Table 1. Bond lengths (Å) for the conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	1.67	1.67	1.67	1.67	1.67	1.67	1.67
O1 - C5'	1.22	1.21	1.21	1.22	1.22	1.21	1.21
O2 - C5'	1.36	1.36	1.36	1.36	1.36	1.36	1.36
N1 - C2	1.38	1.38	1.38	1.38	1.38	1.38	1.38
C2 - N3	1.34	1.34	1.34	1.34	1.34	1.34	1.34
N3 - C4	1.47	1.47	1.47	1.47	1.47	1.47	1.47
C4 - C5	1.52	1.52	1.52	1.52	1.52	1.52	1.52
C5 - C6	1.36	1.36	1.36	1.36	1.36	1.36	1.36
C6 - N1	1.39	1.39	1.39	1.39	1.39	1.39	1.39
C4 - C4'	1.54	1.54	1.54	1.54	1.54	1.54	1.54
C5 - C5'	1.47	1.47	1.47	1.47	1.47	1.47	1.47
C6 - C6'	1.50	1.50	1.50	1.50	1.50	1.50	1.50
O2 - C7	1.45	1.45	1.45	1.45	1.45	1.45	1.45
C7 - C8	1.52	1.52	1.52	1.52	1.52	1.52	1.52
N1 - H1	1.01	1.01	1.01	1.01	1.01	1.01	1.01
N3 - H3	1.01	1.01	1.01	1.01	1.01	1.01	1.01
C4 - H4	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C4' - H41'	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C4' - H42'	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C4' - H43'	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C6' - H61'	1.09	1.10	1.10	1.08	1.08	1.10	1.09
C6' - H62'	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C6' - H63'	1.08	1.08	1.08	1.09	1.09	1.08	1.09
C7 - H71	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C7 - H72	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C8 - H81	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C8 - H82	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C8 - H83	1.09	1.09	1.09	1.09	1.09	1.09	1.09

Table 2. Electron densities at the bond critical points (a.u.) for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	0.21	0.21	0.21	0.21	0.21	0.21	0.21
O1 - C5'	0.41	0.41	0.41	0.41	0.41	0.41	0.41
O2 - C5'	0.30	0.29	0.29	0.30	0.30	0.29	0.29
N1 - C2	0.31	0.31	0.31	0.31	0.31	0.31	0.31
C2 - N3	0.33	0.33	0.33	0.33	0.33	0.33	0.33
N3 - C4	0.25	0.25	0.25	0.25	0.25	0.25	0.25
C4 - C5	0.25	0.25	0.25	0.25	0.25	0.25	0.25
C5 - C6	0.33	0.33	0.33	0.33	0.33	0.33	0.33
C6 - N1	0.30	0.30	0.30	0.30	0.30	0.30	0.30
C4 - C4'	0.24	0.24	0.24	0.24	0.24	0.24	0.24
C5 - C5'	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C6 - C6'	0.25	0.25	0.25	0.25	0.25	0.25	0.25
O2 - C7	0.23	0.23	0.23	0.23	0.23	0.23	0.23
C7 - C8	0.25	0.25	0.25	0.25	0.25	0.25	0.25
N1 - H1	0.34	0.34	0.34	0.34	0.34	0.34	0.34
N3 - H3	0.34	0.34	0.34	0.34	0.34	0.34	0.34
C4 - H4	0.29	0.29	0.29	0.29	0.29	0.29	0.29
C4' - H41'	0.28	0.28	0.28	0.28	0.28	0.28	0.28
C4' - H42'	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C4' - H43'	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C6' - H61'	0.27	0.27	0.27	0.28	0.28	0.27	0.27
C6' - H62'	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C6' - H63'	0.28	0.28	0.28	0.27	0.27	0.28	0.28
C7 - H71	0.28	0.29	0.29	0.29	0.29	0.28	0.29
C7 - H72	0.28	0.29	0.29	0.29	0.29	0.28	0.29
C8 - H81	0.27	0.28	0.27	0.27	0.28	0.27	0.28
C8 - H82	0.27	0.27	0.28	0.28	0.27	0.27	0.27
C8 - H83	0.27	0.27	0.27	0.27	0.27	0.27	0.27

Table 3. Laplacian of electron density at the bond critical points (a.u.) for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	-0.04	-0.04	-0.04	-0.04	-0.04	-0.04	-0.04
O1 - C5'	-0.31	-0.32	-0.31	-0.32	-0.32	-0.31	-0.31
O2 - C5'	-0.51	-0.52	-0.52	-0.52	-0.52	-0.51	-0.51
N1 - C2	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90
C2 - N3	-0.98	-0.98	-0.98	-0.98	-0.98	-0.98	-0.98
N3 - C4	-0.63	-0.62	-0.63	-0.63	-0.63	-0.63	-0.63
C4 - C5	-0.58	-0.57	-0.57	-0.58	-0.58	-0.57	-0.57
C5 - C6	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92
C6 - N1	-0.80	-0.80	-0.81	-0.80	-0.80	-0.80	-0.80
C4 - C4'	-0.54	-0.54	-0.53	-0.54	-0.54	-0.53	-0.54
C5 - C5'	-0.69	-0.69	-0.69	-0.69	-0.69	-0.68	-0.69
C6 - C6'	-0.61	-0.61	-0.61	-0.61	-0.61	-0.61	-0.61
O2 - C7	-0.32	-0.31	-0.31	-0.31	-0.31	-0.32	-0.32
C7 - C8	-0.60	-0.58	-0.58	-0.58	-0.58	-0.60	-0.59
N1 - H1	-1.72	-1.72	-1.72	-1.72	-1.72	-1.72	-1.72
N3 - H3	-1.68	-1.68	-1.68	-1.68	-1.68	-1.68	-1.68
C4 - H4	-0.99	-0.99	-0.99	-0.99	-0.99	-0.99	-0.99
C4' - H41'	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92	-0.92
C4' - H42'	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90
C4' - H43'	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91
C6' - H61'	-0.89	-0.89	-0.89	-0.97	-0.96	-0.89	-0.91
C6' - H62'	-0.90	-0.90	-0.89	-0.89	-0.90	-0.89	-0.90
C6' - H63'	-0.97	-0.98	-0.98	-0.90	-0.91	-0.98	-0.95
C7 - H71	-0.98	-0.99	-0.99	-0.99	-1.00	-0.98	-0.99
C7 - H72	-0.98	-0.99	-0.99	-1.00	-0.99	-0.98	-0.99
C8 - H81	-0.91	-0.92	-0.91	-0.91	-0.92	-0.91	-0.92
C8 - H82	-0.91	-0.91	-0.92	-0.92	-0.91	-0.91	-0.92
C8 - H83	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90	-0.90

Table 4. Electron density curvature λ_1 for conformers of **I** (a.u.)

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	-0.20	-0.20	-0.20	-0.20	-0.20	-0.20	-0.20
O1 - C5'	-1.09	-1.09	-1.09	-1.09	-1.09	-1.09	-1.09
O2 - C5'	-0.63	-0.61	-0.61	-0.63	-0.63	-0.62	-0.62
N1 - C2	-0.65	-0.66	-0.66	-0.65	-0.65	-0.66	-0.66
C2 - N3	-0.75	-0.74	-0.74	-0.75	-0.75	-0.74	-0.75
N3 - C4	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47	-0.47
C4 - C5	-0.48	-0.48	-0.48	-0.48	-0.48	-0.48	-0.48
C5 - C6	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
C6 - N1	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60
C4 - C4'	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46	-0.46
C5 - C5'	-0.56	-0.57	-0.56	-0.56	-0.57	-0.56	-0.56
C6 - C6'	-0.49	-0.49	-0.49	-0.49	-0.49	-0.49	-0.49
O2 - C7	-0.39	-0.38	-0.38	-0.38	-0.38	-0.39	-0.38
C7 - C8	-0.49	-0.48	-0.48	-0.48	-0.48	-0.49	-0.48
N1 - H1	-1.33	-1.33	-1.33	-1.33	-1.33	-1.33	-1.33
N3 - H3	-1.31	-1.31	-1.31	-1.31	-1.31	-1.31	-1.31
C4 - H4	-0.78	-0.78	-0.78	-0.78	-0.78	-0.78	-0.78
C4' - H41'	-0.72	-0.72	-0.72	-0.72	-0.72	-0.71	-0.72
C4' - H42'	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70
C4' - H43'	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71
C6' - H61'	-0.70	-0.70	-0.70	-0.76	-0.76	-0.70	-0.72
C6' - H62'	-0.70	-0.70	-0.70	-0.70	-0.71	-0.70	-0.70
C6' - H63'	-0.76	-0.77	-0.77	-0.70	-0.71	-0.77	-0.75
C7 - H71	-0.78	-0.79	-0.78	-0.78	-0.79	-0.78	-0.78
C7 - H72	-0.78	-0.78	-0.79	-0.79	-0.78	-0.78	-0.78
C8 - H81	-0.71	-0.72	-0.71	-0.71	-0.72	-0.71	-0.71
C8 - H82	-0.71	-0.71	-0.72	-0.72	-0.71	-0.71	-0.71
C8 - H83	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70	-0.70

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

Table 6. Electron density curvature λ_3 for conformers of **I** (a.u.)

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	0.35	0.35	0.35	0.35	0.35	0.35	0.35
O1 - C5'	1.78	1.78	1.78	1.77	1.77	1.79	1.78
O2 - C5'	0.75	0.71	0.70	0.73	0.73	0.72	0.72
N1 - C2	0.36	0.36	0.36	0.36	0.36	0.36	0.36
C2 - N3	0.41	0.41	0.41	0.41	0.41	0.41	0.41
N3 - C4	0.29	0.30	0.30	0.29	0.29	0.30	0.29
C4 - C5	0.36	0.36	0.36	0.36	0.36	0.36	0.36
C5 - C6	0.30	0.30	0.30	0.30	0.30	0.30	0.30
C6 - N1	0.35	0.36	0.36	0.35	0.36	0.36	0.36
C4 - C4'	0.36	0.37	0.37	0.36	0.36	0.37	0.36
C5 - C5'	0.36	0.36	0.36	0.36	0.36	0.36	0.36
C6 - C6'	0.35	0.34	0.34	0.35	0.35	0.34	0.35
O2 - C7	0.44	0.44	0.44	0.43	0.43	0.44	0.44
C7 - C8	0.36	0.36	0.36	0.36	0.36	0.36	0.36
N1 - H1	0.87	0.87	0.87	0.87	0.87	0.87	0.87
N3 - H3	0.88	0.88	0.88	0.88	0.88	0.88	0.88
C4 - H4	0.56	0.55	0.56	0.56	0.56	0.56	0.56
C4' - H41'	0.51	0.51	0.51	0.51	0.51	0.51	0.51
C4' - H42'	0.50	0.50	0.50	0.50	0.50	0.50	0.50
C4' - H43'	0.50	0.50	0.50	0.50	0.50	0.50	0.50
C6' - H61'	0.51	0.50	0.50	0.54	0.54	0.50	0.52
C6' - H62'	0.50	0.50	0.50	0.51	0.51	0.50	0.50
C6' - H63'	0.54	0.55	0.56	0.50	0.50	0.56	0.53
C7 - H71	0.55	0.56	0.54	0.54	0.56	0.55	0.55
C7 - H72	0.55	0.54	0.56	0.56	0.54	0.55	0.55
C8 - H81	0.50	0.51	0.50	0.50	0.51	0.50	0.51
C8 - H82	0.50	0.50	0.51	0.51	0.50	0.50	0.51
C8 - H83	0.50	0.50	0.50	0.50	0.50	0.50	0.50

Table 7. Bond ellipticity (λ_1/λ_2 - 1) for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	0.08	0.08	0.08	0.08	0.08	0.08	0.08
O1 - C5'	0.09	0.08	0.08	0.09	0.09	0.08	0.08
O2 - C5'	0.01	0.01	0.01	0.01	0.01	0.01	0.01
N1 - C2	0.09	0.09	0.09	0.09	0.09	0.09	0.09
C2 - N3	0.16	0.16	0.16	0.16	0.16	0.16	0.16
N3 - C4	0.04	0.04	0.04	0.04	0.04	0.04	0.04
C4 - C5	0.07	0.06	0.07	0.07	0.07	0.06	0.07
C5 - C6	0.36	0.37	0.37	0.36	0.36	0.37	0.36
C6 - N1	0.07	0.06	0.06	0.07	0.07	0.06	0.07
C4 - C4'	0.02	0.03	0.03	0.02	0.02	0.03	0.02
C5 - C5'	0.17	0.18	0.18	0.18	0.18	0.18	0.18
C6 - C6'	0.04	0.04	0.04	0.04	0.04	0.04	0.04
O2 - C7	0.04	0.03	0.03	0.03	0.03	0.04	0.03
C7 - C8	0.03	0.04	0.04	0.04	0.04	0.03	0.04
N1 - H1	0.05	0.05	0.05	0.05	0.05	0.05	0.05
N3 - H3	0.05	0.05	0.05	0.05	0.05	0.05	0.05
C4 - H4	0.02	0.02	0.02	0.02	0.02	0.02	0.02
C4' - H41'	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C4' - H42'	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C4' - H43'	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C6' - H61'	0.01	0.01	0.02	0.01	0.01	0.02	0.01
C6' - H62'	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C6' - H63'	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C7 - H71	0.03	0.03	0.04	0.04	0.03	0.03	0.04
C7 - H72	0.03	0.04	0.03	0.03	0.04	0.03	0.04
C8 - H81	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C8 - H82	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C8 - H83	0.01	0.01	0.01	0.01	0.01	0.01	0.01

Table 8. Kinetic energy density at the bond critical points (a.u.) for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	0.238	0.239	0.239	0.238	0.238	0.239	0.239
O1 - C5'	0.623	0.623	0.623	0.621	0.621	0.625	0.623
O2 - C5'	0.294	0.282	0.281	0.290	0.290	0.286	0.287
N1 - C2	0.178	0.178	0.178	0.178	0.178	0.178	0.178
C2 - N3	0.221	0.219	0.220	0.221	0.221	0.219	0.220
N3 - C4	0.126	0.124	0.124	0.126	0.126	0.124	0.125
C4 - C5	0.057	0.057	0.057	0.057	0.057	0.057	0.057
C5 - C6	0.129	0.128	0.128	0.128	0.128	0.128	0.128
C6 - N1	0.193	0.196	0.196	0.193	0.194	0.196	0.195
C4 - C4'	0.055	0.055	0.055	0.055	0.055	0.055	0.055
C5 - C5'	0.071	0.071	0.071	0.071	0.072	0.071	0.071
C6 - C6'	0.062	0.063	0.063	0.062	0.061	0.063	0.062
O2 - C7	0.209	0.210	0.210	0.207	0.207	0.211	0.209
C7 - C8	0.057	0.057	0.057	0.057	0.057	0.057	0.057
N1 - H1	0.050	0.050	0.050	0.050	0.050	0.050	0.050
N3 - H3	0.052	0.052	0.052	0.052	0.052	0.052	0.052
C4 - H4	0.037	0.037	0.037	0.037	0.037	0.037	0.037
C4' - H41'	0.041	0.042	0.042	0.041	0.041	0.042	0.042
C4' - H42'	0.043	0.043	0.043	0.043	0.043	0.043	0.043
C4' - H43'	0.043	0.042	0.042	0.043	0.043	0.042	0.042
C6' - H61'	0.042	0.042	0.042	0.039	0.040	0.043	0.041
C6' - H62'	0.043	0.043	0.043	0.042	0.042	0.043	0.043
C6' - H63'	0.039	0.038	0.038	0.043	0.043	0.038	0.040
C7 - H71	0.036	0.036	0.037	0.036	0.036	0.036	0.036
C7 - H72	0.036	0.036	0.036	0.036	0.037	0.036	0.036
C8 - H81	0.042	0.042	0.043	0.043	0.041	0.042	0.042
C8 - H82	0.043	0.043	0.042	0.041	0.043	0.042	0.042
C8 - H83	0.043	0.043	0.043	0.043	0.043	0.043	0.043

