

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	8ZZQ
PDB-Dev ID	PDBDEV_00000026
Structure Title	The proteasome-interacting Ecm29 protein disassembles the 26S proteasome in response to oxidative stress
Structure Authors	Wang X; Chemmama IE; Yu C; Huszagh A; Xu Y; Viner R; Block SA; Cimerancic P; Rychnovsky SD; Ye Y; Sali A; Huang L
Deposited on	2018-10-05

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

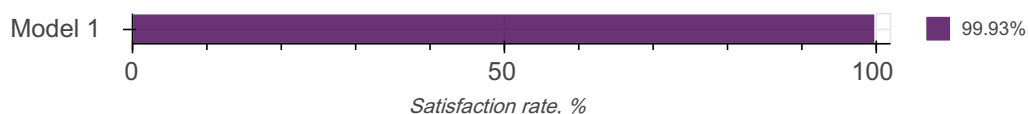
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

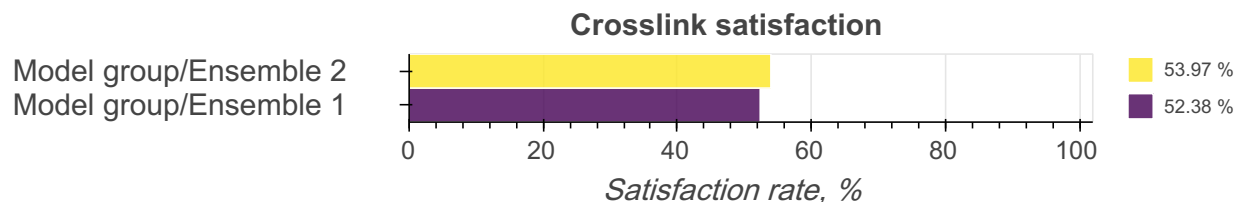
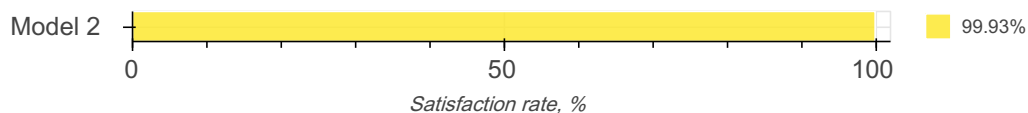
List of references used to build this report is available [here](#).

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 2 distinct ensemble(s).

Summary ?

This entry consists of 2 model(s). A total of 7 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	1-2	1	Rpt6	A	406	-	1-23, 24-250, 251-266, 267-397, 398-406	100.00 / 88.18	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		2	Rpt4	B	389	-	1-14, 15-389	100.00 / 96.40	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	Rpt5	C	439	-	1-43, 44-99, 100-119, 120-439	100.00 / 85.65	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		4	Rpt2	D	440	-	1-64, 65-84, 85-90, 91-429, 430-440	100.00 / 81.59	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		5	Rpt3	E	418	-	1-38, 39-418	100.00 / 90.91	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		6	Rpt1	F	433	-	1-46, 47-72, 73-79, 80-433	100.00 / 87.76	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		7	Rpn12	G	350	-	1-88, 89-130, 131-134, 135-350	100.00 / 73.71	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		8	Rpn10	H	377	-	1-193, 194-377	100.00 / 51.19	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
		9	Rpn11	I	310	-	1-27, 28-163, 164-189, 190-310	100.00 / 82.90	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		10	Rpn15	J	70	-	1-2, 3-27, 28-34, 35-68, 69-70	100.00 / 84.29	Multiscale: Coarse-grained: 1 - 7 residue(s) per bead
		11	Rpn1	K	908	-	1-105, 106-170, 171-178, 179-301, 302-308, 309-618, 619-652, 653-848, 849-870, 871-908	100.00 / 80.62	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		12	Rpn2	L	953	-	1-2, 3-272, 273-320, 321-750, 751-752, 753-816, 817-877, 878-917, 918-922, 923-939, 940-953	100.00 / 86.15	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		13	Rpn3	M	534	-	1-56, 57-101, 102-103, 104-116, 117-159, 160-496, 497-499, 500-525, 526-534	100.00 / 78.84	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		14	Rpn5	N	456	-	1-4, 5-24, 25-39, 40-94, 95-98, 99-112, 113-116, 117-132, 133-138, 139-332, 333-340, 341-454, 455-456	100.00 / 90.57	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		15	Rpn6	O	422	-	1, 2-422	100.00 / 99.76	Coarse-grained: 1 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
		16	Rpn7	P	389	-	1-13, 14-389	100.00 / 96.66	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		17	Rpn8	Q	324	-	1-3, 4-142, 143-151, 152-295, 296-324	100.00 / 87.35	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
		18	Rpn9	R	376	-	1-2, 3-54, 55-56, 57-376	100.00 / 98.94	Multiscale: Coarse-grained: 1 - 2 residue(s) per bead
		19	ecm29	S	1845	352-504, 686-760, 788-911, 934-1035, 1062-1306, 1331-1666, 1689-1738	1-351, 505-685, 761-787, 912-933, 1036-1061, 1307-1330, 1667-1688, 1739-1845	100.00 / 58.81	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead

Datasets used for modeling ?

