

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