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Automated Ligand Refinement with a Combined Force Field and Shape Potential. S. Wlodek, A.G. Skillman, A. Nicholls, OpenEye Scientific Software, 3600 Cerrillos Rd., Santa Fe, NM 87507, USA.

An automated computational procedure for fitting a ligand into its electron density with the use of the MMFF94 force field and a Gaussian shape description has been developed. It employs a series of adiabatic optimizations of gradually increasing shape potential. Starting from a set of energy-relaxed ligand conformations, the final results are structures realistically strained to fit the crystallographic data.