Table 51. Electron density curvature λ_3 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	1.66	1.96	1.43	2.34
O2 – C5'	1.77	2.15	1.49	2.64
N1 – C2	0.36	0.35	0.40	0.49
N1 – C6	0.36	0.41	0.36	0.55
N3 – C2	0.39	0.40	0.41	0.52
N3 – C4	0.29	0.27	0.34	0.37
C4 – C4'	0.36	0.34	0.38	0.29
C4 – C5	0.36	0.33	0.38	0.28
C5 – C6	0.30	0.24	0.33	0.15
C6 – C6'	0.35	0.32	0.37	0.26
C5 – C5'	0.37	0.34	0.39	0.28
C5' – C5"	0.37	0.34	0.39	0.28
N1 – H1	0.88	0.83	0.91	0.76
N3 – H3	0.88	0.84	0.92	0.77
C4 – H4	0.56	0.53	0.58	0.46
C4' – H41	0.49	0.46	0.51	0.39
C4' – H42	0.51	0.48	0.53	0.42
C4' – H43	0.50	0.46	0.52	0.39
C6' – H61	0.50	0.47	0.52	0.41
C6' – H62	0.53	0.50	0.54	0.43
C6' – H63	0.51	0.48	0.52	0.42
C5" – H51"	0.53	0.50	0.54	0.43
C5" – H52"	0.50	0.47	0.52	0.40
C5" – H53"	0.49	0.46	0.51	0.40