

Integrative Structure Validation Report ?

February 18, 2025 - 08:30 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	9A0T
PDB-Dev ID	PDBDEV_00000065
Structure Title	Molecular architecture of the endocytic TPLATE/TSET complex
Structure Authors	Yperman K; Wang J; Eeckhout D; Winkler J; Vu LD; Vandorpe M; Grones P; Mylle E; Kraus M; Merceron R; Nolf J; Mor E; De Bruyn P; Loris R; Potocky M; Savvides SN; De Rybel B; De Jager G; Van Damme D; Pleskot R
Deposited on	2020-12-04

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

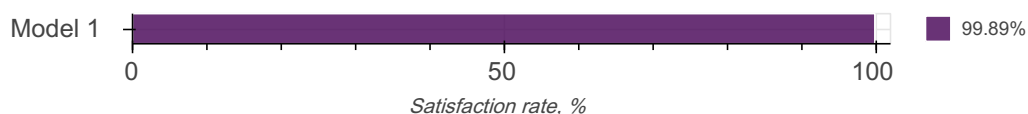
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

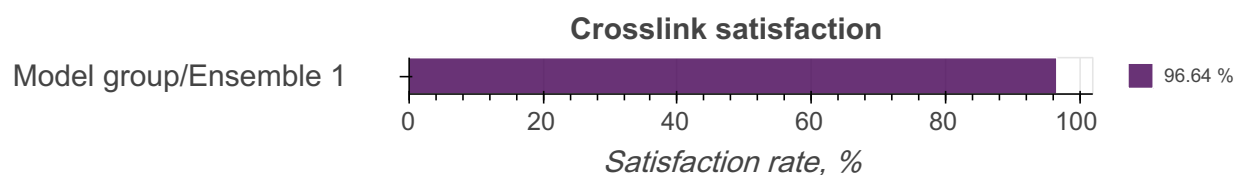
List of references used to build this report is available [here](#).

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 28 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	lol	A	147	1-147	-	100.00 / 100.00	Coarse-grained: 1 residue(s) per bead
		2	tash3	B	1198	104-171, 205-258, 281-419, 464-499, 551-686, 716-734, 766-812, 1131-1198	1-103, 172-204, 259-280, 420-463, 500-550, 687-715, 735-765, 813-1130	100.00 / 47.33	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		3	tplate	C	1176	1-467, 771-1045	468-770, 1046-1176	100.00 / 63.10	Multiscale: Coarse-grained: 1 - 50 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
		4	tml	D	646	1-40, 96-191, 407-646	41-95, 192-406	100.00 / 58.20	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		5	wd1	E	1592	18-349, 450-1002, 1303-1592	1-17, 350-449, 1003-1302	100.00 / 73.81	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		6	wd2	F	1376	1-52, 125-534, 676-752, 771-974, 1012-1167	53-124, 535-675, 753-770, 975-1011, 1168-1376	100.00 / 65.33	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		7	eh1	G	1019	1-110, 346-449	111-345, 450-1019	100.00 / 21.00	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
		8	eh2	H	1218	1-112, 400-512	113-399, 513-1218	100.00 / 18.47	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead

Datasets used for modeling ?

There are 28 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Comparative model	Zenodo	10.5281/zenodo.3979550
2	Comparative model	Zenodo	10.5281/zenodo.3979550
3	Comparative model	Zenodo	10.5281/zenodo.3979550

ID	Dataset type	Database name	Data access code
4	Comparative model	Zenodo	10.5281/zenodo.3979550
5	Comparative model	Zenodo	10.5281/zenodo.3979550
6	Comparative model	Zenodo	10.5281/zenodo.3979550
7	Comparative model	Zenodo	10.5281/zenodo.3979550
8	Comparative model	Zenodo	10.5281/zenodo.3979550
9	Comparative model	Zenodo	10.5281/zenodo.3979550
10	Comparative model	Zenodo	10.5281/zenodo.3979550
11	Comparative model	Zenodo	10.5281/zenodo.3979550
12	Comparative model	Zenodo	10.5281/zenodo.3979550
13	Comparative model	Zenodo	10.5281/zenodo.3979550
14	Comparative model	Zenodo	10.5281/zenodo.3979550
15	Crosslinking-MS data	Zenodo	10.5281/zenodo.3979550
16	Experimental model	PDB	5NZR
17	Experimental model	PDB	5MU7
18	Experimental model	PDB	6OWT
19	Experimental model	PDB	2KYM
20	Experimental model	PDB	2JKR
21	Experimental model	PDB	5JP2
22	Experimental model	PDB	5AWS
23	Experimental model	PDB	3G9H
24	Experimental model	PDB	3MKQ
25	Experimental model	PDB	3MKR
26	Experimental model	PDB	2YNP
27	Experimental model	PDB	6YEU
28	Experimental model	PDB	6YET