Table 9. Potential energy density at the bond critical points (a.u.) for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	-0.486	-0.488	-0.487	-0.487	-0.487	-0.488	-0.487
O1 - C5'	-1.325	-1.324	-1.325	-1.321	-1.320	-1.328	-1.324
O2 - C5'	-0.716	-0.694	-0.692	-0.710	-0.710	-0.700	-0.704
N1 - C2	-0.580	-0.581	-0.582	-0.580	-0.579	-0.582	-0.581
C2 - N3	-0.687	-0.684	-0.684	-0.688	-0.687	-0.683	-0.685
N3 - C4	-0.408	-0.404	-0.404	-0.409	-0.408	-0.405	-0.406
C4 - C5	-0.258	-0.257	-0.257	-0.259	-0.259	-0.257	-0.258
C5 - C6	-0.486	-0.486	-0.485	-0.486	-0.486	-0.486	-0.486
C6 - N1	-0.587	-0.594	-0.593	-0.587	-0.589	-0.592	-0.590
C4 - C4'	-0.244	-0.244	-0.243	-0.244	-0.245	-0.243	-0.244
C5 - C5'	-0.314	-0.315	-0.313	-0.314	-0.316	-0.312	-0.314
C6 - C6'	-0.276	-0.279	-0.279	-0.276	-0.275	-0.279	-0.277
O2 - C7	-0.497	-0.498	-0.498	-0.492	-0.492	-0.503	-0.497
C7 - C8	-0.263	-0.259	-0.259	-0.259	-0.259	-0.263	-0.261
N1 - H1	-0.531	-0.530	-0.530	-0.531	-0.531	-0.530	-0.531
N3 - H3	-0.524	-0.523	-0.523	-0.524	-0.524	-0.524	-0.524
C4 - H4	-0.321	-0.323	-0.323	-0.321	-0.321	-0.323	-0.322
C4' - H41'	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313
C4' - H42'	-0.311	-0.311	-0.311	-0.311	-0.311	-0.311	-0.311
C4' - H43'	-0.312	-0.313	-0.312	-0.312	-0.312	-0.312	-0.312
C6' - H61'	-0.307	-0.307	-0.307	-0.321	-0.320	-0.307	-0.311
C6' - H62'	-0.312	-0.311	-0.310	-0.307	-0.307	-0.310	-0.310
C6' - H63'	-0.322	-0.320	-0.321	-0.312	-0.313	-0.321	-0.318
C7 - H71	-0.318	-0.320	-0.320	-0.320	-0.320	-0.317	-0.319
C7 - H72	-0.318	-0.320	-0.320	-0.320	-0.320	-0.318	-0.319
C8 - H81	-0.313	-0.314	-0.313	-0.313	-0.314	-0.313	-0.313
C8 - H82	-0.313	-0.313	-0.314	-0.314	-0.313	-0.313	-0.313
C8 - H83	-0.312	-0.311	-0.311	-0.311	-0.310	-0.312	-0.311

Table 10. Electronic energy density $h(\mathbf{r})$ at the bond critical points (a.u.) for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	-0.248	-0.248	-0.248	-0.248	-0.248	-0.248	-0.248
O1 - C5'	-0.701	-0.701	-0.702	-0.700	-0.700	-0.703	-0.701
O2 - C5'	-0.422	-0.411	-0.411	-0.420	-0.419	-0.413	-0.416
N1 - C2	-0.402	-0.403	-0.403	-0.402	-0.402	-0.404	-0.403
C2 - N3	-0.466	-0.464	-0.464	-0.466	-0.466	-0.464	-0.465
N3 - C4	-0.282	-0.280	-0.280	-0.283	-0.282	-0.281	-0.281
C4 - C5	-0.201	-0.200	-0.200	-0.201	-0.202	-0.200	-0.201
C5 - C6	-0.358	-0.358	-0.358	-0.357	-0.357	-0.358	-0.358
C6 - N1	-0.394	-0.398	-0.397	-0.394	-0.395	-0.397	-0.396
C4 - C4'	-0.189	-0.189	-0.189	-0.189	-0.189	-0.189	-0.189
C5 - C5'	-0.243	-0.243	-0.242	-0.243	-0.244	-0.242	-0.243
C6 - C6'	-0.214	-0.216	-0.216	-0.214	-0.213	-0.216	-0.215
O2 - C7	-0.289	-0.288	-0.288	-0.285	-0.286	-0.291	-0.288
C7 - C8	-0.207	-0.202	-0.202	-0.202	-0.202	-0.207	-0.204
N1 - H1	-0.481	-0.480	-0.480	-0.481	-0.481	-0.480	-0.481
N3 - H3	-0.472	-0.472	-0.472	-0.472	-0.472	-0.472	-0.472
C4 - H4	-0.285	-0.286	-0.286	-0.285	-0.284	-0.286	-0.285
C4' - H41'	-0.272	-0.271	-0.271	-0.271	-0.272	-0.271	-0.271
C4' - H42'	-0.268	-0.268	-0.268	-0.268	-0.268	-0.268	-0.268
C4' - H43'	-0.270	-0.270	-0.270	-0.270	-0.270	-0.270	-0.270
C6' - H61'	-0.265	-0.264	-0.264	-0.282	-0.280	-0.264	-0.270
C6' - H62'	-0.269	-0.268	-0.267	-0.265	-0.266	-0.267	-0.267
C6' - H63'	-0.282	-0.282	-0.283	-0.269	-0.270	-0.283	-0.278
C7 - H71	-0.282	-0.284	-0.284	-0.284	-0.284	-0.281	-0.283
C7 - H72	-0.281	-0.284	-0.284	-0.284	-0.284	-0.282	-0.283
C8 - H81	-0.271	-0.273	-0.270	-0.270	-0.273	-0.271	-0.271
C8 - H82	-0.270	-0.270	-0.272	-0.273	-0.270	-0.271	-0.271
C8 - H83	-0.269	-0.267	-0.268	-0.267	-0.267	-0.269	-0.268

Table 11. Variation of the covalent bond orders for conformers of **I**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
C2 - S	1.55	1.56	1.56	1.55	1.55	1.56	1.56
O1 - C5'	1.27	1.27	1.28	1.27	1.27	1.28	1.28
O2 - C5'	0.87	0.86	0.87	0.87	0.87	0.86	0.87
N1 - C2	1.02	1.03	1.03	1.02	1.02	1.03	1.02
C2 - N3	1.14	1.14	1.14	1.14	1.14	1.14	1.14
N3 - C4	0.89	0.89	0.89	0.89	0.89	0.89	0.89
C4 - C5	0.95	0.95	0.96	0.95	0.95	0.96	0.95
C5 - C6	1.53	1.52	1.52	1.53	1.52	1.52	1.52
C6 - N1	1.03	1.03	1.03	1.03	1.03	1.03	1.03
C4 - C4'	0.95	0.95	0.95	0.95	0.95	0.95	0.95
C5 - C5'	1.02	1.02	1.02	1.02	1.02	1.02	1.02
C6 - C6'	0.99	1.00	1.00	0.99	0.99	1.00	1.00
O2 - C7	0.82	0.82	0.82	0.82	0.82	0.82	0.82
C7 - C8	0.98	0.98	0.98	0.98	0.98	0.98	0.98
N1 - H1	0.77	0.77	0.77	0.77	0.77	0.77	0.77
N3 - H3	0.79	0.79	0.79	0.79	0.79	0.79	0.79
C4 - H4	0.89	0.89	0.89	0.89	0.89	0.89	0.89
C4' - H41'	0.95	0.95	0.95	0.95	0.95	0.95	0.95
C4' - H42'	0.96	0.96	0.96	0.96	0.96	0.96	0.96
C4' - H43'	0.95	0.95	0.95	0.95	0.95	0.95	0.95
C6' - H61'	0.94	0.94	0.94	0.92	0.92	0.94	0.93
C6' - H62'	0.95	0.95	0.95	0.94	0.94	0.95	0.95
C6' - H63'	0.92	0.91	0.91	0.95	0.95	0.91	0.93
C7 - H71	0.91	0.90	0.92	0.92	0.90	0.91	0.91
C7 - H72	0.91	0.92	0.90	0.90	0.93	0.91	0.91
C8 - H81	0.96	0.95	0.96	0.96	0.95	0.96	0.96
C8 - H82	0.96	0.96	0.95	0.95	0.96	0.96	0.95
C8 - H83	0.96	0.96	0.96	0.96	0.96	0.96	0.96

Table 12. Variation of the atomic free valence indexes for conformers of **I**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S1	0.45	0.44	0.44	0.45	0.45	0.44	0.44
O1	0.73	0.73	0.72	0.73	0.73	0.72	0.72
O2	0.31	0.31	0.31	0.31	0.31	0.32	0.31
N1	0.17	0.17	0.17	0.17	0.17	0.17	0.17
N3	0.17	0.18	0.18	0.17	0.17	0.18	0.17
C2	0.28	0.28	0.27	0.28	0.28	0.28	0.28
C4	0.31	0.31	0.31	0.31	0.31	0.31	0.31
C4'	0.19	0.19	0.19	0.19	0.19	0.19	0.19
C5	0.50	0.51	0.50	0.50	0.50	0.51	0.50
C5'	0.84	0.84	0.83	0.84	0.84	0.84	0.84
C6	0.44	0.46	0.45	0.44	0.45	0.45	0.45
C6'	0.19	0.20	0.20	0.19	0.19	0.20	0.20
C7	0.37	0.37	0.37	0.37	0.37	0.37	0.37
C8	0.14	0.15	0.15	0.15	0.15	0.14	0.15
H1	0.23	0.23	0.23	0.23	0.23	0.23	0.23
H3	0.21	0.21	0.21	0.21	0.21	0.21	0.21
H4	0.11	0.11	0.11	0.11	0.11	0.11	0.11
H41'	0.05	0.05	0.05	0.05	0.05	0.05	0.05
H42'	0.04	0.04	0.04	0.04	0.04	0.04	0.04
H43'	0.05	0.05	0.05	0.05	0.05	0.05	0.05
H61'	0.06	0.06	0.06	0.08	0.08	0.06	0.07
H62'	0.05	0.05	0.05	0.06	0.06	0.05	0.05
H63'	0.08	0.09	0.09	0.05	0.05	0.09	0.07
H71	0.09	0.10	0.08	0.08	0.10	0.09	0.09
H72	0.09	0.08	0.10	0.10	0.07	0.09	0.09
H81	0.04	0.05	0.04	0.04	0.05	0.04	0.04
H82	0.04	0.04	0.05	0.05	0.04	0.04	0.05
H83	0.04	0.04	0.04	0.04	0.04	0.04	0.04

Table 13. Variation of the atomic volumes ($Å^3$) for conformers of **I**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S1	37.448	37.390	37.405	37.389	37.419	37.411	37.410
O1	18.944	18.560	18.554	18.773	18.790	18.720	18.724
O2	14.044	14.240	14.176	14.060	14.103	14.204	14.138
N1	13.892	13.873	13.884	13.936	13.894	13.879	13.893
N3	13.758	13.721	13.724	13.753	13.768	13.695	13.737
C2	8.509	8.492	8.543	8.490	8.468	8.525	8.504
C4	6.550	6.573	6.519	6.535	6.580	6.558	6.552
C4'	10.003	10.002	10.033	10.018	10.016	10.045	10.019
C5	10.663	10.621	10.648	10.626	10.640	10.642	10.640
C5'	5.969	6.024	6.125	6.012	5.982	6.105	6.036
C6	9.038	8.948	8.975	9.093	9.027	8.987	9.011
C6'	10.208	10.218	10.258	10.133	10.017	10.283	10.186
C7	7.581	7.790	7.832	7.788	7.830	7.578	7.733
C8	10.141	10.262	10.282	10.218	10.201	10.195	10.216
H1	4.385	4.380	4.409	4.374	4.358	4.410	4.386
H3	4.501	4.508	4.506	4.497	4.489	4.501	4.500
H4	6.476	6.459	6.437	6.461	6.483	6.434	6.458
H41'	7.125	7.192	7.161	7.155	7.131	7.210	7.162
H42'	7.629	7.630	7.637	7.619	7.626	7.624	7.628
H43'	7.565	7.521	7.509	7.550	7.560	7.519	7.537
H61'	7.267	7.275	7.316	6.083	6.240	7.309	6.915
H62'	7.335	7.401	7.405	7.278	7.229	7.406	7.342
H63'	6.141	5.895	5.771	7.332	7.308	5.777	6.371
H71	7.003	6.606	7.267	7.252	6.584	7.099	6.969
H72	7.039	7.268	6.590	6.593	7.275	6.972	6.956
H81	7.518	7.191	7.556	7.577	7.189	7.532	7.427
H82	7.576	7.572	7.195	7.159	7.552	7.519	7.429
H83	7.537	7.590	7.585	7.584	7.587	7.558	7.574
Σ	271.844	271.203	271.301	271.336	271.348	271.697	271.455

Table 14. Variation of atomic charges for conformers of **I**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S1	0.00	0.00	0.00	0.00	0.00	0.00	0.00
O1	-1.14	-1.15	-1.15	-1.14	-1.14	-1.15	-1.15
O2	-1.06	-1.06	-1.06	-1.06	-1.06	-1.06	-1.06
N1	-1.13	-1.13	-1.13	-1.13	-1.13	-1.13	-1.13
N3	-1.10	-1.10	-1.10	-1.10	-1.10	-1.10	-1.10
C2	0.58	0.58	0.58	0.58	0.58	0.58	0.58
C4	0.38	0.38	0.38	0.37	0.37	0.38	0.38
C4'	0.02	0.02	0.02	0.02	0.02	0.02	0.02
C5	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01	-0.01
C5'	1.47	1.46	1.45	1.46	1.46	1.46	1.46
C6	0.39	0.39	0.39	0.39	0.39	0.39	0.39
C6'	0.03	0.02	0.02	0.03	0.04	0.02	0.03
C7	0.45	0.45	0.44	0.44	0.44	0.45	0.45
C8	0.04	0.03	0.03	0.03	0.03	0.04	0.04
H1	0.41	0.41	0.41	0.41	0.41	0.41	0.41
H3	0.41	0.41	0.40	0.41	0.41	0.40	0.41
H4	0.05	0.04	0.04	0.05	0.05	0.04	0.05
H41'	0.03	0.02	0.02	0.03	0.03	0.02	0.02
H42'	0.00	0.00	0.00	0.00	0.00	0.00	0.00
H43'	0.00	0.01	0.01	0.00	0.00	0.01	0.00
H61'	0.03	0.03	0.03	0.07	0.06	0.03	0.04
H62'	0.01	0.01	0.01	0.03	0.04	0.01	0.02
H63'	0.07	0.09	0.09	0.01	0.00	0.10	0.06
H71	0.04	0.05	0.02	0.02	0.05	0.03	0.03
H72	0.03	0.02	0.05	0.05	0.02	0.04	0.03
H81	0.01	0.02	0.00	0.00	0.02	0.01	0.01
H82	0.00	0.00	0.02	0.02	0.00	0.01	0.01
H83	0.01	0.00	0.00	0.01	0.00	0.01	0.01
Σ	0.01	0.01	0.00	0.01	0.01	0.01	0.01

