Suppl. Table 1. Contributions to the ionization energy of residue C24 at pH 7.

| Terms | t=10ns | t=142.5ns |
|---|---|---|
| ebkb | -6.18 | -2.62 |
| dsol | 4.96 | 1.84 |
| pH&pK0 | 2.86 | 2.86 |
| -TS | 0.21 | 0.63 |
| residues | -1.64 | -0.69 |
| TOTAL | 0.26 | 2.06 |
| LYS 13 | -0.63 | -0.67 |
| ASP 17 | | 0.22 |
| SER 27 | -1.52 | |
| GLN 28 | 0.21 | |
| ARG 29 | -0.50 | -0.24 |
| GLU 63 | 0.27 | 0.21 |
| ASP 76 | 0.26 | |
| LYS 183 | -0.35 | -0.35 |
| TYR 233 | | -0.43 |
| GLU 228 | 0.32 | 0.26 |

Breakdown of energy terms that influence the free energy of ionization of the residue C24 thiol at pH 7. Values are in kcal/M, only terms greater than 0.2 kcal/M are shown. Negative values favour ionization. "ebkb" is the electrostatic interaction of the side chain to the backbone. "dsolv" is the loss of solvation energy. "pH&pK0" is the pH effect, which equals solution pH minus solution pKa of the residue if the residue is an acid. "-TS" is entropy effect. "residues" refers to the mean field interaction with residues at this pH. The bottom section of the table gives the breakdown of the residue contributions. Columns of values refer to analysis of two frames from the apo1 simulation at the indicated time points.