

Integrative Structure Validation Report

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

IHMValidation Version 3.2

Python-IHM Version 2.9

PDB ID	9AAA pdb_00009aaa
Structure Title	Integrative model of mTORC2-AKT1
Structure Authors	Hancock, M.; Mondal, D.; Taylor, M.S.; Cole, P.A.
Deposited on	2025-10-01

This is a PDB-IHM Structure Validation Report.

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](#).

1. Overview

1.1. Summary

This entry consists of 1 model(s). A total of 7 dataset(s) were used to build this entry.

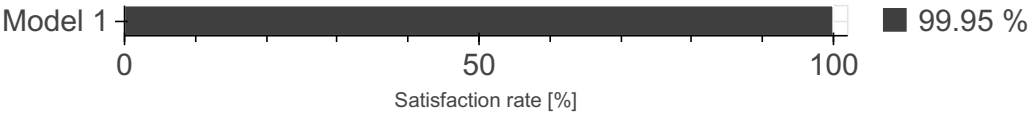
Name	Type	Count
3DEM volume	Experimental data	2
Crosslinking-MS data	Experimental data	2
De Novo model	Starting model	1

Name	Type	Count
Experimental model	Starting model	2

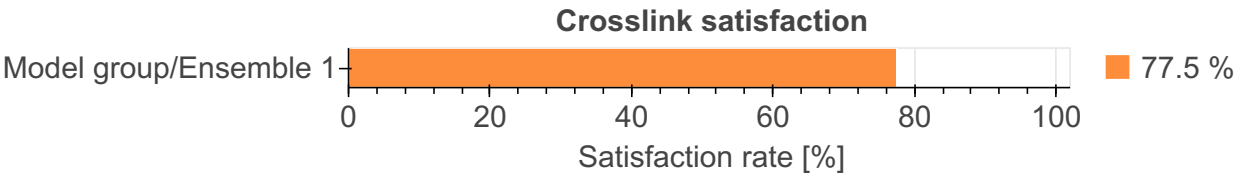
1.2. Overall quality ?

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 ?



Fit to Data Used for Modeling ?



2. Model Details ?

2.1. Ensemble information ?

This entry consists of 1 distinct ensemble(s).

2.2. 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	MTOR	A	2549	14-22, 46-53, 80-93, 120-135, 141-157, 162-197, 203-226, 233-245, 257-295, 360-551, 570-595, 599-637, 646-905, 926-1240, 1262-1814, 1870-2434, 2492-2549	1-13, 23-45, 54-79, 94-119, 136-140, 158-161, 198-202, 227-232, 246-256, 296-359, 552-569, 596-598, 638-645, 906-925, 1241-1261, 1815-1869, 2435-2491	100.00 / 85.68	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				B					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
		2	RICTOR	C	1708	22-858, 866-1017, 1419-1449, 1478-1539, 1606-1694	1-21, 859-865, 1018-1418, 1450-1477, 1540-1605, 1695-1708	100.00 / 68.56	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				D					
		3	MLST8	E	326	8-324	1-7, 325-326	100.00 / 97.24	Multiscale: Coarse-grained: 1 - 7 residue(s) per bead
				F					
		4	MSIN1	G	522	1-39, 66-154, 155-267, 278-353, 383-415, 421-481	40-65, 184-191, 268-277, 354-382, 416-420, 482-522	100.00 / 78.74	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				H					
		5	AKT1	I	480	1-123, 144-229, 234-425	124-143, 208-209	87.71 / 95.25	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				J					

2.3. 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	pdb_00009zbk
2	Experimental model	PDB	pdb_00007lc1
3	De Novo model	AlphaFoldDB	AF-P31749-F1
4	Crosslinking-MS data	Zenodo	10.5281/zenodo.17237325
5	Crosslinking-MS data	Zenodo	10.5281/zenodo.17237325
6	3DEM volume	EMDB	EMD-44037
7	3DEM volume	Zenodo	10.5281/zenodo.17237325

2.4. 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	Not available	1	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.21.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.21.0	integrative model building	https://integrativemodeling.org

3. Data quality ?

3.2. 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.

3.3. 3DEM ?

This section describes quality of the 3DEM datasets

3DEM dataset is not available in the *EMDB* database.

4. 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.

4.1a. Excluded Volume Analysis ?

