Supporting Information

Molecular Dynamics of Fibrinogen Adsorption onto Graphene, but not onto Poly(ethylene glycol) Surface, Increases Exposure of Recognition Sites that Trigger Immune Response

Nadiya Dragneva[†,‡], *Oleg Rubel*[†,§] *and Wely B. Floriano*[†,‡,¶,*]

[†]Thunder Bay Regional Research Institute, 290 Munro St, Thunder Bay, Ontario P7A 7T1, Canada.

[‡]Biotechnology PhD program, Faculty of Science and Environment Studies, Lakehead University, 955 Oliver Road, Thunder Bay, Ontario P7B 5E1, Canada.

[§] McMaster University, Department of Materials Science and Engineering, 1280 Main Street West, Hamilton, ON L8S 4L8, Canada.

[¶]Lakehead University, Department of Chemistry, 955 Oliver Road, Thunder Bay, Ontario P7B 5E1, Canada.

[*]To whom correspondence should be addressed. Phone: (807) 766-7215. E-mail: wely.floriano@lakeheadu.ca

Figure S1. Potential energy (kJ/mol) of fibrinogen D-domain as a function of simulation time. Here, unbound (Unbound-D), top (Top-D), side (Side-D), and perpendicular 1-3 (Perp1-D, Perp2-D, Perp3-D) are initial orientations of D-domain on graphene, and PEG-D is a perpendicular orientation of D-domain on a monolayer of PEG. For time plot, the 6,000 (or 3,000) data points were smoothed over 60 (30) points using a moving window average approach.

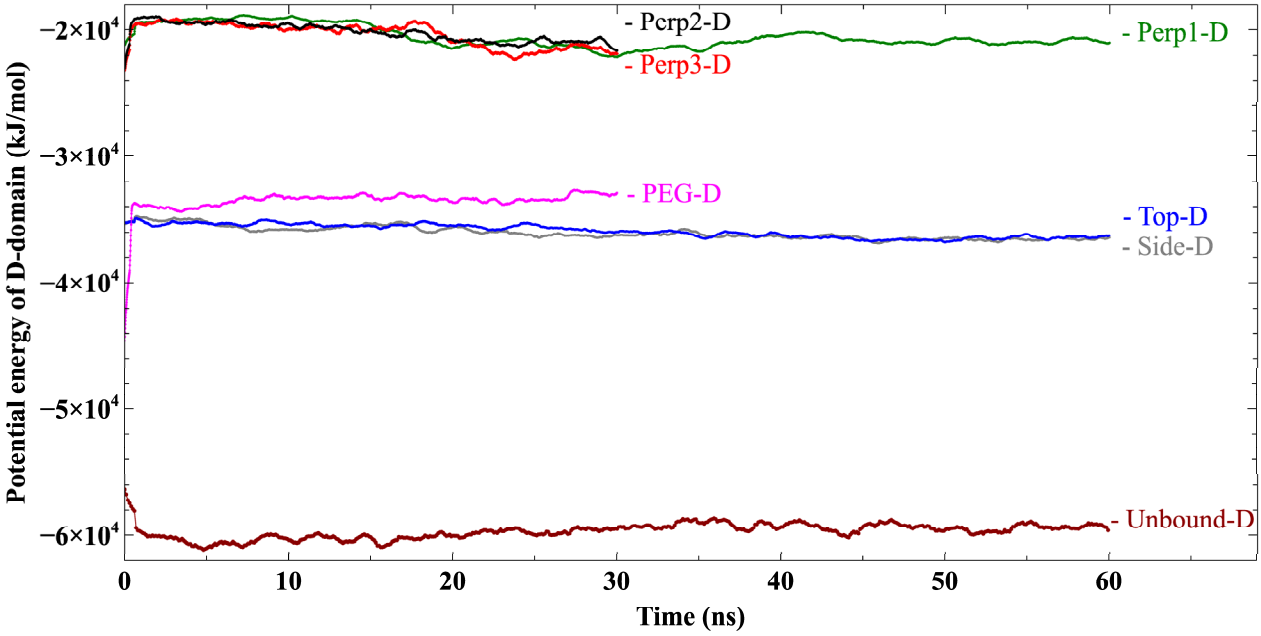


Figure S2. Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on graphene, for top orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

