

## Summary of integrative structure determination of molecular architecture of human fibrin clots (PDBDEV00000030)

1. Model Composition	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- RGD-containing Alpha Domain Alpha_558-620: Chain A (63 residues)</li> <li>- Subunit Beta: Chain J (401 residues)</li> <li>- Subunit Alpha_220-249: Chain H (30 residues)</li> <li>- Subunit Gamma: Chain K (381 residues)</li> <li>- Interactive Alpha Domain Alpha_432-491: Chain L (60 residues)</li> <li>- Subunit Alpha_220-249: Chain C (30 residues)</li> <li>- Subunit Alpha_46-219: Chain B (174 residues)</li> <li>- Subunit Beta: Chain D (401 residues)</li> <li>- Beta N-term Beta_55-84: Chain I (34 residues)</li> <li>- Subunit Gamma: Chain E (381 residues)</li> <li>- RGD-containing Alpha Domain Alpha_558-620: Chain M (63 residues)</li> <li>- Subunit Alpha_46-219: Chain G (174 residues)</li> <li>- Interactive Alpha Domain Alpha_432-491: Chain F (60 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 3GHG</li> <li>- De Novo model, Not listed</li> <li>- De Novo model, Not listed</li> <li>- De Novo model, Not listed</li> <li>- De Novo model, Not listed</li> <li>- CX-MS data, Linker name and number of cross-links: DSSO, 1 cross-links</li> <li>- De Novo model, Not listed</li> <li>- De Novo model, Not listed</li> <li>- De Novo model, Not listed</li> </ul>
2. Representation	
<a href="#">Atomic structural coverage</a>	100%
Number of <a href="#">rigid bodies</a> , <a href="#">flexible units</a>	14, 7
Rigid bodies	<ul style="list-style-type: none"> <li>- A: -</li> <li>- B: 13-35:Experimental model/3GHG, 53-63:Experimental model/3GHG. 13-35:Experimental model/3GHG, 53-63:Experimental model/3GHG.</li> <li>- C: -</li> <li>- D: 1-174:Experimental model/3GHG. 1-174:Experimental model/3GHG.</li> <li>- E: 1-30:Experimental model/3GHG. 1-30:Experimental model/3GHG.</li> <li>- F: -</li> <li>- G: 1-401:Experimental model/3GHG. 1-401:Experimental model/3GHG.</li> <li>- H: -</li> <li>- I: -</li> <li>- J: 1-381:Experimental model/3GHG. 1-381:Experimental model/3GHG.</li> <li>- K: 29-60:Experimental model/3GHG. 29-60:Experimental model/3GHG.</li> <li>- L: -</li> <li>- M: -</li> </ul>

<i>Flexible units</i>	<ul style="list-style-type: none"> <li>- A: 1-12, 36-52.</li> <li>- B: -</li> <li>- C: -</li> <li>- D: -</li> <li>- E: -</li> <li>- F: 1-28.</li> <li>- G: -</li> <li>- H: -</li> <li>- I: 1-34.</li> <li>- J: -</li> <li>- K: -</li> <li>- L: 1-28.</li> <li>- M: 1-12, 36-52.</li> </ul>
<a href="#"><i>Resolution</i></a>	<ul style="list-style-type: none"> <li>- Rigid bodies: 1 residue per bead.</li> <li>- Flexible regions: N/A</li> </ul>
<b>3. Restraints</b>	
<a href="#"><i>Physical principles</i></a>	Information about physical principles was not provided
<a href="#"><i>Experimental data</i></a>	- 1 unique CrossLinkRestraint: DSSO, 1 cross-links
<b>4. Validation</b>	
<a href="#"><i>Sampling validation</i></a>	- Information related to sampling validation has not been provided
<a href="#"><i>Clustering algorithm ,clustering feature</i></a>	Distance threshold-based clustering used if ensembles are deposited, Not applicable
<a href="#"><i>Number of ensembles</i></a>	0
<a href="#"><i>Number of models in ensembles</i></a>	Not applicable
<a href="#"><i>Model precision (uncertainty of models)</i></a>	Model precision can not be calculated with one structure
<a href="#"><i>Quality of data</i></a>	- Quality of input data has not be assessed
<a href="#"><i>Model quality: assessment of atomic segments</i></a>	Clashscore: 9.38, Ramachandran outliers: 1.17% , Sidechain outliers: 9.64%
<a href="#"><i>Model quality: assessment of excluded volume</i></a>	- Not applicable
<a href="#"><i>Fit of the model to information used to compute it</i></a>	- Fit of model to information used to compute it has not been determined
<a href="#"><i>Fit of the model to information not used to compute it</i></a>	- Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<a href="#"><i>Method</i></a>	?
<a href="#"><i>Name</i></a>	?
<a href="#"><i>Details</i></a>	- Method details unspecified

Software

- ThreaDomEx (version None)
- Robetta (version None)
- HHalign-Kbest (version None)
- I-TASSER (version None)
- RaptorX (version None)
- HADDOCK (version 2.2)
- CPORT (version None)
- DisVis (version None)
- No location specified