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	42168336	21371	99.95

5. Fit to Data Used for Modeling Assessment ?

5.2. Crosslinking-MS ?

5.2.1. Restraint types ?

This table summarizes information about crosslinker(s) used for data generation, and how crosslinking information was translated into

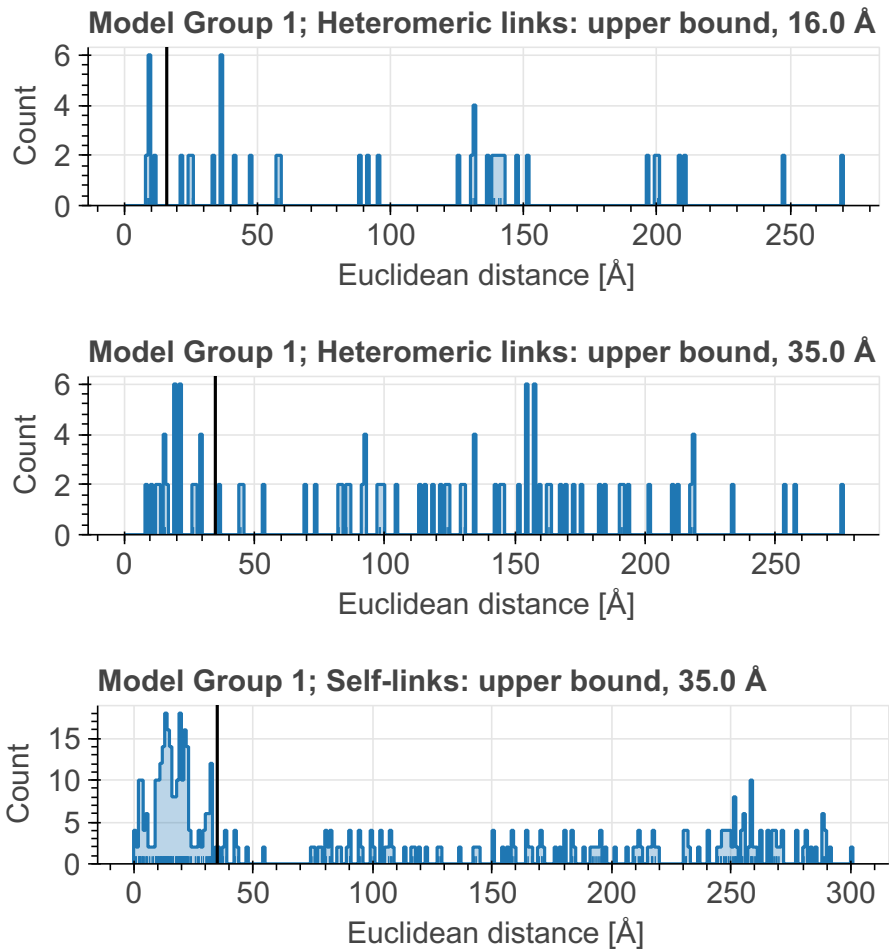
actual modeling restraints. Restraints assigned "by-residue" are interpreted as between CA atoms. Restraints between coarse-grained beads are indicated as "coarse-grained". *Restraint group* represents a set of crosslinking restraints applied collectively in the modeling.

There are 800 crosslinking restraints combined in 200 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
DSS	LYS	CA	LYS	CA	upper bound	35.00	500
DSS	LYS	coarse-grained	LYS	coarse-grained	upper bound	35.00	224
EDC	GLU	CA	LYS	CA	upper bound	16.00	24
EDC	ASP	CA	LYS	CA	upper bound	16.00	16
EDC	GLU	coarse-grained	LYS	coarse-grained	upper bound	16.00	8
EDC	ASP	coarse-grained	LYS	coarse-grained	upper bound	16.00	28

Distograms of individual restraints

Distograms (i.e., histogram plots of distances) provide an overview of distributions of distances between residues for which chemical crosslinks were identified. The shift of the distogram relative to the threshold value may indicate a poor model. 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.



5.2.2. 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=200)
1	1	1	1/1	All	77.50	22.50	200
				Self-links/ Ambiguous	93.01	6.99	143
				Heteromeric links/ Intermolecular	38.60	61.40	57

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.



5.3. 3DEM

This section describes fit of models to the 3DEM data. Only results for the representative model, selected as a first model with the largest number of asymmetric units.

3DEM validation for coarse-grained structures is under development.

6. Fit to Data Used for Validation Assessment ?

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

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