Supplemental Material for

Albumin (BSA) adsorption onto graphite stepped surfaces

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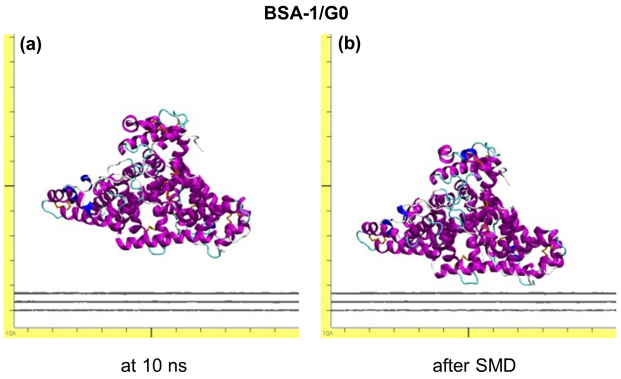

Figure S1. Snapshots of the configuration of the BSA-1 adsorption on the G0 substrate. The left image shows the configuration after 10 ns of the MD simulation. The right image shows the configuration after applying the SMD procedure to promote the approach of the BSA molecule towards the flat surface. The protein structure is not perturbed after carrying out this procedure.

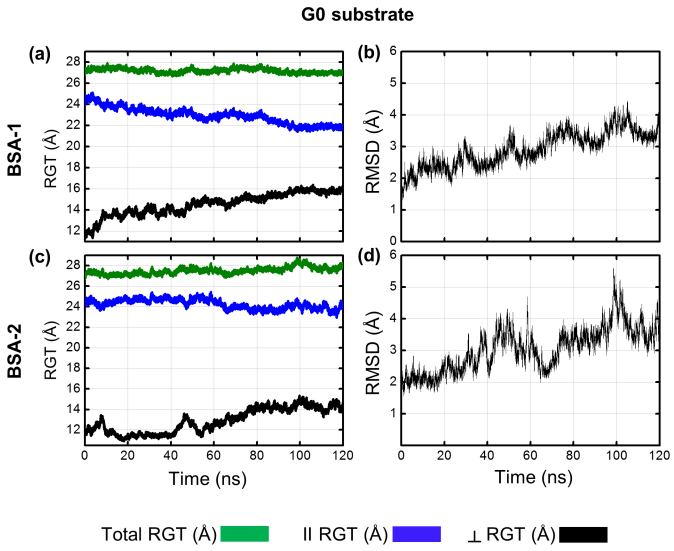

Figure S2. Time evolution of: (a) the parallel and perpendicular components of the radius of gyration tensor (RGT) for the BSA-1/G0 system, (b) the root-mean-square-distance (RMSD) of the α-carbon atoms for the BSA-1/G0 system, (c) RGT measurements of BSA-2/G0, and (d) RMSD measurements of BSA-2/G0.

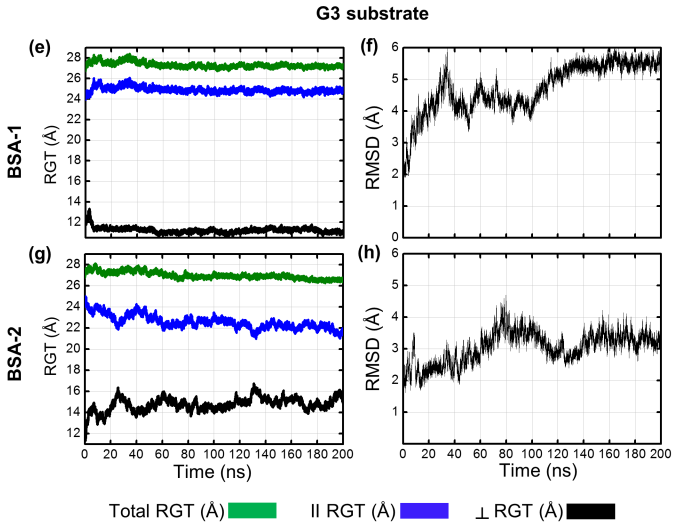

Figure S3. Time evolution of: (a) the parallel and perpendicular components of the radius of gyration tensor (RGT) for the BSA-1/G3 system, (b) the root-mean-square-distance (RMSD) of the α-carbon atoms for the BSA 1/G3 system, (c) RGT measurements of BSA-2/G3, and (d) RMSD measurements of BSA-2/G3.

