

Integrative Structure Validation Report ?

February 18, 2025 - 08:28 AM PST

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

Integrative Modeling Validation Version 2.0

Python-IHM Version 1.8

PDB ID	8ZZP
PDB-Dev ID	PDBDEV_00000025
Structure Title	Architecture of Pol II(G) and molecular mechanism of transcription regulation by Gdown1
Structure Authors	Jishage M; Yu X; Shi Y; Ganesan SJ; Chen WY; Sali A; Chait BT; Asturias FJ; Roeder RG
Deposited on	2018-09-28

This is a PDB-IHM IM Structure Validation Report for a publicly released PDB-IHM entry.

We welcome your comments at helpdesk@pdb-ihm.org

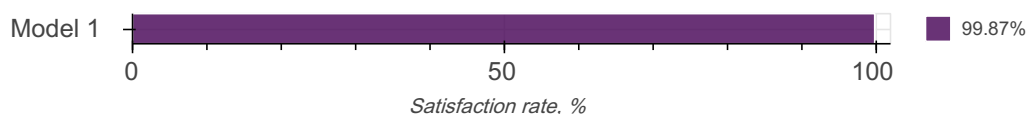
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

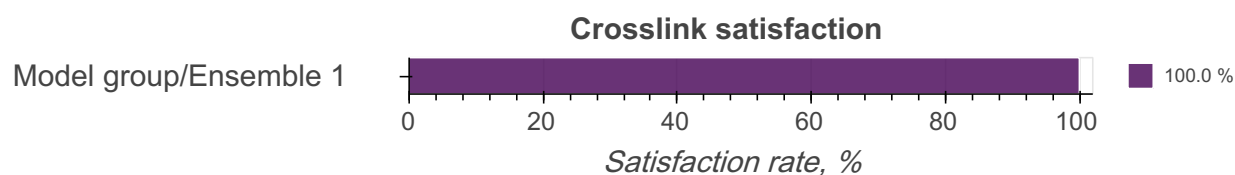
List of references used to build this report is available [here](#).

Overall quality ?

This validation report contains model quality assessments for all structures, data quality and fit to model assessments for SAS and crosslinking-MS datasets. Data quality and fit to model assessments for other datasets and model uncertainty are under development. Number of plots is limited to 256.

Model Quality: Excluded Volume Analysis





Ensemble information ?

This entry consists of 1 distinct ensemble(s).

Summary ?

This entry consists of 1 model(s). A total of 3 datasets were used to build this entry.

Representation ?

This entry has 1 representation(s).

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
1	1	1	RPB1	A	1970	-	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, 1429-1450, 1451-1458, 1459-1460, 1461-1487, 1488-1970	100.00 / 55.58	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		2	RPB2	B	1174	-	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	100.00 / 88.93	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		3	RPB3	C	275	-	1, 2-73, 74, 75-132, 133-145, 146-271, 272-275	100.00 / 93.09	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		4	RPB4	D	142	-	1-13, 14-141, 142	100.00 / 90.14	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		5	RPB5	E	210	-	1, 2-31, 32, 33-45, 46, 47-111, 112-113, 114-131, 132, 133-156, 157, 158-185, 186, 187-210	100.00 / 96.19	Multiscale: Coarse-grained: 1 - 2 residue(s) per bead
		6	RPB6	F	127	-	1-45, 46-127	100.00 / 64.57	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		7	RPB7	G	172	-	1-171, 172	100.00 / 99.42	Coarse-grained: 1 residue(s) per bead
		8	RPB8	H	150	-	1, 2-149, 150	100.00 / 98.67	Coarse-grained: 1 residue(s) per bead
		9	RPB9	I	125	-	1-11, 12-125	100.00 / 91.20	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		10	RPB10	J	67	-	1-67	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
		11	RPB11	K	117	-	1-115, 116-117	100.00 / 98.29	Multiscale: Coarse-grained: 1 - 2 residue(s) per bead
		12	RPB12	L	58	-	1-14, 15-58	100.00 / 75.86	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		13	GDOWN1	M	368	-	1-368	100.00 / 0.00	Multiscale: Coarse-grained: 8 - 10 residue(s) per bead

Datasets used for modeling ?

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

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	5FLM
2	Experimental model	Zenodo	10.5281/zenodo.1438479
3	Crosslinking-MS data	Zenodo	10.5281/zenodo.1438479

Methodology and software ?

This entry is a result of 1 distinct protocol(s).

Step number	Protocol ID	Method name	Method type	Method description	Number of computed models	Multi state modeling	Multi scale modeling
1	1	Sampling	Replica exchange monte carlo	None	5000000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	develop-7c7c0f4348	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	develop-0a5706e202	integrative model building	https://integrativemodeling.org

Data quality ?

Crosslinking-MS

At the moment, data validation is only available for crosslinking-MS data deposited as a fully [compliant](#) dataset in the [PRIDE Crosslinking](#) database. Correspondence between crosslinking-MS and entry entities is established using [pyHMMER](#). Only residue pairs that passed the reported threshold are used for the analysis. The values in the report have to be interpreted in the context of the experiment (i.e. only a minor fraction of in-situ or in-vivo dataset can be used for modeling).