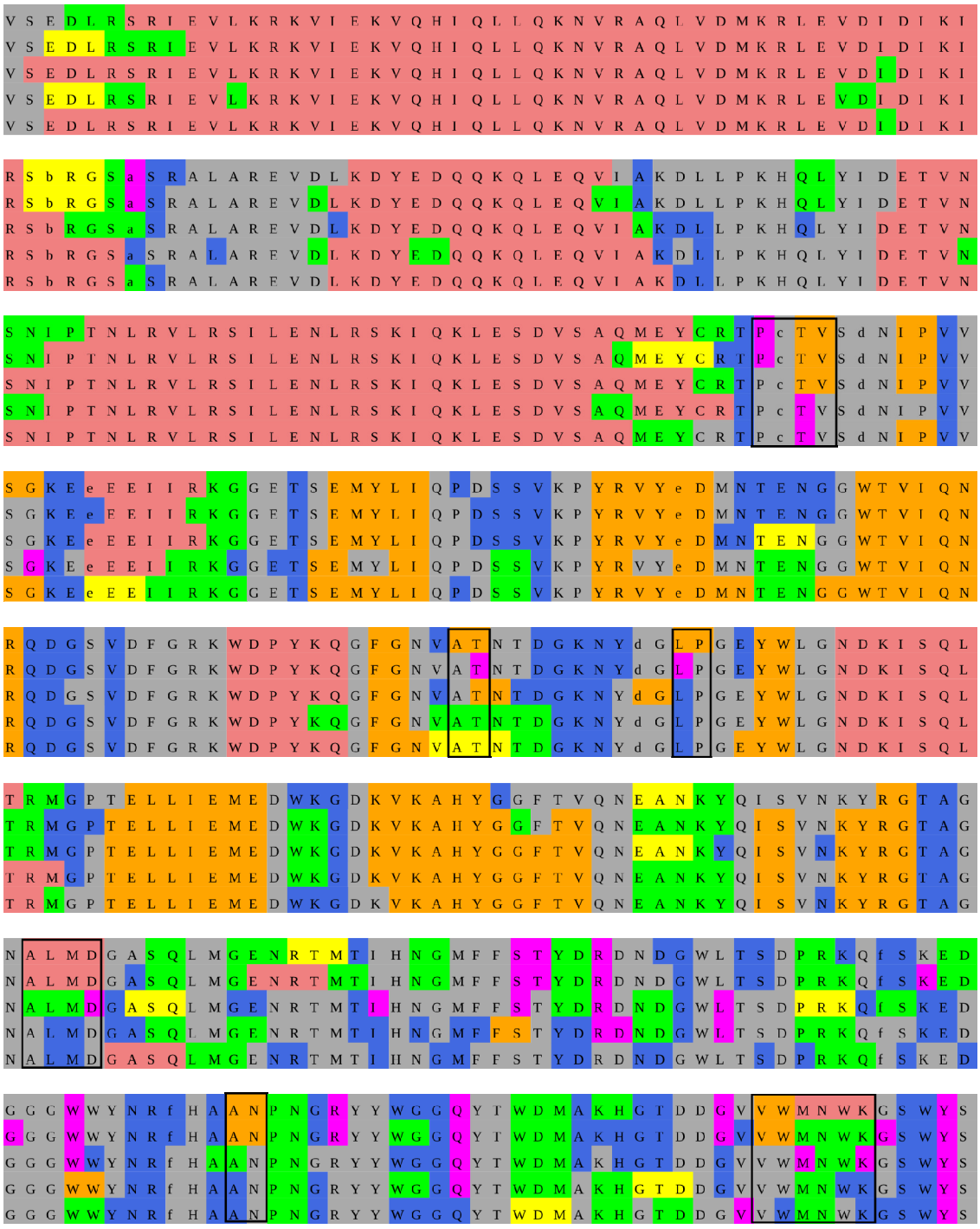


Figure S2. (Continued) Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on graphene, for top orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

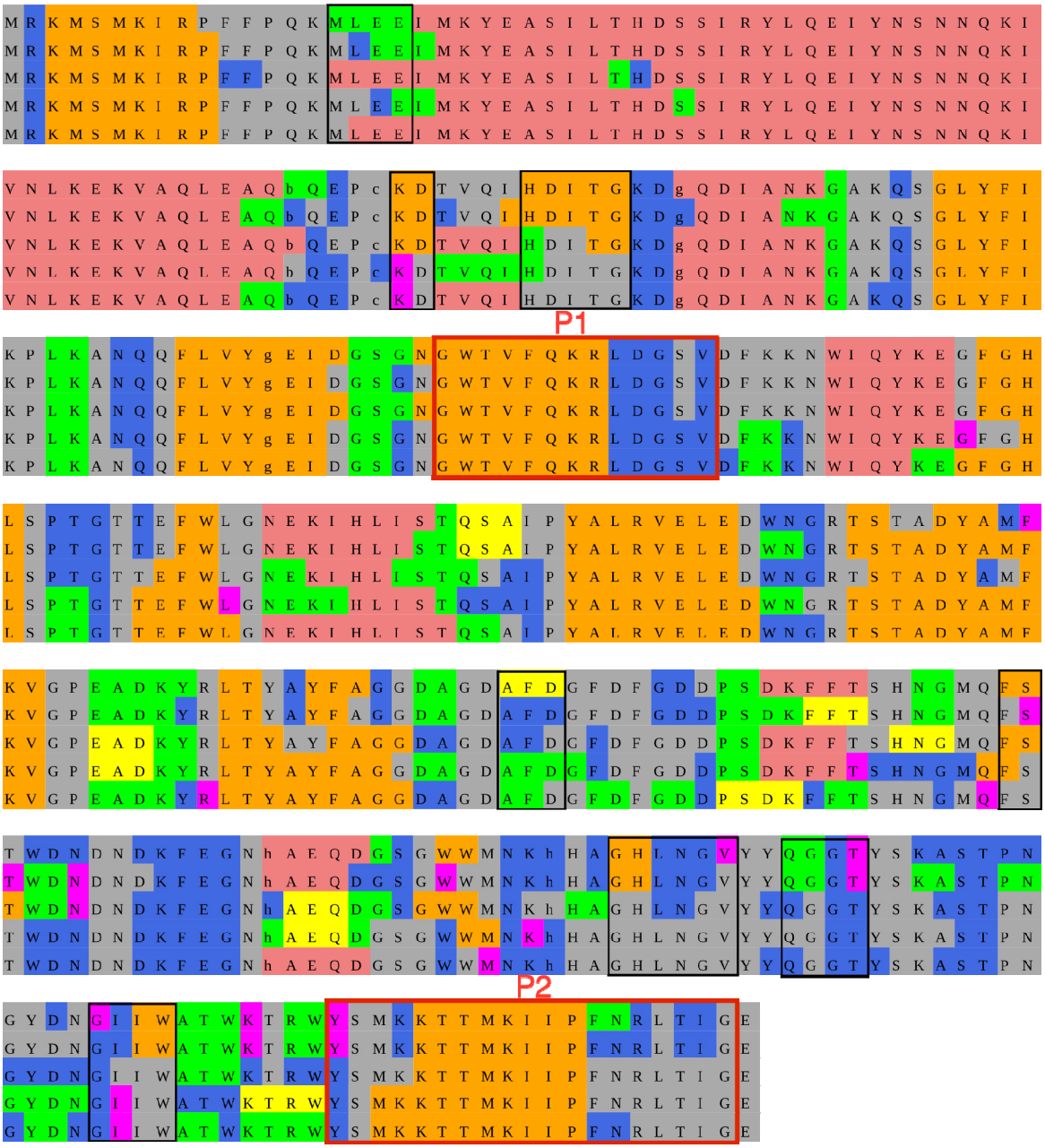


Figure S3. Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on graphene, for side orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

