

Table 58. Variation of the atomic volumes (\AA^3) for different methods of computation

Atom	DFT B3LYP/ 6-311++G**	DFT BHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1	20.651	20.543	20.793	20.540
O2	19.298	19.179	19.527	19.214
N1	14.183	14.402	14.074	14.865
N3	14.092	14.211	14.079	14.594
C2	4.905	4.128	5.534	3.156
C4	6.496	6.226	6.734	5.995
C4'	10.105	9.750	10.302	9.282
C5	10.813	10.711	10.932	10.782
C6	9.130	8.923	9.395	9.061
C6'	9.987	9.705	10.153	9.365
C5'	7.480	7.038	7.912	6.645
C5''	10.205	9.959	10.368	9.589
H1	4.393	4.156	4.597	3.951
H3	4.519	4.293	4.723	4.104
H4	6.387	6.336	6.493	6.411
H41	7.655	7.615	7.752	7.677
H42	7.094	6.975	7.261	6.999
H43	7.601	7.533	7.718	7.576
H61	7.223	7.100	7.345	7.109
H62	6.408	6.270	6.602	6.356
H63	7.303	7.212	7.446	7.245
H51''	7.026	6.903	7.185	6.899
H52''	7.156	7.052	7.306	7.106
H53''	7.240	7.114	7.375	7.145
Σ	217.350	213.334	221.606	211.665