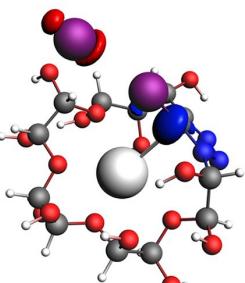


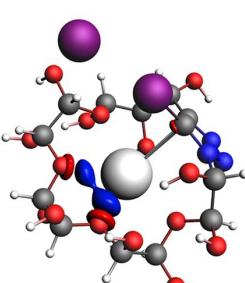
$\Delta\rho_1^*$

$$\Delta q_1 = 0.153 \text{ a.u.}$$



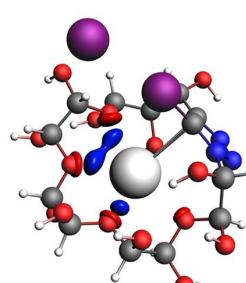
$\Delta\rho_2^*$

$$\Delta q_2 = 0.119 \text{ a.u.}$$



$\Delta\rho_4^*$

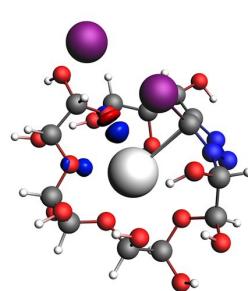
$$\Delta q_4 = 0.096 \text{ a.u.}$$



$\Delta\rho_5^*$

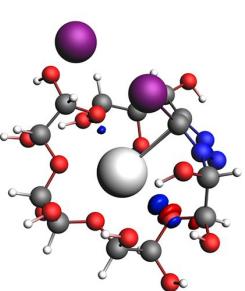
$$\Delta q_5 = 0.090 \text{ a.u.}$$

$$\Delta E_{\text{oi},1} = -4.32 \text{ kcal mol}^{-1} \quad \Delta E_{\text{oi},2} = -2.06 \text{ kcal mol}^{-1} \quad \Delta E_{\text{oi},4} = -2.46 \text{ kcal mol}^{-1} \quad \Delta E_{\text{oi},5} = -2.36 \text{ kcal mol}^{-1}$$



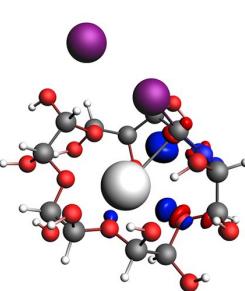
$\Delta\rho_6^*$

$$\Delta q_6 = 0.077 \text{ a.u.}$$



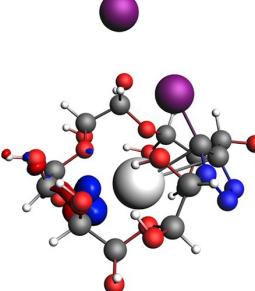
$\Delta\rho_7^*$

$$\Delta q_7 = 0.074 \text{ a.u.}$$



$\Delta\rho_8^\ominus$

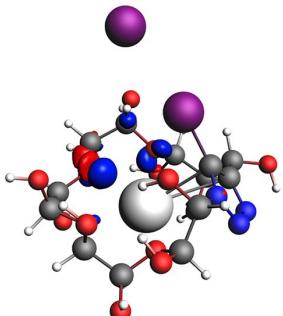
$$\Delta q_8 = 0.069 \text{ a.u.}$$



$\Delta\rho_9^\ominus$

$$\Delta q_9 = 0.059 \text{ a.u.}$$

$$\Delta E_{\text{oi},6} = -1.85 \text{ kcal mol}^{-1} \quad \Delta E_{\text{oi},7} = -1.69 \text{ kcal mol}^{-1} \quad \Delta E_{\text{oi},8} = -1.43 \text{ kcal mol}^{-1} \quad \Delta E_{\text{oi},9} = -1.06 \text{ kcal mol}^{-1}$$



$\Delta\rho_{10}^\ddagger$

$$\Delta q_{10} = 0.054 \text{ a.u.}$$

$$\Delta E_{\text{oi},10} = -0.77 \text{ kcal mol}^{-1}$$