There are 7 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	5GJR
2	Experimental model	Zenodo	10.5281/zenodo.1445841
3	Experimental model	PDB	1U6G
4	Comparative model	Zenodo	10.5281/zenodo.1445841
5	Experimental model	PDB	3W3W
6	Comparative model	Zenodo	10.5281/zenodo.1445841
7	Crosslinking-MS data	Zenodo	10.5281/zenodo.1445841

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	3750000	False	True

There are 3 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
3	MODELLER	9.17	comparative modeling	https://salilab.org/modeller/

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	33142011	22257	99.93

Model ID	Analysed	Number of violations	Excluded Volume Satisfaction (%)
2	33142011	22180	99.93

Fit of model to data used for modeling ?

Fit of model(s) to crosslinking-MS data

Restraint types

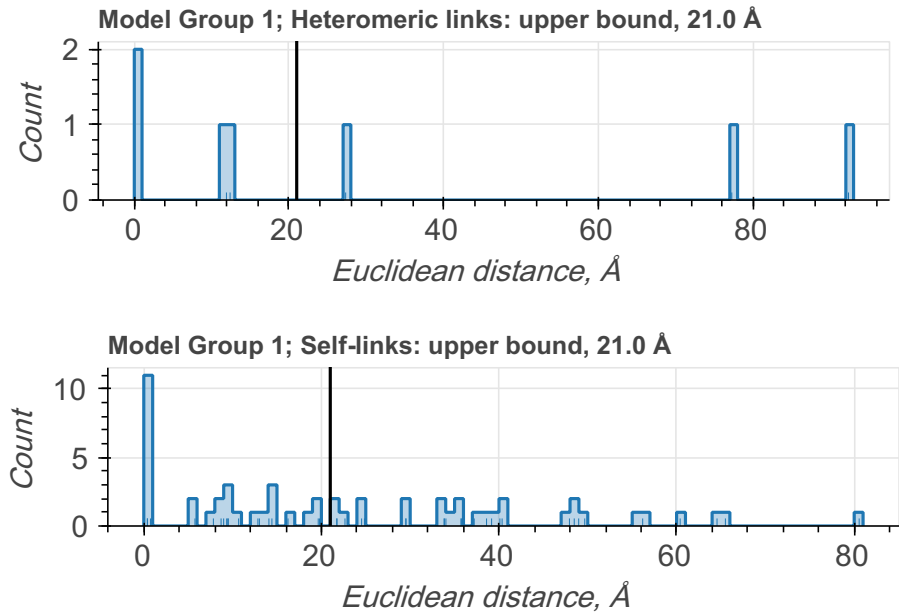
Restraint types are summarized in the table below. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

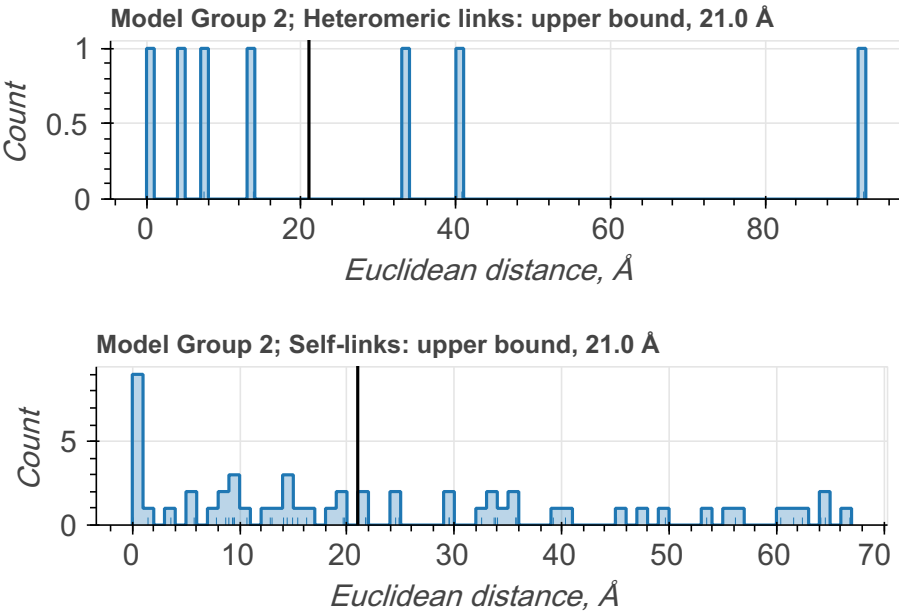
There are 63 crosslinking restraints combined in 63 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSSO	LYS	CA	LYS	CA	upper bound	21.0	39
DSSO	LYS	coarse-grained	LYS	coarse-grained	upper bound	21.0	24

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.





