Table 4. Electron density curvature $\lambda_1$ 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 |