Table 15. Variation of atomic electronic energies (a.u.) for conformers of **I**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S1	-398.686	-398.685	-398.685	-398.686	-398.686	-398.685	-398.685
O1	-75.929	-75.941	-75.942	-75.932	-75.931	-75.939	-75.936
O2	-75.893	-75.879	-75.880	-75.886	-75.886	-75.887	-75.885
N1	-55.391	-55.395	-55.395	-55.390	-55.391	-55.394	-55.393
N3	-55.357	-55.354	-55.355	-55.358	-55.357	-55.355	-55.356
C2	-37.654	-37.656	-37.655	-37.654	-37.655	-37.655	-37.655
C4	-37.797	-37.793	-37.794	-37.798	-37.797	-37.794	-37.795
C4'	-37.998	-37.998	-37.998	-37.998	-37.998	-37.998	-37.998
C5	-38.061	-38.061	-38.060	-38.061	-38.063	-38.060	-38.061
C5'	-37.140	-37.140	-37.137	-37.140	-37.142	-37.137	-37.139
C6	-37.825	-37.829	-37.829	-37.825	-37.825	-37.830	-37.827
C6'	-37.993	-37.997	-38.000	-37.994	-37.991	-38.000	-37.996
C7	-37.748	-37.745	-37.746	-37.748	-37.747	-37.745	-37.747
C8	-37.981	-37.986	-37.986	-37.987	-37.987	-37.981	-37.985
H1	-0.461	-0.460	-0.460	-0.461	-0.461	-0.460	-0.460
H3	-0.465	-0.465	-0.465	-0.465	-0.465	-0.465	-0.465
H4	-0.621	-0.625	-0.625	-0.621	-0.621	-0.625	-0.623
H41'	-0.611	-0.615	-0.615	-0.612	-0.611	-0.615	-0.613
H42'	-0.621	-0.621	-0.622	-0.621	-0.621	-0.621	-0.621
H43'	-0.621	-0.619	-0.619	-0.621	-0.621	-0.619	-0.620
H61'	-0.605	-0.605	-0.607	-0.604	-0.605	-0.607	-0.606
H62'	-0.619	-0.619	-0.617	-0.605	-0.604	-0.616	-0.613
H63'	-0.605	-0.595	-0.593	-0.620	-0.621	-0.593	-0.604
H71	-0.620	-0.615	-0.626	-0.626	-0.615	-0.621	-0.620
H72	-0.620	-0.626	-0.615	-0.614	-0.627	-0.620	-0.620
H81	-0.618	-0.614	-0.620	-0.620	-0.614	-0.619	-0.617
H82	-0.620	-0.620	-0.614	-0.614	-0.619	-0.619	-0.618
H83	-0.616	-0.617	-0.617	-0.616	-0.617	-0.617	-0.617
Σ	-1009.777	-1009.777	-1009.774	-1009.775	-1009.775	-1009.776	-1009.776

Table 16. Bond lengths (Å) for the conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	1.67	1.67	1.67	1.67	1.67	1.68	1.67
O – C5'	1.22	1.22	1.22	1.22	1.22	1.22	1.22
N1 – C2	1.38	1.38	1.38	1.38	1.39	1.38	1.38
N1 – C6	1.39	1.39	1.39	1.38	1.39	1.39	1.39
N3 – C2	1.34	1.35	1.35	1.34	1.34	1.34	1.34
N3 – C4	1.47	1.47	1.47	1.47	1.47	1.47	1.47
C4 – C4'	1.54	1.55	1.55	1.55	1.55	1.55	1.55
C4' – C4"	1.53	1.53	1.53	1.53	1.53	1.53	1.53
C4 – C5	1.52	1.52	1.52	1.52	1.52	1.52	1.52
C5 – C6	1.36	1.36	1.36	1.36	1.36	1.36	1.36
C6 – C6'	1.51	1.50	1.50	1.50	1.51	1.51	1.50
C5 – C5'	1.48	1.47	1.48	1.48	1.48	1.48	1.48
C5' – C5"	1.52	1.52	1.52	1.53	1.52	1.52	1.52
N1 – H1	1.01	1.01	1.01	1.01	1.01	1.01	1.01
N3 – H3	1.01	1.01	1.01	1.01	1.01	1.01	1.01
C4 – H4	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C4' – H41	1.09	1.09	1.09	1.10	1.10	1.10	1.10
C4' – H42	1.10	1.09	1.10	1.10	1.10	1.09	1.10
C4" – H43	1.09	1.10	1.09	1.09	1.09	1.09	1.09
C4" – H44	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C4" – H45	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C6' – H61	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C6' – H62	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C6' – H63	1.08	1.09	1.09	1.09	1.08	1.08	1.09
C5" – H51"	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C5" – H52"	1.09	1.09	1.09	1.09	1.09	1.09	1.09
C5" – H53"	1.09	1.09	1.09	1.09	1.09	1.09	1.09

Table 17. Electron densities at the bond critical points (a.u.) for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	0.21	0.21	0.21	0.21	0.21	0.21	0.21
O – C5'	0.40	0.40	0.40	0.40	0.40	0.40	0.40
N1 – C2	0.31	0.31	0.31	0.31	0.30	0.31	0.31
N1 – C6	0.30	0.30	0.30	0.30	0.30	0.30	0.30
N3 – C2	0.34	0.33	0.33	0.33	0.34	0.34	0.33
N3 – C4	0.25	0.25	0.25	0.25	0.25	0.25	0.25
C4 – C4'	0.24	0.24	0.24	0.24	0.24	0.24	0.24
C4' – C4"	0.24	0.24	0.24	0.24	0.24	0.24	0.24
C4 – C5	0.25	0.25	0.25	0.25	0.25	0.25	0.25
C5 – C6	0.32	0.32	0.32	0.32	0.32	0.32	0.32
C6 – C6'	0.25	0.25	0.25	0.25	0.25	0.25	0.25
C5 – C5'	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C5' – C5"	0.25	0.25	0.25	0.25	0.25	0.25	0.25
N1 – H1	0.34	0.34	0.34	0.34	0.34	0.34	0.34
N3 – H3	0.34	0.34	0.34	0.34	0.34	0.34	0.34
C4 – H4	0.29	0.28	0.28	0.28	0.29	0.29	0.29
C4' – H41	0.28	0.27	0.28	0.27	0.27	0.27	0.27
C4' – H42	0.27	0.28	0.27	0.27	0.27	0.28	0.28
C4" – H43	0.27	0.27	0.27	0.27	0.28	0.27	0.27
C4" – H44	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C4" – H45	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C6' – H61	0.27	0.27	0.28	0.28	0.27	0.27	0.27
C6' – H62	0.27	0.27	0.27	0.27	0.27	0.27	0.27
C6' – H63	0.28	0.28	0.28	0.28	0.28	0.28	0.28
C5" – H51"	0.28	0.28	0.28	0.28	0.27	0.27	0.28
C5" – H52"	0.27	0.27	0.27	0.27	0.27	0.28	0.27
C5" – H53"	0.27	0.27	0.27	0.27	0.28	0.27	0.27

Table 18. Laplacian of electron density at the bond critical points (a.u.) for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	-0.04	-0.03	-0.03	-0.03	-0.04	-0.04	-0.04
O – C5'	-0.22	-0.22	-0.22	-0.22	-0.22	-0.22	-0.22
N1 – C2	-0.89	-0.90	-0.90	-0.91	-0.89	-0.90	-0.90
N1 – C6	-0.80	-0.80	-0.80	-0.80	-0.80	-0.81	-0.80
N3 – C2	-0.99	-0.98	-0.98	-0.97	-0.99	-0.98	-0.98
N3 – C4	-0.62	-0.63	-0.63	-0.62	-0.61	-0.61	-0.62
C4 – C4'	-0.53	-0.52	-0.52	-0.51	-0.52	-0.52	-0.52
C4' – C4"	-0.53	-0.53	-0.53	-0.53	-0.53	-0.54	-0.53
C4 – C5	-0.57	-0.57	-0.57	-0.56	-0.57	-0.57	-0.57
C5 – C6	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91
C6 – C6'	-0.60	-0.61	-0.61	-0.61	-0.60	-0.60	-0.61
C5 – C5'	-0.66	-0.66	-0.66	-0.66	-0.65	-0.65	-0.66
C5' – C5"	-0.58	-0.58	-0.58	-0.58	-0.58	-0.58	-0.58
N1 – H1	-1.72	-1.73	-1.73	-1.73	-1.72	-1.72	-1.72
N3 – H3	-1.69	-1.69	-1.68	-1.68	-1.68	-1.68	-1.68
C4 – H4	-0.99	-0.97	-0.97	-0.97	-1.00	-0.99	-0.98
C4' – H41	-0.93	-0.91	-0.92	-0.90	-0.91	-0.90	-0.91
C4' – H42	-0.91	-0.92	-0.91	-0.91	-0.91	-0.93	-0.91
C4" – H43	-0.90	-0.89	-0.90	-0.91	-0.92	-0.91	-0.90
C4" – H44	-0.91	-0.91	-0.91	-0.90	-0.91	-0.90	-0.91
C4" – H45	-0.90	-0.91	-0.91	-0.91	-0.90	-0.90	-0.90
C6' – H61	-0.89	-0.92	-0.93	-0.92	-0.89	-0.89	-0.91
C6' – H62	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91	-0.91
C6' – H63	-0.95	-0.93	-0.92	-0.93	-0.95	-0.95	-0.94
C5" – H51"	-0.94	-0.94	-0.94	-0.94	-0.91	-0.88	-0.92
C5" – H52"	-0.91	-0.89	-0.89	-0.89	-0.88	-0.94	-0.90
C5" – H53"	-0.88	-0.88	-0.89	-0.88	-0.94	-0.91	-0.90

Table 19. Electron density curvature λ_1 for conformers of **II** (a.u.)

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	-0.20	-0.20	-0.20	-0.20	-0.20	-0.20	-0.20
O – C5'	-1.03	-1.02	-1.03	-1.03	-1.03	-1.03	-1.03
N1 – C2	-0.65	-0.66	-0.65	-0.66	-0.65	-0.65	-0.65
N1 – C6	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60	-0.60
N3 – C2	-0.75	-0.74	-0.74	-0.74	-0.76	-0.75	-0.75
N3 – C4	-0.46	-0.47	-0.47	-0.47	-0.46	-0.46	-0.47
C4 – C4'	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45	-0.45
C4' – C4"	-0.44	-0.44	-0.44	-0.44	-0.44	-0.45	-0.44
C4 – C5	-0.48	-0.48	-0.47	-0.48	-0.48	-0.48	-0.48
C5 – C6	-0.69	-0.69	-0.69	-0.69	-0.69	-0.69	-0.69
C6 – C6'	-0.49	-0.49	-0.49	-0.49	-0.49	-0.48	-0.49
C5 – C5'	-0.55	-0.55	-0.55	-0.55	-0.54	-0.54	-0.55
C5' – C5"	-0.49	-0.49	-0.49	-0.49	-0.48	-0.48	-0.49
N1 – H1	-1.33	-1.33	-1.33	-1.33	-1.33	-1.33	-1.33
N3 – H3	-1.32	-1.32	-1.31	-1.31	-1.31	-1.31	-1.31
C4 – H4	-0.78	-0.76	-0.76	-0.76	-0.79	-0.78	-0.77
C4' – H41	-0.72	-0.71	-0.71	-0.70	-0.71	-0.70	-0.71
C4' – H42	-0.71	-0.71	-0.71	-0.71	-0.70	-0.73	-0.71
C4" – H43	-0.70	-0.70	-0.70	-0.71	-0.72	-0.71	-0.70
C4" – H44	-0.71	-0.71	-0.71	-0.70	-0.71	-0.70	-0.71
C4" – H45	-0.70	-0.71	-0.71	-0.71	-0.70	-0.70	-0.70
C6' – H61	-0.71	-0.73	-0.73	-0.73	-0.71	-0.71	-0.72
C6' – H62	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71	-0.71
C6' – H63	-0.74	-0.74	-0.73	-0.73	-0.74	-0.74	-0.74
C5" – H51"	-0.73	-0.73	-0.73	-0.73	-0.71	-0.69	-0.72
C5" – H52"	-0.71	-0.69	-0.70	-0.70	-0.69	-0.74	-0.70
C5" – H53"	-0.69	-0.69	-0.69	-0.69	-0.74	-0.71	-0.70

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

Table 21. Electron density curvature λ_3 for conformers of **II** (a.u.)

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	0.35	0.35	0.36	0.35	0.35	0.35	0.35
O – C5'	1.78	1.78	1.78	1.78	1.79	1.78	1.78
N1 – C2	0.35	0.36	0.35	0.36	0.35	0.36	0.36
N1 – C6	0.35	0.37	0.36	0.37	0.35	0.36	0.36
N3 – C2	0.41	0.41	0.40	0.41	0.41	0.42	0.41
N3 – C4	0.29	0.30	0.30	0.30	0.29	0.29	0.29
C4 – C4'	0.37	0.37	0.37	0.37	0.37	0.37	0.37
C4' – C4"	0.35	0.35	0.35	0.35	0.35	0.35	0.35
C4 – C5	0.36	0.36	0.36	0.36	0.36	0.36	0.36
C5 – C6	0.30	0.30	0.30	0.30	0.30	0.30	0.30
C6 – C6'	0.35	0.35	0.35	0.35	0.35	0.35	0.35
C5 – C5'	0.37	0.37	0.37	0.37	0.37	0.37	0.37
C5' – C5"	0.37	0.37	0.37	0.37	0.37	0.37	0.37
N1 – H1	0.87	0.87	0.87	0.87	0.87	0.87	0.87
N3 – H3	0.88	0.88	0.88	0.88	0.88	0.88	0.88
C4 – H4	0.56	0.54	0.54	0.54	0.56	0.56	0.55
C4' – H41	0.51	0.50	0.51	0.50	0.50	0.49	0.50
C4' – H42	0.50	0.51	0.50	0.50	0.50	0.52	0.50
C4" – H43	0.50	0.49	0.49	0.50	0.51	0.50	0.50
C4" – H44	0.50	0.50	0.50	0.50	0.50	0.50	0.50
C4" – H45	0.50	0.50	0.50	0.50	0.50	0.50	0.50
C6' – H61	0.51	0.53	0.53	0.53	0.51	0.51	0.52
C6' – H62	0.50	0.50	0.50	0.50	0.50	0.50	0.50
C6' – H63	0.53	0.53	0.52	0.53	0.53	0.53	0.53
C5" – H51"	0.53	0.53	0.53	0.53	0.50	0.49	0.52
C5" – H52"	0.50	0.49	0.50	0.49	0.49	0.53	0.50
C5" – H53"	0.49	0.49	0.49	0.49	0.53	0.50	0.50

