

3D Interaction Homology: Computational Titration of Aspartic Acid, Glutamic Acid and Histidine Residues Can Create pH-Tunable Hydrophobic Environment Maps

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Figure S20. Hydrophathic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 300^\circ$ parse of the **f6** chess square at pH = 3.345.

Figure S21: Character interaction chart for the GLU **b1.300.180** parse at pH 4.224.

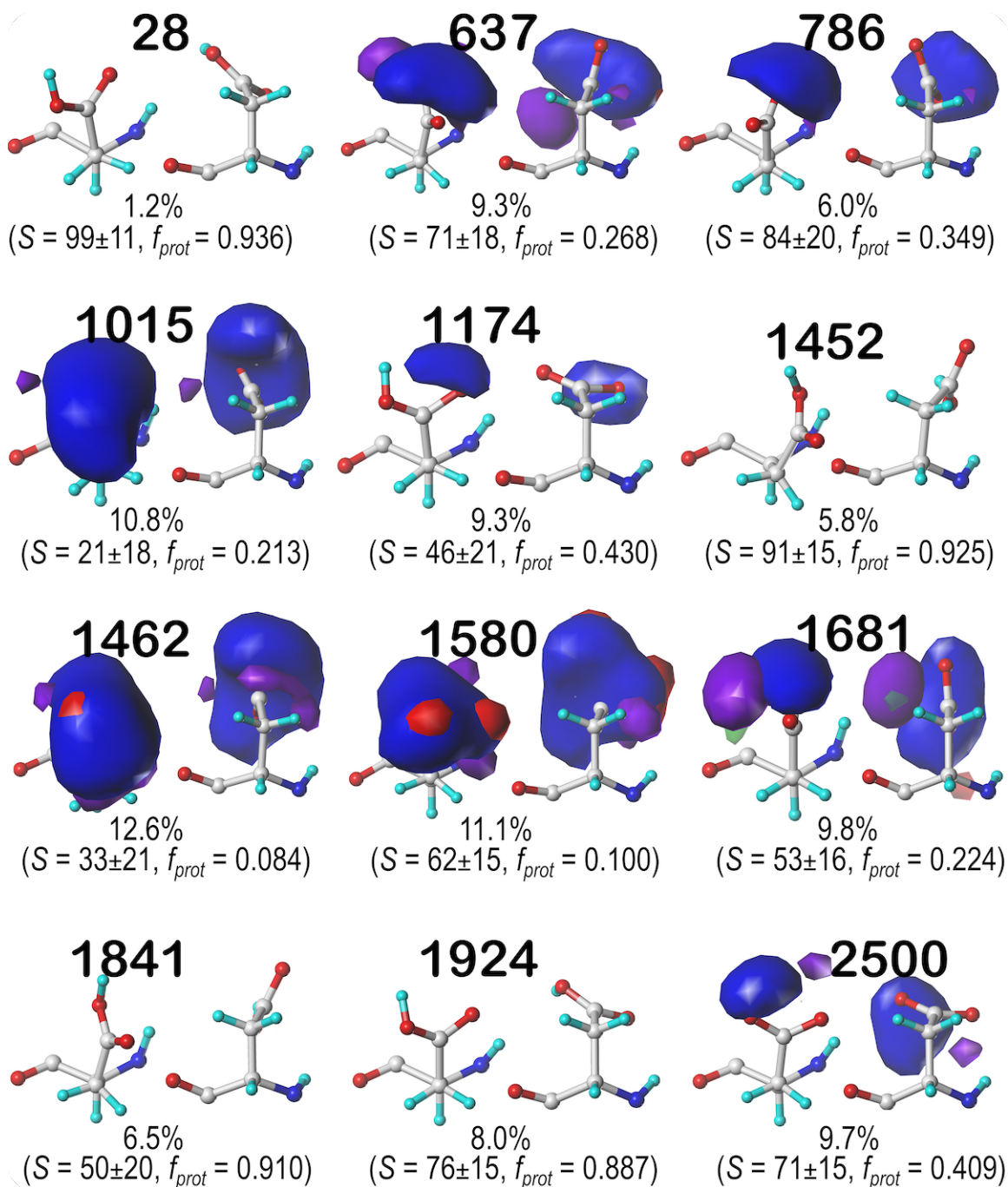


Figure S1: Hydrophathic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 60^\circ$ parse of the c5 chess square at pH = 3.345. Two map viewpoints are given for each cluster, whose ID is given in bold. The left map in each pair is oriented such that the CA-CB z-axis bond points upward, while the right is oriented to point it out of the page. The x-axis is oriented horizontally in both. The percentage indicates the fraction of the parse represented by that cluster. S represents the solvent accessible surface area in Å², and f_{prot} indicates the fraction of the cluster protonated at pH₅₀. Blue contours indicate positive polar interactions made with the sidechain, and red indicates negative polar interactions, while green and purple indicate positive and negative hydrophobic interactions, respectively.

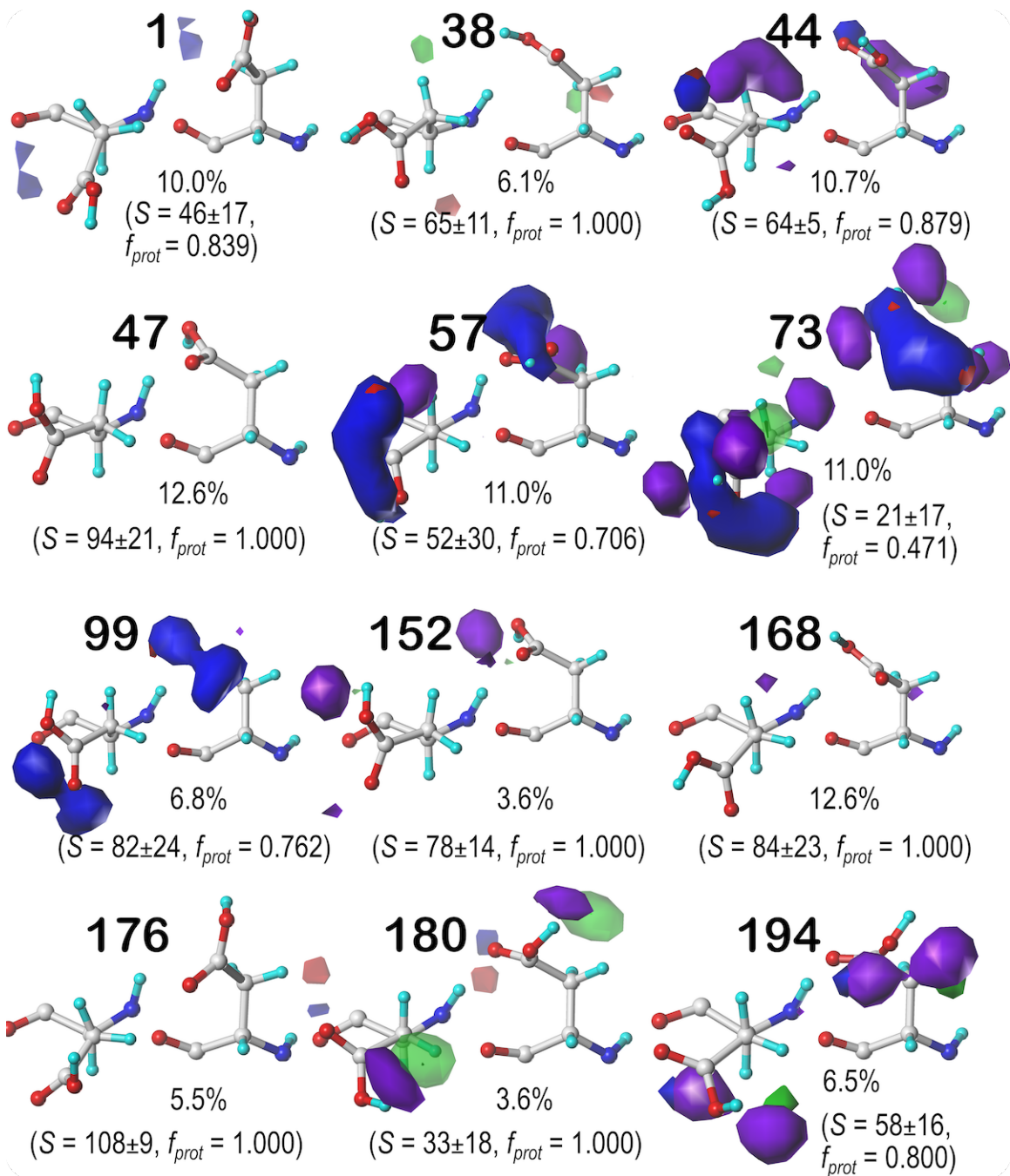


Figure S2: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 180^\circ$ parse of the c5 chess square at pH = 3.345. See caption for Figure S1.

