Structure, Volume *26*

Supplemental Information

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Keywords: fibrinogen; fibrin; fibrin polymerization; fibrin oligomers; fibrin protofibrils; GPU computing; multiscale modeling; MD simulations

Table S1. Crystal structures of human fibrinogen and fibrin from Protein Data Bank. Related to STAR Methods. The table includes various portions of WT fibrin(ogen) and fibrinogen used in the reconstruction of fibrin oligomers.

PDB code	Structure
Fibrinogen	
3GHG	Human fibrinogen co-crystallized with GPRP and GHRP
D-dimer fragments from crosslinked fibrin	
1FZB	Crosslinked double D fragment
1FZC	Fragment double-D from human fibrin with bound ligands
1FZE	Fragment double-D from human fibrin
1FZF	Fragment double-D from human fibrin with GHRP
1N86	Human D-dimer from cross-linked fibrin with GPR and GHRPLDK
1N8E	Fragment double-D from human fibrin
2HLO	Fragment D-dimer from human fibrin with G-hydroxyP-RP
2HOD	Fragment D-dimer from human fibrin with G-hydroxyP-RP
2HPC	Fragment D-dimer from human fibrin with GPRP
2Q9I	D-dimer from human fibrin with MHRPY
2Z4E	D-dimer from human fibrin with GHRPY
3H32	D-dimer from human fibrin with GHRPY
Fragments D (D-D interactions in a crystal as a result of molecular packing)	
1FZG	Fragment D from human fibrinogen with GHRP
2H43	Fragment D co-complexed with AHRP
2FFD	Fibrinogen fragment D with GPRVVE
3BVH	Recombinant γD364A fibrinogen fragment D with GPRP
3E1I	BβD432A variant fibrinogen fragment D with GHRP
2OYH	Fragment D of γD298,301A fibrinogen variant with GHRP
2OYI	Fragment D of γD298,301A fibrinogen variant with GHRP
1LT9	Recombinant human fibrinogen fragment D
1LTJ	Recombinant human fibrinogen fragment D with GPRP and GHRP
1FZA	Fibrinogen fragment D
1RE3	Fragment D of BβD398A fibrinogen variant with GHRP
1RE4	Fragment D of BβD398A variant fibrinogen
1RF1	Fragment D of γE132A fibrinogen variant with GHRP
1RF0	Fragment D of γE132A fibrinogen variant

Table S2. Structure and shape characteristics of fibrin protofibrils obtained from AFM experiment and equilibrium Molecular Dynamics simulations. Related to Figure 4. Shown are the average quantities and standard deviations of the D-D, D-E, and DED-DED distances and the DED-DED-DED angle (distances and angles are calculated using the centers of mass in the simulations and geometric centers in AFM experiments).

Metric	AFM	Simulations
D-D distance, nm	9.2 ± 1.7	9.0 ± 0.1
D-E distance, nm	6.7 ± 1.2	6.3 ± 0.5
DED-DED distance, nm	22.9 ± 2.5	22.1 ± 1.7
DED-DED-DED angle, degrees	162 ± 12	162 ± 10

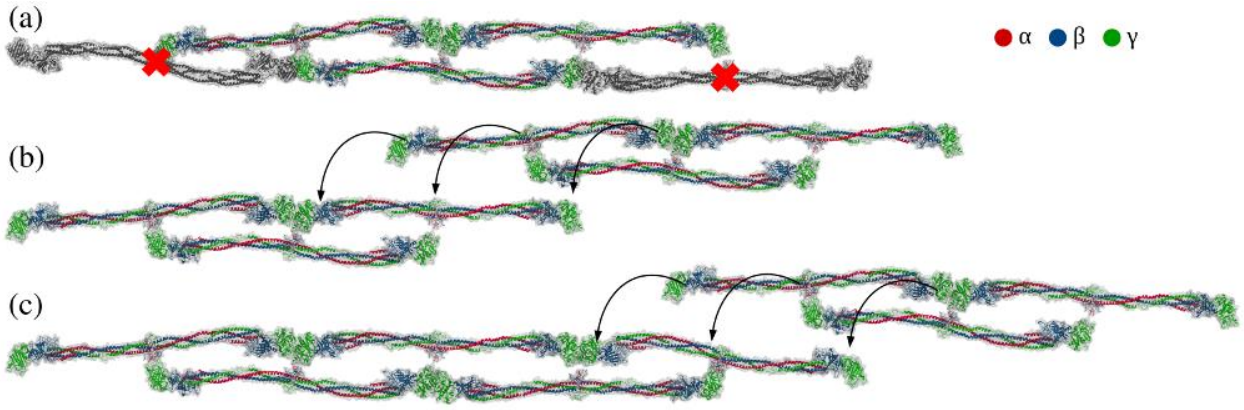

Figure S1: Schematic illustration of the reconstruction of fibrin protofibril $FP_{n/m}$. Related to Figure 1 and STAR Methods.

