

Summary of integrative structure determination of Integrative structure of cGMP-GAFab complex (PDB ID: 9A0M, PDB-Dev ID: PDBDEV_0000058)

| 1. Model Composition | |
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| Entry composition | <ul style="list-style-type: none"> - GAFab: Chain A (399 residues) - GUANOSINE-3',5'-MONOPHOSPHATE: Chain C (Not available residues) - GAFab: Chain B (399 residues) - GUANOSINE-3',5'-MONOPHOSPHATE: Chain D (Not available residues) |
| Datasets used for modeling | <ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: sulfo-SDA, 40 cross-links - Experimental model, PDB ID: 6X88 - Experimental model, PDB ID: 6MZB |
| 2. Representation | |
| Resolution | Atomic |
| Number of rigid bodies, flexible units | 2, 2 |
| Rigid bodies | <ul style="list-style-type: none"> - C: None-None - D: None-None - A: - - B: - |
| Flexible units | <ul style="list-style-type: none"> - C: - - D: - - A: 1-399 - B: 1-399 |
| 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: sulfo-SDA, 40 cross-links - 1 unique CrossLinkRestraint: BS3, 24 cross-links - 1 unique CrossLinkRestraint: EDC, 5 cross-links |
| 4. Validation | |
| Number of ensembles | 0 |
| Number of models in ensembles | Not applicable |
| Number of deposited models | 1 |
| Model precision (uncertainty of models) | Model precision can not be calculated with one structure |

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| <i>Data quality</i> | Data quality has not been assessed |
| <i>Model quality: assessment of atomic segments</i> | Model-1: Clashescore = 104.67, Number of Ramachandran outliers = 36, Number of sidechain outliers = 32 |
| <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) |