

Summary of integrative structure determination of Integrative structure of Pg-cGMP-GAFab complex (PDB ID: 9A0N, PDB-Dev ID: PDBDEV_0000059)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - PDE GAFab: Chain B (399 residues) - GUANOSINE-3',5'-MONOPHOSPHATE: Chain E (Not available residues) - PDE GAFab: Chain A (399 residues) - GUANOSINE-3',5'-MONOPHOSPHATE: Chain F (Not available residues) - PDE gamma subunit: Chain D (51 residues) - PDE gamma subunit: Chain C (51 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: EDC, 45 cross-links - Experimental model, PDB ID: 6X88 - Experimental model, PDB ID: 6MZB - Comparative model, template PDB ID: Not available
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	2, 4
Rigid bodies	<ul style="list-style-type: none"> - E: None-None - F: None-None - A: - - B: - - C: - - D: -
Flexible units	<ul style="list-style-type: none"> - E: - - F: - - A: 1-399 - B: 1-399 - C: 1-51 - D: 1-51
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: EDC, 45 cross-links - 1 unique CrossLinkRestraint: BS3, 31 cross-links - 1 unique CrossLinkRestraint: sulfo-SDA, 45 cross-links
4. Validation	
Number of ensembles	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 = 210.32, Number of Ramachandran outliers = 39, Number of sidechain outliers = 55
<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	
<i>1. 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)