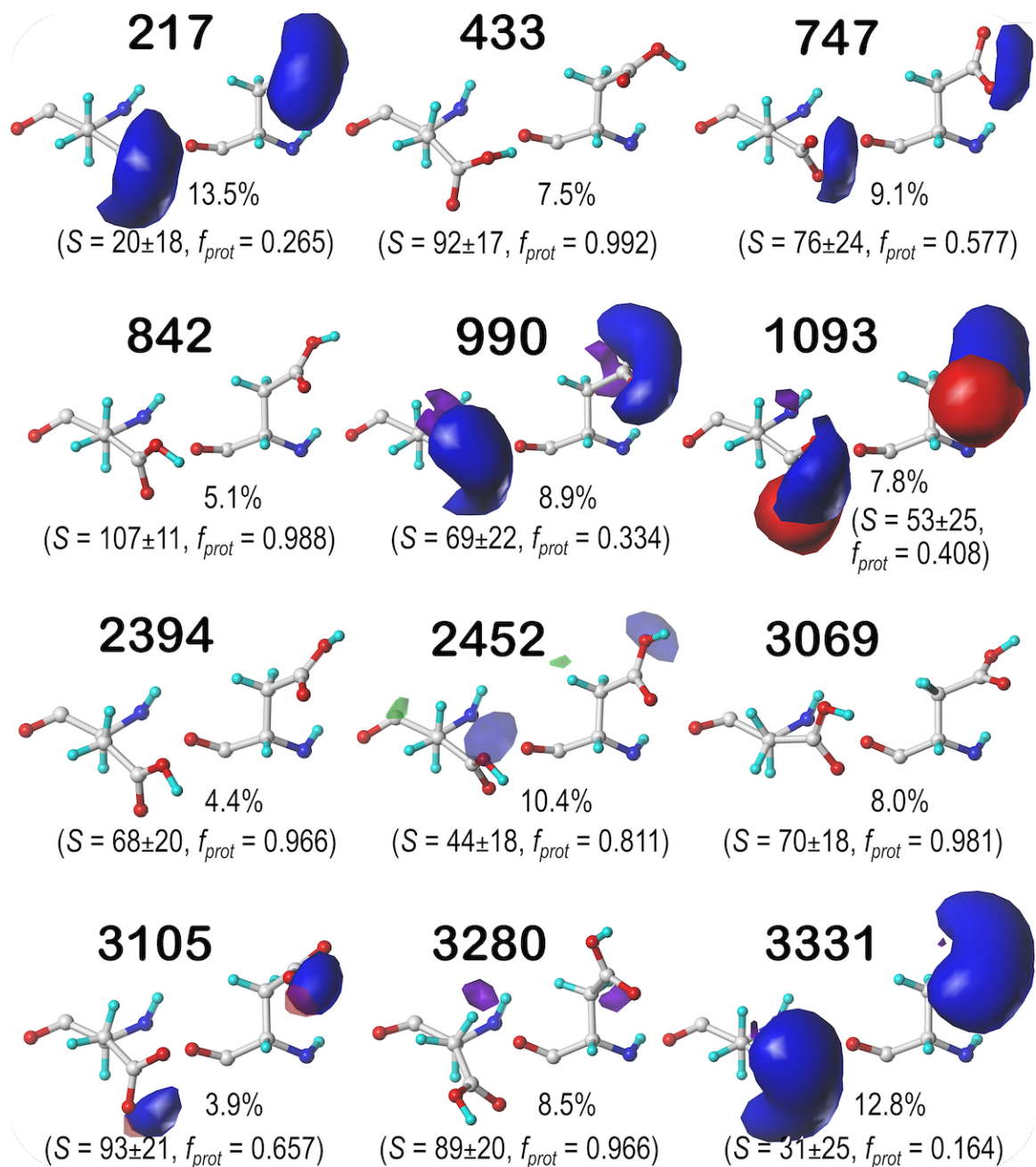


Figure S3: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 300^\circ$ parse of the c5 chess square at pH = 3.345. See caption for Figure S1.

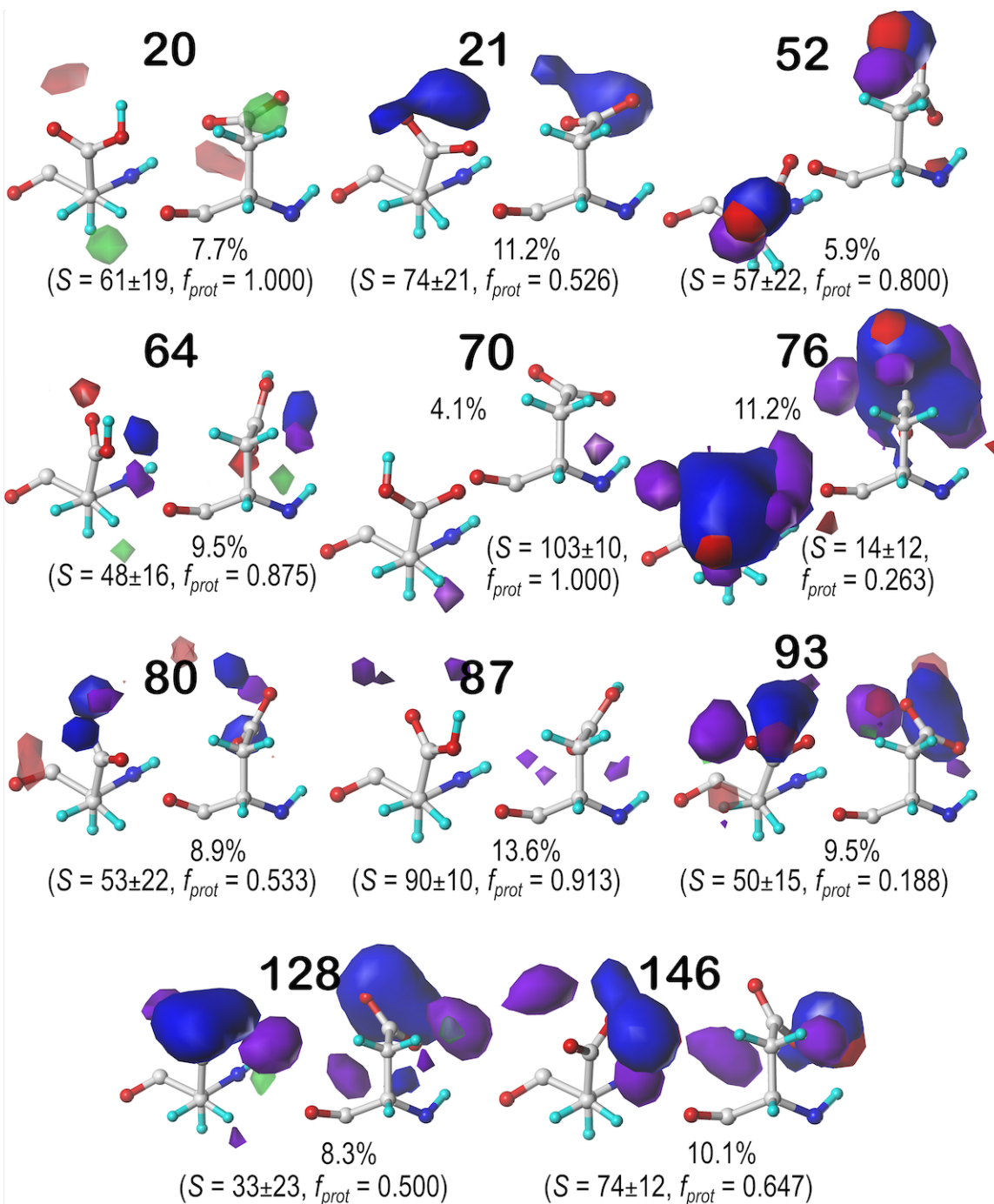


Figure S4: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 60^\circ$ parse of the $d5$ chess square at pH = 3.345. See caption for Figure S1.