Table 22. Bond ellipticity (λ_1/λ_2 - 1) for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	0.08	0.08	0.08	0.08	0.08	0.08	0.08
O – C5'	0.05	0.05	0.05	0.05	0.05	0.05	0.05
N1 – C2	0.09	0.10	0.10	0.10	0.09	0.09	0.09
N1 – C6	0.08	0.06	0.06	0.06	0.08	0.08	0.07
N3 – C2	0.16	0.15	0.15	0.15	0.16	0.16	0.16
N3 – C4	0.04	0.04	0.04	0.04	0.04	0.05	0.04
C4 – C4'	0.02	0.03	0.04	0.02	0.04	0.02	0.03
C4' – C4"	0.01	0.00	0.00	0.00	0.00	0.01	0.00
C4 – C5	0.06	0.06	0.05	0.06	0.05	0.07	0.06
C5 – C6	0.35	0.34	0.34	0.35	0.34	0.35	0.35
C6 – C6'	0.04	0.05	0.05	0.05	0.04	0.04	0.05
C5 – C5'	0.14	0.16	0.15	0.16	0.14	0.14	0.15
C5' – C5"	0.04	0.04	0.04	0.04	0.04	0.04	0.04
N1 – H1	0.05	0.05	0.05	0.05	0.05	0.05	0.05
N3 – H3	0.05	0.05	0.05	0.05	0.05	0.05	0.05
C4 – H4	0.02	0.02	0.02	0.02	0.02	0.03	0.02
C4' – H41	0.01	0.01	0.00	0.01	0.01	0.01	0.01
C4' – H42	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C4" – H43	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C4" – H44	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C4" – H45	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C6' – H61	0.01	0.01	0.01	0.02	0.01	0.01	0.01
C6' – H62	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C6' – H63	0.01	0.02	0.02	0.02	0.01	0.01	0.01
C5" – H51"	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C5" – H52"	0.01	0.01	0.01	0.01	0.01	0.01	0.01
C5" – H53"	0.01	0.01	0.01	0.01	0.01	0.01	0.01

Table 23. Kinetic energy density at the bond critical points (a.u.) for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	0.239	0.241	0.241	0.240	0.239	0.238	0.239
O – C5'	0.615	0.614	0.615	0.614	0.616	0.614	0.615
N1 – C2	0.177	0.178	0.176	0.180	0.174	0.179	0.177
N1 – C6	0.192	0.200	0.199	0.203	0.192	0.196	0.197
N3 – C2	0.223	0.217	0.216	0.220	0.223	0.226	0.221
N3 – C4	0.129	0.124	0.123	0.124	0.129	0.129	0.126
C4 – C4'	0.055	0.054	0.054	0.054	0.054	0.054	0.054
C4' – C4"	0.055	0.055	0.055	0.055	0.055	0.055	0.055
C4 – C5	0.057	0.058	0.058	0.058	0.057	0.057	0.057
C5 – C6	0.128	0.126	0.126	0.126	0.128	0.128	0.127
C6 – C6'	0.060	0.063	0.063	0.062	0.060	0.060	0.061
C5 – C5'	0.070	0.072	0.071	0.071	0.070	0.070	0.071
C5' – C5"	0.057	0.057	0.057	0.057	0.057	0.057	0.057
N1 – H1	0.050	0.050	0.050	0.050	0.050	0.050	0.050
N3 – H3	0.052	0.052	0.052	0.052	0.051	0.052	0.052
C4 – H4	0.037	0.039	0.039	0.039	0.036	0.037	0.038
C4' – H41	0.042	0.043	0.042	0.043	0.043	0.044	0.043
C4' – H42	0.043	0.042	0.043	0.043	0.043	0.041	0.043
C4" – H43	0.043	0.044	0.044	0.043	0.042	0.043	0.043
C4" – H44	0.043	0.043	0.043	0.043	0.044	0.044	0.043
C4" – H45	0.044	0.043	0.043	0.043	0.044	0.044	0.043
C6' – H61	0.042	0.040	0.040	0.040	0.042	0.042	0.041
C6' – H62	0.043	0.043	0.043	0.043	0.043	0.043	0.043
C6' – H63	0.042	0.040	0.040	0.040	0.042	0.042	0.041
C5" – H51"	0.040	0.040	0.040	0.040	0.043	0.044	0.041
C5" – H52"	0.043	0.044	0.044	0.044	0.044	0.040	0.043
C5" – H53"	0.044	0.044	0.043	0.044	0.040	0.043	0.043

Table 24. Potential energy density at the bond critical points (a.u.) for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	-0.487	-0.489	-0.490	-0.488	-0.487	-0.485	-0.488
O – C5'	-1.285	-1.284	-1.284	-1.284	-1.287	-1.284	-1.285
N1 – C2	-0.576	-0.581	-0.576	-0.587	-0.570	-0.582	-0.579
N1 – C6	-0.586	-0.600	-0.598	-0.605	-0.586	-0.593	-0.595
N3 – C2	-0.692	-0.678	-0.678	-0.683	-0.693	-0.698	-0.687
N3 – C4	-0.412	-0.405	-0.403	-0.403	-0.411	-0.410	-0.407
C4 – C4'	-0.242	-0.240	-0.237	-0.236	-0.238	-0.238	-0.238
C4' – C4"	-0.243	-0.243	-0.244	-0.244	-0.243	-0.244	-0.244
C4 – C5	-0.258	-0.258	-0.257	-0.256	-0.257	-0.255	-0.257
C5 – C6	-0.484	-0.480	-0.479	-0.479	-0.482	-0.482	-0.481
C6 – C6'	-0.271	-0.278	-0.278	-0.277	-0.271	-0.270	-0.274
C5 – C5'	-0.304	-0.309	-0.307	-0.307	-0.302	-0.303	-0.305
C5' – C5"	-0.261	-0.259	-0.259	-0.259	-0.261	-0.260	-0.260
N1 – H1	-0.530	-0.531	-0.531	-0.532	-0.530	-0.531	-0.531
N3 – H3	-0.526	-0.526	-0.523	-0.523	-0.523	-0.523	-0.524
C4 – H4	-0.320	-0.320	-0.321	-0.321	-0.321	-0.321	-0.321
C4' – H41	-0.315	-0.314	-0.314	-0.312	-0.314	-0.312	-0.313
C4' – H42	-0.313	-0.313	-0.313	-0.314	-0.313	-0.315	-0.314
C4" – H43	-0.311	-0.311	-0.313	-0.313	-0.314	-0.313	-0.313
C4" – H44	-0.313	-0.313	-0.313	-0.313	-0.314	-0.313	-0.313
C4" – H45	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313	-0.313
C6' – H61	-0.307	-0.310	-0.311	-0.310	-0.307	-0.307	-0.309
C6' – H62	-0.312	-0.314	-0.314	-0.315	-0.312	-0.313	-0.313
C6' – H63	-0.321	-0.312	-0.311	-0.312	-0.322	-0.322	-0.317
C5" – H51"	-0.314	-0.315	-0.314	-0.315	-0.313	-0.309	-0.313
C5" – H52"	-0.314	-0.310	-0.311	-0.311	-0.309	-0.314	-0.312
C5" – H53"	-0.309	-0.308	-0.309	-0.308	-0.315	-0.314	-0.310

Table 25. Electronic energy density $h(\mathbf{r})$ at the bond critical points (a.u.) for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	-0.248	-0.249	-0.249	-0.248	-0.248	-0.248	-0.248
O – C5'	-0.670	-0.670	-0.670	-0.670	-0.671	-0.669	-0.670
N1 – C2	-0.400	-0.403	-0.400	-0.407	-0.396	-0.403	-0.401
N1 – C6	-0.394	-0.400	-0.399	-0.403	-0.393	-0.398	-0.398
N3 – C2	-0.469	-0.461	-0.461	-0.463	-0.470	-0.472	-0.466
N3 – C4	-0.283	-0.281	-0.280	-0.280	-0.282	-0.282	-0.281
C4 – C4'	-0.187	-0.185	-0.183	-0.182	-0.184	-0.184	-0.184
C4' – C4"	-0.188	-0.188	-0.189	-0.189	-0.188	-0.189	-0.189
C4 – C5	-0.201	-0.200	-0.199	-0.199	-0.199	-0.198	-0.199
C5 – C6	-0.356	-0.354	-0.353	-0.353	-0.354	-0.354	-0.354
C6 – C6'	-0.211	-0.215	-0.215	-0.215	-0.211	-0.210	-0.213
C5 – C5'	-0.234	-0.237	-0.236	-0.236	-0.232	-0.233	-0.235
C5' – C5"	-0.203	-0.202	-0.202	-0.202	-0.203	-0.203	-0.203
N1 – H1	-0.480	-0.482	-0.481	-0.482	-0.480	-0.481	-0.481
N3 – H3	-0.475	-0.474	-0.471	-0.471	-0.472	-0.472	-0.472
C4 – H4	-0.283	-0.281	-0.282	-0.281	-0.285	-0.284	-0.283
C4' – H41	-0.274	-0.271	-0.272	-0.269	-0.271	-0.268	-0.271
C4' – H42	-0.270	-0.271	-0.270	-0.270	-0.270	-0.274	-0.271
C4" – H43	-0.268	-0.267	-0.268	-0.271	-0.272	-0.270	-0.269
C4" – H44	-0.270	-0.270	-0.270	-0.270	-0.270	-0.269	-0.270
C4" – H45	-0.269	-0.270	-0.270	-0.270	-0.269	-0.269	-0.270
C6' – H61	-0.265	-0.270	-0.271	-0.271	-0.265	-0.265	-0.268
C6' – H62	-0.270	-0.271	-0.271	-0.271	-0.269	-0.270	-0.270
C6' – H63	-0.280	-0.272	-0.271	-0.272	-0.280	-0.280	-0.276
C5" – H51"	-0.274	-0.274	-0.274	-0.274	-0.270	-0.265	-0.272
C5" – H52"	-0.270	-0.266	-0.267	-0.267	-0.265	-0.274	-0.268
C5" – H53"	-0.265	-0.264	-0.266	-0.265	-0.275	-0.270	-0.267

Table 26. Variation of the covalent bond orders for conformers of **II**

Bond	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S – C2	1.55	1.56	1.56	1.55	1.56	1.55	1.56
O – C5'	1.38	1.38	1.38	1.38	1.38	1.38	1.38
N1 – C2	1.02	1.03	1.03	1.03	1.01	1.02	1.02
N1 – C6	1.04	1.04	1.04	1.04	1.04	1.04	1.04
N3 – C2	1.15	1.13	1.14	1.13	1.15	1.15	1.14
N3 – C4	0.89	0.89	0.89	0.89	0.89	0.89	0.89
C4 – C4'	0.93	0.93	0.93	0.93	0.93	0.93	0.93
C4' – C4"	0.99	0.99	0.99	0.99	0.99	0.99	0.99
C4 – C5	0.95	0.96	0.96	0.96	0.95	0.95	0.96
C5 – C6	1.52	1.49	1.49	1.49	1.52	1.52	1.51
C6 – C6'	0.99	1.00	1.00	1.00	0.99	0.99	0.99
C5 – C5'	1.05	1.06	1.05	1.05	1.04	1.05	1.05
C5' – C5"	0.95	0.95	0.95	0.95	0.95	0.95	0.95
N1 – H1	0.77	0.77	0.77	0.77	0.77	0.77	0.77
N3 – H3	0.79	0.79	0.79	0.79	0.79	0.79	0.79
C4 – H4	0.88	0.89	0.89	0.89	0.88	0.89	0.89
C4' – H41	0.93	0.93	0.93	0.94	0.93	0.94	0.93
C4' – H42	0.94	0.93	0.94	0.93	0.94	0.93	0.93
C4" – H43	0.96	0.96	0.95	0.95	0.95	0.95	0.95
C4" – H44	0.96	0.96	0.95	0.96	0.95	0.96	0.96
C4" – H45	0.96	0.95	0.96	0.95	0.96	0.95	0.96
C6' – H61	0.94	0.92	0.92	0.92	0.94	0.94	0.93
C6' – H62	0.94	0.95	0.95	0.95	0.94	0.95	0.95
C6' – H63	0.93	0.93	0.93	0.93	0.93	0.93	0.93
C5" – H51"	0.94	0.95	0.95	0.95	0.95	0.94	0.95
C5" – H52"	0.95	0.94	0.94	0.94	0.94	0.94	0.94
C5" – H53"	0.94	0.95	0.95	0.95	0.94	0.95	0.95

Table 27. Variation of the atomic free valence indexes for conformers of **II**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S	0.45	0.44	0.44	0.45	0.44	0.45	0.44
O	0.62	0.62	0.62	0.62	0.62	0.62	0.62
N1	0.17	0.17	0.17	0.17	0.17	0.17	0.17
N3	0.18	0.19	0.18	0.18	0.17	0.18	0.18
C2	0.28	0.28	0.27	0.29	0.28	0.29	0.28
C4	0.35	0.32	0.32	0.32	0.35	0.34	0.33
C4'	0.21	0.21	0.21	0.21	0.20	0.21	0.21
C4"	0.13	0.13	0.14	0.15	0.14	0.14	0.14
C5	0.48	0.49	0.50	0.49	0.49	0.48	0.49
C5'	0.63	0.62	0.63	0.62	0.63	0.62	0.62
C5"	0.22	0.21	0.22	0.22	0.22	0.22	0.22
C6	0.45	0.47	0.47	0.48	0.45	0.45	0.46
C6'	0.19	0.20	0.20	0.20	0.19	0.19	0.20
H1	0.23	0.23	0.23	0.23	0.23	0.23	0.23
H3	0.21	0.21	0.21	0.21	0.21	0.21	0.21
H4	0.12	0.11	0.11	0.11	0.12	0.11	0.11
H41	0.07	0.07	0.07	0.06	0.07	0.06	0.07
H42	0.06	0.07	0.06	0.07	0.06	0.07	0.07
H43	0.04	0.04	0.05	0.05	0.05	0.05	0.05
H44	0.04	0.04	0.05	0.04	0.05	0.04	0.04
H45	0.04	0.05	0.04	0.05	0.04	0.05	0.04
H51"	0.06	0.05	0.05	0.05	0.05	0.06	0.05
H52"	0.05	0.06	0.06	0.06	0.06	0.06	0.06
H53"	0.06	0.05	0.05	0.05	0.06	0.05	0.05
H61	0.06	0.08	0.08	0.08	0.06	0.06	0.07
H62	0.06	0.05	0.05	0.05	0.06	0.05	0.05
H63	0.07	0.07	0.07	0.07	0.07	0.07	0.07

Table 28. Variation of the atomic volumes ($Å^3$) for conformers of **II**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S	37.407	37.300	37.322	37.404	37.433	37.489	37.393
O	19.276	19.124	19.145	19.077	19.078	19.121	19.137
N1	13.790	13.801	13.740	13.692	13.731	13.749	13.751
N3	13.454	13.440	13.628	13.412	13.604	13.480	13.503
C2	8.477	8.510	8.563	8.305	8.474	8.347	8.446
C4	6.430	6.454	6.515	6.538	6.515	6.468	6.487
C4'	8.341	8.364	8.370	8.286	8.374	8.349	8.347
C4"	10.142	10.156	9.969	10.069	10.043	10.093	10.079
C5	10.703	10.710	10.487	10.552	10.619	10.597	10.611
C5'	7.503	7.427	7.318	7.405	7.458	7.536	7.441
C5"	7.503	7.427	7.318	7.405	7.458	7.536	7.441
C6	9.157	8.911	8.914	8.818	9.137	9.048	8.998
C6'	10.016	9.975	9.977	9.938	9.979	10.020	9.984
H1	4.377	4.339	4.348	4.330	4.391	4.366	4.358
H3	4.492	4.509	4.512	4.520	4.465	4.500	4.500
H4	6.405	6.637	6.567	6.608	6.198	6.393	6.468
H41	7.031	7.334	7.266	7.575	7.364	7.582	7.359
H42	7.510	7.368	7.507	7.249	7.521	6.876	7.339
H43	7.648	7.705	7.561	7.254	7.292	7.362	7.470
H44	7.576	7.550	7.303	7.582	7.440	7.599	7.508
H45	7.475	7.398	7.545	7.364	7.627	7.489	7.483
H51"	7.016	7.036	7.055	7.036	7.116	7.221	7.080
H52"	7.148	7.214	7.059	7.117	7.231	7.000	7.128
H53"	7.228	7.369	7.365	7.361	6.998	7.114	7.239
H61	7.251	6.676	6.496	6.600	7.252	7.235	6.918
H62	7.174	7.337	7.342	7.328	7.178	7.161	7.253
H63	6.465	6.687	6.873	6.746	6.443	6.432	6.608
Σ	256.994	256.758	256.066	255.571	256.420	256.163	256.329