(A) Two fibrin molecules in the lower strand are removed from the atomic model of oligomer $FO_{2/3}$ (shown in gray color and marked by the cross).

(B) Two copies of the obtained oligomer $FO_{1/2}$ are aligned using Kabsch algorithm (Elongation procedure; see Figure 1B). We overlapped the monomer from $FO_{1/2}$ at the top with the monomer from $FO_{1/2}$ at the bottom (connected by the curved arrows).

(C) The result of this operation described in panel B – the fibrin oligomer $FO_{1/2}$ (bottom structure). This same procedure can be repeated to reconstruct fibrin oligomers $FO_{3/4}$, $FO_{4/5}$, etc., up to a protofibril of arbitrary length.

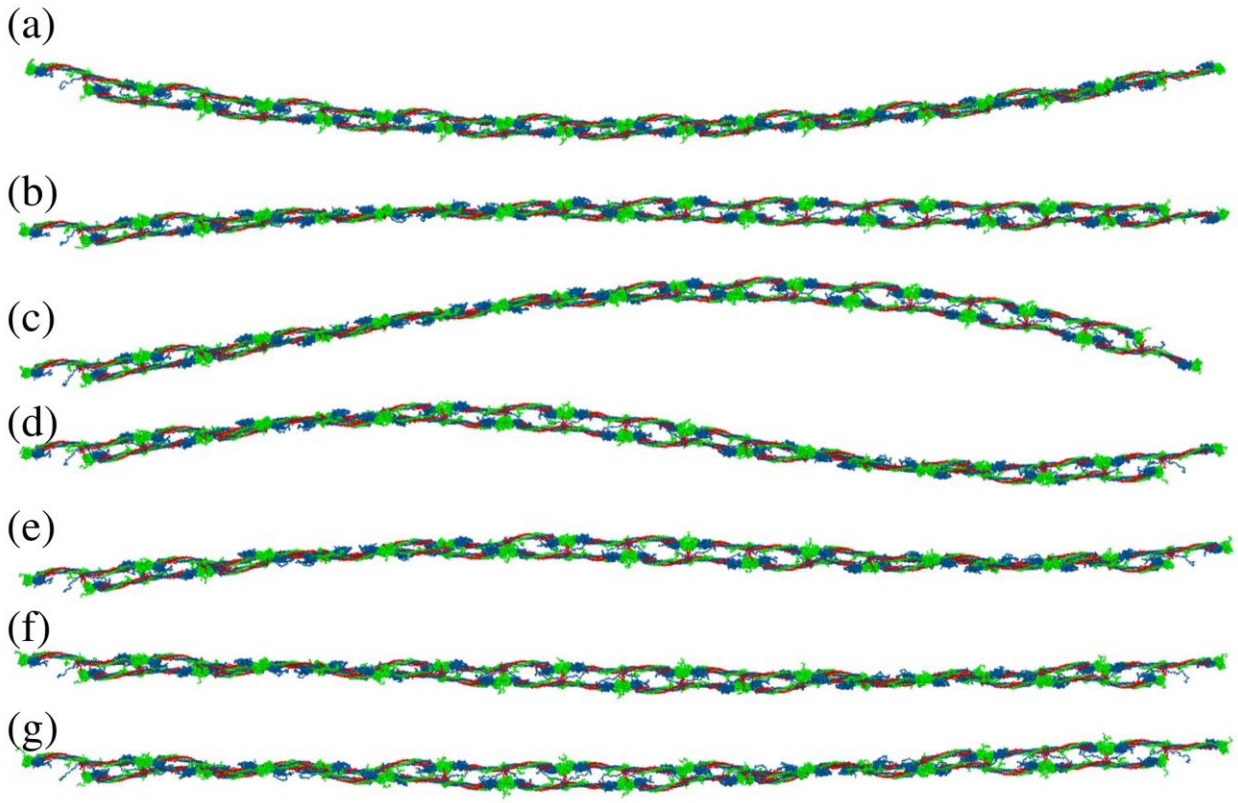

Figure S2: Twisting of fibrin protofibrils upon transition from the straight to the bent configuration of D:D interface. Related to Figure 3.

(A) Structures of fibrin protofibril $FP_{10/9}$ that correspond to the straight conformation of D:D interface (based on PDB structure 1N86).

(B-F) Transient structures detected in the course of transition from the straight to the bent configuration of D:D interface.

(G) Structure of $FP_{10/9}$ that correspond to the bent configuration of D:D interface (based on PDB structure 1FZG).