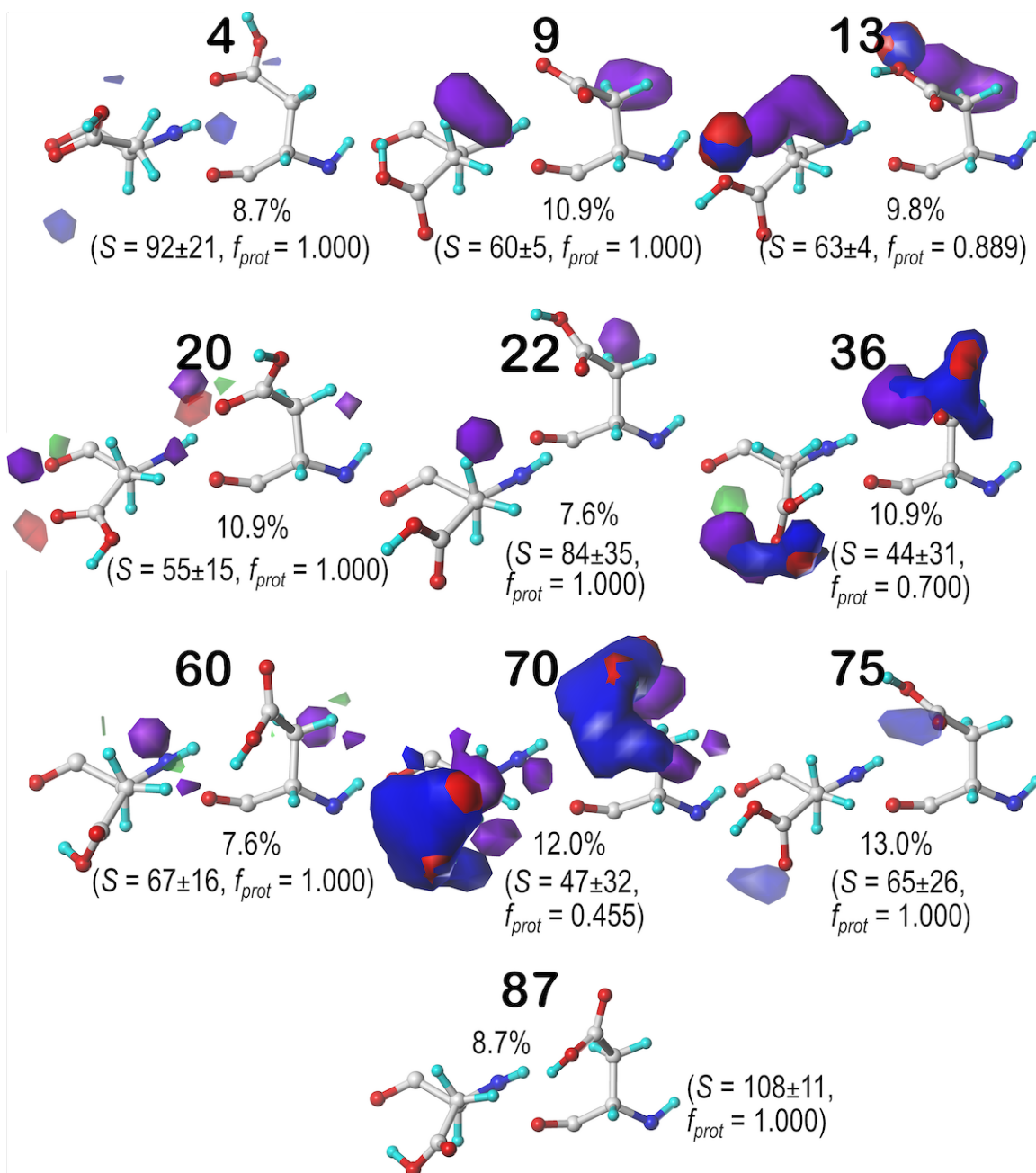


Figure S5: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 180^\circ$ parse of the *d5* chess square at pH = 3.345. See caption for Figure S1.

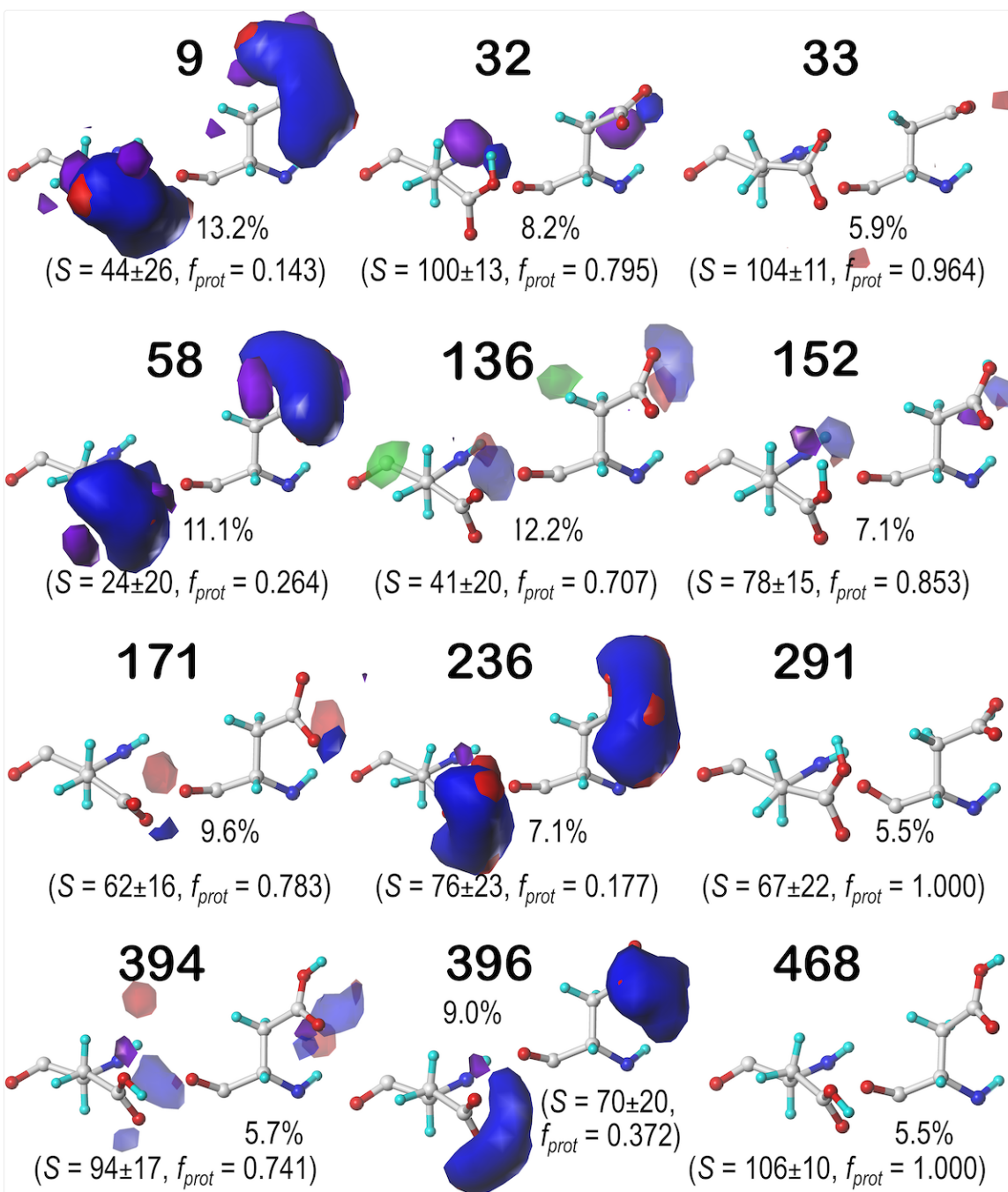


Figure S6: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 300^\circ$ parse of the *d5* chess square at pH = 3.345. See caption for Figure S1.

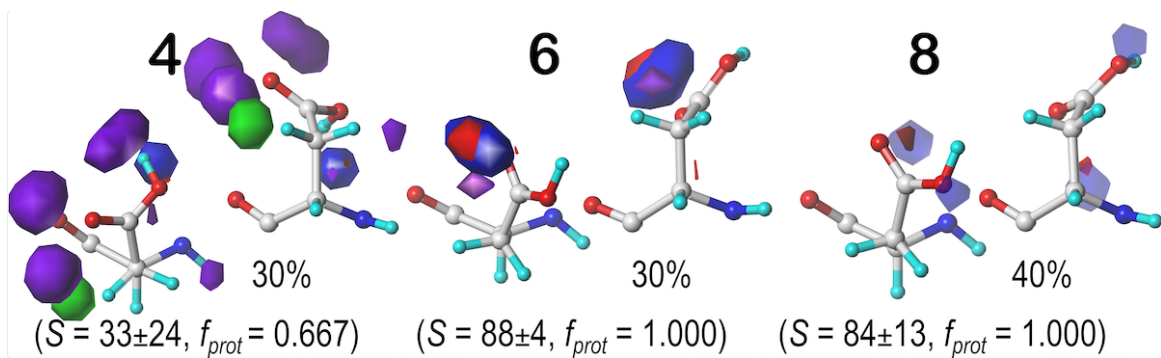


Figure S7: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 60^\circ$ parse of the *f6* chess square at pH = 3.345. See caption for Figure S1.

