Table 49. Electron density curvature λ_1 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	-1.08	-1.18	-1.01	-1.27
O2 – C5'	-1.02	-1.12	-0.95	-1.22
N1 – C2	-0.64	-0.67	-0.61	-0.70
N1 – C6	-0.61	-0.62	-0.60	-0.64
N3 – C2	-0.75	-0.79	-0.72	-0.82
N3 – C4	-0.47	-0.48	-0.46	-0.46
C4 – C4'	-0.46	-0.48	-0.43	-0.50
C4 – C5	-0.48	-0.50	-0.46	-0.51
C5 – C6	-0.69	-0.73	-0.66	-0.76
C6 – C6'	-0.49	-0.51	-0.47	-0.52
C5 – C5'	-0.55	-0.57	-0.53	-0.57
C5' – C5"	-0.48	-0.51	-0.46	-0.53
N1 – H1	-1.31	-1.38	-1.26	-1.43
N3 – H3	-1.29	-1.36	-1.24	-1.41
C4 – H4	-0.79	-0.81	-0.77	-0.81
C4' – H41	-0.70	-0.71	-0.69	-0.71
C4' – H42	-0.72	-0.74	-0.71	-0.73
C4' – H43	-0.70	-0.72	-0.69	-0.71
C6' – H61	-0.71	-0.73	-0.69	-0.72
C6' – H62	-0.74	-0.76	-0.73	-0.76
C6' – H63	-0.70	-0.72	-0.69	-0.72
C5" – H51"	-0.73	-0.75	-0.72	-0.75
C5" – H52"	-0.71	-0.73	-0.69	-0.72
C5" – H53"	-0.69	-0.71	-0.68	-0.70