Table 29. Variation of atomic charges for conformers of **II**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S	0.00	0.01	0.01	0.01	0.01	0.00	0.01
O	-1.10	-1.11	-1.11	-1.11	-1.10	-1.10	-1.11
N1	-1.12	-1.13	-1.13	-1.13	-1.12	-1.13	-1.13
N3	-1.10	-1.09	-1.09	-1.10	-1.10	-1.10	-1.10
C2	0.58	0.57	0.57	0.58	0.58	0.59	0.58
C4	0.36	0.36	0.36	0.36	0.36	0.36	0.36
C4'	0.05	0.05	0.05	0.05	0.06	0.05	0.05
C4"	0.03	0.02	0.03	0.02	0.03	0.02	0.03
C5	-0.03	-0.04	-0.04	-0.04	-0.03	-0.03	-0.04
C5'	0.94	0.95	0.95	0.95	0.94	0.94	0.94
C5"	-0.01	-0.01	-0.02	-0.01	0.00	-0.01	-0.01
C6	0.37	0.39	0.39	0.39	0.37	0.38	0.38
C6'	0.03	0.04	0.04	0.04	0.03	0.03	0.03
H1	0.41	0.41	0.41	0.42	0.41	0.41	0.41
H3	0.41	0.41	0.40	0.40	0.41	0.41	0.41
H4	0.05	0.01	0.02	0.01	0.06	0.05	0.03
H41	0.02	-0.01	0.00	-0.02	-0.01	-0.02	-0.01
H42	-0.01	0.00	-0.01	-0.01	-0.01	0.02	0.00
H43	-0.01	-0.01	-0.02	0.00	0.01	0.00	0.00
H44	0.00	0.01	0.00	0.00	-0.01	0.00	0.00
H45	-0.01	0.00	0.00	0.00	-0.01	-0.01	-0.01
H51"	0.04	0.04	0.04	0.04	0.01	0.01	0.03
H52"	0.01	0.01	0.02	0.01	0.01	0.04	0.02
H53"	0.01	0.01	0.01	0.01	0.04	0.01	0.02
H61	0.03	0.06	0.07	0.07	0.03	0.03	0.05
H62	0.02	-0.01	-0.01	-0.01	0.02	0.02	0.00
H63	0.03	0.06	0.05	0.06	0.03	0.03	0.05
Σ	0.01	0.01	0.01	0.01	0.01	0.01	0.01

Table 30. Variation of atomic electronic energies (a.u.) for conformers of **II**

Atom	Conformer						Mean value
	1R, 1S	2R, 2S	3R, 3S	4R, 4S	5R, 5S	6R, 6S	
S	-398.704	-398.703	-398.702	-398.704	-398.703	-398.705	-398.704
O	-75.897	-75.902	-75.902	-75.903	-75.901	-75.899	-75.901
N1	-55.391	-55.398	-55.394	-55.407	-55.387	-55.401	-55.396
N3	-55.366	-55.357	-55.354	-55.356	-55.363	-55.366	-55.360
C2	-37.658	-37.663	-37.666	-37.658	-37.662	-37.652	-37.660
C4	-37.816	-37.807	-37.806	-37.800	-37.817	-37.810	-37.809
C4'	-37.988	-37.989	-37.988	-37.986	-37.983	-37.987	-37.987
C4"	-37.973	-37.974	-37.973	-37.976	-37.970	-37.974	-37.973
C5	-38.075	-38.079	-38.080	-38.075	-38.072	-38.068	-38.075
C5'	-37.448	-37.445	-37.446	-37.445	-37.446	-37.448	-37.446
C5"	-38.023	-38.026	-38.026	-38.026	-38.024	-38.023	-38.025
C6	-37.831	-37.833	-37.834	-37.829	-37.831	-37.827	-37.831
C6'	-37.994	-37.989	-37.990	-37.990	-37.995	-37.995	-37.992
H1	-0.461	-0.460	-0.460	-0.459	-0.462	-0.461	-0.461
H3	-0.465	-0.465	-0.465	-0.466	-0.464	-0.465	-0.465
H4	-0.619	-0.635	-0.635	-0.637	-0.616	-0.621	-0.627
H41	-0.623	-0.632	-0.629	-0.632	-0.633	-0.633	-0.630
H42	-0.632	-0.627	-0.632	-0.633	-0.633	-0.620	-0.629
H43	-0.623	-0.626	-0.628	-0.622	-0.618	-0.624	-0.624
H44	-0.621	-0.619	-0.623	-0.621	-0.627	-0.622	-0.622
H45	-0.626	-0.624	-0.620	-0.624	-0.624	-0.628	-0.624
H51"	-0.605	-0.606	-0.606	-0.606	-0.618	-0.615	-0.609
H52"	-0.619	-0.617	-0.615	-0.617	-0.616	-0.605	-0.615
H53"	-0.614	-0.613	-0.615	-0.613	-0.605	-0.619	-0.613
H61	-0.606	-0.597	-0.596	-0.597	-0.606	-0.606	-0.602
H62	-0.617	-0.626	-0.626	-0.627	-0.617	-0.618	-0.622
H63	-0.617	-0.600	-0.601	-0.600	-0.617	-0.617	-0.609
Σ	-934.512	-934.512	-934.510	-934.511	-934.510	-934.510	-934.511

Table 31. Bond lengths (Å) for the conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	1.22	1.21	1.21
O2 – C5'	1.22	1.22	1.22
N1 – C2	1.41	1.40	1.41
N1 – C6	1.39	1.38	1.38
N3 – C2	1.36	1.36	1.36
N3 – C4	1.47	1.47	1.47
C4 – C4'	1.54	1.54	1.54
C4 – C5	1.52	1.52	1.52
C5 – C6	1.36	1.37	1.36
C6 – C6'	1.51	1.50	1.50
C5 – C5'	1.48	1.47	1.47
C5' – C5"	1.52	1.53	1.52
N1 – H1	1.01	1.01	1.01
N3 – H3	1.01	1.01	1.01
C4 – H4	1.09	1.09	1.09
C4' – H41	1.09	1.09	1.09
C4' – H42	1.09	1.09	1.09
C4' – H43	1.09	1.09	1.09
C6' – H61	1.09	1.09	1.09
C6' – H62	1.08	1.09	1.09
C6' – H63	1.09	1.09	1.09
C5" – H51"	1.09	1.09	1.09
C5" – H52"	1.09	1.09	1.09
C5" – H53"	1.09	1.09	1.09

Table 32. Electron densities at the bond critical points (a.u.) for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	0.42	0.42	0.42
O2 – C5'	0.40	0.40	0.40
N1 – C2	0.29	0.30	0.30
N1 – C6	0.30	0.30	0.30
N3 – C2	0.33	0.32	0.33
N3 – C4	0.25	0.25	0.25
C4 – C4'	0.24	0.24	0.24
C4 – C5	0.25	0.25	0.25
C5 – C6	0.32	0.32	0.32
C6 – C6'	0.25	0.25	0.25
C5 – C5'	0.27	0.27	0.27
C5' – C5"	0.25	0.25	0.25
N1 – H1	0.34	0.34	0.34
N3 – H3	0.34	0.34	0.34
C4 – H4	0.29	0.28	0.29
C4' – H41	0.27	0.27	0.27
C4' – H42	0.28	0.27	0.27
C4' – H43	0.27	0.27	0.27
C6' – H61	0.27	0.27	0.27
C6' – H62	0.28	0.27	0.28
C6' – H63	0.27	0.28	0.27
C5" – H51"	0.28	0.28	0.28
C5" – H52"	0.27	0.27	0.27
C5" – H53"	0.27	0.27	0.27

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

Table 34. Electron density curvature λ_1 for conformers of **III** (a.u.)

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	-1.08	-1.09	-1.09
O2 – C5'	-1.02	-1.02	-1.02
N1 – C2	-0.64	-0.65	-0.64
N1 – C6	-0.61	-0.61	-0.61
N3 – C2	-0.75	-0.74	-0.74
N3 – C4	-0.47	-0.48	-0.47
C4 – C4'	-0.46	-0.45	-0.45
C4 – C5	-0.48	-0.48	-0.48
C5 – C6	-0.69	-0.69	-0.69
C6 – C6'	-0.49	-0.49	-0.49
C5 – C5'	-0.55	-0.55	-0.55
C5' – C5"	-0.48	-0.49	-0.48
N1 – H1	-1.31	-1.31	-1.31
N3 – H3	-1.29	-1.29	-1.29
C4 – H4	-0.79	-0.77	-0.78
C4' – H41	-0.70	-0.70	-0.70
C4' – H42	-0.72	-0.70	-0.71
C4' – H43	-0.70	-0.71	-0.71
C6' – H61	-0.71	-0.72	-0.72
C6' – H62	-0.74	-0.71	-0.73
C6' – H63	-0.70	-0.74	-0.72
C5" – H51"	-0.73	-0.73	-0.73
C5" – H52"	-0.71	-0.69	-0.70
C5" – H53"	-0.69	-0.69	-0.69

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

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

Table 37. Bond ellipticity (λ_1/λ_2 - 1) for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	0.10	0.10	0.10
O2 – C5'	0.05	0.05	0.05
N1 – C2	0.11	0.12	0.12
N1 – C6	0.07	0.05	0.06
N3 – C2	0.18	0.18	0.18
N3 – C4	0.04	0.03	0.04
C4 – C4'	0.03	0.03	0.03
C4 – C5	0.06	0.06	0.06
C5 – C6	0.35	0.35	0.35
C6 – C6'	0.04	0.05	0.05
C5 – C5'	0.15	0.16	0.16
C5' – C5"	0.04	0.04	0.04
N1 – H1	0.05	0.05	0.05
N3 – H3	0.06	0.06	0.06
C4 – H4	0.03	0.02	0.02
C4' – H41	0.01	0.01	0.01
C4' – H42	0.01	0.01	0.01
C4' – H43	0.01	0.01	0.01
C6' – H61	0.01	0.02	0.01
C6' – H62	0.01	0.01	0.01
C6' – H63	0.01	0.02	0.01
C5" – H51"	0.01	0.01	0.01
C5" – H52"	0.01	0.01	0.01
C5" – H53"	0.01	0.01	0.01

Table 38. Kinetic energy density at the bond critical points (a.u.) for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	0.602	0.605	0.604
O2 – C5'	0.613	0.609	0.611
N1 – C2	0.150	0.151	0.151
N1 – C6	0.195	0.203	0.199
N3 – C2	0.187	0.182	0.185
N3 – C4	0.127	0.122	0.124
C4 – C4'	0.055	0.054	0.055
C4 – C5	0.057	0.057	0.057
C5 – C6	0.128	0.126	0.127
C6 – C6'	0.060	0.062	0.061
C5 – C5'	0.071	0.072	0.072
C5' – C5"	0.057	0.057	0.057
N1 – H1	0.052	0.051	0.052
N3 – H3	0.054	0.054	0.054
C4 – H4	0.037	0.039	0.038
C4' – H41	0.043	0.043	0.043
C4' – H42	0.041	0.043	0.042
C4' – H43	0.043	0.042	0.043
C6' – H61	0.043	0.040	0.042
C6' – H62	0.042	0.043	0.043
C6' – H63	0.042	0.040	0.041
C5" – H51"	0.040	0.040	0.040
C5" – H52"	0.043	0.044	0.044
C5" – H53"	0.044	0.044	0.044

Table 39. Potential energy density at the bond critical points (a.u.) for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	-1.309	-1.314	-1.311
O2 – C5'	-1.281	-1.277	-1.279
N1 – C2	-0.512	-0.517	-0.515
N1 – C6	-0.595	-0.609	-0.602
N3 – C2	-0.624	-0.610	-0.617
N3 – C4	-0.412	-0.404	-0.408
C4 – C4'	-0.243	-0.241	-0.242
C4 – C5	-0.256	-0.256	-0.256
C5 – C6	-0.482	-0.478	-0.480
C6 – C6'	-0.270	-0.277	-0.274
C5 – C5'	-0.307	-0.311	-0.309
C5' – C5"	-0.259	-0.258	-0.259
N1 – H1	-0.523	-0.524	-0.524
N3 – H3	-0.516	-0.516	-0.516
C4 – H4	-0.322	-0.322	-0.322
C4' – H41	-0.311	-0.311	-0.311
C4' – H42	-0.313	-0.312	-0.313
C4' – H43	-0.312	-0.312	-0.312
C6' – H61	-0.312	-0.309	-0.311
C6' – H62	-0.322	-0.314	-0.318
C6' – H63	-0.307	-0.313	-0.310
C5" – H51"	-0.314	-0.315	-0.314
C5" – H52"	-0.314	-0.311	-0.312
C5" – H53"	-0.309	-0.308	-0.308

Table 40. Electronic energy density $h(\mathbf{r})$ at the bond critical points (a.u.) for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	-0.707	-0.708	-0.708
O2 – C5'	-0.669	-0.667	-0.668
N1 – C2	-0.362	-0.366	-0.364
N1 – C6	-0.400	-0.406	-0.403
N3 – C2	-0.437	-0.428	-0.432
N3 – C4	-0.285	-0.282	-0.284
C4 – C4'	-0.189	-0.187	-0.188
C4 – C5	-0.199	-0.199	-0.199
C5 – C6	-0.354	-0.352	-0.353
C6 – C6'	-0.210	-0.215	-0.213
C5 – C5'	-0.236	-0.239	-0.237
C5' – C5"	-0.202	-0.201	-0.202
N1 – H1	-0.471	-0.473	-0.472
N3 – H3	-0.463	-0.462	-0.462
C4 – H4	-0.285	-0.283	-0.284
C4' – H41	-0.268	-0.268	-0.268
C4' – H42	-0.272	-0.269	-0.271
C4' – H43	-0.269	-0.270	-0.270
C6' – H61	-0.269	-0.269	-0.269
C6' – H62	-0.280	-0.271	-0.275
C6' – H63	-0.265	-0.273	-0.269
C5" – H51"	-0.274	-0.274	-0.274
C5" – H52"	-0.271	-0.267	-0.269
C5" – H53"	-0.265	-0.264	-0.264