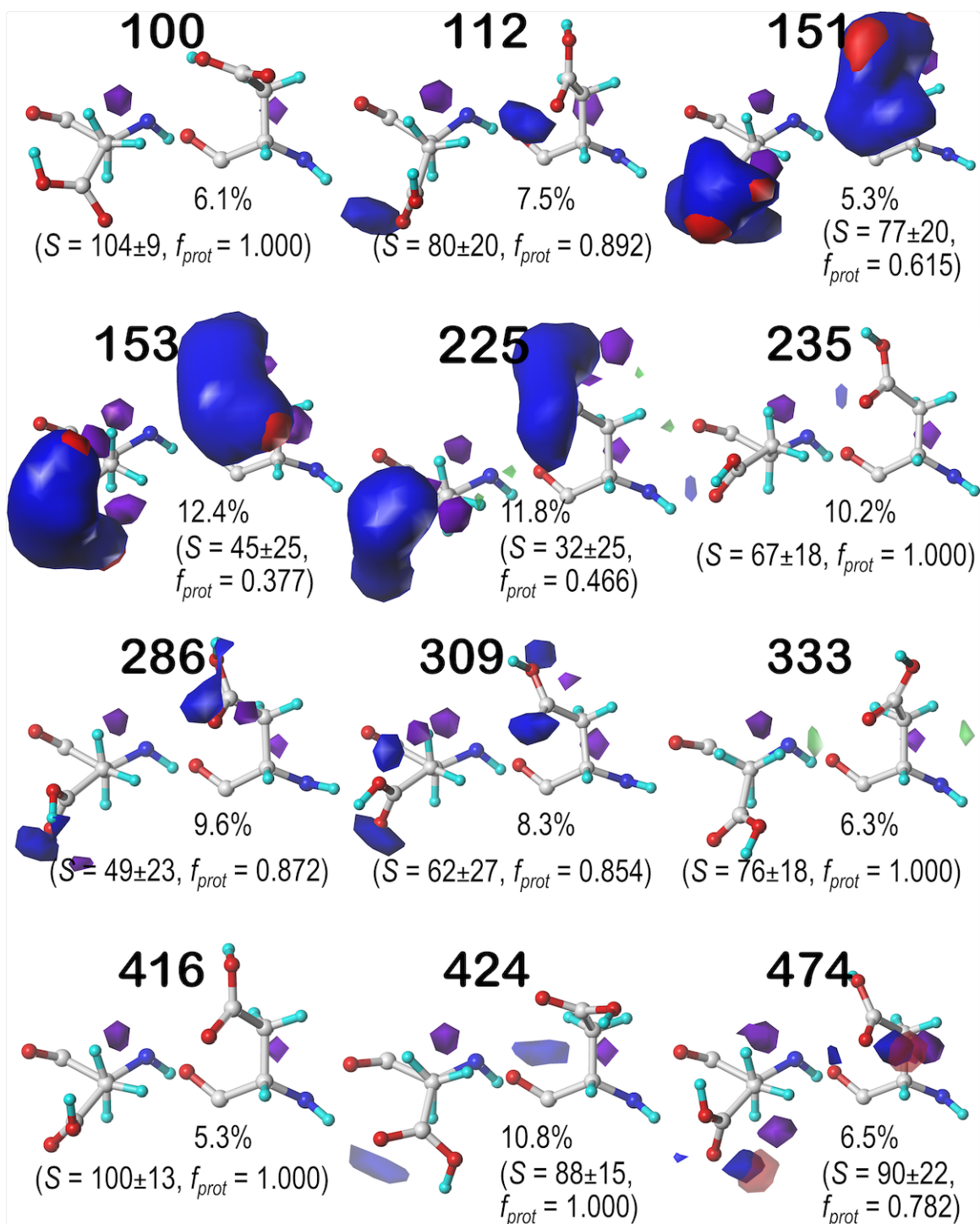


Figure S8: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 180^\circ$ parse of the *f6* chess square at pH = 3.345. See caption for Figure S1.

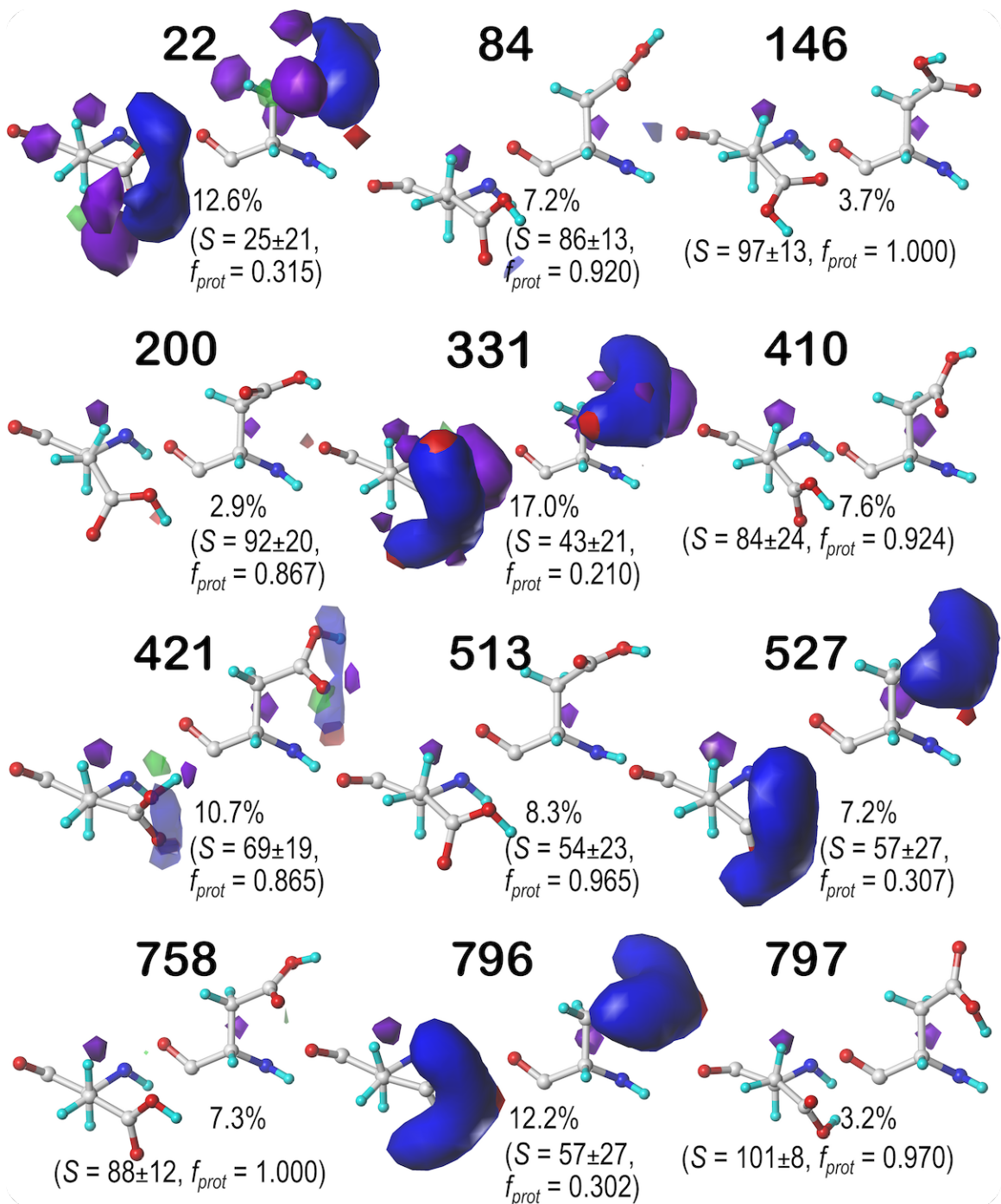


Figure S9: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of aspartic acid in the $\chi_1 = 300^\circ$ parse of the *f6* chess square at pH = 3.345. See caption for Figure S1.

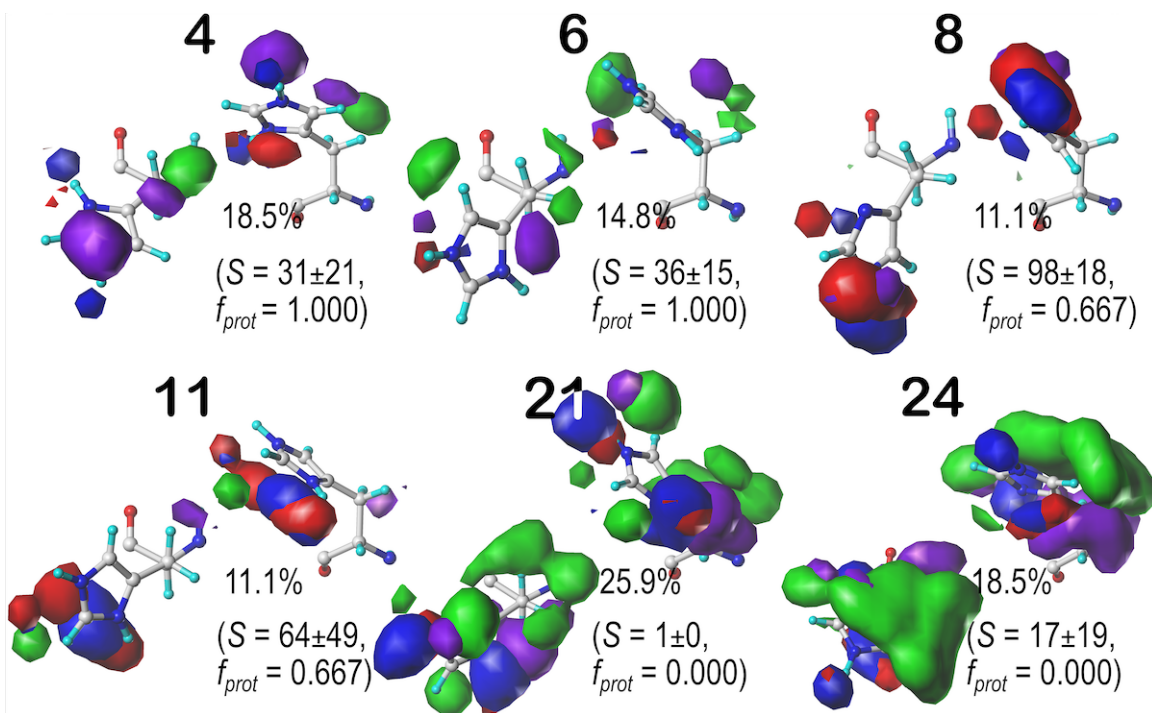


Figure S10: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 180^\circ$ parse of the *b1* chess square at pH = 5.174. See caption for Figure S1.