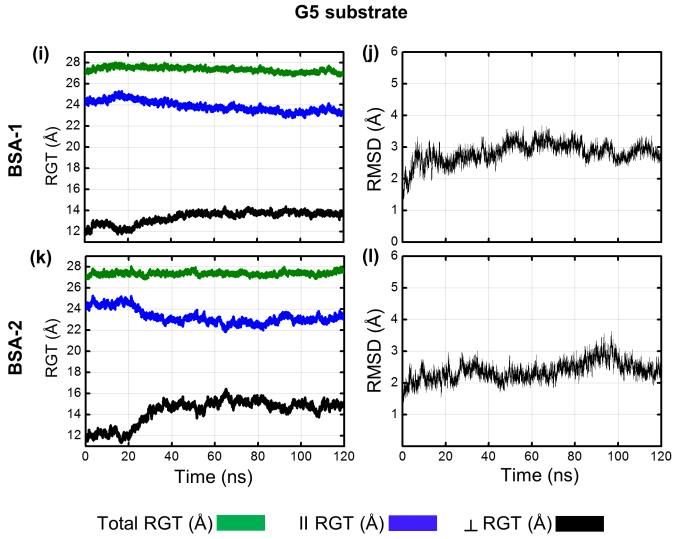

Figure S4. Time evolution of: (a) the parallel and perpendicular components of the radius of gyration tensor (RGT) for the BSA-1/G5 system, (b) the root-mean-square-distance (RMSD) of the α-carbon atoms for the BSA 1/G5 system, (c) RGT measurements of BSA-2/G5, and (d) RMSD measurements of BSA-2/G5.

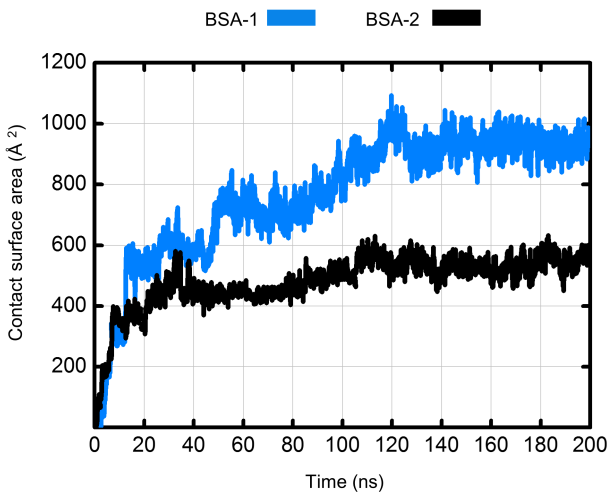

Figure S5. Time evolution of the contact surface area (CSA) in Å^2 for protein adsorbed in orientation BSA-1 (blue) and BSA-2 (black) on the G3 substrate with a step height of three graphene layers.