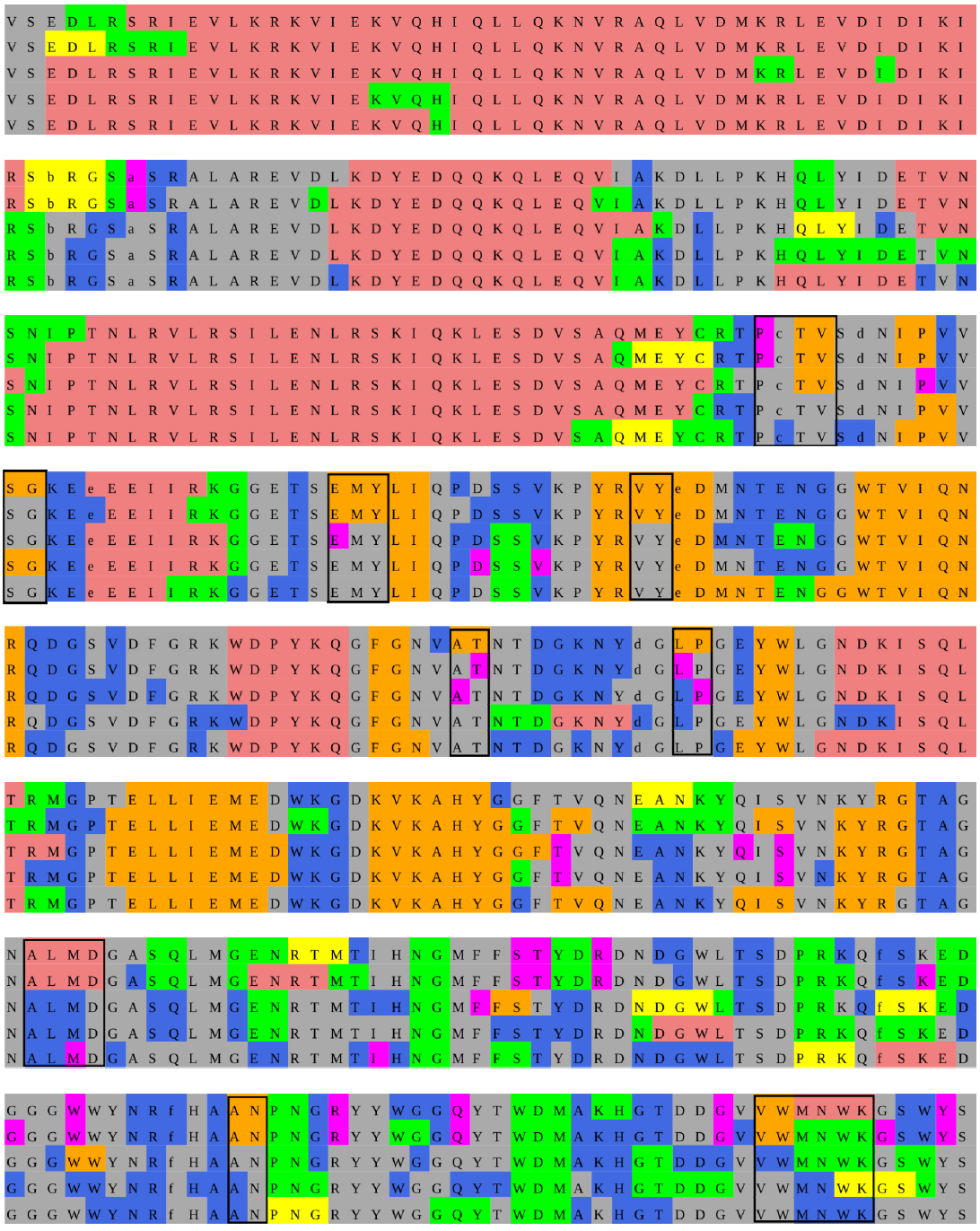


Figure S3. (Continued) Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on graphene, for side orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

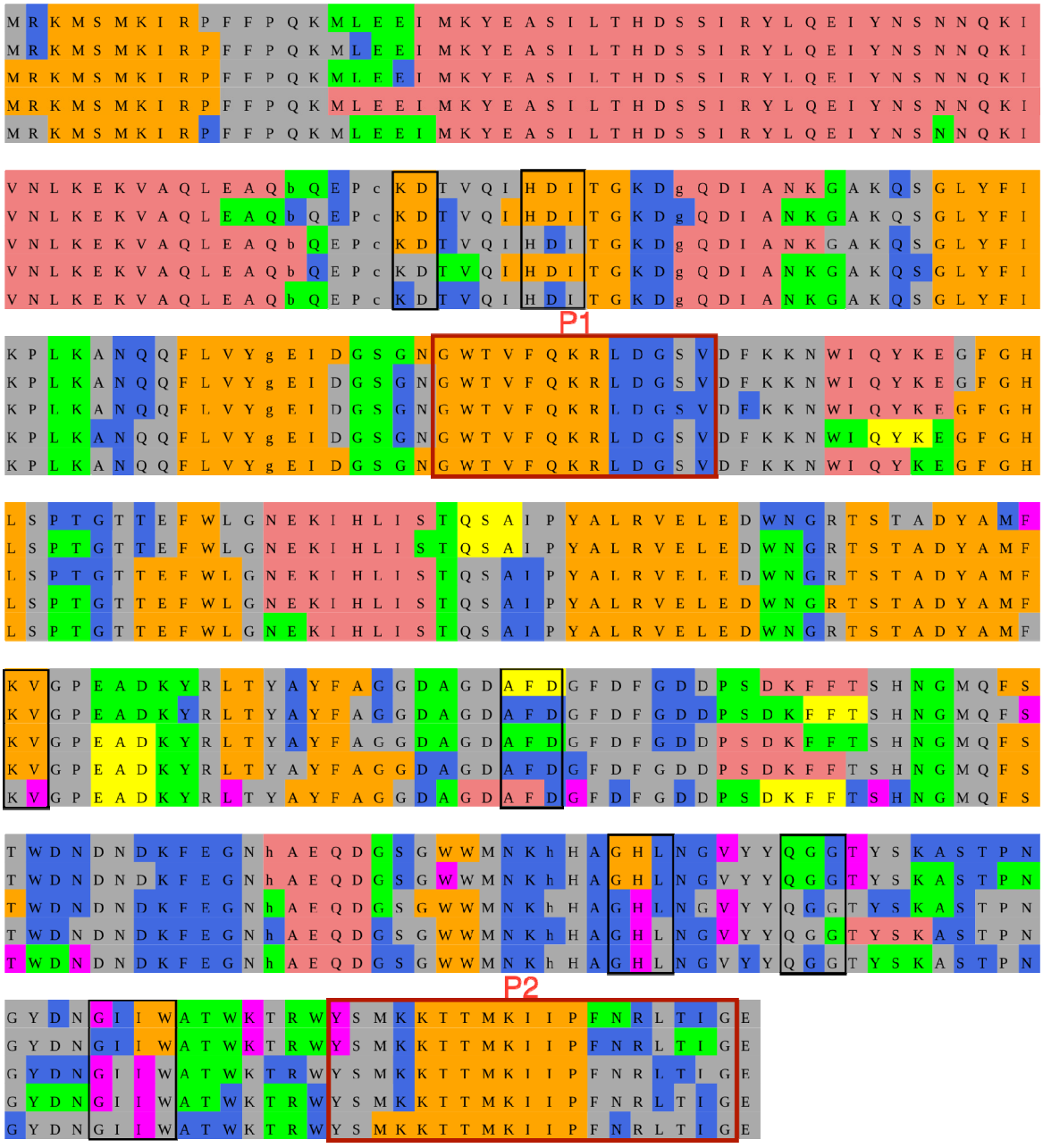


Figure S4. Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on graphene, for perpendicular orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

