

Summary of integrative structure determination of Molecular Architecture of Human Fibrin Clots (PDB ID: 8ZZU, PDB-Dev ID: PDBDEV_00000030)

1. Model Composition	
<i>Entry composition</i>	<ul style="list-style-type: none"> - RGD-containing Alpha Domain Alpha_558-620: chain(s) A [I], M [J] (63 residues) - Subunit Alpha_46-219: chain(s) B [A], G [D] (174 residues) - Subunit Alpha_220-249: chain(s) C [Z], H [Y] (30 residues) - Subunit Beta: chain(s) D [B], J [E] (401 residues) - Subunit Gamma: chain(s) E [C], K [F] (381 residues) - Interactive Alpha Domain Alpha_432-491: chain(s) F [H], L [G] (60 residues) - Beta N-term Beta_55-84: chain(s) I [K] (34 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - Experimental model, PDB: 3GHG - De Novo model, Not available - Crosslinking-MS data, PRIDE: PXD011680 - De Novo model, Not available - De Novo model, Not available - De Novo model, Not available
2. Representation	
<i>Number of representations</i>	1
<i>Scale</i>	Atomic
<i>Number of rigid and flexible segments</i>	14, 7
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSSO, 156 crosslinks
4. Validation	
<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	Not available

<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	<ul style="list-style-type: none"> - Clashscore: 9.26 - Ramachandran outliers: 26 - Sidechain outliers: 192
<u>Fit to data used for modeling</u>	Satisfaction of crosslinks: 51.28%
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. <u>Name</u>	?
<u>Method</u>	?
<u>Number of computed models</u>	?
<u>Software</u>	<ul style="list-style-type: none"> - ThreaDomEx (version Not available) - Robetta (version Not available) - HHalign-Kbest (version Not available) - I-TASSER (version Not available) - RaptorX (version Not available) - HADDOCK (version 2.2) - CPORt (version Not available) - DisVis (version Not available)