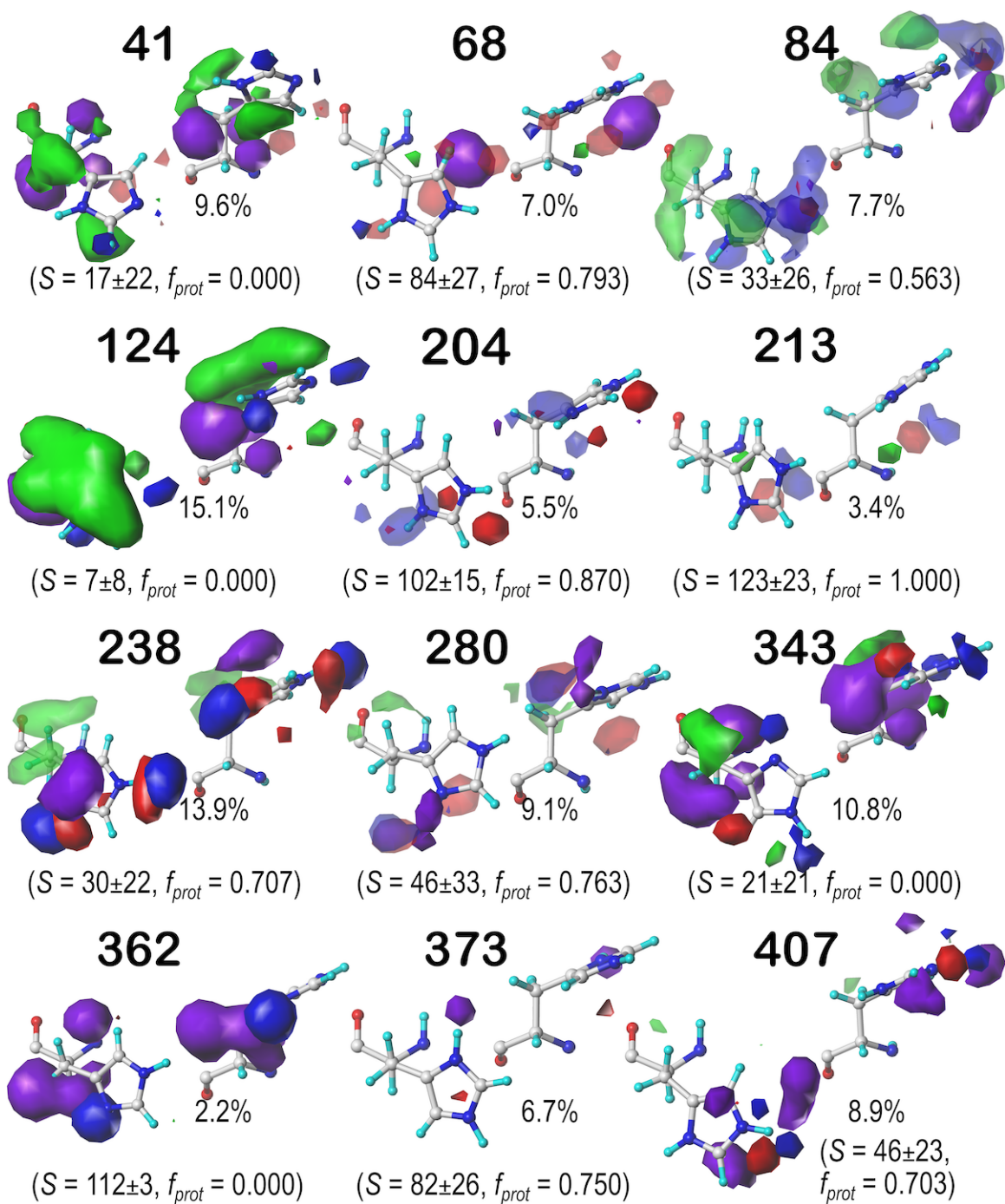


Figure S11: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 300^\circ$ parse of the *b1* chess square at pH = 5.174. See caption for Figure S1.

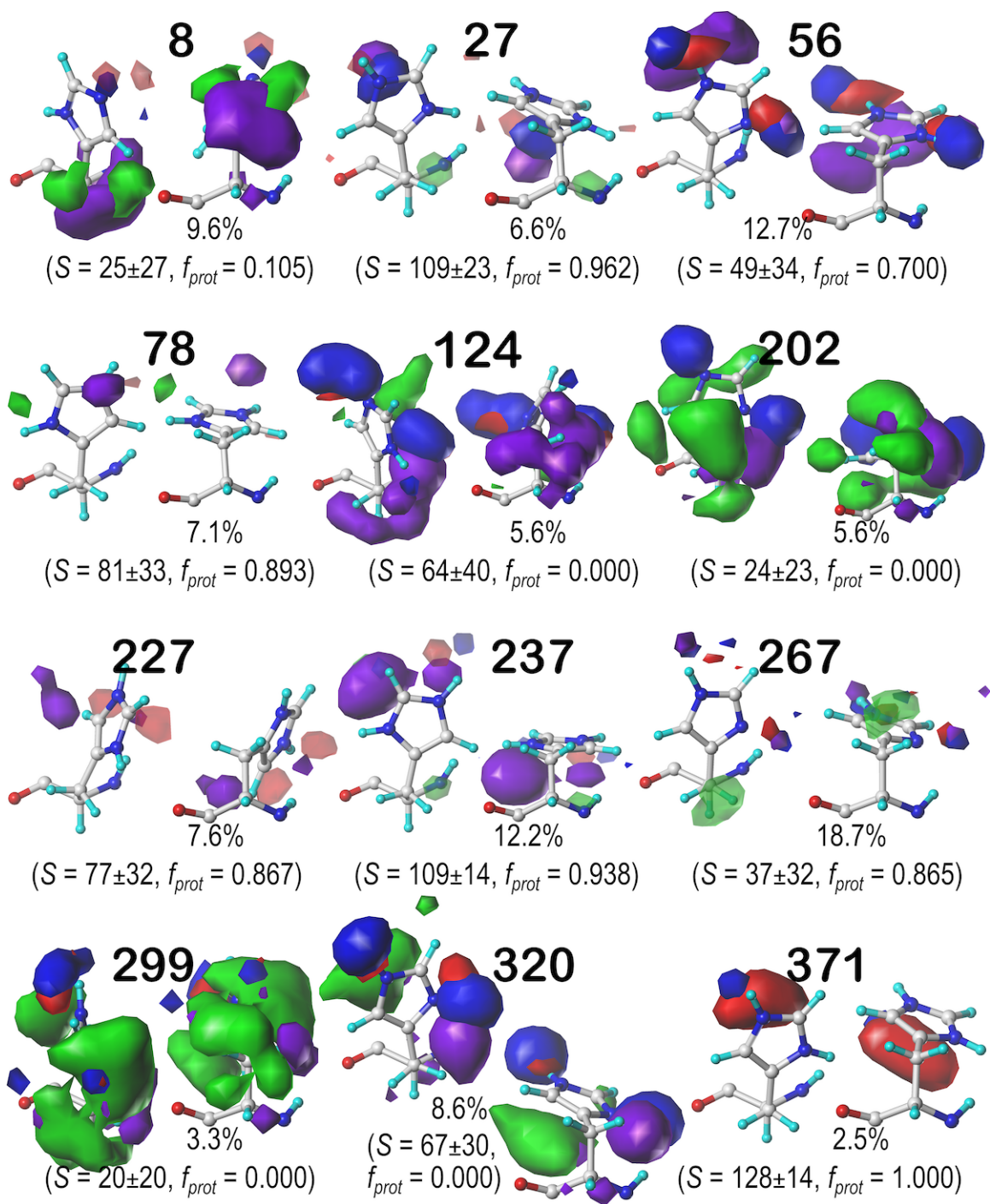


Figure S12: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 60^\circ$ parse of the c5 chess square at pH = 5.174. See caption for Figure S1.