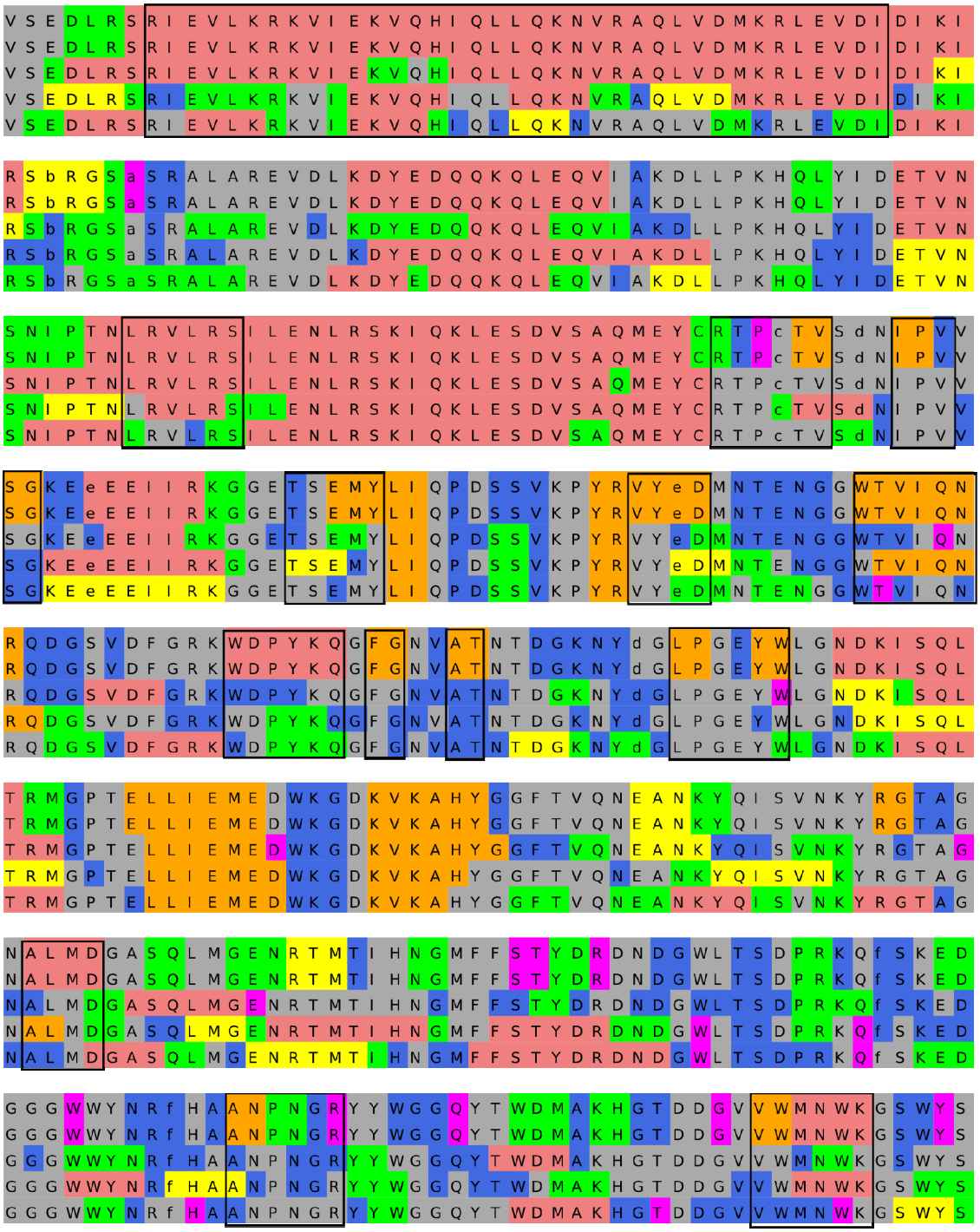


Figure S4. (Continued) Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on graphene, for perpendicular orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

