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