"	-0.202	-0.224	-0.184	-0.241
N1 – H1	-0.471	-0.515	-0.438	-0.558
N3 – H3	-0.463	-0.504	-0.430	-0.544
C4 – H4	-0.285	-0.304	-0.272	-0.321
C4' – H41	-0.268	-0.284	-0.256	-0.298
C4' – H42	-0.272	-0.289	-0.260	-0.303
C4' – H43	-0.269	-0.285	-0.257	-0.299
C6' – H61	-0.269	-0.286	-0.258	-0.300
C6' – H62	-0.280	-0.298	-0.267	-0.314
C6' – H63	-0.265	-0.282	-0.253	-0.295
C5" – H51"	-0.274	-0.291	-0.262	-0.304
C5" – H52"	-0.271	-0.288	-0.258	-0.303
C5" – H53"	-0.265	-0.281	-0.253	-0.295