

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 | 9A15 |
| PDB-Dev ID | PDBDEV_00000077 |
| Structure Title | Integrative structure of the yeast gammaTuSC-Spc110 monomer 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

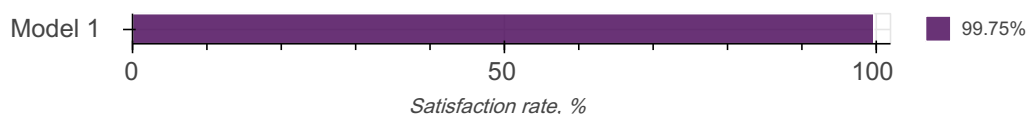
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

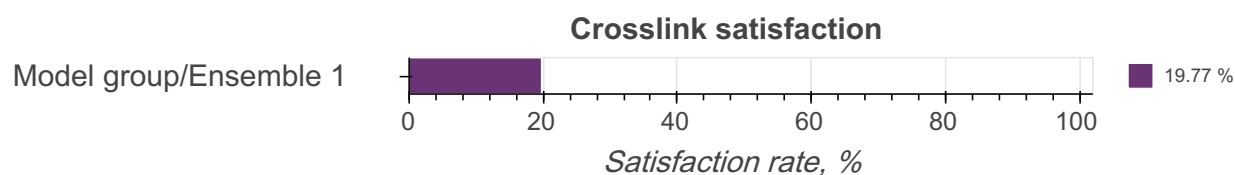
List of references used to build this report is available [here](#).

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 |

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 | 2295153 | 5721 | 99.75 |

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

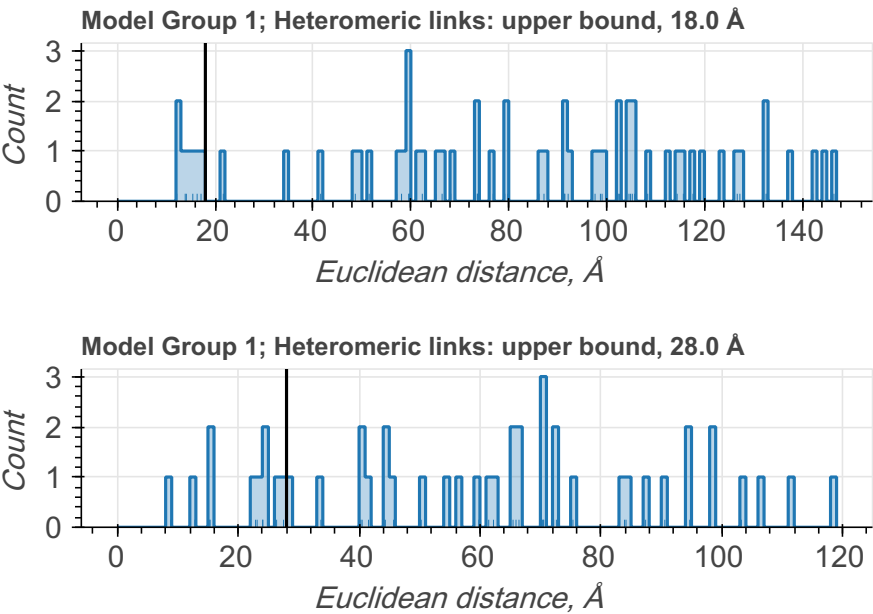
Restraint types are summarized in the table below. Restraints assigned "[by-residue](#)" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "[coarse-grained](#)". [Restraint group](#) represents a set of crosslinking restraints applied collectively in the modeling.

There are 103 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 | 6 |
| EDC | ASP | coarse-grained | LYS | coarse-grained | upper bound | 18.0 | 33 |
| EDC | ASP | CA | LYS | CA | upper bound | 18.0 | 3 |
| EDC | GLU | coarse-grained | LYS | coarse-grained | upper bound | 18.0 | 15 |
| DSS | LYS | coarse-grained | LYS | coarse-grained | upper bound | 28.0 | 41 |
| DSS | LYS | CA | LYS | CA | upper bound | 28.0 | 5 |

[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.



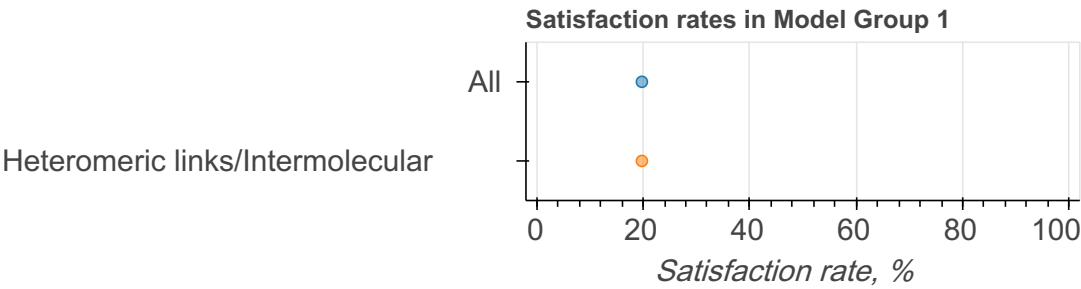
Satisfaction of restraints

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 | 1/1621 | All | 19.77 | 80.23 | 86 |
| | | | | Heteromeric links/ Intermolecular | 19.77 | 80.23 | 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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