Crosslinking-MS dataset is not available in the [PRIDE Crosslinking](#) database.

Model quality ?

For models with atomic structures, MolProbity analysis is performed. For models with coarse-grained or multi-scale structures, excluded volume analysis is performed.

Excluded volume satisfaction ?

Excluded volume satisfaction for the models in the entry are listed below. The Analysed column shows the number of particle-particle or particle-atom pairs for which excluded volume was analysed.

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
1	6622980	8765	99.87

Fit of model to data used for modeling ?

[Fit of model\(s\) to crosslinking-MS data](#)

Restraint types

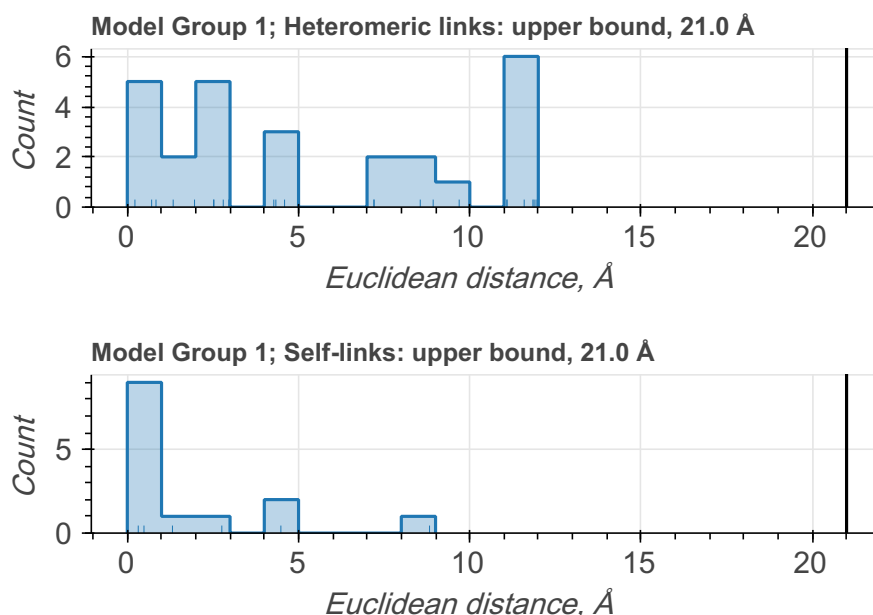
Restraint types are summarized in the table below. Restraints assigned "*by-residue*" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "*coarse-grained*". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 40 crosslinking restraints combined in 40 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	coarse-grained	LYS	coarse-grained	upper bound	21.0	40

Distograms of individual restraints

Restraints with identical thresholds are grouped into one plot. Only the best distance per restraint per model group/ensemble is plotted. Inter- and intramolecular (including self-links) restraints are also grouped into one plot. Distance for a restraint between coarse-grained beads is calculated as a minimal distance between shells; if beads intersect, the distance will be reported as 0.0. A bead with the highest available resolution for a given residue is used for the assessment.



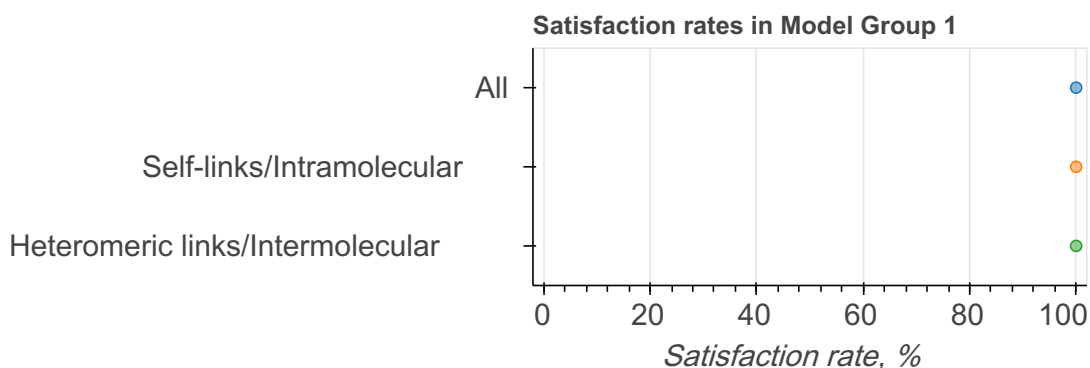
Satisfaction of restraints

Satisfaction of restraints is calculated on a *restraint group* (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (*all/any*). A restraint group is considered satisfied, if the condition was met in at least one model of the model group/ensemble. The number of measured restraints can be smaller than the total number of restraint groups if crosslinks involve non-modeled residues. Only deposited models are used for validation right now.

State group	State	Model group	# of Deposited models/Total	Restraint group type	Satisfied (%)	Violated (%)	Count (Total=40)
1	1	1	1/1640	All	100.00	0.00	40
				Self-links/ Intramolecular	100.00	0.00	14
				Heteromeric links/ Intermolecular	100.00	0.00	26

Per-model satisfaction rates in ensembles

Every point represents one model in a model group/ensemble. Where possible, boxplots with quartile marks are also plotted.



Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgments

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