

Table 35. Electron density curvature λ_2 for conformers of **III** (a.u.)

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	-0.99	-0.99	-0.99
O2 – C5'	-0.97	-0.97	-0.97
N1 – C2	-0.57	-0.58	-0.58
N1 – C6	-0.57	-0.58	-0.57
N3 – C2	-0.63	-0.63	-0.63
N3 – C4	-0.45	-0.46	-0.46
C4 – C4'	-0.44	-0.44	-0.44
C4 – C5	-0.45	-0.45	-0.45
C5 – C6	-0.51	-0.51	-0.51
C6 – C6'	-0.47	-0.47	-0.47
C5 – C5'	-0.48	-0.48	-0.48
C5' – C5''	-0.47	-0.47	-0.47
N1 – H1	-1.24	-1.25	-1.25
N3 – H3	-1.22	-1.22	-1.22
C4 – H4	-0.77	-0.75	-0.76
C4' – H41	-0.69	-0.69	-0.69
C4' – H42	-0.72	-0.70	-0.71
C4' – H43	-0.70	-0.71	-0.70
C6' – H61	-0.70	-0.71	-0.71
C6' – H62	-0.74	-0.70	-0.72
C6' – H63	-0.69	-0.73	-0.71
C5'' – H51''	-0.73	-0.73	-0.73
C5'' – H52''	-0.70	-0.69	-0.70
C5'' – H53''	-0.68	-0.69	-0.68