

**Summary of integrative structure determination of architecture of pol ii(g) and molecular mechanism of transcription regulation by gdown1 (PDBDEV00000025)**

| 1. Model Composition                                                    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
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| <a href="#">Entry composition</a>                                       | <ul style="list-style-type: none"> <li>- RPB7: Chain G (172 residues)</li> <li>- RPB10: Chain J (67 residues)</li> <li>- RPB12: Chain L (58 residues)</li> <li>- RPB9: Chain I (125 residues)</li> <li>- RPB2: Chain B (1174 residues)</li> <li>- RPB1: Chain A (1970 residues)</li> <li>- RPB6: Chain F (127 residues)</li> <li>- RPB11: Chain K (117 residues)</li> <li>- RPB3: Chain C (275 residues)</li> <li>- RPB8: Chain H (150 residues)</li> <li>- RPB4: Chain D (142 residues)</li> <li>- GDOWN1: Chain M (368 residues)</li> <li>- RPB5: Chain E (210 residues)</li> </ul> |
| <a href="#">Datasets used for modeling</a>                              | <ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 5FLM</li> <li>- Experimental model, PDB ID: Not listed</li> <li>- CX-MS data, Linker name and number of cross-links: DSS, 40 cross-links</li> </ul>                                                                                                                                                                                                                                                                                                                                                              |
| 2. Representation                                                       |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| <a href="#">Atomic structural coverage</a>                              | 0%                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| Number of <a href="#">rigid bodies</a> , <a href="#">flexible units</a> | 0, 71                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| Rigid bodies                                                            | <ul style="list-style-type: none"> <li>- A: -</li> <li>- B: -</li> <li>- C: -</li> <li>- D: -</li> <li>- E: -</li> <li>- F: -</li> <li>- G: -</li> <li>- H: -</li> <li>- I: -</li> <li>- J: -</li> <li>- K: -</li> <li>- L: -</li> <li>- M: -</li> </ul>                                                                                                                                                                                                                                                                                                                              |

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| <i>Flexible units</i>                                                  | <ul style="list-style-type: none"> <li>- A: 1-265, 266-270, 271-320, 321-336, 337-354, 355-421, 422-437, 438-1108, 1109-1114, 1115-1267, 1268-1277, 1278-1424, 1425-1427, 1428-1428, 1429-1450, 1451-1458, 1459-1460, 1461-1487, 1488-1970.</li> <li>- B: 1-15, 16-68, 69-80, 81-833, 834-843, 844-874, 875-888, 889-1063, 1064-1076, 1077-1080, 1081-1082, 1083-1110, 1111-1174.</li> <li>- C: 1-1, 2-73, 74-74, 75-132, 133-145, 146-271, 272-275.</li> <li>- D: 1-13, 14-141, 142-142.</li> <li>- E: 1-1, 2-31, 32-32, 33-45, 46-46, 47-111, 112-113, 114-131, 132-132, 133-156, 157-157, 158-185, 186-186, 187-210.</li> <li>- F: 1-45, 46-127.</li> <li>- G: 1-171, 172-172.</li> <li>- H: 1-1, 2-149, 150-150.</li> <li>- I: 1-11, 12-125.</li> <li>- J: 1-67.</li> <li>- K: 1-115, 116-117.</li> <li>- L: 1-14, 15-58.</li> <li>- M: 1-368.</li> </ul> |
| <a href="#">Resolution</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="#">Physical principles</a>                                    | Information about physical principles was not provided                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| <a href="#">Experimental data</a>                                      | - 1 unique CrossLinkRestraint: DSS, 40 cross-links                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| <b>4. Validation</b>                                                   |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <a href="#">Sampling validation</a>                                    | - Information related to sampling validation has not been provided                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| <a href="#">Clustering algorithm ,clustering feature</a>               | Distance threshold-based clustering used if ensembles are deposited, dRMSD                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| <a href="#">Number of ensembles</a>                                    | 1                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| <a href="#">Number of models in ensembles</a>                          | 1640                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| <a href="#">Model precision (uncertainty of models)</a>                | 12.2Å                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| <a href="#">Quality of data</a>                                        | - Quality of input data has not be assessed                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| <a href="#">Model quality: assessment of atomic segments</a>           | Not applicable                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| <a href="#">Model quality: assessment of excluded volume</a>           | - Model-1: Number of violations-8765.0                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
| <a href="#">Fit of the model to information used to compute it</a>     | - CX-MS Fit of mediod: model # 1, percentage satisfied 100.0%                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| <a href="#">Fit of the model to information not used to compute it</a> | - Fit of model to information not used to compute it has not been determined                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| <b>5. Methodology and Software</b>                                     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| <a href="#">Method</a>                                                 | Sampling                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |

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| <a href="#"><i>Name</i></a>     | Replica exchange Monte Carlo                                                                                                                                                                             |
| <a href="#"><i>Details</i></a>  | - Method details unspecified                                                                                                                                                                             |
| <a href="#"><i>Software</i></a> | <ul style="list-style-type: none"><li>- IMP PMI module (version develop-7c7c0f4348)</li><li>- Integrative Modeling Platform (IMP) (version develop-0a5706e202)</li><li>- No location specified</li></ul> |