Table 41. Variation of the covalent bond orders for conformers of **III**

Bond	Conformer		Mean value
	1R, 1S	2R, 2S	
O1 – C2	1.24	1.24	1.24
O2 – C5'	1.37	1.37	1.37
N1 – C2	0.89	0.90	0.89
N1 – C6	1.05	1.05	1.05
N3 – C2	1.02	1.01	1.02
N3 – C4	0.90	0.91	0.90
C4 – C4'	0.95	0.95	0.95
C4 – C5	0.95	0.96	0.95
C5 – C6	1.52	1.49	1.51
C6 – C6'	0.99	1.00	0.99
C5 – C5'	1.05	1.06	1.06
C5' – C5"	0.95	0.95	0.95
N1 – H1	0.79	0.79	0.79
N3 – H3	0.81	0.81	0.81
C4 – H4	0.89	0.90	0.89
C4' – H41	0.96	0.96	0.96
C4' – H42	0.95	0.96	0.95
C4' – H43	0.96	0.95	0.95
C6' – H61	0.94	0.92	0.93
C6' – H62	0.93	0.95	0.94
C6' – H63	0.94	0.93	0.93
C5" – H51"	0.94	0.95	0.95
C5" – H52"	0.95	0.94	0.95
C5" – H53"	0.94	0.95	0.94

Table 42. Variation of the atomic free valence indexes for conformers of **III**

Atom	Conformer		Mean value
	1R, 1S	2R, 2S	
O1	0.76	0.76	0.76
O2	0.63	0.63	0.63
N1	0.28	0.27	0.27
N3	0.27	0.28	0.27
C2	0.85	0.85	0.85
C4	0.31	0.29	0.30
C4'	0.19	0.19	0.19
C5	0.48	0.49	0.48
C6	0.44	0.47	0.45
C6'	0.19	0.20	0.20
C5'	0.63	0.62	0.62
C5"	0.22	0.21	0.22
H1	0.21	0.21	0.21
H3	0.19	0.19	0.19
H4	0.11	0.10	0.11
H41	0.04	0.04	0.04
H42	0.05	0.04	0.05
H43	0.04	0.05	0.05
H61	0.06	0.08	0.07
H62	0.07	0.05	0.06
H63	0.06	0.07	0.07
H51"	0.06	0.05	0.05
H52"	0.05	0.06	0.05
H53"	0.06	0.05	0.06

Table 43. Variation of the atomic volumes ($Å^3$) for conformers of **III**

Atom	Conformer		Mean value
	1R, 1S	2R, 2S	
O1	20.651	20.601	20.626
O2	19.298	19.137	19.218
N1	14.183	14.173	14.178
N3	14.092	13.987	14.039
C2	4.905	4.883	4.894
C4	6.496	6.573	6.534
C4'	10.105	9.971	10.038
C5	10.813	10.803	10.808
C6	9.130	8.893	9.011
C6'	9.987	9.976	9.982
C5'	7.480	7.426	7.453
C5"	10.205	10.294	10.249
H1	4.393	4.337	4.365
H3	4.519	4.544	4.532
H4	6.387	6.615	6.501
H41	7.655	7.647	7.651
H42	7.094	7.430	7.262
H43	7.601	7.442	7.522
H61	7.223	6.768	6.995
H62	6.408	7.370	6.889
H63	7.303	6.614	6.959
H51"	7.026	7.062	7.044
H52"	7.156	7.221	7.188
H53"	7.240	7.391	7.316
Σ	217.350	217.158	217.254

Table 44. Variation of atomic charges for conformers of **III**

Atom	Conformer		Mean value
	1R, 1S	2R, 2S	
O1	-1.16	-1.16	-1.16
O2	-1.11	-1.11	-1.11
N1	-1.12	-1.13	-1.12
N3	-1.10	-1.09	-1.09
C2	1.78	1.77	1.77
C4	0.38	0.38	0.38
C4'	0.02	0.02	0.02
C5	-0.03	-0.04	-0.04
C6	0.38	0.40	0.39
C6'	0.03	0.04	0.03
C5'	0.94	0.95	0.94
C5"	-0.01	-0.01	-0.01
H1	0.40	0.41	0.41
H3	0.40	0.39	0.40
H4	0.05	0.01	0.03
H41	-0.01	-0.01	-0.01
H42	0.03	0.00	0.01
H43	-0.01	0.01	0.00
H61	0.01	0.06	0.04
H62	0.03	-0.01	0.01
H63	0.03	0.06	0.05
H51"	0.04	0.04	0.04
H52"	0.01	0.01	0.01
H53"	0.01	0.01	0.01
Σ	0.01	0.01	0.01

Table 45. Variation of atomic electronic energies (a.u.) for conformers of **III**

Atom	Conformer		Mean value
	1R, 1S	2R, 2S	
O1	-75.963	-75.965	-75.964
O2	-75.956	-75.961	-75.958
N1	-55.422	-55.430	-55.426
N3	-55.386	-55.375	-55.381
C2	-37.036	-37.039	-37.038
C4	-37.827	-37.818	-37.822
C4'	-38.028	-38.030	-38.029
C5	-38.102	-38.106	-38.104
C6	-37.852	-37.855	-37.853
C6'	-38.025	-38.020	-38.023
C5'	-37.479	-37.476	-37.478
C5"	-38.053	-38.056	-38.054
H1	-0.466	-0.464	-0.465
H3	-0.470	-0.471	-0.471
H4	-0.622	-0.638	-0.630
H41	-0.623	-0.622	-0.623
H42	-0.612	-0.622	-0.617
H43	-0.623	-0.619	-0.621
H61	-0.618	-0.599	-0.608
H62	-0.618	-0.628	-0.623
H63	-0.608	-0.600	-0.604
H51"	-0.606	-0.607	-0.606
H52"	-0.621	-0.619	-0.620
H53"	-0.615	-0.614	-0.615
Σ	-572.232	-572.233	-572.232

Table 46. Bond lengths (Å) for the different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**	MP2/ 6-311++G**
O1 – C2	1.22	1.20	1.23	1.19	1.22
O2 – C5'	1.22	1.21	1.24	1.20	1.23
N1 – C2	1.41	1.39	1.43	1.38	1.41
N1 – C6	1.39	1.38	1.39	1.39	1.39
N3 – C2	1.36	1.35	1.37	1.35	1.37
N3 – C4	1.47	1.46	1.48	1.46	1.46
C4 – C4'	1.54	1.53	1.55	1.53	1.53
C4 – C5	1.52	1.51	1.54	1.52	1.51
C5 – C6	1.36	1.35	1.38	1.34	1.36
C6 – C6'	1.51	1.50	1.52	1.51	1.50
C5 – C5'	1.48	1.47	1.48	1.49	1.48
C5' – C5"	1.52	1.51	1.54	1.52	1.52
N1 – H1	1.01	1.00	1.02	0.99	1.01
N3 – H3	1.01	1.00	1.02	0.99	1.01
C4 – H4	1.09	1.08	1.10	1.08	1.09
C4' – H41	1.09	1.09	1.10	1.09	1.10
C4' – H42	1.09	1.08	1.10	1.08	1.09
C4' – H43	1.09	1.09	1.10	1.09	1.09
C6' – H61	1.09	1.09	1.10	1.09	1.09
C6' – H62	1.08	1.08	1.09	1.07	1.09
C6' – H63	1.09	1.09	1.10	1.09	1.10
C5" – H51"	1.09	1.08	1.10	1.08	1.09
C5" – H52"	1.09	1.08	1.10	1.08	1.09
C5" – H53"	1.09	1.09	1.10	1.09	1.09

Table 47. Electron densities at the bond critical points (a.u.) for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	0.42	0.43	0.40	0.44
O2 – C5'	0.40	0.41	0.39	0.43
N1 – C2	0.29	0.31	0.28	0.31
N1 – C6	0.30	0.31	0.29	0.30
N3 – C2	0.33	0.34	0.32	0.34
N3 – C4	0.25	0.26	0.24	0.26
C4 – C4'	0.24	0.25	0.23	0.26
C4 – C5	0.25	0.26	0.24	0.26
C5 – C6	0.32	0.34	0.31	0.35
C6 – C6'	0.25	0.26	0.24	0.26
C5 – C5'	0.27	0.28	0.26	0.28
C5' – C5"	0.25	0.26	0.24	0.26
N1 – H1	0.34	0.35	0.33	0.36
N3 – H3	0.34	0.35	0.33	0.36
C4 – H4	0.29	0.29	0.28	0.30
C4' – H41	0.27	0.28	0.27	0.28
C4' – H42	0.28	0.28	0.27	0.29
C4' – H43	0.27	0.28	0.27	0.28
C6' – H61	0.27	0.28	0.27	0.28
C6' – H62	0.28	0.29	0.28	0.29
C6' – H63	0.27	0.28	0.27	0.28
C5" – H51"	0.28	0.28	0.27	0.29
C5" – H52"	0.27	0.28	0.27	0.29
C5" – H53"	0.27	0.28	0.26	0.28

Table 48. Laplacian of electron density at the bond critical points (a.u.) for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	-0.42	-0.31	-0.50	-0.12
O2 – C5'	-0.22	-0.03	-0.36	0.25
N1 – C2	-0.85	-0.94	-0.74	-0.89
N1 – C6	-0.82	-0.81	-0.78	-0.69
N3 – C2	-1.00	-1.07	-0.91	-1.05
N3 – C4	-0.63	-0.67	-0.56	-0.53
C4 – C4'	-0.53	-0.61	-0.47	-0.69
C4 – C5	-0.57	-0.64	-0.51	-0.71
C5 – C6	-0.90	-1.01	-0.82	-1.11
C6 – C6'	-0.60	-0.68	-0.54	-0.75
C5 – C5'	-0.66	-0.74	-0.60	-0.80
C5' – C5"	-0.58	-0.67	-0.51	-0.75
N1 – H1	-1.68	-1.85	-1.54	-2.03
N3 – H3	-1.64	-1.80	-1.51	-1.97
C4 – H4	-0.99	-1.07	-0.94	-1.14
C4' – H41	-0.90	-0.96	-0.85	-1.01
C4' – H42	-0.92	-0.99	-0.88	-1.05
C4' – H43	-0.90	-0.96	-0.86	-1.02
C6' – H61	-0.91	-0.97	-0.86	-1.03
C6' – H62	-0.95	-1.02	-0.90	-1.09
C6' – H63	-0.89	-0.95	-0.85	-1.01
C5" – H51"	-0.93	-1.00	-0.89	-1.05
C5" – H52"	-0.91	-0.97	-0.86	-1.04
C5" – H53"	-0.88	-0.94	-0.84	-1.00

Table 49. Electron density curvature λ_1 for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	-1.08	-1.18	-1.01	-1.27
O2 – C5'	-1.02	-1.12	-0.95	-1.22
N1 – C2	-0.64	-0.67	-0.61	-0.70
N1 – C6	-0.61	-0.62	-0.60	-0.64
N3 – C2	-0.75	-0.79	-0.72	-0.82
N3 – C4	-0.47	-0.48	-0.46	-0.46
C4 – C4'	-0.46	-0.48	-0.43	-0.50
C4 – C5	-0.48	-0.50	-0.46	-0.51
C5 – C6	-0.69	-0.73	-0.66	-0.76
C6 – C6'	-0.49	-0.51	-0.47	-0.52
C5 – C5'	-0.55	-0.57	-0.53	-0.57
C5' – C5"	-0.48	-0.51	-0.46	-0.53
N1 – H1	-1.31	-1.38	-1.26	-1.43
N3 – H3	-1.29	-1.36	-1.24	-1.41
C4 – H4	-0.79	-0.81	-0.77	-0.81
C4' – H41	-0.70	-0.71	-0.69	-0.71
C4' – H42	-0.72	-0.74	-0.71	-0.73
C4' – H43	-0.70	-0.72	-0.69	-0.71
C6' – H61	-0.71	-0.73	-0.69	-0.72
C6' – H62	-0.74	-0.76	-0.73	-0.76
C6' – H63	-0.70	-0.72	-0.69	-0.72
C5" – H51"	-0.73	-0.75	-0.72	-0.75
C5" – H52"	-0.71	-0.73	-0.69	-0.72
C5" – H53"	-0.69	-0.71	-0.68	-0.70

Table 50. Electron density curvature λ_2 for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	-0.99	-1.09	-0.92	-1.19
O2 – C5'	-0.97	-1.07	-0.90	-1.17
N1 – C2	-0.57	-0.63	-0.53	-0.69
N1 – C6	-0.57	-0.60	-0.54	-0.61
N3 – C2	-0.63	-0.69	-0.60	-0.75
N3 – C4	-0.45	-0.46	-0.44	-0.44
C4 – C4'	-0.44	-0.47	-0.42	-0.48
C4 – C5	-0.45	-0.47	-0.43	-0.48
C5 – C6	-0.51	-0.52	-0.50	-0.51
C6 – C6'	-0.47	-0.49	-0.45	-0.50
C5 – C5'	-0.48	-0.50	-0.46	-0.51
C5' – C5"	-0.47	-0.49	-0.44	-0.51
N1 – H1	-1.24	-1.31	-1.20	-1.35
N3 – H3	-1.22	-1.28	-1.18	-1.33
C4 – H4	-0.77	-0.79	-0.75	-0.79
C4' – H41	-0.69	-0.71	-0.68	-0.70
C4' – H42	-0.72	-0.73	-0.70	-0.73
C4' – H43	-0.70	-0.71	-0.69	-0.70
C6' – H61	-0.70	-0.72	-0.69	-0.71
C6' – H62	-0.74	-0.75	-0.72	-0.75
C6' – H63	-0.69	-0.71	-0.68	-0.71
C5" – H51"	-0.73	-0.74	-0.71	-0.74
C5" – H52"	-0.70	-0.72	-0.69	-0.72
C5" – H53"	-0.68	-0.70	-0.67	-0.70

Table 51. Electron density curvature λ_3 for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	1.66	1.96	1.43	2.34
O2 – C5'	1.77	2.15	1.49	2.64
N1 – C2	0.36	0.35	0.40	0.49
N1 – C6	0.36	0.41	0.36	0.55
N3 – C2	0.39	0.40	0.41	0.52
N3 – C4	0.29	0.27	0.34	0.37
C4 – C4'	0.36	0.34	0.38	0.29
C4 – C5	0.36	0.33	0.38	0.28
C5 – C6	0.30	0.24	0.33	0.15
C6 – C6'	0.35	0.32	0.37	0.26
C5 – C5'	0.37	0.34	0.39	0.28
C5' – C5"	0.37	0.34	0.39	0.28
N1 – H1	0.88	0.83	0.91	0.76
N3 – H3	0.88	0.84	0.92	0.77
C4 – H4	0.56	0.53	0.58	0.46
C4' – H41	0.49	0.46	0.51	0.39
C4' – H42	0.51	0.48	0.53	0.42
C4' – H43	0.50	0.46	0.52	0.39
C6' – H61	0.50	0.47	0.52	0.41
C6' – H62	0.53	0.50	0.54	0.43
C6' – H63	0.51	0.48	0.52	0.42
C5" – H51"	0.53	0.50	0.54	0.43
C5" – H52"	0.50	0.47	0.52	0.40
C5" – H53"	0.49	0.46	0.51	0.40

Table 52. Bond ellipticity (λ_1/λ_2 - 1) for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	0.10	0.08	0.11	0.06
O2 – C5'	0.05	0.05	0.06	0.04
N1 – C2	0.11	0.07	0.14	0.02
N1 – C6	0.07	0.03	0.10	0.05
N3 – C2	0.18	0.15	0.20	0.08
N3 – C4	0.04	0.04	0.04	0.05
C4 – C4'	0.03	0.03	0.03	0.03
C4 – C5	0.06	0.07	0.06	0.07
C5 – C6	0.35	0.40	0.32	0.50
C6 – C6'	0.04	0.04	0.04	0.04
C5 – C5'	0.15	0.14	0.15	0.13
C5' – C5"	0.04	0.04	0.04	0.04
N1 – H1	0.05	0.06	0.05	0.06
N3 – H3	0.06	0.06	0.05	0.06
C4 – H4	0.03	0.03	0.02	0.03
C4' – H41	0.01	0.01	0.01	0.01
C4' – H42	0.01	0.01	0.01	0.01
C4' – H43	0.01	0.01	0.01	0.01
C6' – H61	0.01	0.01	0.01	0.01
C6' – H62	0.01	0.01	0.01	0.01
C6' – H63	0.01	0.01	0.01	0.01
C5" – H51"	0.01	0.01	0.01	0.01
C5" – H52"	0.01	0.01	0.01	0.01
C5" – H53"	0.01	0.01	0.01	0.01