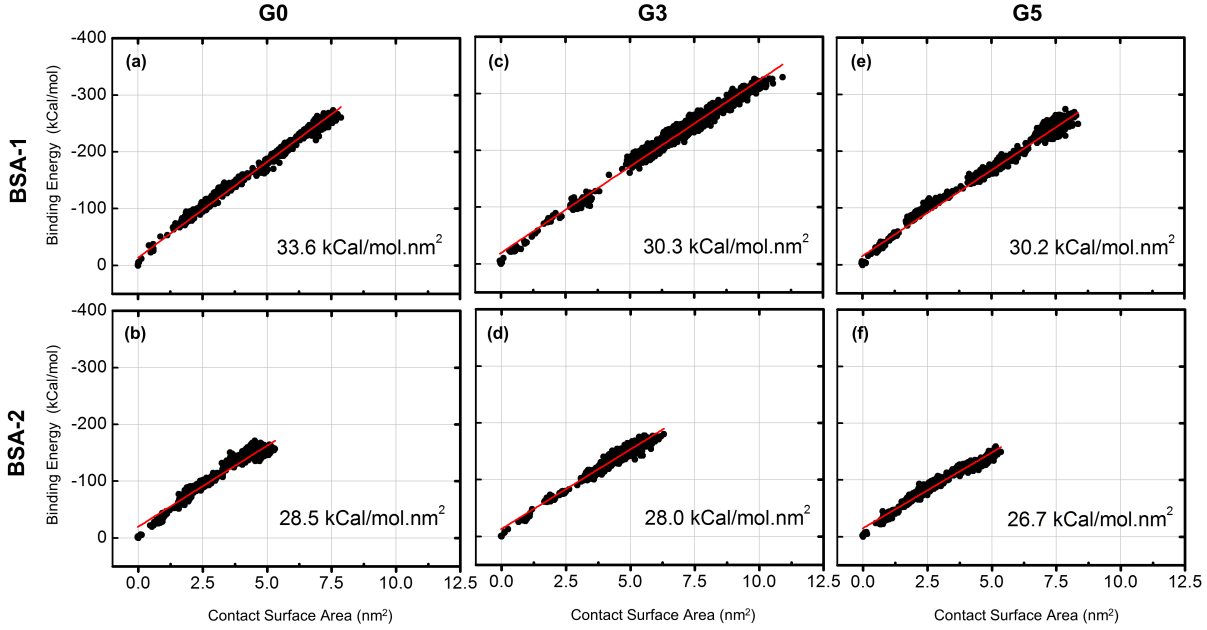

Figure S6. Correlation between the binding energy (kcal/mol) and the contact surface area (CSA) in nm^2 for the protein adsorbed in orientations BSA-1 and BSA-2. The G0, G3 and G5 graphite substrates were considered.

