



Full wwPDB Integrative Structure Validation Report

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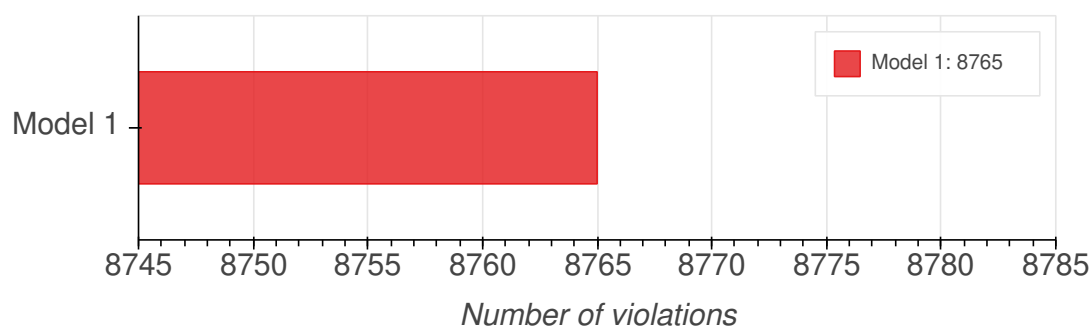
<i>PDB ID</i>	<i>PDBDEV00000025</i>
Molecule Name	Architecture of Pol II(G) and molecular mechanism of transcription regulation by Gdown1
Title	Architecture of Pol II(G) and molecular mechanism of transcription regulation by Gdown1.
Authors	Jishage M;Yu X;Shi Y;Ganesan SJ;Chen WY;Sali A;Chait BT;Asturias FJ;Roeder RG

The following software were used in the production of this report:

Integrative Modeling Validation Package : Version 1.0

1. Overall quality at a glance

Model quality: Excluded Volume Analysis



2. Ensemble information

This entry consists of 1 distinct ensemble.

<i>Ensemble number</i>	<i>Ensemble name</i>	<i>Model ID</i>	<i>Number of models</i>	<i>Clustering method</i>	<i>Clustering feature</i>	<i>Cluster precision</i>
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1	Cluster 0 in state State_0	1	1640	None	dRMSD	12.2
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3. Model composition

3.1 Summary

This entry consists of 1 unique models, with 13 subunits in each model. A total of 3 datasets or restraints was used to build this entry. Each model is represented by 0 rigid bodies and 71 flexible or non-rigid units.

3.2 Entry composition

There is 1 unique type of model in this entry. This model is titled Cluster 0 in state State_0/None respectively.

<i>Model ID</i>	<i>Subunit number</i>	<i>Subunit ID</i>	<i>Subunit name</i>	<i>Chain ID</i>	<i>Total residues</i>
1	1	1	RPB1	A	1970
1	2	2	RPB2	B	1174
1	3	3	RPB3	C	275
1	4	4	RPB4	D	142
1	5	5	RPB5	E	210
1	6	6	RPB6	F	127
1	7	7	RPB7	G	172
1	8	8	RPB8	H	150
1	9	9	RPB9	I	125
1	10	10	RPB10	J	67
1	11	11	RPB11	K	117
1	12	12	RPB12	L	58
1	13	13	GDOWN1	M	368

3.3 Datasets used for modeling

There are 3 unique datasets used to build the models in this entry.

<i>ID</i>	<i>Dataset type</i>	<i>Database name</i>	<i>Data access code</i>
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1	Experimental model	PDB	5FLM
2	Experimental model	Not listed	None
3	CX-MS data	Not listed	None

4. Representation

This entry has only one representation and includes 0 rigid bodies and 71 flexible units.

Chain ID	Rigid bodies	Non-rigid segments
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.
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.
C	-	1-1, 2-73, 74-74, 75-132, 133-145, 146-271, 272-275.
D	-	1-13, 14-141, 142-142.
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.
F	-	1-45, 46-127.
G	-	1-171, 172-172.
H	-	1-1, 2-149, 150-150.
I	-	1-11, 12-125.
J	-	1-67.
K	-	1-115, 116-117.
L	-	1-14, 15-58.
M	-	1-368.

5. Methodology and software

<i>Step number</i>	<i>Protocol ID</i>	<i>Method name</i>	<i>Method type</i>	<i>Number of computed models</i>	<i>Multi state modeling</i>	<i>Multi scale modeling</i>
1	1	Replica exchange monte carlo	Sampling	5000000	False	True

There are 2 software packages reported in this entry.

<i>ID</i>	<i>Software name</i>	<i>Software version</i>	<i>Software classification</i>
1	IMP PMI module	develop-7c7c0f4348	integrative model building
2	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building

6. Data quality

7. Model quality

7.1 Excluded volume satisfaction

Excluded volume satisfaction for the models in the entry are listed below.

<i>Models</i>	<i>Excluded Volume Satisfaction</i>	<i>Number of violations</i>
1	99.87	8765

8. Fit of model to data used for modeling

9. Fit of model to data not used for modeling

10. Uncertainty of model