

Table 36. Electron density curvature λ_3 for conformers of **III** (a.u.)

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	1.66	1.67	1.66
O2 – C5'	1.77	1.76	1.77
N1 – C2	0.36	0.36	0.36
N1 – C6	0.36	0.37	0.36
N3 – C2	0.39	0.38	0.38
N3 – C4	0.29	0.30	0.30
C4 – C4'	0.36	0.37	0.37
C4 – C5	0.36	0.36	0.36
C5 – C6	0.30	0.30	0.30
C6 – C6'	0.35	0.35	0.35
C5 – C5'	0.37	0.37	0.37
C5' – C5''	0.37	0.37	0.37
N1 – H1	0.88	0.88	0.88
N3 – H3	0.88	0.88	0.88
C4 – H4	0.56	0.54	0.55
C4' – H41	0.49	0.50	0.49
C4' – H42	0.51	0.50	0.51
C4' – H43	0.50	0.50	0.50
C6' – H61	0.50	0.52	0.51
C6' – H62	0.53	0.49	0.51
C6' – H63	0.51	0.53	0.52
C5'' – H51''	0.53	0.53	0.53
C5'' – H52''	0.50	0.49	0.50
C5'' – H53''	0.49	0.49	0.49