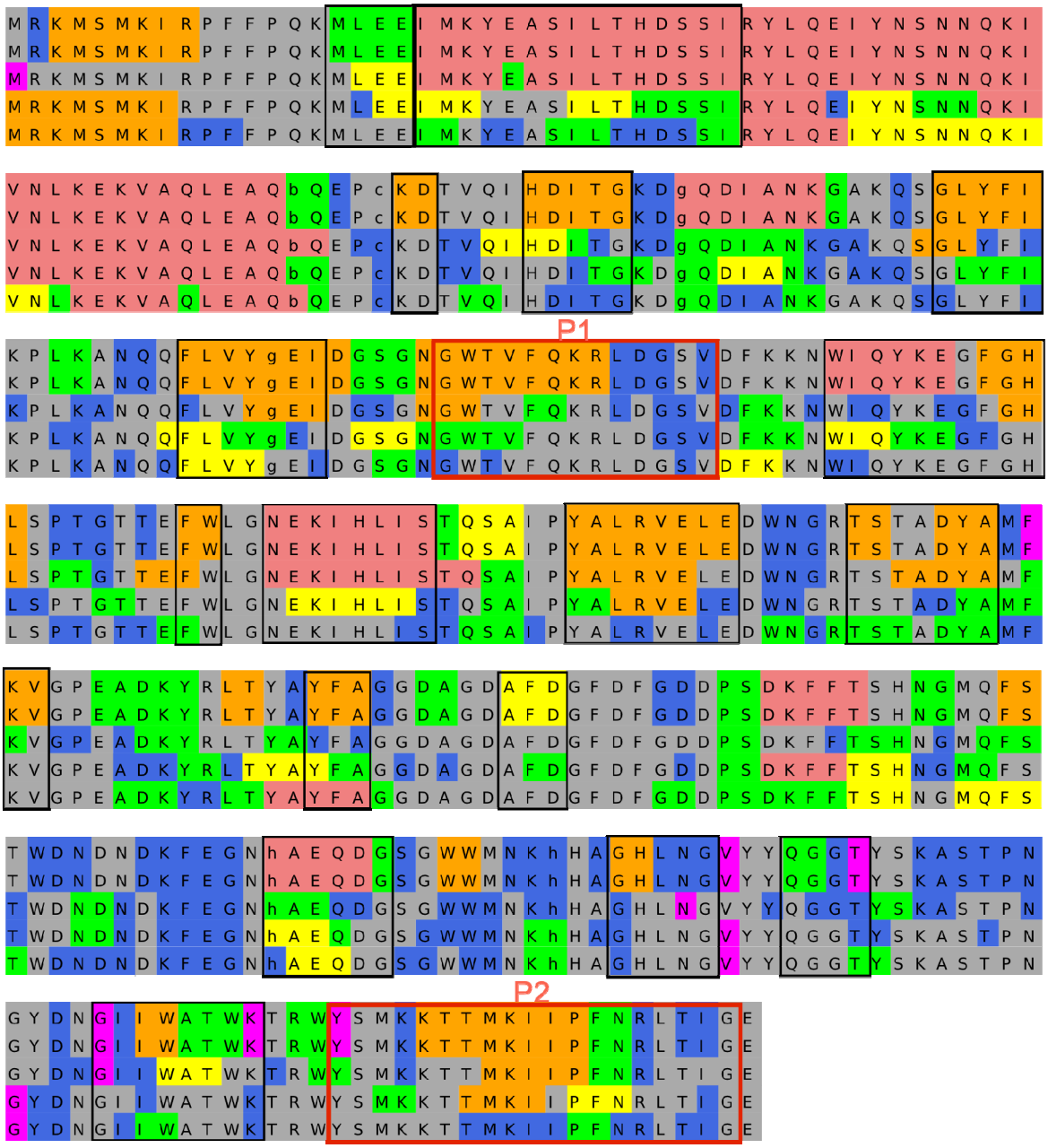


Figure S5. Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on PEG, for perpendicular orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns and 30 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

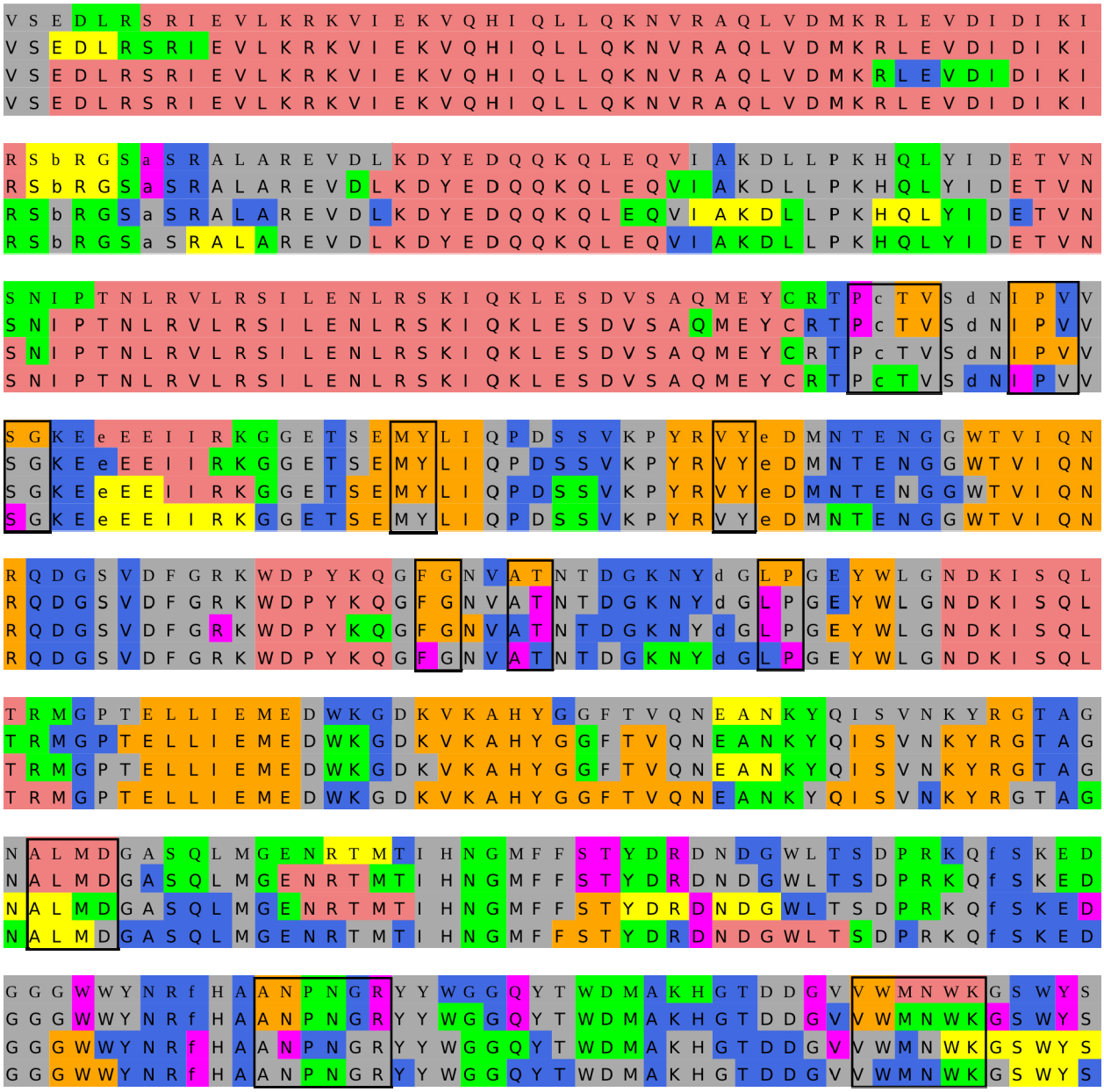


Figure S5. (Continued) Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD on PEG, for perpendicular orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns and 30 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