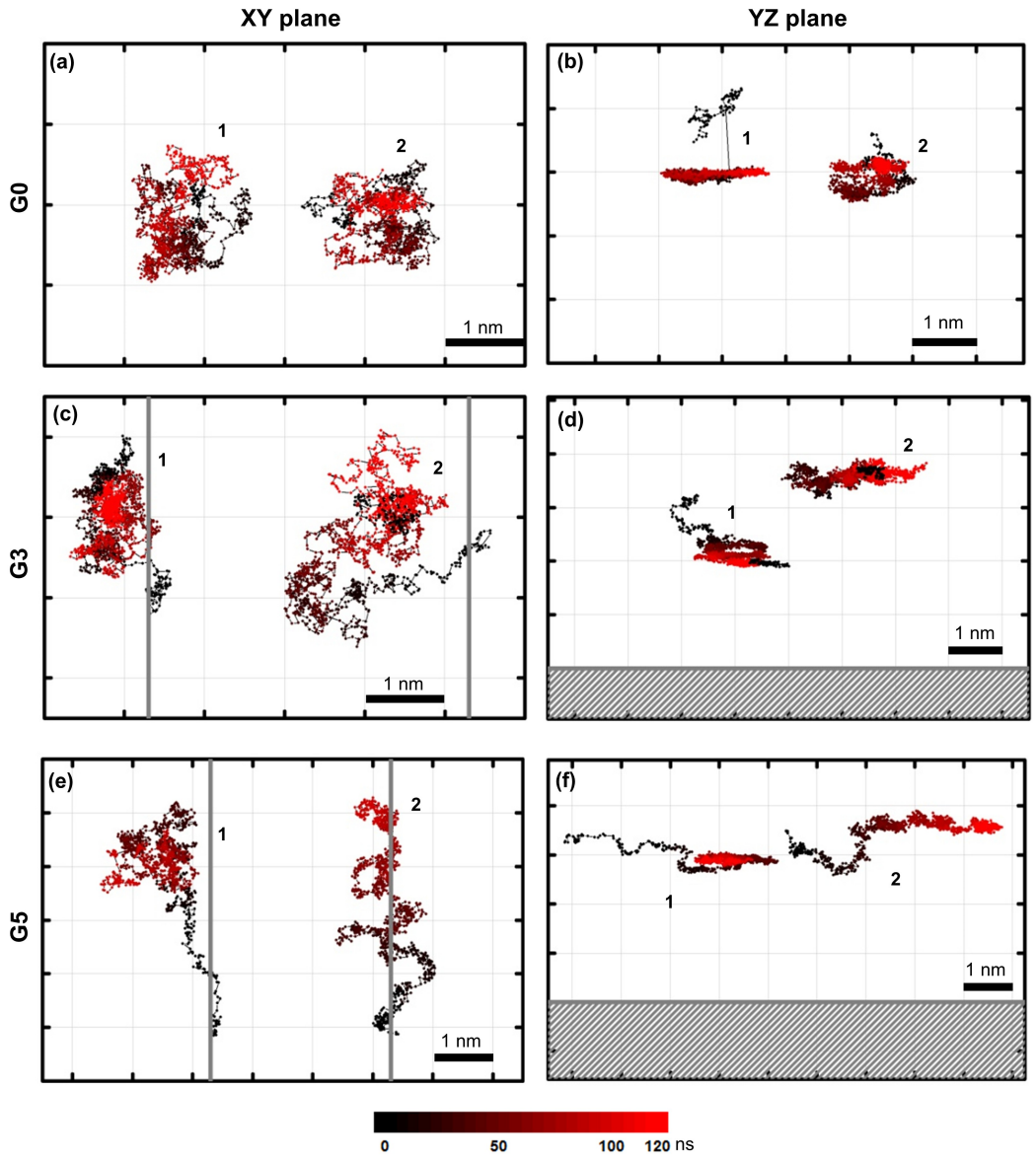

Figure S7. Trajectories of the center of mass (CM) for the BSA protein in orientations BSA-1 and BSA-2 on the G0, G3 and G5 graphite substrates for the complete (120 ns) molecular dynamics (MD) simulations.

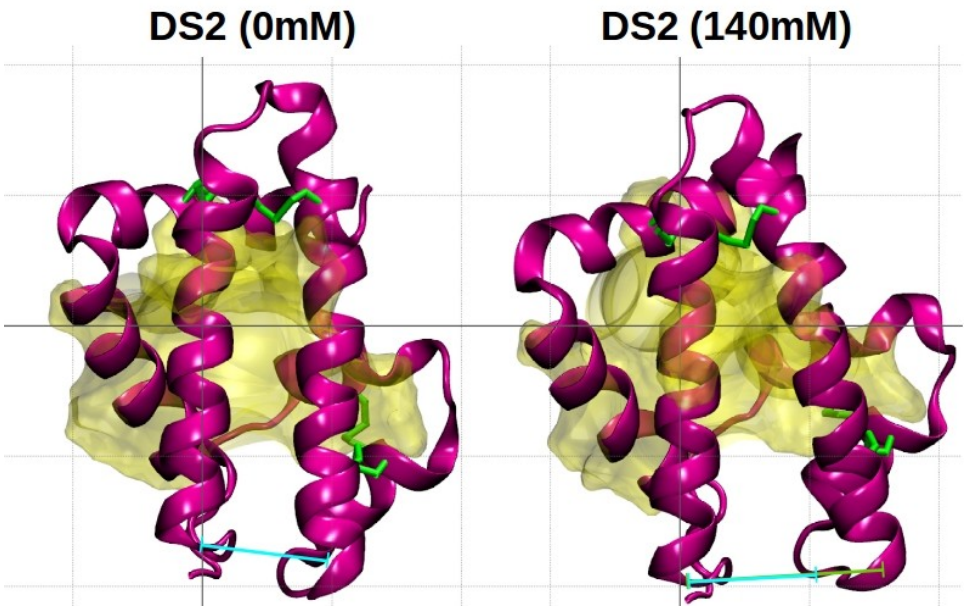

Figure S8. Configuration of DS2 site at 0mM (left) and at 140mM (right). DS2 and surrounding residues are represented using their secondary structure as in Figs.3,4 and 5 of the main text. The light green rods, seen on top and right hand side of the structure, are the S-S bridges. Note that they are very rigid and therefore so shall be the surrounding area. At the bottom of both images we drew scale bars to visualize the opening of the bottom part of DS2 site occurring at 140mM which allowed the extrusion of hydrophilic residues as shown in Fig.10 in the main text.