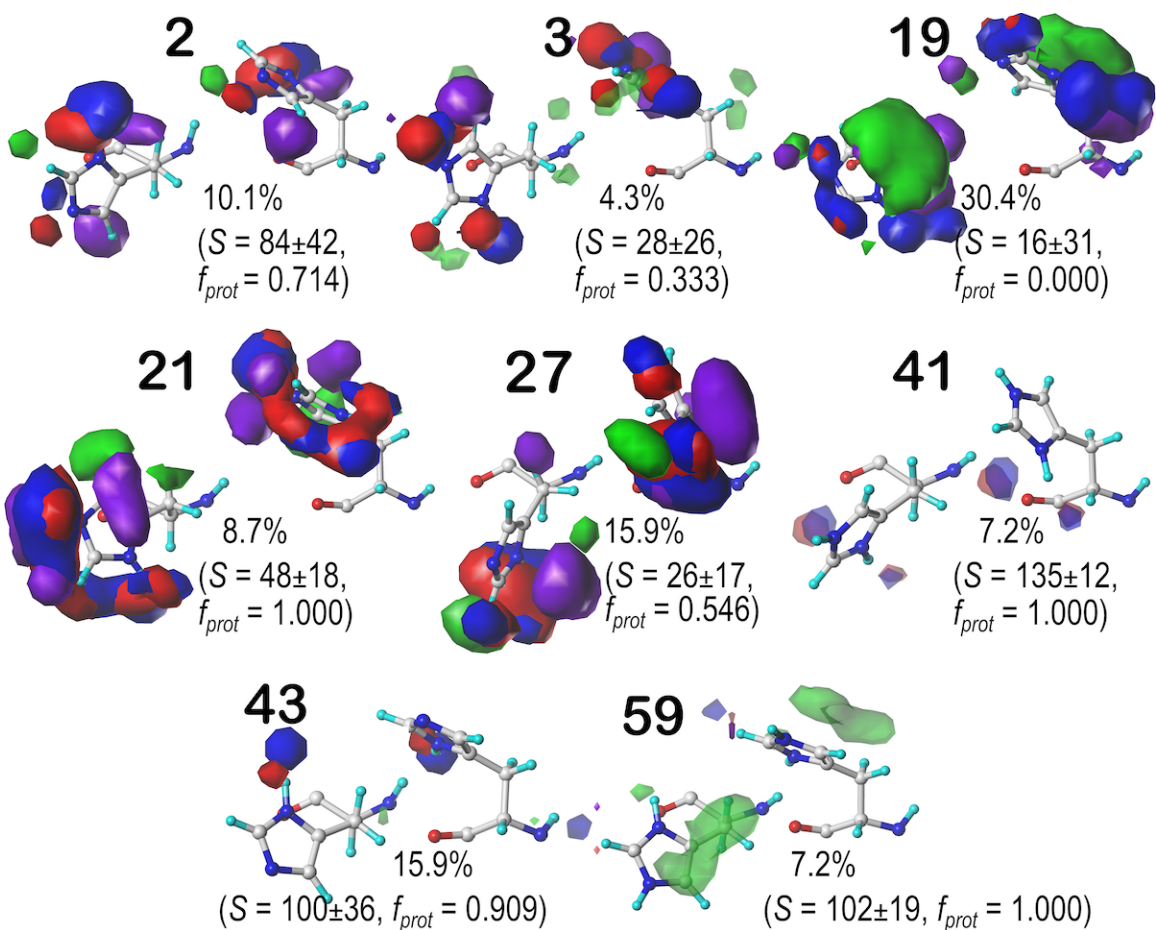


Figure S13: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 180^\circ$ parse of the c5 chess square at pH = 5.174. See caption for Figure S1.

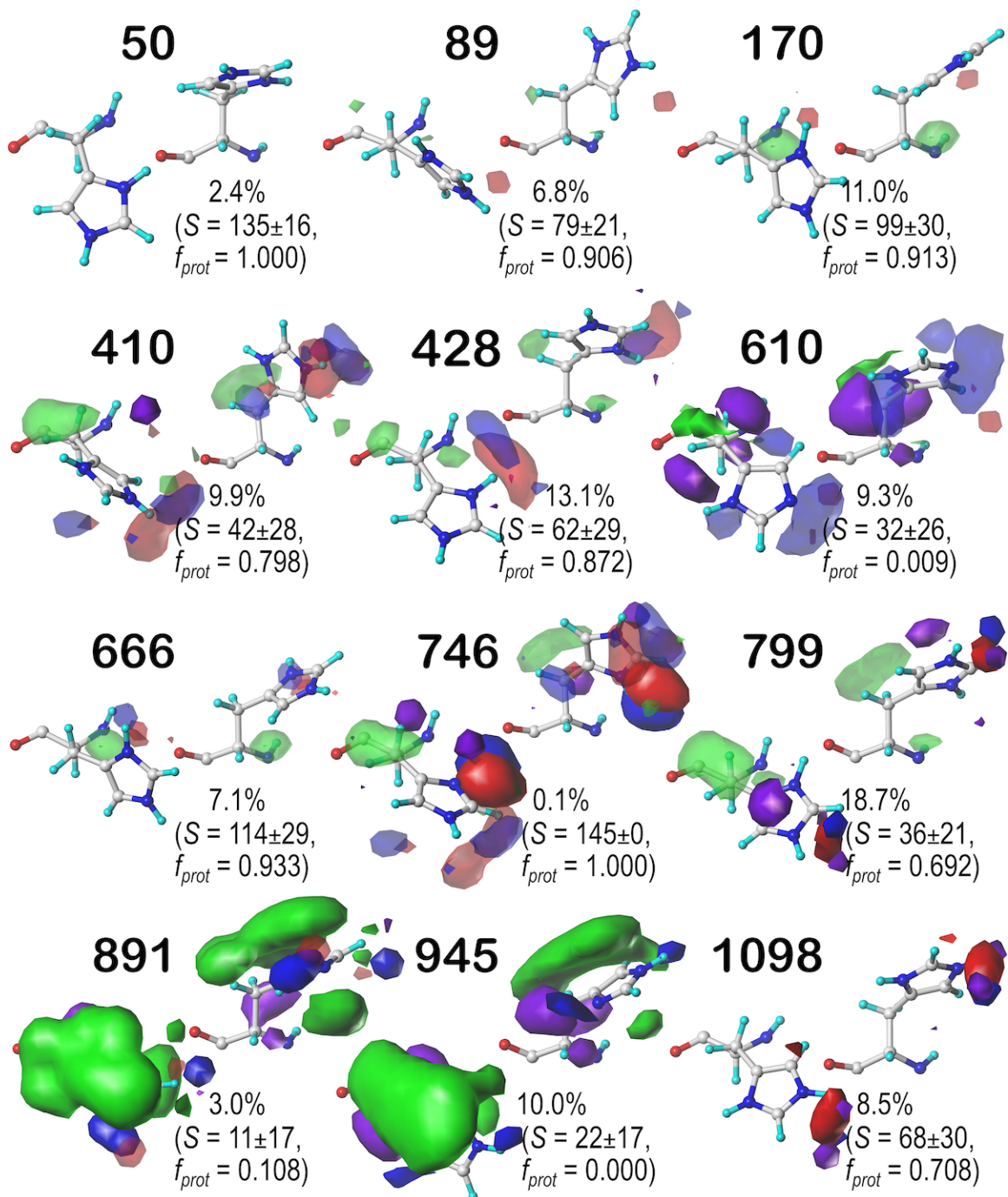


Figure S14: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 300^\circ$ parse of the *c5* chess square at pH = 5.174. See caption for Figure S1.

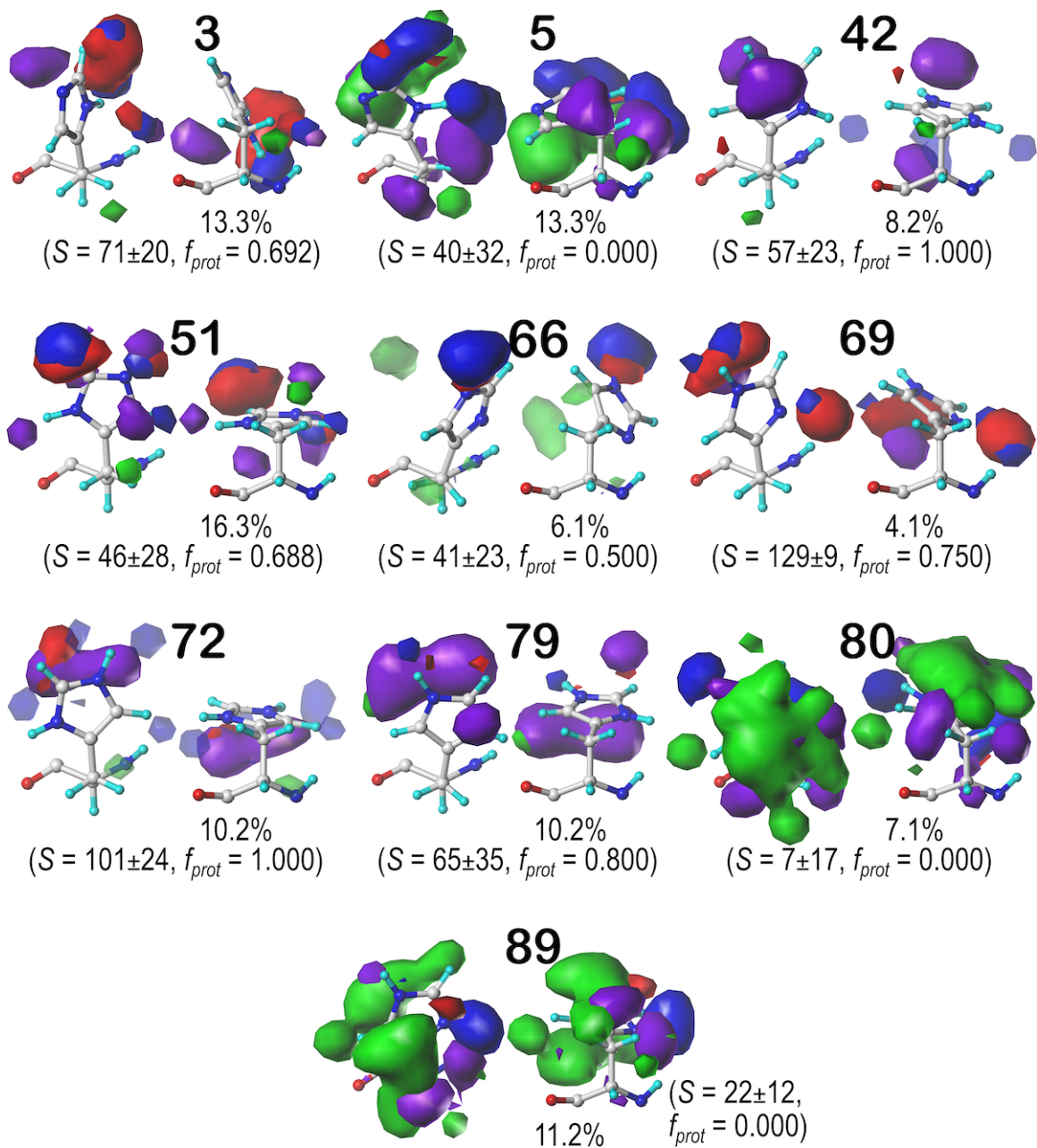


Figure S15: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 60^\circ$ parse of the *d5* chess square at pH = 5.174. See caption for Figure S1.

