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Supporting Material

Polarizable Atomic Multipole X-Ray Refinement: Hydration Geometry and Application to Macromolecules

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Supplemental Information

Table 1. Lysozyme (2VB1) timings for computing force field and X-ray energies.

	Time (seconds)
AMOEBA (no electrostatics)	0.2
AMOEBA (PME electrostatics)	3.6
Structure factor calculation (IAM)	160.5

Table 2. Lysozyme (2VB1) electrostatic timings using either a PME based method or using cutoffs of various sizes, and the corresponding permanent and polarization energies.

Cutoff size (Å)	Time (seconds)	Permanent (Kcal/mol)	Polarization (Kcal/mol)
NA (PME)	1.8	-5292	-1169
7.0	1.3	-2906	-1496
8.0	1.8	-6312	-1464
9.0	2.3	-4905	-1371
10.0	7.1	-5012	-1349
11.0	7.9	-5227	-1314
12.0	13.7	-4791	-1311
13.0	15.2	-4768	-1275
14.0	17.5	-4913	-1266
15.0	27.0	-6294	-1242
25.0	109.2	-5453	-1197

Figure 1: Final model of the lysozyme (PDB ID 2VB1) active site for the deposited structure **(A)** and following addition of hydrogens using either PDB2PQR **(B)** or using AMOEBA forces and the X-ray data **(C)**. Shown are the nucleophile (Asp52), general acid (Glu35) and surrounding water molecules. Water molecules without hydrogens are depicted as red crosses. Hydrogen bonds are drawn as dashed lines and electron density represents $2F_o$-F_c σ_A weighted maps contoured at 3.0 σ. Glu35 was modeled as protonated based on bonds lengths, available data and crystallization conditions.

Figure 2: Zig-zag spine of hydration in the DNA minor groove. Bases in gray are from the 3'→5' strand, while bases in black are derived from the 5'→3' strand. Shown is the AATT subsequence of the deposited structure **(A)** and after adding hydrogens using PDB2PQR **(B)** or following AMOEBA-assisted refinement with the X-ray data **(C)** with the primary and secondary layer of water forming the zig-zag pattern. Green arrows represent polarization vectors originating from the water oxygens, and a 3.0 Å vector length corresponds to 1 Debye (average vector length: 1.5 Å).

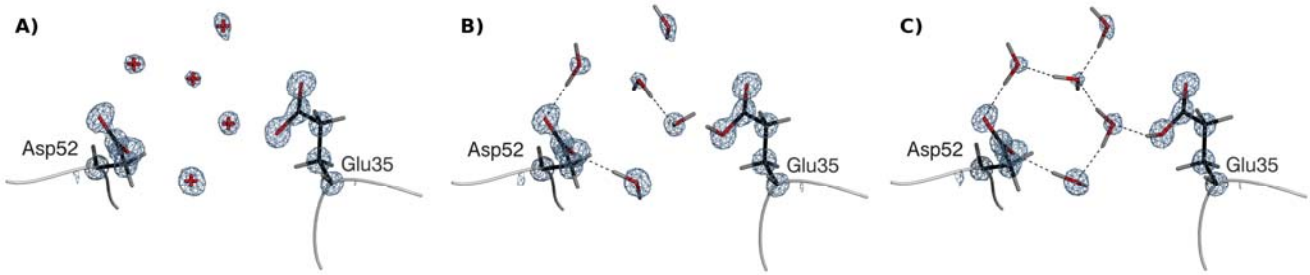

Figure 1

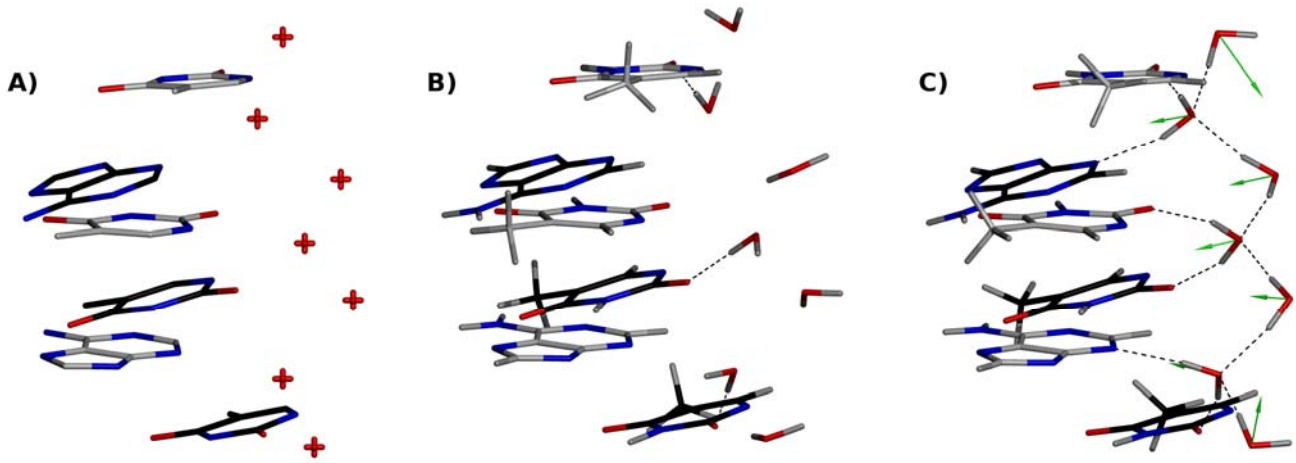

Figure 2