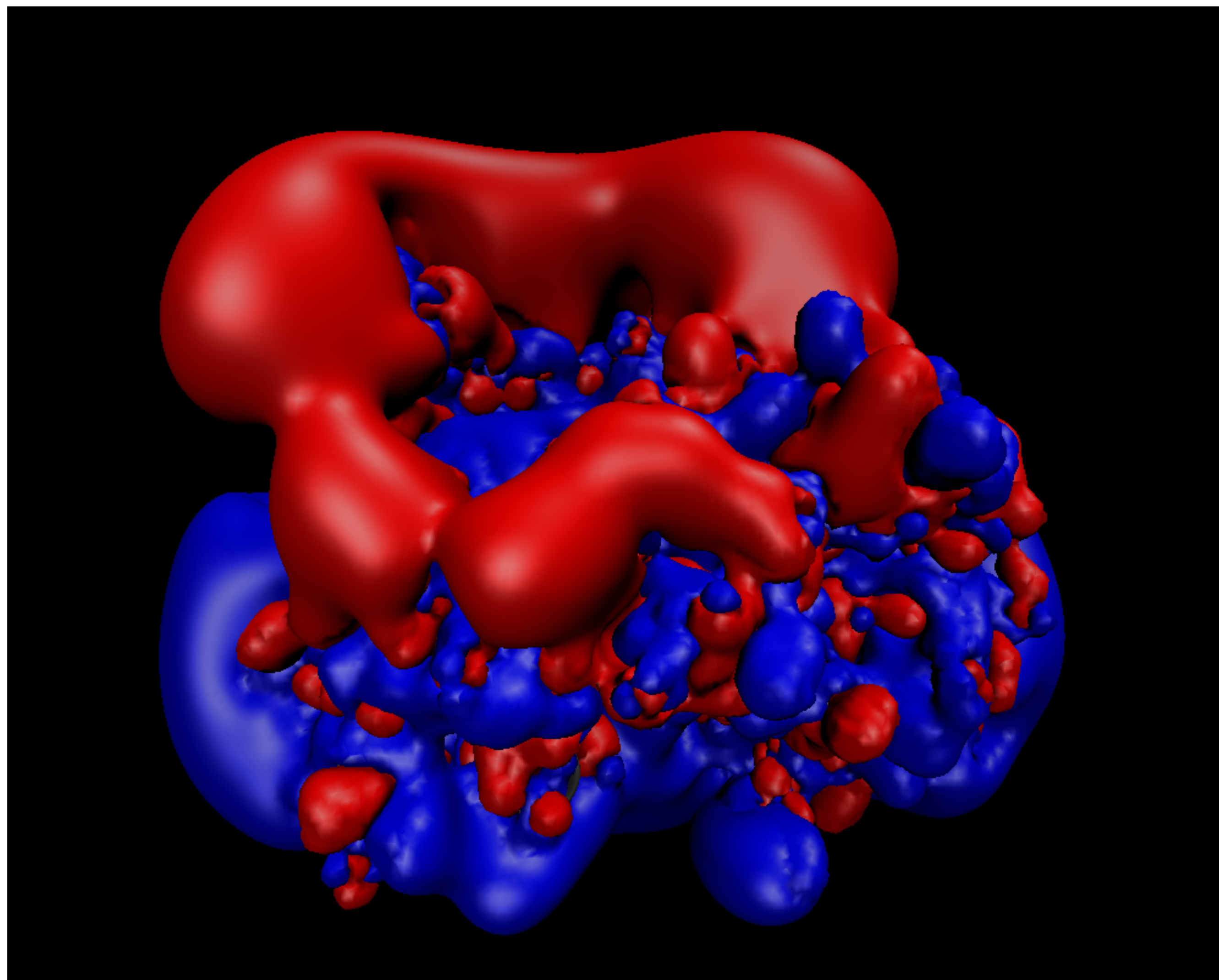


- The isosurfaces are a reasonable reproduction of Fig.1 from Garg *et al.* (2015).
- However, the charges here seem to have a larger magnitude than in the paper. This may be because of charge assignment or including the ligands in the PQR file.





- Electric field lines show the path that a massless positive charge would take. The density of lines shows the intensity of the electric field.
- There is clearly a major electrostatic sink pulling negative ligands into the active site.

