

**Summary of integrative structure determination of Integrative structure of Apo-GAFab
(PDB ID: 9A0L, PDB-Dev ID: PDBDEV_00000057)**

1. Model Composition	
<u>Entry composition</u>	- GAFab: Chain B (399 residues) - GAFab: Chain A (399 residues)
<u>Datasets used for modeling</u>	- Crosslinking-MS data, Linker name and number of cross-links: sulfo-SDA, 55 cross-links - Experimental model, PDB ID: 6X88
2. Representation	
<u>Resolution</u>	Atomic
<u>Number of rigid bodies, flexible units</u>	0, 2
<u>Flexible units</u>	- A: 1-399 - B: 1-399
<u>Structural coverage (rigid bodies)</u>	100%
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	- 1 unique CrossLinkRestraint: sulfo-SDA, 55 cross-links - 1 unique CrossLinkRestraint: BS3, 22 cross-links - 1 unique CrossLinkRestraint: EDC, 7 cross-links
4. Validation	
<u>Number of ensembles</u>	0
<u>Number of models in ensembles</u>	Not applicable
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	Model precision can not be calculated with one structure
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of atomic segments</u>	Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 42, Number of sidechain outliers = 30
<u>Model quality: assessment of excluded volume</u>	Not applicable
<u>Fit to data used for modeling</u>	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. <i>Method</i>	None
<i>Name</i>	None
<i>Software</i>	<ul style="list-style-type: none"> - Integrative Modeling Platform (IMP) (version Not available) - Modeller (version Not available)