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	1000000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.12.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.12.0	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	9845703	11105	99.89

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

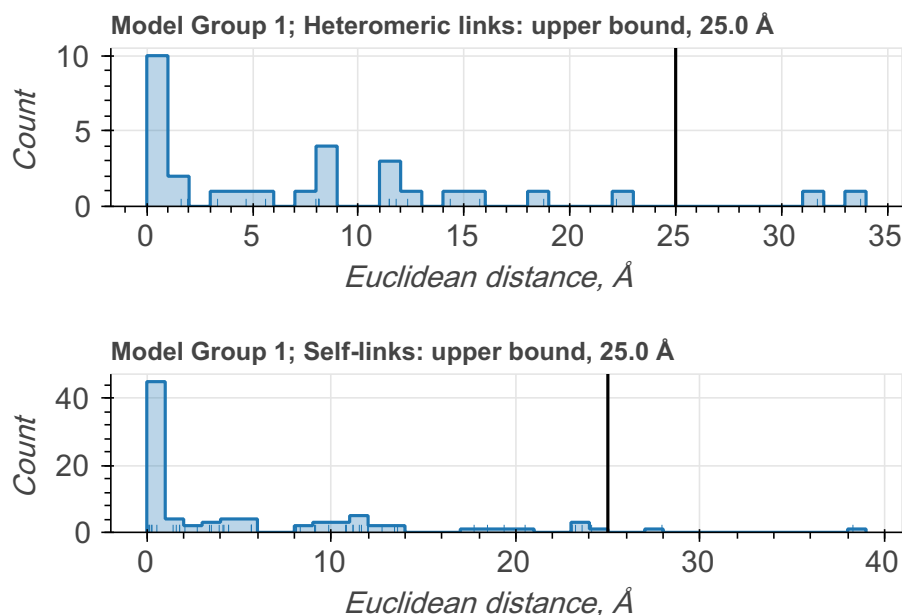
Restraint types are summarized in the table below. Restraints assigned "[by-residue](#)" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "[coarse-grained](#)". [Restraint group](#) represents a set of crosslinking restraints applied collectively in the modeling.

There are 119 crosslinking restraints combined in 119 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
BS3	LYS	CA	LYS	CA	upper bound	25.0	19
BS3	LYS	coarse-grained	LYS	coarse-grained	upper bound	25.0	99
BS3	ALA	coarse-grained	LYS	coarse-grained	upper bound	25.0	1

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

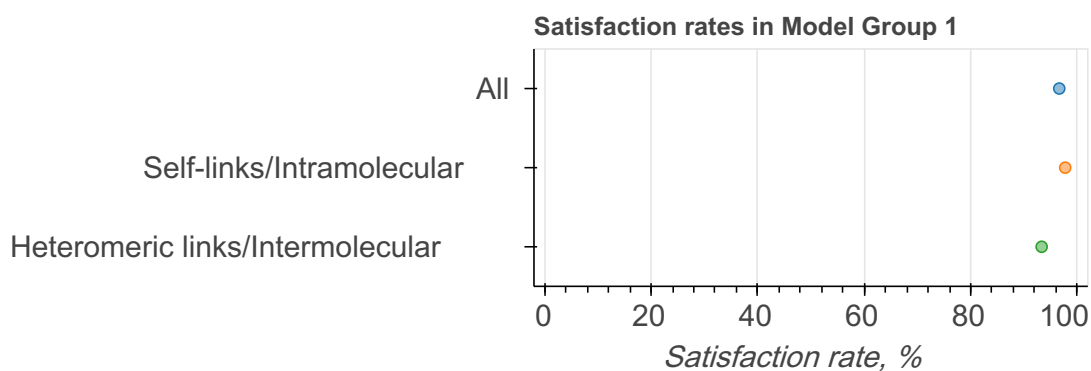
Satisfaction of restraints is calculated on a [restraint group](#) (a set of crosslinking restraints applied collectively in the modeling) level. Satisfaction of a restraint group depends on satisfaction of individual restraints in the group and the conditionality (all/any). A restraint group is considered 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=119)
1	1	1	1/3981	All	96.64	3.36	119
				Self-links/ Intramolecular	97.75	2.25	89
				Heteromeric links/ Intermolecular	93.33	6.67	30

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.

Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods. Team members from the labs of Dr. Juri Rappsilber, Dr. Alexander Leitner, Dr. Andrea Graziadei, and members of [PRIDE](#) database are acknowledged for their advice and support in implementing crosslinking-MS validation methods. We are grateful to Dr. Shruthi Viswanath for discussions about uncertainty assessment of integrative structural models.

Members of the [wwPDB Integrative/Hybrid Methods Task Force](#) provided recommendations and community support for the project.