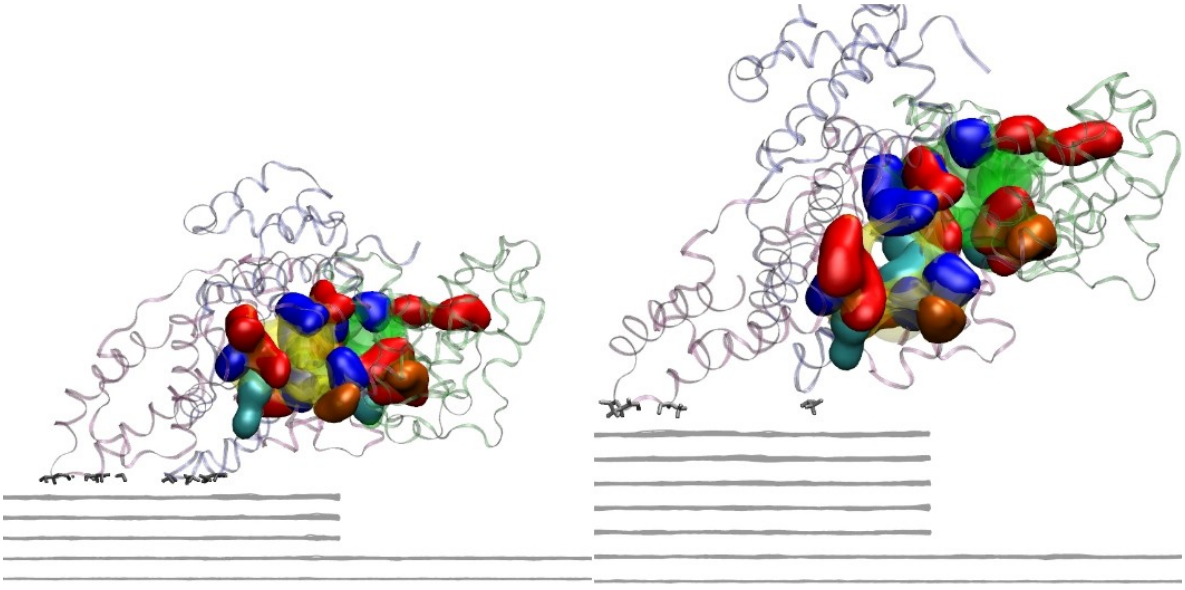

Figure S9. Early stages (at 10ns) of adsorption of BSA-1 for G3 (left) and G5 (right) substrates. The representation used here is the same as in Fig.10 in the main text.

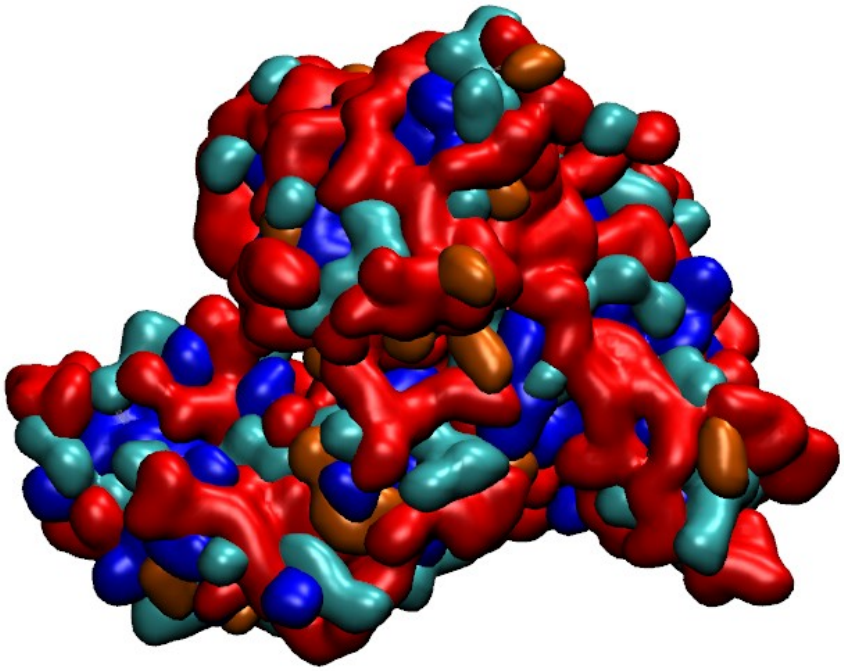

Figure S10. Distribution of aminoacids on the BSA surface. The residues (aminoacids) color is in accordance with their hydrophobicity index: very hydrophobic, hydrophobic, neutral and hydrophilic residues are colored in blue, cyan, orange and red respectively. BSA is charged protein, whose surface aminoaccids are mostly hydrophilic. In fact, BSA is a blood plasma protein (thus water soluble, i.e. hydrophilic) and it works as a carrier of hydrophobic molecules in the bloodstream. Therefore, as a whole, BSA is a hydrophilic protein.