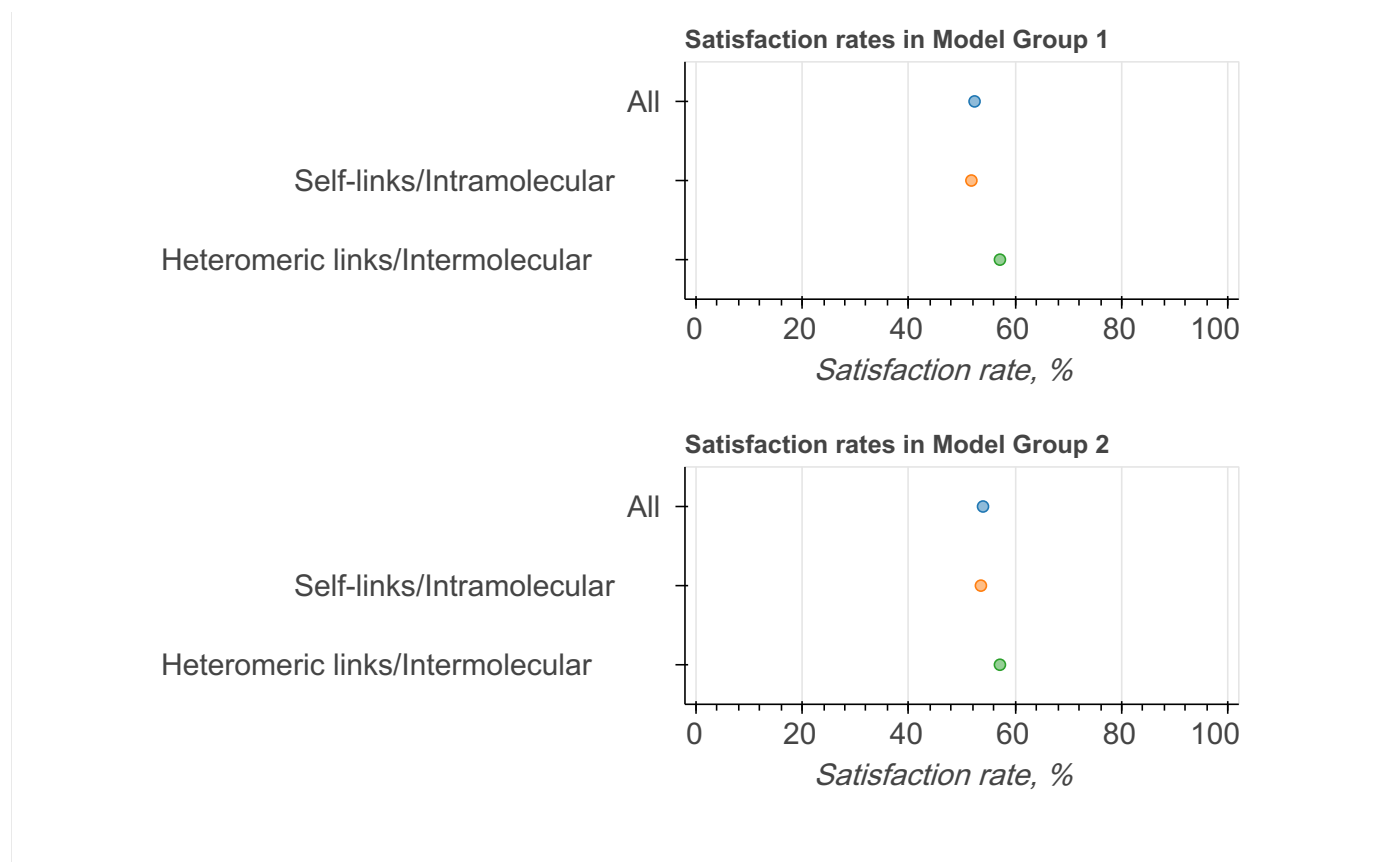
Satisfaction of restraints

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=63)
1	1	1	1/11980	All	52.38	47.62	63
				Self-links/ Intramolecular	51.79	48.21	56
				Heteromeric links/ Intermolecular	57.14	42.86	7
1	1	2	1/6261	All	53.97	46.03	63
				Self-links/ Intramolecular	53.57	46.43	56
				Heteromeric links/ Intermolecular	57.14	42.86	7

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.

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