Table 53. Kinetic energy density at the bond critical points (a.u.) for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	0.602	0.671	0.546	0.746
O2 – C5'	0.613	0.700	0.543	0.799
N1 – C2	0.150	0.184	0.133	0.247
N1 – C6	0.195	0.232	0.172	0.282
N3 – C2	0.187	0.219	0.169	0.270
N3 – C4	0.127	0.160	0.110	0.227
C4 – C4'	0.055	0.055	0.054	0.051
C4 – C5	0.057	0.057	0.056	0.052
C5 – C6	0.128	0.139	0.120	0.155
C6 – C6'	0.060	0.060	0.059	0.057
C5 – C5'	0.071	0.068	0.072	0.060
C5' – C5"	0.057	0.057	0.056	0.053
N1 – H1	0.052	0.052	0.052	0.051
N3 – H3	0.054	0.054	0.054	0.053
C4 – H4	0.037	0.037	0.036	0.037
C4' – H41	0.043	0.045	0.042	0.045
C4' – H42	0.041	0.042	0.041	0.042
C4' – H43	0.043	0.044	0.042	0.044
C6' – H61	0.043	0.044	0.042	0.043
C6' – H62	0.042	0.043	0.041	0.042
C6' – H63	0.042	0.043	0.041	0.042
C5" – H51"	0.040	0.041	0.040	0.040
C5" – H52"	0.043	0.044	0.043	0.044
C5" – H53"	0.044	0.045	0.043	0.045

Table 54. Potential energy density at the bond critical points (a.u.) for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	-1.309	-1.419	-1.216	-1.523
O2 – C5'	-1.281	-1.408	-1.175	-1.534
N1 – C2	-0.512	-0.603	-0.450	-0.717
N1 – C6	-0.595	-0.668	-0.539	-0.736
N3 – C2	-0.624	-0.707	-0.565	-0.802
N3 – C4	-0.412	-0.488	-0.361	-0.586
C4 – C4'	-0.243	-0.263	-0.226	-0.275
C4 – C5	-0.256	-0.275	-0.239	-0.283
C5 – C6	-0.482	-0.530	-0.446	-0.587
C6 – C6'	-0.270	-0.290	-0.253	-0.302
C5 – C5'	-0.307	-0.321	-0.293	-0.319
C5' – C5"	-0.259	-0.282	-0.240	-0.294
N1 – H1	-0.523	-0.567	-0.490	-0.609
N3 – H3	-0.516	-0.558	-0.484	-0.597
C4 – H4	-0.322	-0.341	-0.308	-0.358
C4' – H41	-0.311	-0.329	-0.298	-0.343
C4' – H42	-0.313	-0.331	-0.300	-0.345
C4' – H43	-0.312	-0.330	-0.300	-0.343
C6' – H61	-0.312	-0.330	-0.300	-0.343
C6' – H62	-0.322	-0.341	-0.308	-0.356
C6' – H63	-0.307	-0.324	-0.295	-0.338
C5" – H51"	-0.314	-0.332	-0.302	-0.344
C5" – H52"	-0.314	-0.332	-0.300	-0.347
C5" – H53"	-0.309	-0.326	-0.296	-0.340

Table 55. Electronic energy density $h(\mathbf{r})$ at the bond critical points (a.u.) for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	-0.707	-0.748	-0.671	-0.777
O2 – C5'	-0.669	-0.708	-0.632	-0.736
N1 – C2	-0.362	-0.419	-0.318	-0.470
N1 – C6	-0.400	-0.436	-0.367	-0.454
N3 – C2	-0.437	-0.488	-0.396	-0.532
N3 – C4	-0.285	-0.328	-0.251	-0.359
C4 – C4'	-0.189	-0.208	-0.172	-0.224
C4 – C5	-0.199	-0.218	-0.183	-0.230
C5 – C6	-0.354	-0.391	-0.326	-0.432
C6 – C6'	-0.210	-0.230	-0.194	-0.245
C5 – C5'	-0.236	-0.252	-0.221	-0.259
C5' – C5"	-0.202	-0.224	-0.184	-0.241
N1 – H1	-0.471	-0.515	-0.438	-0.558
N3 – H3	-0.463	-0.504	-0.430	-0.544
C4 – H4	-0.285	-0.304	-0.272	-0.321
C4' – H41	-0.268	-0.284	-0.256	-0.298
C4' – H42	-0.272	-0.289	-0.260	-0.303
C4' – H43	-0.269	-0.285	-0.257	-0.299
C6' – H61	-0.269	-0.286	-0.258	-0.300
C6' – H62	-0.280	-0.298	-0.267	-0.314
C6' – H63	-0.265	-0.282	-0.253	-0.295
C5" – H51"	-0.274	-0.291	-0.262	-0.304
C5" – H52"	-0.271	-0.288	-0.258	-0.303
C5" – H53"	-0.265	-0.281	-0.253	-0.295

Table 56. Variation of the covalent bond orders for different methods of computation

Bond	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1 – C2	1.24	1.14	1.30	1.00
O2 – C5'	1.37	1.32	1.41	1.25
N1 – C2	0.89	0.83	0.92	0.73
N1 – C6	1.05	1.00	1.08	0.93
N3 – C2	1.02	0.95	1.07	0.82
N3 – C4	0.90	0.87	0.91	0.82
C4 – C4'	0.95	0.95	0.95	0.94
C4 – C5	0.95	0.95	0.95	0.94
C5 – C6	1.52	1.55	1.50	1.59
C6 – C6'	0.99	0.99	0.99	0.97
C5 – C5'	1.05	1.03	1.07	0.99
C5' – C5"	0.95	0.94	0.95	0.93
N1 – H1	0.79	0.78	0.80	0.77
N3 – H3	0.81	0.80	0.82	0.79
C4 – H4	0.89	0.89	0.89	0.90
C4' – H41	0.96	0.96	0.96	0.96
C4' – H42	0.95	0.95	0.94	0.95
C4' – H43	0.96	0.96	0.95	0.96
C6' – H61	0.94	0.95	0.94	0.95
C6' – H62	0.93	0.94	0.93	0.94
C6' – H63	0.94	0.94	0.94	0.95
C5" – H51"	0.94	0.95	0.94	0.95
C5" – H52"	0.95	0.95	0.95	0.96
C5" – H53"	0.94	0.95	0.94	0.95

Table 57. Variation of the atomic free valence indexes for different methods of computation

Atom	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1	0.76	0.86	0.70	1.00
O2	0.63	0.68	0.59	0.75
N1	0.28	0.39	0.20	0.57
N3	0.27	0.38	0.20	0.57
C2	0.85	1.08	0.72	1.45
C4	0.31	0.34	0.31	0.41
C4'	0.19	0.19	0.19	0.19
C5	0.48	0.47	0.49	0.48
C6	0.44	0.46	0.43	0.51
C6'	0.19	0.19	0.19	0.19
C5'	0.63	0.70	0.57	0.83
C5"	0.22	0.21	0.22	0.21
H1	0.21	0.22	0.20	0.23
H3	0.19	0.20	0.18	0.21
H4	0.11	0.11	0.11	0.10
H41	0.04	0.04	0.04	0.04
H42	0.05	0.05	0.06	0.05
H43	0.04	0.04	0.05	0.04
H61	0.06	0.05	0.06	0.05
H62	0.07	0.06	0.07	0.06
H63	0.06	0.06	0.06	0.05
H51"	0.06	0.05	0.06	0.05
H52"	0.05	0.05	0.05	0.04
H53"	0.06	0.05	0.06	0.05

Table 58. Variation of the atomic volumes ($Å^3$) for different methods of computation

Atom	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1	20.651	20.543	20.793	20.540
O2	19.298	19.179	19.527	19.214
N1	14.183	14.402	14.074	14.865
N3	14.092	14.211	14.079	14.594
C2	4.905	4.128	5.534	3.156
C4	6.496	6.226	6.734	5.995
C4'	10.105	9.750	10.302	9.282
C5	10.813	10.711	10.932	10.782
C6	9.130	8.923	9.395	9.061
C6'	9.987	9.705	10.153	9.365
C5'	7.480	7.038	7.912	6.645
C5"	10.205	9.959	10.368	9.589
H1	4.393	4.156	4.597	3.951
H3	4.519	4.293	4.723	4.104
H4	6.387	6.336	6.493	6.411
H41	7.655	7.615	7.752	7.677
H42	7.094	6.975	7.261	6.999
H43	7.601	7.533	7.718	7.576
H61	7.223	7.100	7.345	7.109
H62	6.408	6.270	6.602	6.356
H63	7.303	7.212	7.446	7.245
H51"	7.026	6.903	7.185	6.899
H52"	7.156	7.052	7.306	7.106
H53"	7.240	7.114	7.375	7.145
Σ	217.350	213.334	221.606	211.665

Table 59. Variation of atomic charges for different methods of computation

Atom	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1	-1.16	-1.25	-1.09	-1.37
O2	-1.11	-1.19	-1.04	-1.31
N1	-1.12	-1.29	-1.00	-1.51
N3	-1.10	-1.26	-0.99	-1.47
C2	1.78	2.02	1.60	2.37
C4	0.38	0.45	0.34	0.57
C4'	0.02	0.05	0.02	0.14
C5	-0.03	-0.02	-0.04	0.04
C6	0.38	0.41	0.35	0.40
C6'	0.03	0.06	0.02	0.16
C5'	0.94	1.03	0.87	1.15
C5"	-0.01	0.02	-0.01	0.11
H1	0.40	0.42	0.39	0.44
H3	0.40	0.42	0.38	0.43
H4	0.05	0.04	0.05	0.01
H41	-0.01	-0.02	-0.01	-0.05
H42	0.03	0.02	0.03	-0.01
H43	-0.01	-0.02	0.00	-0.05
H61	0.01	0.01	0.01	-0.01
H62	0.03	0.03	0.03	0.00
H63	0.03	0.02	0.03	0.00
H51"	0.04	0.04	0.04	0.02
H52"	0.01	0.00	0.01	-0.03
H53"	0.01	0.01	0.01	-0.02
Σ	0.01	0.01	0.01	0.01

Table 60. Variation of atomic electronic energies (a.u.) for different methods of computation

Atom	DFT B3LYP/ 6-311++G**	DFT BHHLYP/ 6-311++G**	DFT BLYP/ 6-311++G**	HF/ 6-311++G**
O1	-75.963	-75.966	-75.885	-75.671
O2	-75.956	-75.960	-75.878	-75.668
N1	-55.422	-55.499	-55.324	-55.361
N3	-55.386	-55.457	-55.294	-55.315
C2	-37.036	-36.828	-37.154	-36.355
C4	-37.827	-37.756	-37.844	-37.455
C4'	-38.028	-37.993	-38.020	-37.731
C5	-38.102	-38.073	-38.092	-37.815
C6	-37.852	-37.806	-37.864	-37.586
C6'	-38.025	-37.989	-38.015	-37.724
C5'	-37.479	-37.388	-37.525	-37.086
C5"	-38.053	-38.021	-38.041	-37.761
H1	-0.466	-0.457	-0.474	-0.443
H3	-0.470	-0.461	-0.477	-0.449
H4	-0.622	-0.630	-0.618	-0.642
H41	-0.623	-0.631	-0.620	-0.642
H42	-0.612	-0.618	-0.610	-0.627
H43	-0.623	-0.631	-0.621	-0.641
H61	-0.618	-0.623	-0.617	-0.630
H62	-0.618	-0.625	-0.616	-0.635
H63	-0.608	-0.613	-0.606	-0.620
H51"	-0.606	-0.610	-0.605	-0.616
H52"	-0.621	-0.627	-0.618	-0.636
H53"	-0.615	-0.621	-0.614	-0.628
Σ	-572.232	-571.883	-572.032	-568.739

Table 61. Characteristics of N1 – C2 bond for conformers of **I** – **III**

Conformer	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_1	λ_2	λ_3	ε	$g(\mathbf{r})$	$v(\mathbf{r})$	$h(\mathbf{r})$	n
I (1R, 1S)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.178	-0.580	-0.402	1.02
I (2R, 2S)	0.31	-0.90	-0.66	-0.60	0.36	0.09	0.178	-0.581	-0.403	1.03
I (3R, 3S)	0.31	-0.90	-0.66	-0.60	0.36	0.09	0.178	-0.582	-0.403	1.03
I (4R, 4S)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.178	-0.580	-0.402	1.02
I (5R, 5S)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.178	-0.579	-0.402	1.02
I (6R, 6S)	0.31	-0.90	-0.66	-0.60	0.36	0.09	0.178	-0.582	-0.404	1.03
II (1R, 1S)	0.31	-0.89	-0.65	-0.60	0.35	0.09	0.177	-0.576	-0.400	1.02
II (2R, 2S)	0.31	-0.90	-0.66	-0.60	0.36	0.10	0.178	-0.581	-0.403	1.03
II (3R, 3S)	0.31	-0.90	-0.65	-0.60	0.35	0.10	0.176	-0.576	-0.400	1.03
II (4R, 4S)	0.31	-0.91	-0.66	-0.60	0.36	0.10	0.180	-0.587	-0.407	1.03
II (5R, 5S)	0.30	-0.89	-0.65	-0.59	0.35	0.09	0.174	-0.570	-0.396	1.01
II (6R, 6S)	0.31	-0.90	-0.65	-0.60	0.36	0.09	0.179	-0.582	-0.403	1.02
III (1R, 1S)	0.29	-0.85	-0.64	-0.57	0.36	0.11	0.150	-0.512	-0.362	0.89
III (2R, 2S)	0.30	-0.86	-0.65	-0.58	0.36	0.12	0.151	-0.517	-0.366	0.90
Mean value	0.31	-0.89	-0.65	-0.60	0.36	0.10	0.174	-0.570	-0.397	1.00

