

Table 46. Bond lengths (Å) for the different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**	MP2/ 6-311++G**
O1 – C2	1.22	1.20	1.23	1.19	1.22
O2 – C5'	1.22	1.21	1.24	1.20	1.23
N1 – C2	1.41	1.39	1.43	1.38	1.41
N1 – C6	1.39	1.38	1.39	1.39	1.39
N3 – C2	1.36	1.35	1.37	1.35	1.37
N3 – C4	1.47	1.46	1.48	1.46	1.46
C4 – C4'	1.54	1.53	1.55	1.53	1.53
C4 – C5	1.52	1.51	1.54	1.52	1.51
C5 – C6	1.36	1.35	1.38	1.34	1.36
C6 – C6'	1.51	1.50	1.52	1.51	1.50
C5 – C5'	1.48	1.47	1.48	1.49	1.48
C5' – C5''	1.52	1.51	1.54	1.52	1.52
N1 – H1	1.01	1.00	1.02	0.99	1.01
N3 – H3	1.01	1.00	1.02	0.99	1.01
C4 – H4	1.09	1.08	1.10	1.08	1.09
C4' – H41	1.09	1.09	1.10	1.09	1.10
C4' – H42	1.09	1.08	1.10	1.08	1.09
C4' – H43	1.09	1.09	1.10	1.09	1.09
C6' – H61	1.09	1.09	1.10	1.09	1.09
C6' – H62	1.08	1.08	1.09	1.07	1.09
C6' – H63	1.09	1.09	1.10	1.09	1.10
C5'' – H51''	1.09	1.08	1.10	1.08	1.09
C5'' – H52''	1.09	1.08	1.10	1.08	1.09
C5'' – H53''	1.09	1.09	1.10	1.09	1.09