

Table 20. Electron density curvature λ_2 for conformers of **II** (a.u.)

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19
O – C5'	-0.98	-0.98	-0.98	-0.98	-0.98	-0.97	-0.98
N1 – C2	-0.60	-0.60	-0.60	-0.60	-0.59	-0.60	-0.60
N1 – C6	-0.56	-0.56	-0.56	-0.57	-0.56	-0.56	-0.56
N3 – C2	-0.65	-0.64	-0.64	-0.64	-0.65	-0.65	-0.65
N3 – C4	-0.44	-0.45	-0.45	-0.45	-0.44	-0.44	-0.45
C4 – C4'	-0.44	-0.44	-0.43	-0.44	-0.44	-0.44	-0.44
C4' – C4''	-0.44	-0.44	-0.44	-0.44	-0.44	-0.44	-0.44
C4 – C5	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45
C5 – C6	-0.51	-0.52	-0.52	-0.51	-0.51	-0.51	-0.51
C6 – C6'	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47
C5 – C5'	-0.48	-0.48	-0.48	-0.47	-0.47	-0.48	-0.48
C5' – C5''	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47
N1 – H1	-1.26	-1.27	-1.27	-1.27	-1.26	-1.26	-1.27
N3 – H3	-1.25	-1.25	-1.24	-1.24	-1.25	-1.25	-1.25
C4 – H4	-0.76	-0.74	-0.75	-0.74	-0.77	-0.76	-0.76
C4' – H41	-0.72	-0.70	-0.71	-0.70	-0.70	-0.69	-0.70
C4' – H42	-0.70	-0.71	-0.70	-0.70	-0.70	-0.72	-0.71
C4'' – H43	-0.69	-0.69	-0.69	-0.70	-0.71	-0.70	-0.70
C4'' – H44	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
C4'' – H45	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
C6' – H61	-0.70	-0.72	-0.72	-0.72	-0.70	-0.70	-0.71
C6' – H62	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
C6' – H63	-0.73	-0.72	-0.72	-0.72	-0.74	-0.73	-0.73
C5'' – H51''	-0.73	-0.73	-0.73	-0.73	-0.70	-0.69	-0.72
C5'' – H52''	-0.70	-0.69	-0.69	-0.69	-0.69	-0.73	-0.70
C5'' – H53''	-0.69	-0.69	-0.69	-0.69	-0.73	-0.70	-0.70