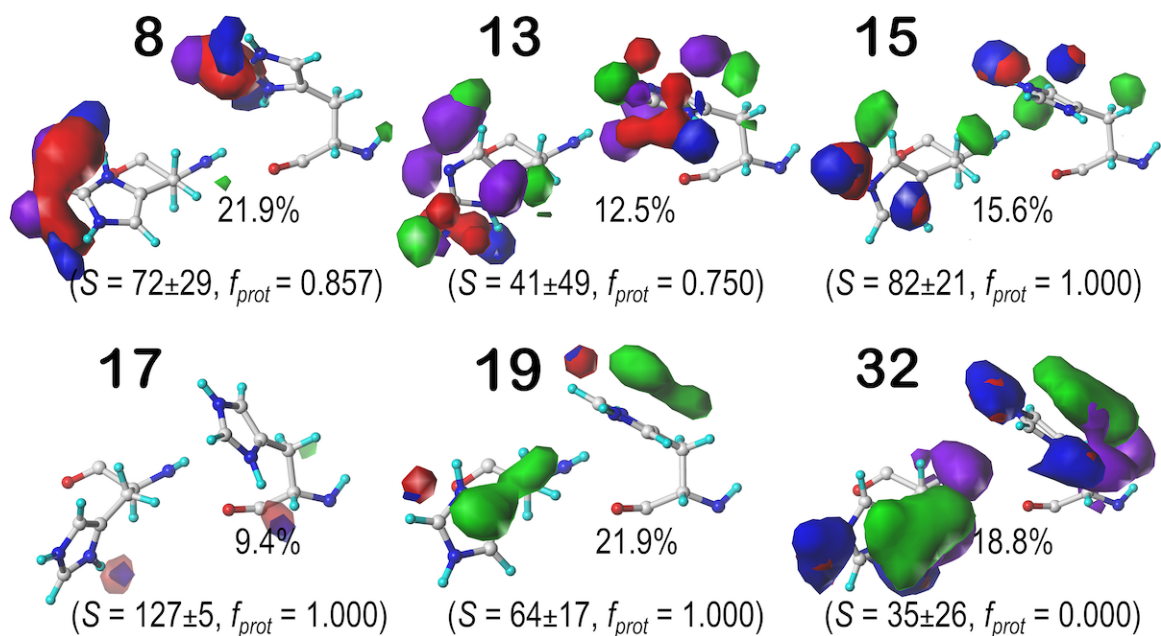


Figure S16: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 180^\circ$ parse of the *d5* chess square at pH = 5.174. See caption for Figure S1.

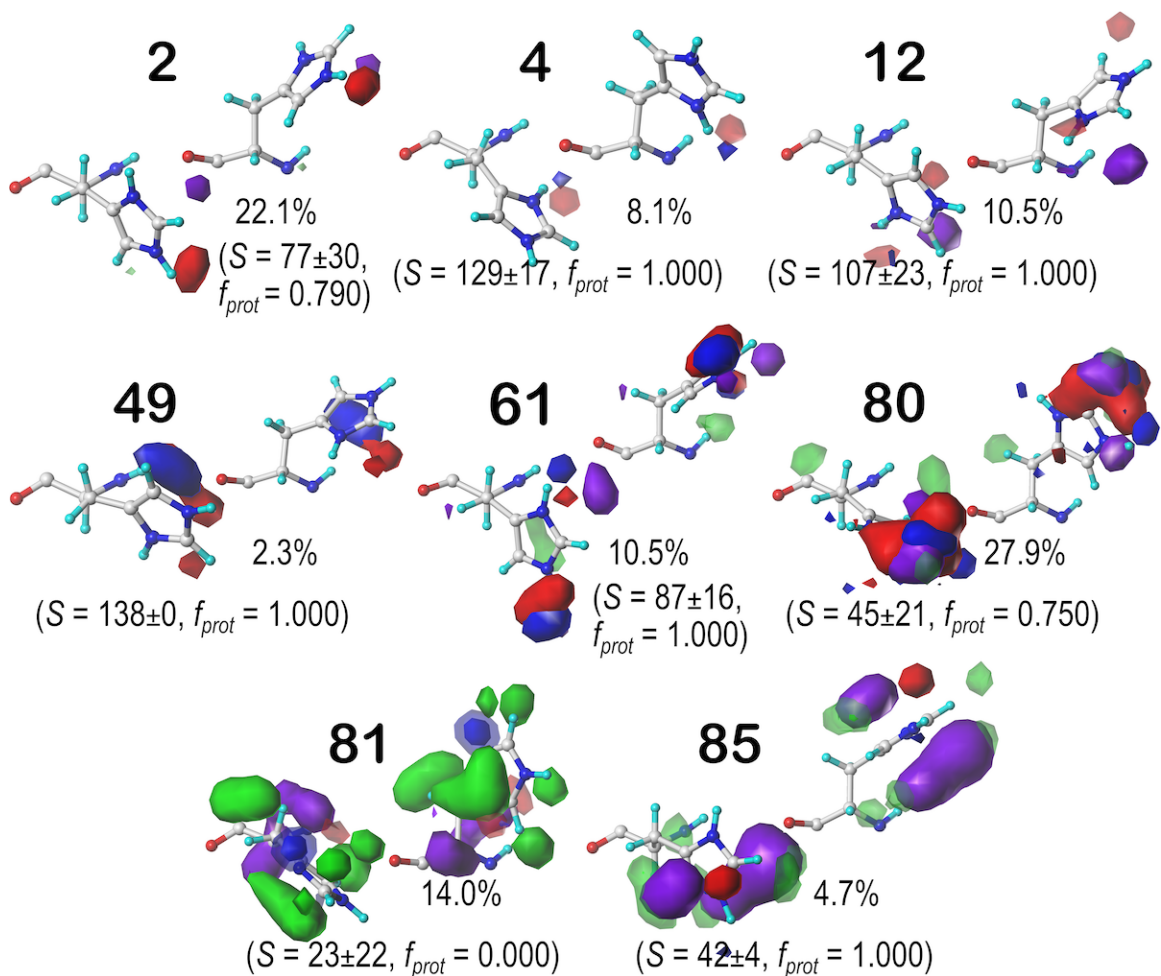


Figure S17: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 300^\circ$ parse of the *d5* chess square at pH = 5.174. See caption for Figure S1.

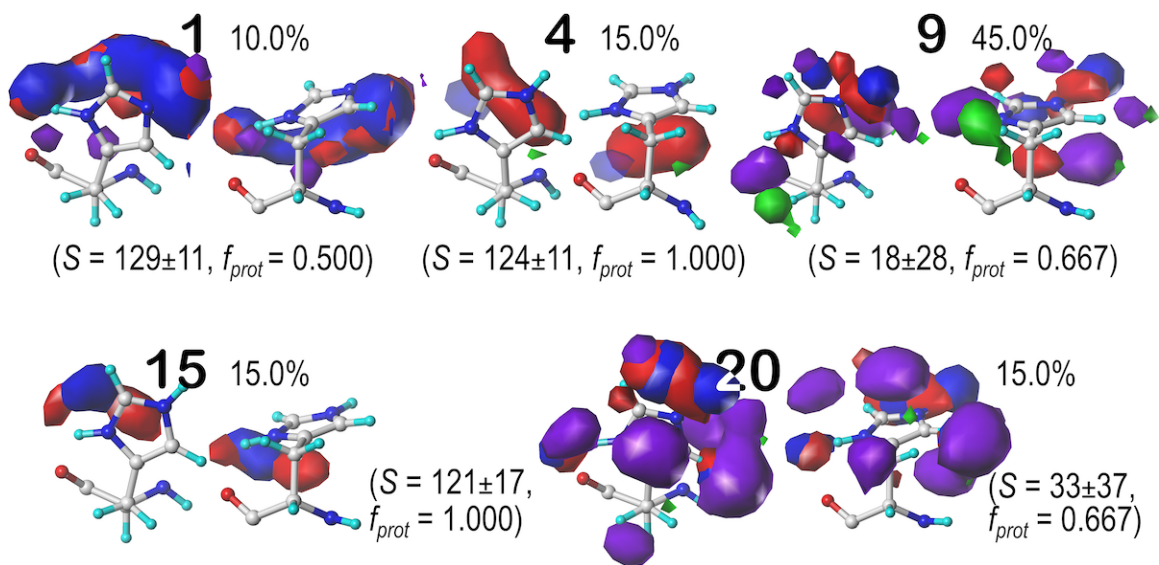


Figure S18: Hydropathic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 60^\circ$ parse of the *f6* chess square at pH = 5.174. See caption for Figure S1.

