

**Summary of integrative structure determination of Architecture of Pol II(G) and molecular mechanism of transcription regulation by Gdown1 (PDB ID: 8ZZP, PDB-Dev ID: PDBDEV\_00000025)**

<b>1. Model Composition</b>	
<i>Entry composition</i>	<ul style="list-style-type: none"> <li>- RPB10: Chain J (67 residues)</li> <li>- RPB3: Chain C (275 residues)</li> <li>- RPB6: Chain F (127 residues)</li> <li>- RPB8: Chain H (150 residues)</li> <li>- RPB9: Chain I (125 residues)</li> <li>- RPB5: Chain E (210 residues)</li> <li>- RPB4: Chain D (142 residues)</li> <li>- RPB2: Chain B (1174 residues)</li> <li>- RPB1: Chain A (1970 residues)</li> <li>- RPB12: Chain L (58 residues)</li> <li>- RPB11: Chain K (117 residues)</li> <li>- GDOWN1: Chain M (368 residues)</li> <li>- RPB7: Chain G (172 residues)</li> </ul>
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 5FLM</li> <li>- Experimental model, PDB ID: Not available</li> <li>- Crosslinking-MS data, Linker name and number of cross-links: DSS, 40 cross-links</li> </ul>
<b>2. Representation</b>	
<i>Resolution</i>	Coarse-grained: 1, 2, 3, 5, 7, 27, 37, 49 residue(s) per bead
<i>Number of rigid bodies, flexible units</i>	0, 71
<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>
<i>Structural coverage (rigid bodies)</i>	0%
<b>3. Restraints</b>	

<u>Physical principles</u>	Information about physical principles was not provided
<u>Experimental data</u>	- 1 unique CrossLinkRestraint: DSS, 40 cross-links
<b>4. Validation</b>	
<u>Number of ensembles</u>	1
<u>Number of models in ensembles</u>	1640
<u>Number of deposited models</u>	1
<u>Model precision (uncertainty of models)</u>	12.2, Å
<u>Data quality</u>	Data quality has not been assessed
<u>Model quality: assessment of excluded volume</u>	Satisfaction: 99.87-99.87%
<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<u>1. Method</u>	Sampling
<u>Name</u>	Replica exchange monte carlo
<u>Number of computed models</u>	5000000
<u>Software</u>	- <a href="#">IMP PMI module</a> (version develop-7c7c0f4348) - <a href="#">Integrative Modeling Platform (IMP)</a> (version develop-0a5706e202)