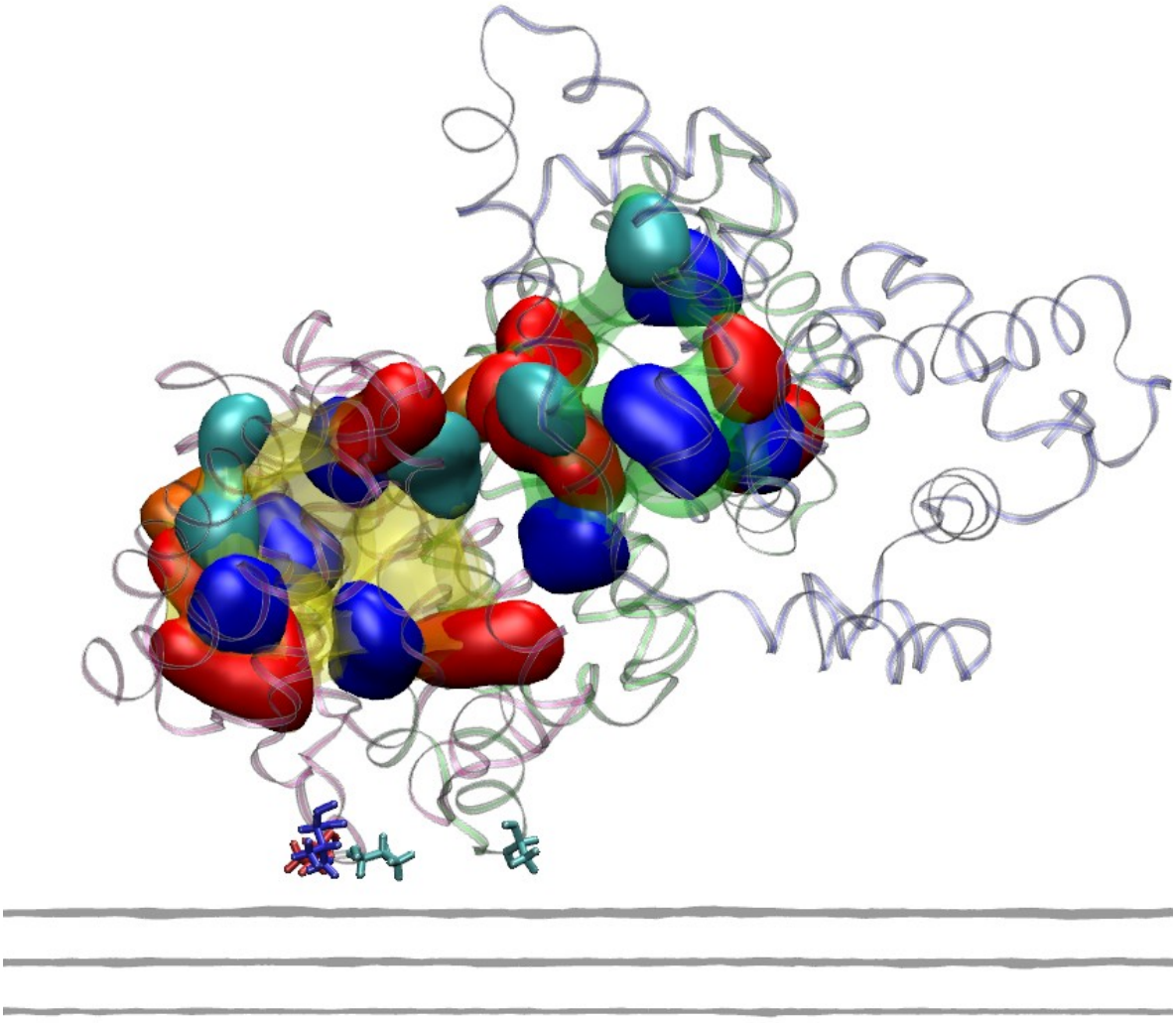

Figure S11. BSA-2 initial stages of adsorption to G0 substrate. The representation used here is the same as in Fig.10 in the main text. The only exception are the aminoacids from BSA in contact with the surface that are represented in liquorice with a coloring scheme in accordance with their hydrophobicity as in Fig.10 in the main text.