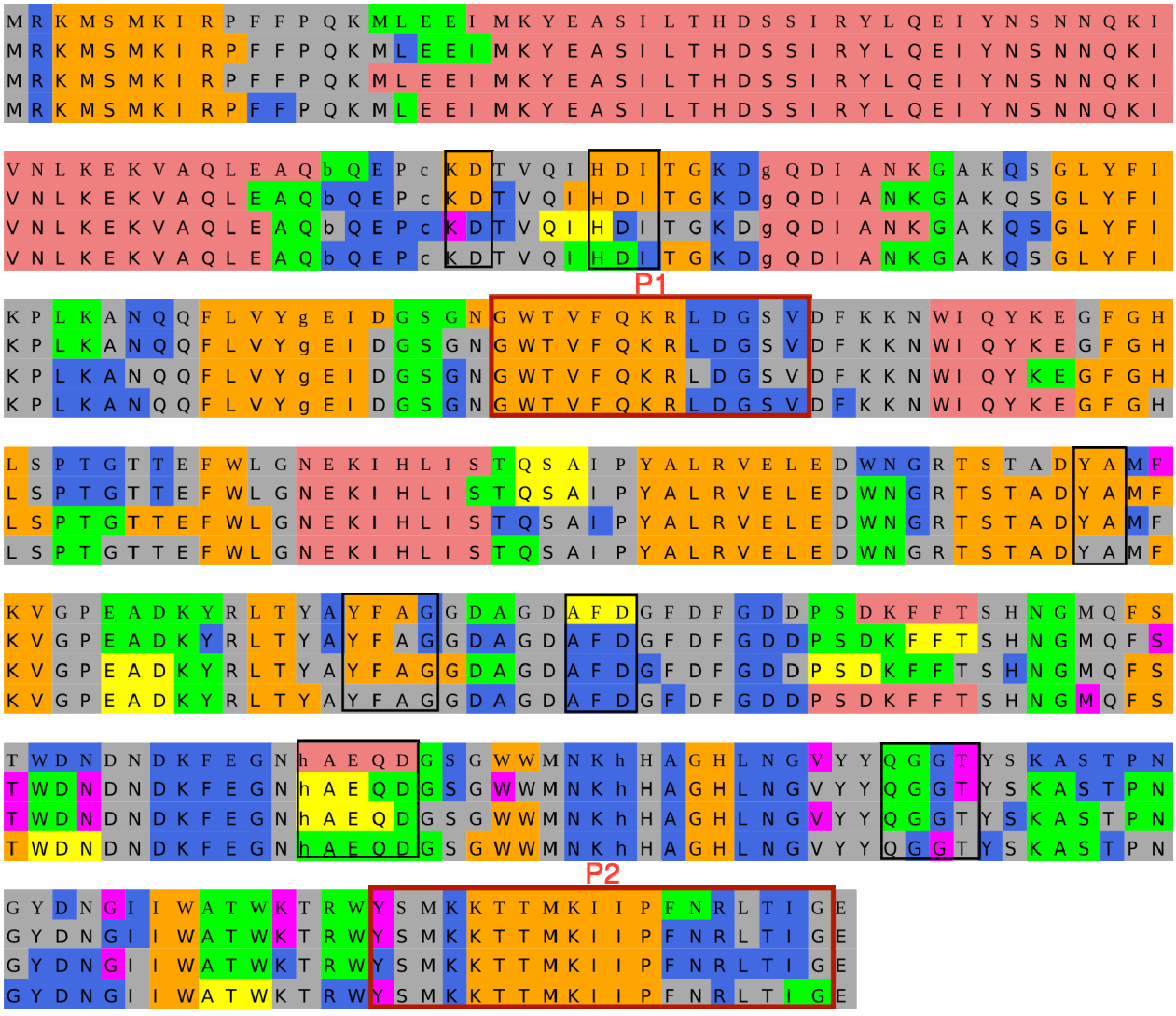


Figure S6. Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD, for unbound orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.

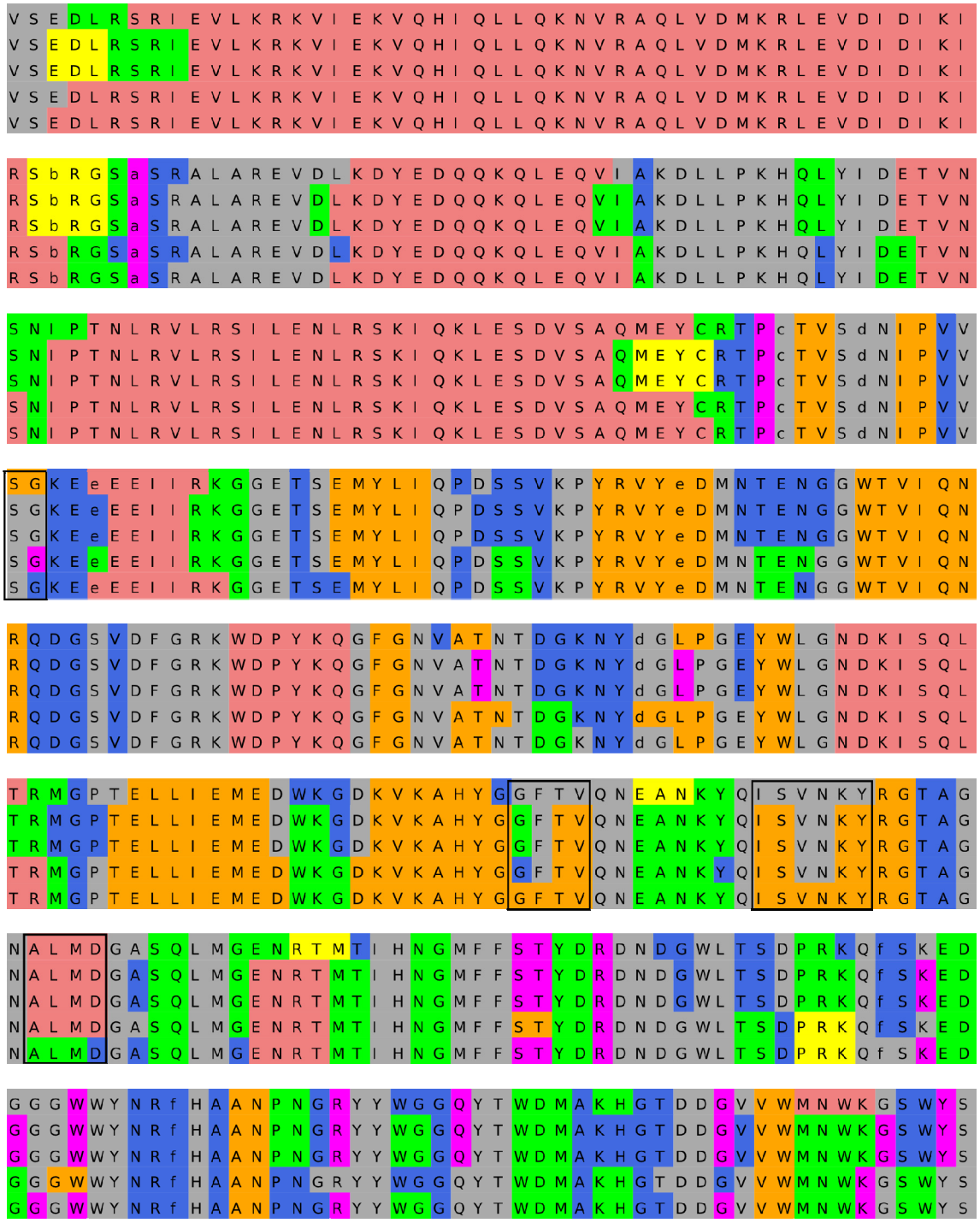
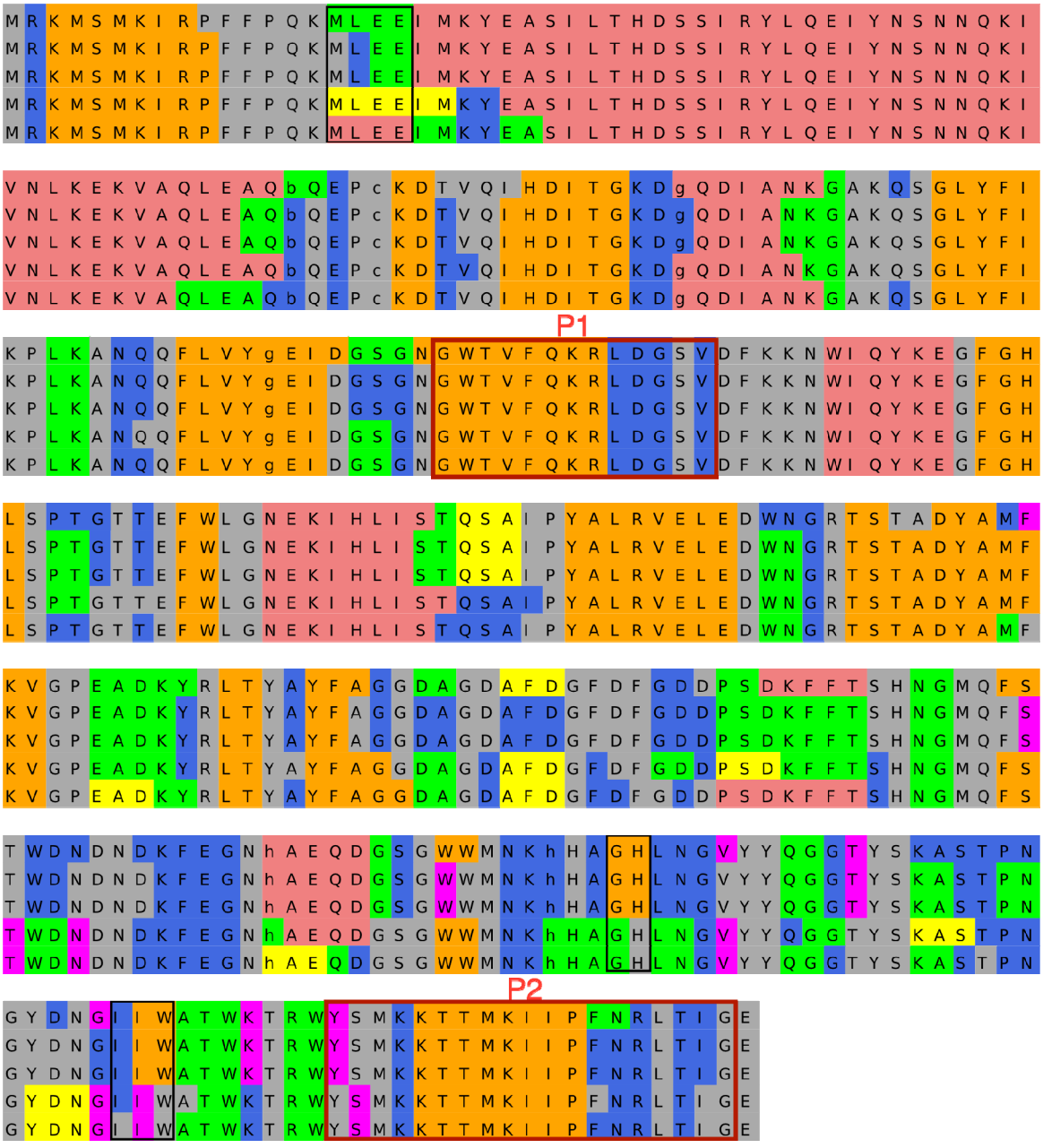


