

Table 33. Laplacian of electron density at the bond critical points (a.u.) for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	-0.42	-0.41	-0.42
O2 – C5'	-0.22	-0.23	-0.23
N1 – C2	-0.85	-0.86	-0.85
N1 – C6	-0.82	-0.81	-0.82
N3 – C2	-1.00	-0.98	-0.99
N3 – C4	-0.63	-0.64	-0.64
C4 – C4'	-0.53	-0.53	-0.53
C4 – C5	-0.57	-0.57	-0.57
C5 – C6	-0.90	-0.91	-0.90
C6 – C6'	-0.60	-0.61	-0.61
C5 – C5'	-0.66	-0.67	-0.66
C5' – C5''	-0.58	-0.58	-0.58
N1 – H1	-1.68	-1.69	-1.68
N3 – H3	-1.64	-1.63	-1.63
C4 – H4	-0.99	-0.98	-0.99
C4' – H41	-0.90	-0.90	-0.90
C4' – H42	-0.92	-0.91	-0.91
C4' – H43	-0.90	-0.91	-0.91
C6' – H61	-0.91	-0.91	-0.91
C6' – H62	-0.95	-0.91	-0.93
C6' – H63	-0.89	-0.93	-0.91
C5'' – H51''	-0.93	-0.94	-0.94
C5'' – H52''	-0.91	-0.89	-0.90
C5'' – H53''	-0.88	-0.88	-0.88