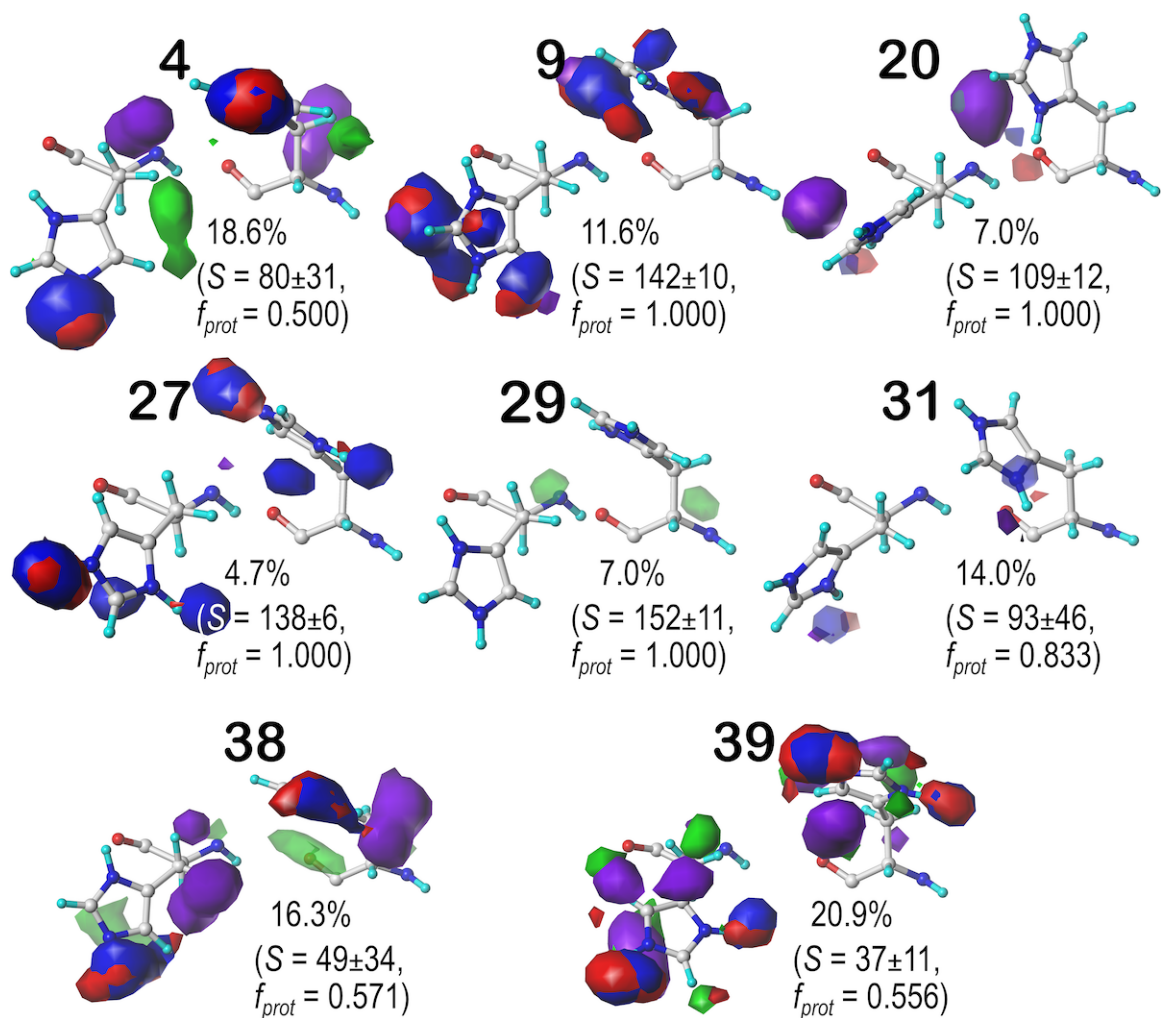


Figure S19: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 180^\circ$ parse of the *f6* chess square at pH = 5.174. See caption for Figure S1.

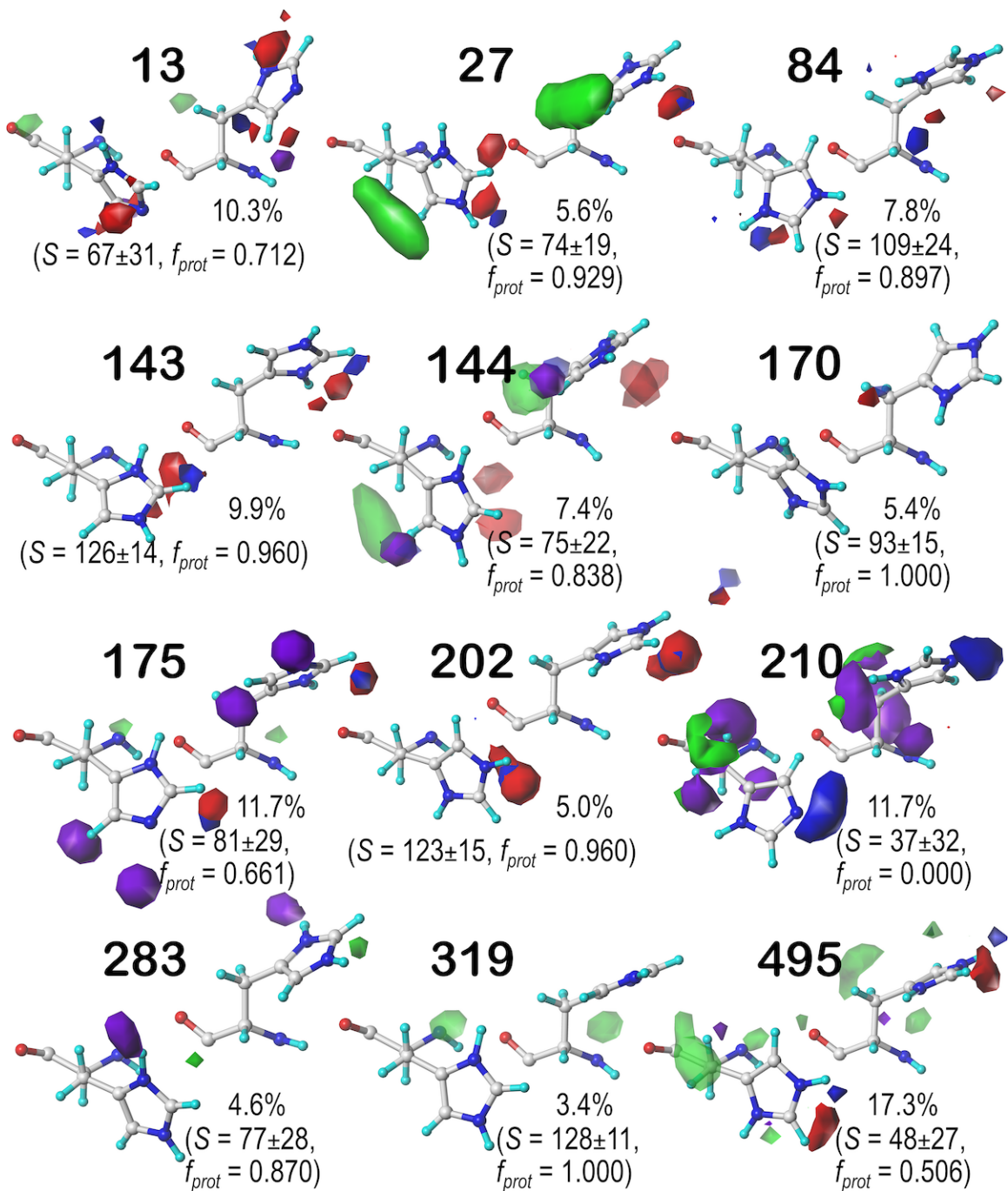


Figure S20: Hydrophobic interaction maps displaying the Gaussian-weighted average sidechain environments of histidine in the $\chi_1 = 300^\circ$ parse of the *f6* chess square at pH = 5.174. See caption for Figure S1.

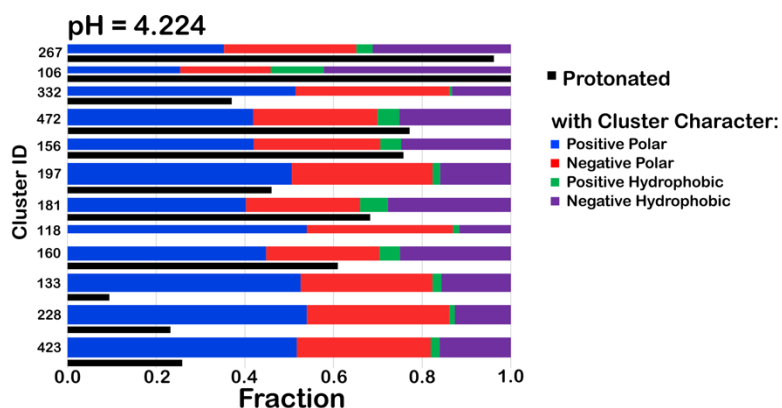


Figure S21: Character interaction chart for the GLU *b1.300.180* parse at pH 4.224. The fraction of each interaction type is given on the x-axis, for each cluster ID on the y-axis. The bars are arranged such that, descending, clusters have smaller SASAs. The thickness of the bars indicates residue population contained within that cluster. The black bars indicate f_{prot} , the fraction of the residues in the cluster protonated.