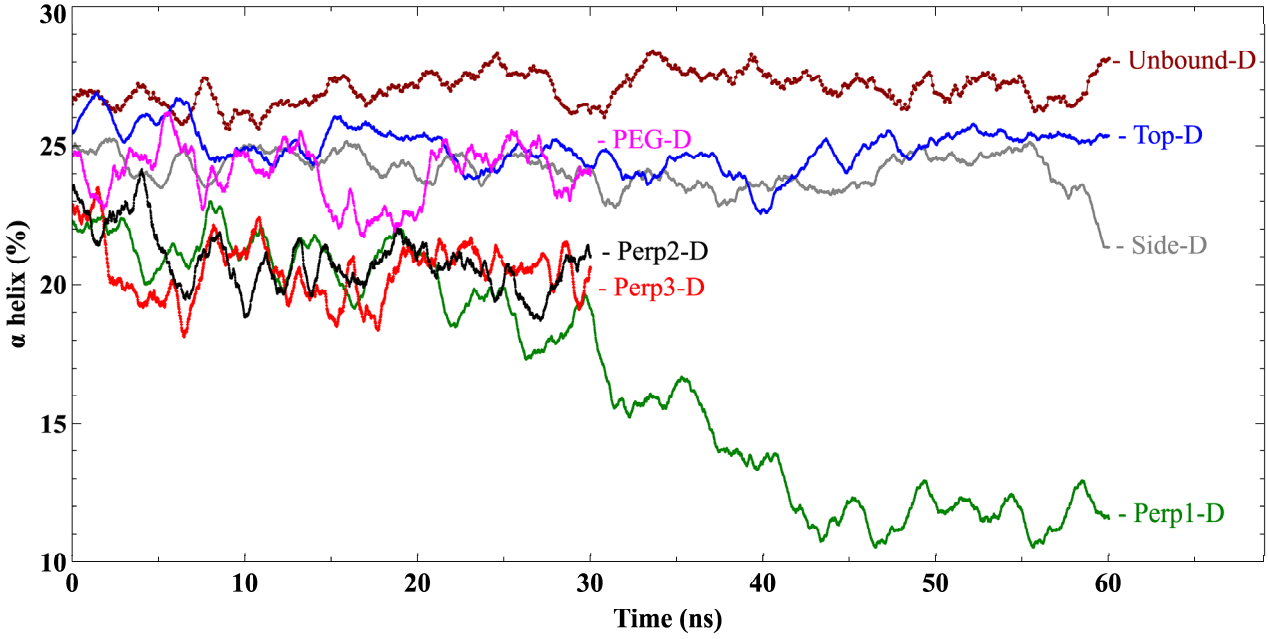
Figure S6. (Continued) Secondary structure assignment per residue for the complete sequence of the D-domain of fibrinogen before and after MD, for unbound orientation simulated. The rows correspond to a D-domain crystal structure, its structure at 0 ns, 20 ns, 40 ns, and 60 ns of the simulation time, respectively. The outlined in black fragments correspond to the most significant changes in the secondary structure content of the D-domain such as unfolding of the α-helix and/or β-extended strand; while the outlined in red fragments are P1 γ190-202 and P2 γ377-395 binding sites.



