

Summary of integrative structure determination of Integrative structure of cGMP-GAFab complex (PDB ID: 9A0M, PDB-Dev ID: PDBDEV_00000058)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - GAFab: chain(s) A, B (399 residues) - GUANOSINE-3',5'-MONOPHOSPHATE: chain(s) C [A], D [B]
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Crosslinking-MS data, PRIDE: PXD020817 - Experimental model, PDB: 6X88 - Experimental model, PDB: 6MZB
2. Representation	
<u>Number of representations</u>	1
<u>Scale</u>	Atomic
<u>Number of rigid and flexible segments</u>	0, 2
3. Restraints	
<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: sulfo-SDA, 40 crosslinks - 1 unique CrossLinkRestraint: BS3, 24 crosslinks - 1 unique CrossLinkRestraint: EDC, 5 crosslinks
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>	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: 104.67 - Ramachandran outliers: 36 - Sidechain outliers: 32
<u>Fit to data used for modeling</u>	Satisfaction of crosslinks: 100.00%
<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>	None
<u>Software</u>	<ul style="list-style-type: none">- Integrative Modeling Platform (IMP) (version Not available)- Modeller (version Not available)