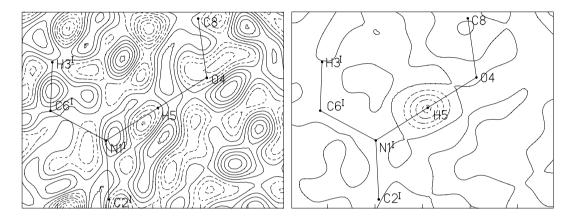
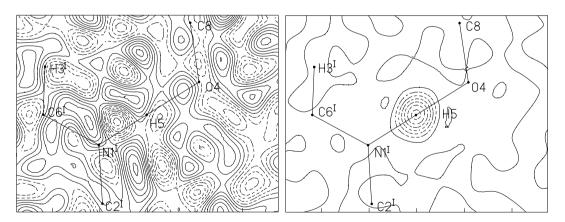
# **Difference Fourier Maps**

Difference Fourier map calculated from the neutron diffraction data. with H2 (figure 3a) or H1 (figure 3b) omitted from the model. The left hand maps are calculated from the final refined structures with the contours at nuclear scattering density intervals of 0.2 fm  $\rm \mathring{A}^{-3}$  and dashed lines indicate negative contours. The right hand maps are calculated with H/D5 omitted and the contours at nuclear scattering density intervals of 3 fm  $\rm \mathring{A}^{-3}$ .

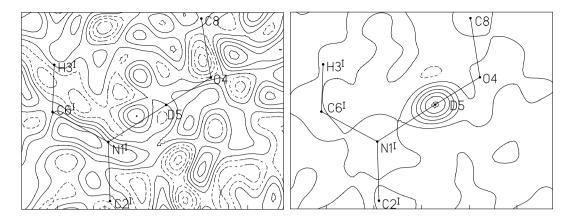
#### Room Temperature Structure, PDA.



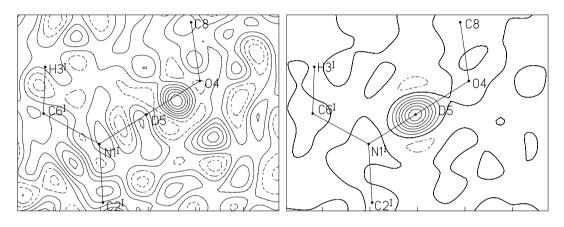
#### 15 K structure, PDA.



# Room temperature deuterated structure, dPDA.



## 150 K deuterated structure, dPDA.



### 15 K deuterated structure, dPDA.

