

Summary of integrative structure determination of Molecular Architecture of Human Fibrin Clots (PDB ID: 8ZZU, PDB-Dev ID: PDBDEV_0000030)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Subunit Alpha_220-249: Chain C (30 residues) - Subunit Beta: Chain D (401 residues) - Subunit Gamma: Chain E (381 residues) - RGD-containing Alpha Domain Alpha_558-620: Chain M (63 residues) - Subunit Beta: Chain J (401 residues) - Subunit Alpha_46-219: Chain G (174 residues) - Interactive Alpha Domain Alpha_432-491: Chain F (60 residues) - Subunit Alpha_220-249: Chain H (30 residues) - RGD-containing Alpha Domain Alpha_558-620: Chain A (63 residues) - Subunit Gamma: Chain K (381 residues) - Beta N-term Beta_55-84: Chain I (34 residues) - Subunit Alpha_46-219: Chain B (174 residues) - Interactive Alpha Domain Alpha_432-491: Chain L (60 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 3GHG - De Novo model, Not available - De Novo model, Not available - De Novo model, Not available - De Novo model, Not available - De Novo model, Not available - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 1 cross-links - De Novo model, Not available - De Novo model, Not available - De Novo model, Not available
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	14, 7
Rigid bodies	<ul style="list-style-type: none"> - A: - - B: 13-35, 53-63 13-35, 53-63 - C: - - D: 1-174 1-174 - E: 1-301 1-301 - F: - - G: 1-401 1-401 - H: - - I: - - J: 1-381 1-381 - K: 29-60 29-60 - L: - - M: -

<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-12, 36-52 - B: - - C: - - D: - - E: - - F: 1-28 - G: - - H: - - I: 1-34 - J: - - K: - - L: 1-28 - M: 1-12, 36-52
<i>Structural coverage (rigid bodies)</i>	100%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	- 1 unique CrossLinkRestraint: DSSO, 1 cross-links
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>	Model precision can not be calculated with one structure
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	Model-1: Clashescore = 9.27, Number of Ramachandran outliers = 26, Number of sidechain outliers = 192
<i>Model quality: assessment of excluded volume</i>	Not applicable
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	?
<i>Name</i>	?
<i>Number of computed models</i>	?

Software

- [ThreaDomEx](#) (version Not available)
- [Robetta](#) (version Not available)
- [HAlign-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)