Table 5. Electron density curvature λ_2 for conformers of **I** (a.u.)

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19	-0.19
O1 - C5'	-1.00	-1.01	-1.01	-1.00	-1.00	-1.01	-1.00
O2 - C5'	-0.62	-0.61	-0.61	-0.62	-0.62	-0.61	-0.62
N1 - C2	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60
C2 - N3	-0.65	-0.64	-0.64	-0.65	-0.64	-0.64	-0.64
N3 - C4	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45
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	-0.52	-0.51
C6 - N1	-0.56	-0.56	-0.56	-0.56	-0.56	-0.56	-0.56
C4 - C4'	-0.45	-0.44	-0.44	-0.45	-0.45	-0.44	-0.44
C5 - C5'	-0.48	-0.48	-0.48	-0.48	-0.48	-0.48	-0.48
C6 - C6'	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47
O2 - C7	-0.37	-0.37	-0.37	-0.37	-0.37	-0.37	-0.37
C7 - C8	-0.47	-0.46	-0.46	-0.46	-0.46	-0.47	-0.47
N1 - H1	-1.26	-1.26	-1.26	-1.26	-1.26	-1.26	-1.26
N3 - H3	-1.25	-1.25	-1.25	-1.25	-1.25	-1.25	-1.25
C4 - H4	-0.77	-0.77	-0.77	-0.77	-0.77	-0.77	-0.77
C4' - H41'	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71
C4' - H42'	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
C4' - H43'	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
C6' - H61'	-0.69	-0.69	-0.69	-0.75	-0.75	-0.69	-0.71
C6' - H62'	-0.70	-0.69	-0.69	-0.69	-0.70	-0.69	-0.69
C6' - H63'	-0.75	-0.76	-0.76	-0.70	-0.70	-0.76	-0.74
C7 - H71	-0.76	-0.77	-0.75	-0.75	-0.77	-0.75	-0.76
C7 - H72	-0.75	-0.75	-0.77	-0.77	-0.75	-0.76	-0.76
C8 - H81	-0.71	-0.72	-0.70	-0.70	-0.72	-0.71	-0.71
C8 - H82	-0.70	-0.70	-0.72	-0.72	-0.70	-0.71	-0.71
C8 - H83	-0.70	-0.69	-0.69	-0.69	-0.69	-0.70	-0.70