

Table 34. Electron density curvature λ_1 for conformers of **III** (a.u.)

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	-1.08	-1.09	-1.09
O2 – C5'	-1.02	-1.02	-1.02
N1 – C2	-0.64	-0.65	-0.64
N1 – C6	-0.61	-0.61	-0.61
N3 – C2	-0.75	-0.74	-0.74
N3 – C4	-0.47	-0.48	-0.47
C4 – C4'	-0.46	-0.45	-0.45
C4 – C5	-0.48	-0.48	-0.48
C5 – C6	-0.69	-0.69	-0.69
C6 – C6'	-0.49	-0.49	-0.49
C5 – C5'	-0.55	-0.55	-0.55
C5' – C5''	-0.48	-0.49	-0.48
N1 – H1	-1.31	-1.31	-1.31
N3 – H3	-1.29	-1.29	-1.29
C4 – H4	-0.79	-0.77	-0.78
C4' – H41	-0.70	-0.70	-0.70
C4' – H42	-0.72	-0.70	-0.71
C4' – H43	-0.70	-0.71	-0.71
C6' – H61	-0.71	-0.72	-0.72
C6' – H62	-0.74	-0.71	-0.73
C6' – H63	-0.70	-0.74	-0.72
C5'' – H51''	-0.73	-0.73	-0.73
C5'' – H52''	-0.71	-0.69	-0.70
C5'' – H53''	-0.69	-0.69	-0.69