Table 62. Characteristics of C2 – N3 bond for conformers of **I** – **III**

Conformer	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_1	λ_2	λ_3	ε	$g(\mathbf{r})$	$v(\mathbf{r})$	$h(\mathbf{r})$	n
I (1R, 1S)	0.33	-0.98	-0.75	-0.65	0.41	0.16	0.221	-0.687	-0.466	1.14
I (2R, 2S)	0.33	-0.98	-0.74	-0.64	0.41	0.16	0.219	-0.684	-0.464	1.14
I (3R, 3S)	0.33	-0.98	-0.74	-0.64	0.41	0.16	0.220	-0.684	-0.464	1.14
I (4R, 4S)	0.33	-0.98	-0.75	-0.65	0.41	0.16	0.221	-0.688	-0.466	1.14
I (5R, 5S)	0.33	-0.98	-0.75	-0.64	0.41	0.16	0.221	-0.687	-0.466	1.14
I (6R, 6S)	0.33	-0.98	-0.74	-0.64	0.41	0.16	0.219	-0.683	-0.464	1.14
II (1R, 1S)	0.34	-0.99	-0.75	-0.65	0.41	0.16	0.223	-0.692	-0.469	1.15
II (2R, 2S)	0.33	-0.98	-0.74	-0.64	0.41	0.15	0.217	-0.678	-0.461	1.13
II (3R, 3S)	0.33	-0.98	-0.74	-0.64	0.40	0.15	0.216	-0.678	-0.461	1.14
II (4R, 4S)	0.33	-0.97	-0.74	-0.64	0.41	0.15	0.220	-0.683	-0.463	1.13
II (5R, 5S)	0.34	-0.99	-0.76	-0.65	0.41	0.16	0.223	-0.693	-0.470	1.15
II (6R, 6S)	0.34	-0.98	-0.75	-0.65	0.42	0.16	0.226	-0.698	-0.472	1.15
III (1R, 1S)	0.33	-1.00	-0.75	-0.63	0.39	0.18	0.187	-0.624	-0.437	1.02
III (2R, 2S)	0.32	-0.98	-0.74	-0.63	0.38	0.18	0.182	-0.610	-0.428	1.01
Mean value	0.33	-0.98	-0.75	-0.64	0.41	0.16	0.215	-0.676	-0.461	1.12

Table 63. Characteristics of N3 – C4 bond for conformers of **I** – **III**

Conformer	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_1	λ_2	λ_3	ε	$g(\mathbf{r})$	$v(\mathbf{r})$	$h(\mathbf{r})$	n
I (1R, 1S)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.126	-0.408	-0.282	0.89
I (2R, 2S)	0.25	-0.62	-0.47	-0.45	0.30	0.04	0.124	-0.404	-0.280	0.89
I (3R, 3S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.124	-0.404	-0.280	0.89
I (4R, 4S)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.126	-0.409	-0.283	0.89
I (5R, 5S)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.126	-0.408	-0.282	0.89
I (6R, 6S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.124	-0.405	-0.281	0.89
II (1R, 1S)	0.25	-0.62	-0.46	-0.44	0.29	0.04	0.129	-0.412	-0.283	0.89
II (2R, 2S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.124	-0.405	-0.281	0.89
II (3R, 3S)	0.25	-0.63	-0.47	-0.45	0.30	0.04	0.123	-0.403	-0.280	0.89
II (4R, 4S)	0.25	-0.62	-0.47	-0.45	0.30	0.04	0.124	-0.403	-0.280	0.89
II (5R, 5S)	0.25	-0.61	-0.46	-0.44	0.29	0.04	0.129	-0.411	-0.282	0.89
II (6R, 6S)	0.25	-0.61	-0.46	-0.44	0.29	0.05	0.129	-0.410	-0.282	0.89
III (1R, 1S)	0.25	-0.63	-0.47	-0.45	0.29	0.04	0.127	-0.412	-0.285	0.90
III (2R, 2S)	0.25	-0.64	-0.48	-0.46	0.30	0.03	0.122	-0.404	-0.282	0.91
Mean value	0.25	-0.62	-0.47	-0.45	0.29	0.04	0.125	-0.407	-0.282	0.89

Table 64. Characteristics of C4 – C5 bond for conformers of **I** – **III**

Conformer	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_1	λ_2	λ_3	ε	$g(\mathbf{r})$	$v(\mathbf{r})$	$h(\mathbf{r})$	n
I (1R, 1S)	0.25	-0.58	-0.48	-0.45	0.36	0.07	0.057	-0.258	-0.201	0.95
I (2R, 2S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.257	-0.200	0.95
I (3R, 3S)	0.25	-0.57	-0.48	-0.45	0.36	0.07	0.057	-0.257	-0.200	0.96
I (4R, 4S)	0.25	-0.58	-0.48	-0.45	0.36	0.07	0.057	-0.259	-0.201	0.95
I (5R, 5S)	0.25	-0.58	-0.48	-0.45	0.36	0.07	0.057	-0.259	-0.202	0.95
I (6R, 6S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.257	-0.200	0.96
II (1R, 1S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.258	-0.201	0.95
II (2R, 2S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.058	-0.258	-0.200	0.96
II (3R, 3S)	0.25	-0.57	-0.47	-0.45	0.36	0.05	0.058	-0.257	-0.199	0.96
II (4R, 4S)	0.25	-0.56	-0.48	-0.45	0.36	0.06	0.058	-0.256	-0.199	0.96
II (5R, 5S)	0.25	-0.57	-0.48	-0.45	0.36	0.05	0.057	-0.257	-0.199	0.95
II (6R, 6S)	0.25	-0.57	-0.48	-0.45	0.36	0.07	0.057	-0.255	-0.198	0.95
III (1R, 1S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.256	-0.199	0.95
III (2R, 2S)	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.256	-0.199	0.96
Mean value	0.25	-0.57	-0.48	-0.45	0.36	0.06	0.057	-0.257	-0.200	0.95

Table 65. Characteristics of C5 – C6 bond for conformers of **I** – **III**

Conformer	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_1	λ_2	λ_3	ε	$g(\mathbf{r})$	$v(\mathbf{r})$	$h(\mathbf{r})$	n
I (1R, 1S)	0.33	-0.92	-0.70	-0.51	0.30	0.36	0.129	-0.486	-0.358	1.53
I (2R, 2S)	0.33	-0.92	-0.70	-0.52	0.30	0.37	0.128	-0.486	-0.358	1.52
I (3R, 3S)	0.33	-0.92	-0.70	-0.52	0.30	0.37	0.128	-0.485	-0.358	1.52
I (4R, 4S)	0.33	-0.92	-0.70	-0.51	0.30	0.36	0.128	-0.486	-0.357	1.53
I (5R, 5S)	0.33	-0.92	-0.70	-0.51	0.30	0.36	0.128	-0.486	-0.357	1.52
I (6R, 6S)	0.33	-0.92	-0.70	-0.52	0.30	0.37	0.128	-0.486	-0.358	1.52
II (1R, 1S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.128	-0.484	-0.356	1.52
II (2R, 2S)	0.32	-0.91	-0.69	-0.52	0.30	0.34	0.126	-0.480	-0.354	1.49
II (3R, 3S)	0.32	-0.91	-0.69	-0.52	0.30	0.34	0.126	-0.479	-0.353	1.49
II (4R, 4S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.126	-0.479	-0.353	1.49
II (5R, 5S)	0.32	-0.91	-0.69	-0.51	0.30	0.34	0.128	-0.482	-0.354	1.52
II (6R, 6S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.128	-0.482	-0.354	1.52
III (1R, 1S)	0.32	-0.90	-0.69	-0.51	0.30	0.35	0.128	-0.482	-0.354	1.52
III (2R, 2S)	0.32	-0.91	-0.69	-0.51	0.30	0.35	0.126	-0.478	-0.352	1.49
Mean value	0.33	-0.91	-0.70	-0.51	0.30	0.35	0.127	-0.483	-0.355	1.51

Table 66. Characteristics of C6 – N1 bond for conformers of **I** – **III**

Conformer	$\rho(\mathbf{r})$	$\nabla^2\rho(\mathbf{r})$	λ_1	λ_2	λ_3	ε	$g(\mathbf{r})$	$v(\mathbf{r})$	$h(\mathbf{r})$	n
I (1R, 1S)	0.30	-0.80	-0.60	-0.56	0.35	0.07	0.193	-0.587	-0.394	1.03
I (2R, 2S)	0.30	-0.80	-0.60	-0.56	0.36	0.06	0.196	-0.594	-0.398	1.03
I (3R, 3S)	0.30	-0.81	-0.60	-0.56	0.36	0.06	0.196	-0.593	-0.397	1.03
I (4R, 4S)	0.30	-0.80	-0.60	-0.56	0.35	0.07	0.193	-0.587	-0.394	1.03
I (5R, 5S)	0.30	-0.80	-0.60	-0.56	0.36	0.07	0.194	-0.589	-0.395	1.03
I (6R, 6S)	0.30	-0.80	-0.60	-0.56	0.36	0.06	0.196	-0.592	-0.397	1.03
II (1R, 1S)	0.30	-0.80	-0.60	-0.56	0.35	0.08	0.192	-0.586	-0.394	1.04
II (2R, 2S)	0.30	-0.80	-0.60	-0.56	0.37	0.06	0.200	-0.600	-0.400	1.04
II (3R, 3S)	0.30	-0.80	-0.60	-0.56	0.36	0.06	0.199	-0.598	-0.399	1.04
II (4R, 4S)	0.30	-0.80	-0.60	-0.57	0.37	0.06	0.203	-0.605	-0.403	1.04
II (5R, 5S)	0.30	-0.80	-0.60	-0.56	0.35	0.08	0.192	-0.586	-0.393	1.04
II (6R, 6S)	0.30	-0.81	-0.60	-0.56	0.36	0.08	0.196	-0.593	-0.398	1.04
III (1R, 1S)	0.30	-0.82	-0.61	-0.57	0.36	0.07	0.195	-0.595	-0.400	1.05
III (2R, 2S)	0.30	-0.81	-0.61	-0.58	0.37	0.05	0.203	-0.609	-0.406	1.05
Mean value	0.30	-0.80	-0.60	-0.56	0.36	0.07	0.196	-0.594	-0.398	1.04

Table 67. Characteristics of N1 atom for conformers of **I** – **III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	2.83	13.892	-1.13	-55.391
I (2R, 2S)	2.83	13.873	-1.13	-55.395
I (3R, 3S)	2.83	13.884	-1.13	-55.395
I (4R, 4S)	2.83	13.936	-1.13	-55.390
I (5R, 5S)	2.83	13.894	-1.13	-55.391
I (6R, 6S)	2.83	13.879	-1.13	-55.394
II (1R, 1S)	2.83	13.790	-1.12	-55.391
II (2R, 2S)	2.83	13.801	-1.13	-55.398
II (3R, 3S)	2.83	13.740	-1.13	-55.394
II (4R, 4S)	2.83	13.692	-1.13	-55.407
II (5R, 5S)	2.83	13.731	-1.12	-55.387
II (6R, 6S)	2.83	13.749	-1.13	-55.401
III (1R, 1S)	2.72	14.183	-1.12	-55.422
III (2R, 2S)	2.73	14.173	-1.13	-55.430
Mean value	2.82	13.873	-1.13	-55.399

Table 68. Characteristics of C2 atom for conformers of **I** – **III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	3.72	8.509	0.58	-37.654
I (2R, 2S)	3.72	8.492	0.58	-37.656
I (3R, 3S)	3.73	8.543	0.58	-37.655
I (4R, 4S)	3.72	8.490	0.58	-37.654
I (5R, 5S)	3.72	8.468	0.58	-37.655
I (6R, 6S)	3.72	8.525	0.58	-37.655
II (1R, 1S)	3.72	8.477	0.58	-37.658
II (2R, 2S)	3.72	8.510	0.57	-37.663
II (3R, 3S)	3.73	8.563	0.57	-37.666
II (4R, 4S)	3.71	8.305	0.58	-37.658
II (5R, 5S)	3.72	8.474	0.58	-37.662
II (6R, 6S)	3.71	8.347	0.59	-37.652
III (1R, 1S)	3.15	4.905	1.78	-37.036
III (2R, 2S)	3.15	4.883	1.77	-37.039
Mean value	3.64	7.964	0.75	-37.569

Table 69. Characteristics of N3 atom for conformers of **I** – **III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	2.83	13.758	-1.10	-55.357
I (2R, 2S)	2.82	13.721	-1.10	-55.354
I (3R, 3S)	2.82	13.724	-1.10	-55.355
I (4R, 4S)	2.83	13.753	-1.10	-55.358
I (5R, 5S)	2.83	13.768	-1.10	-55.357
I (6R, 6S)	2.82	13.695	-1.10	-55.355
II (1R, 1S)	2.82	13.454	-1.10	-55.366
II (2R, 2S)	2.81	13.440	-1.09	-55.357
II (3R, 3S)	2.82	13.628	-1.09	-55.354
II (4R, 4S)	2.82	13.412	-1.10	-55.356
II (5R, 5S)	2.83	13.604	-1.10	-55.363
II (6R, 6S)	2.82	13.480	-1.10	-55.366
III (1R, 1S)	2.73	14.092	-1.10	-55.386
III (2R, 2S)	2.72	13.987	-1.09	-55.375
Mean value	2.81	13.680	-1.10	-55.361

Table 70. Characteristics of C4 atom for conformers of **I** – **III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	3.69	6.550	0.38	-37.797
I (2R, 2S)	3.69	6.573	0.38	-37.793
I (3R, 3S)	3.69	6.519	0.38	-37.794
I (4R, 4S)	3.69	6.535	0.37	-37.798
I (5R, 5S)	3.69	6.580	0.37	-37.797
I (6R, 6S)	3.69	6.558	0.38	-37.794
II (1R, 1S)	3.65	6.430	0.36	-37.816
II (2R, 2S)	3.68	6.454	0.36	-37.807
II (3R, 3S)	3.68	6.515	0.36	-37.806
II (4R, 4S)	3.68	6.538	0.36	-37.800
II (5R, 5S)	3.65	6.515	0.36	-37.817
II (6R, 6S)	3.66	6.468	0.36	-37.810
III (1R, 1S)	3.69	6.496	0.38	-37.827
III (2R, 2S)	3.71	6.573	0.38	-37.818
Mean value	3.68	6.522	0.37	-37.805

Table 71. Characteristics of C5 atom for conformers of **I** – **III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	3.50	10.663	-0.01	-38.061
I (2R, 2S)	3.49	10.621	-0.01	-38.061
I (3R, 3S)	3.50	10.648	-0.01	-38.060
I (4R, 4S)	3.50	10.626	-0.01	-38.061
I (5R, 5S)	3.50	10.640	-0.01	-38.063
I (6R, 6S)	3.49	10.642	-0.01	-38.060
II (1R, 1S)	3.52	10.703	-0.03	-38.075
II (2R, 2S)	3.51	10.710	-0.04	-38.079
II (3R, 3S)	3.50	10.487	-0.04	-38.080
II (4R, 4S)	3.51	10.552	-0.04	-38.075
II (5R, 5S)	3.51	10.619	-0.03	-38.072
II (6R, 6S)	3.52	10.597	-0.03	-38.068
III (1R, 1S)	3.52	10.813	-0.03	-38.102
III (2R, 2S)	3.51	10.803	-0.04	-38.106
Mean value	3.50	10.652	-0.02	-38.073

Table 72. Characteristics of C6 atom for conformers of **I** – **III**

Conformer	Valence index	Volume	Charge	Electronic energy
I (1R, 1S)	3.56	9.038	0.39	-37.825
I (2R, 2S)	3.54	8.948	0.39	-37.829
I (3R, 3S)	3.55	8.975	0.39	-37.829
I (4R, 4S)	3.56	9.093	0.39	-37.825
I (5R, 5S)	3.55	9.027	0.39	-37.825
I (6R, 6S)	3.55	8.987	0.39	-37.830
II (1R, 1S)	3.55	9.157	0.37	-37.831
II (2R, 2S)	3.53	8.911	0.39	-37.833
II (3R, 3S)	3.53	8.914	0.39	-37.834
II (4R, 4S)	3.52	8.818	0.39	-37.829
II (5R, 5S)	3.55	9.137	0.37	-37.831
II (6R, 6S)	3.55	9.048	0.38	-37.827
III (1R, 1S)	3.56	9.130	0.38	-37.852
III (2R, 2S)	3.53	8.893	0.40	-37.855
Mean value	3.54	9.006	0.39	-37.833