

Integrative Structure Validation Report ?

February 18, 2025 - 08:31 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	9A16
PDB-Dev ID	PDBDEV_00000078
Structure Title	Integrative structure of the yeast gammaTuSC-Spc110 dimer complex
Structure Authors	Brilot AF; Lyon A; Zelter A; Viswanath S; Maxwell A; MacCoss MJ; Muller EG; Sali A; Davis TN; Agard DA
Deposited on	2021-03-09

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

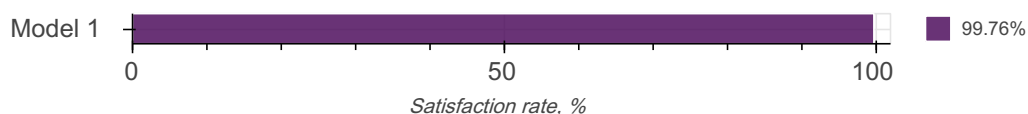
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

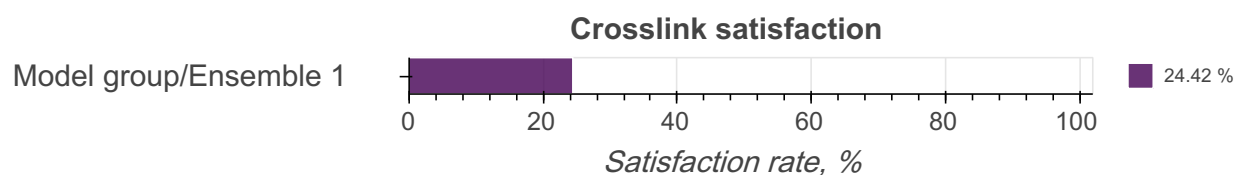
List of references used to build this report is available [here](#).

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	Spc97	A	823	-	1-54, 55-80, 81-89, 90-205, 206-242, 243-304, 305-319, 320-490, 491-553, 554-614, 615-622, 623-714, 715-753, 754-800, 801-823	100.00 / 69.87	Multiscale: Coarse-grained: 1 - 20 residue(s) per bead
		2	Spc98	B	846	-	1-179, 180-367, 368-378, 379-612, 613-627, 628-671, 672-718, 719-743, 744-755, 756-780, 781-797, 798-846	100.00 / 66.78	Multiscale: Coarse-grained: 1 - 20 residue(s) per bead
		3	Tub4	C	473	-	1-445, 446-473	100.00 / 94.08	Multiscale: Coarse-grained: 1 - 20 residue(s) per bead
				D					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		4	Spc110	E	222	-	1-165, 166-205, 206-222	100.00 / 18.02	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
				F					

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	5FLZ
2	Crosslinking-MS data	Zenodo	10.5281/zenodo.4584457
3	Crosslinking-MS data	Zenodo	10.5281/zenodo.4584457

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	500000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.14.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.14.0	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	2463090	5910	99.76

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

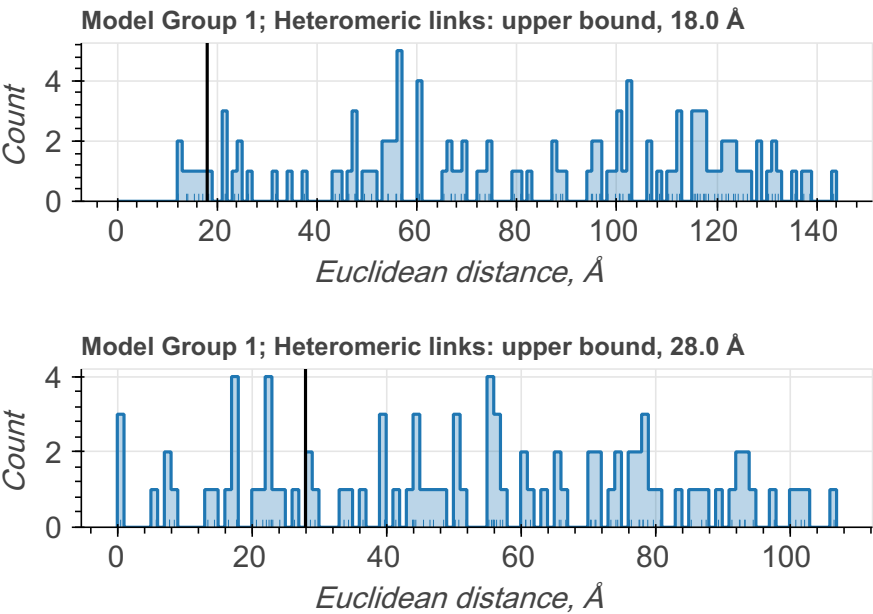
Restraint types are summarized in the table below. Restraints assigned "[by-residue](#)" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "[coarse-grained](#)". [Restraint group](#) represents a set of crosslinking restraints applied collectively in the modeling.

There are 206 crosslinking restraints combined in 86 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
EDC	GLU	CA	LYS	CA	upper bound	18.0	12
EDC	ASP	coarse-grained	LYS	coarse-grained	upper bound	18.0	66
EDC	ASP	CA	LYS	CA	upper bound	18.0	6
EDC	GLU	coarse-grained	LYS	coarse-grained	upper bound	18.0	30
DSS	LYS	coarse-grained	LYS	coarse-grained	upper bound	28.0	82
DSS	LYS	CA	LYS	CA	upper bound	28.0	10

[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.



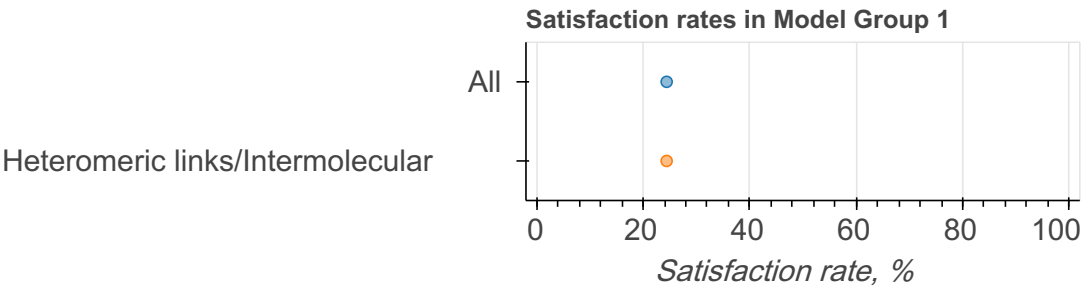
Satisfaction of restraints

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=86)
1	1	1	1/2840	All	24.42	75.58	86
				Heteromeric links/ Intermolecular	24.42	75.58	86

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

The development of integrative model validation metrics, implementation of a model validation pipeline, and creation of a validation report for integrative structures are funded by NSF awards to the [PDB-IHM team](#) (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250) and awards from NSF, NIH, and DOE to the [RCSB PDB](#) (DBI-2321666, R01GM157729, and DE-SC0019749). The PDB-IHM team and members of the [Sali lab](#) contributed model validation metrics and software packages.

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