KEY:


A-Helix
H-Bonded Turn
Bend
G-Helix
Beta Bridge
P-Helix
Extended strand
Undetermined

Figure S7. Percent of secondary structure (α-helix, β-stand) relative to native (initial) state. Here, unbound (Unbound-D), top (Top-D), side (Side-D), and perpendicular 1-3 (Perp1-D, Perp2-D, Perp3-D) are initial orientations of D-domain on graphene, and PEG-D is a perpendicular orientation of D-domain on a monolayer of PEG. For time plots, the 6,000 (or 3,000) data points were smoothed over 60 (30) points using a moving window average approach.



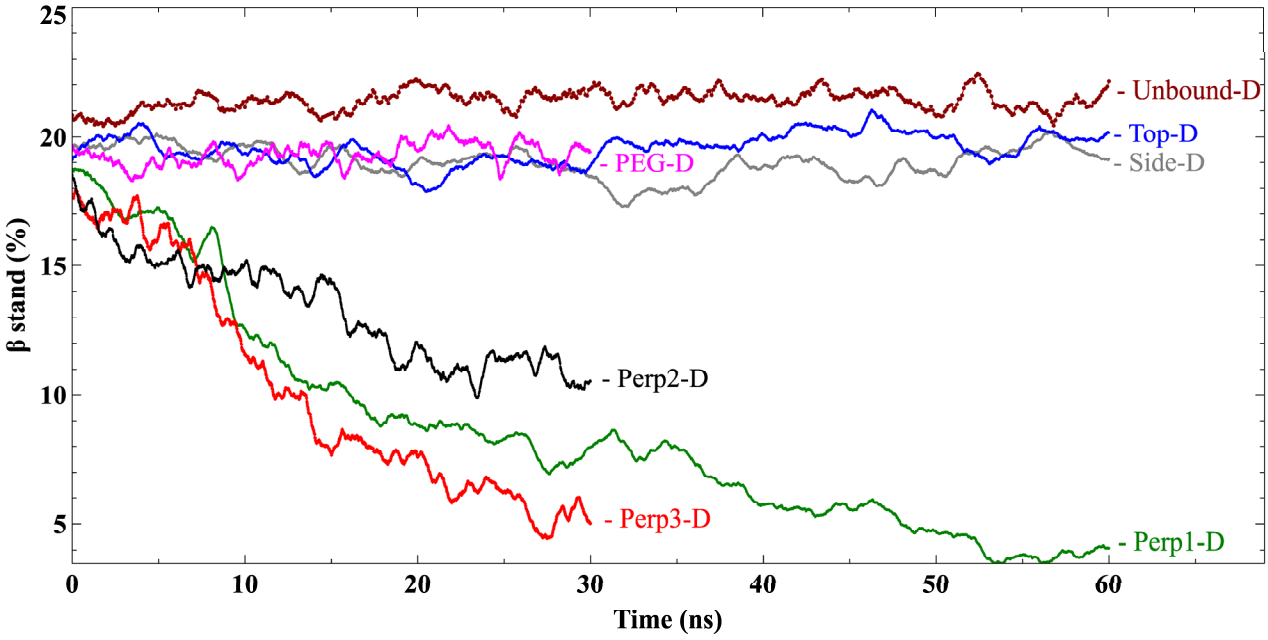


Figure S8. Number of hydrogen bonds (HBs) for initial and final orientations. Here, unbound (Unbound-D), top (Top-D), side (Side-D), and perpendicular 1-3 (Perp1-D, Perp2-D, Perp3-D) are initial orientations of D-domain on graphene, and PEG-D is a perpendicular orientation of D-domain on a monolayer of PEG.

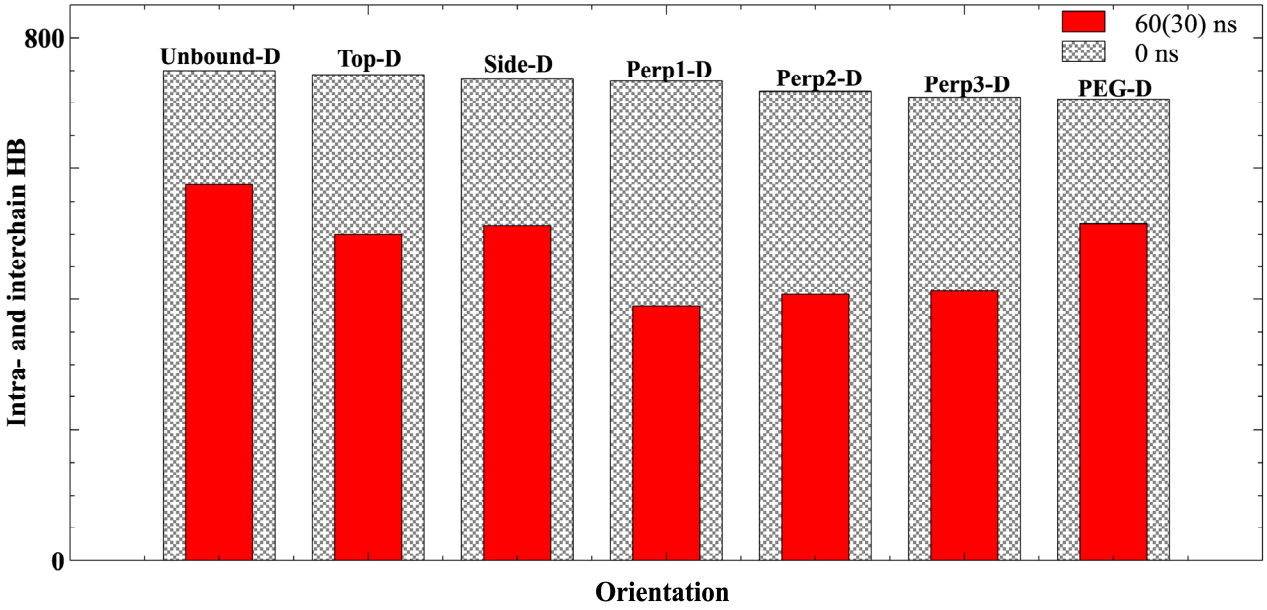


Figure S9. Radius of gyration as a function of simulation time. Here, unbound (Unbound-D), top (Top-D), side (Side-D), and perpendicular 1-3 (Perp1-D, Perp2-D, Perp3-D) are initial orientations of D-domain on graphene, and PEG-D is a perpendicular orientation of D-domain on a monolayer of PEG.