

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	9A12
PDB-Dev ID	PDBDEV_00000074
Structure Title	Modeling of the interaction between doublecortin and microtubule, NDCs fixed at diagonal (#2) orientation
Structure Authors	Rafiei A; Lee L; Crowder A; Saltzberg D; Sali A; Brouhard G; Schreimer DC
Deposited on	2021-02-09

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

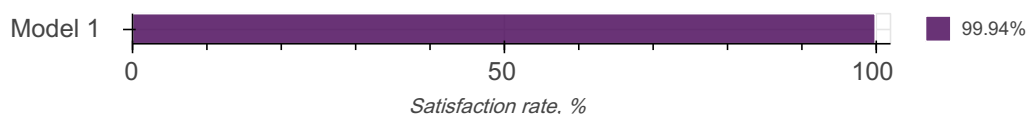
A user guide is available at https://pdb-ihm.org/validation_help.html with specific help available everywhere you see the ? symbol.

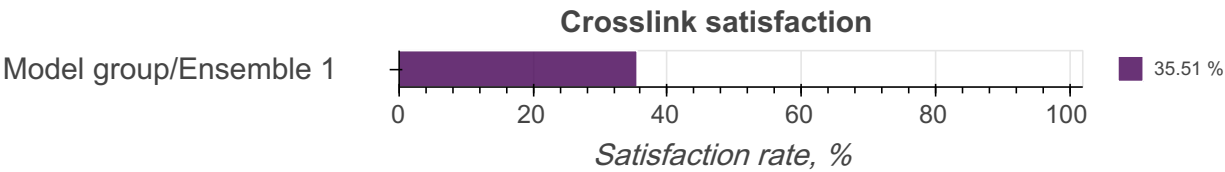
List of references used to build this report is available [here](#).

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 4 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	Doublecortin	A	365	51-140, 177-251	141-176, 252-330	76.71 / 58.93	Multiscale: Coarse-grained: 1 - 10 residue(s) per bead
				B					
		2	Alpha-Tubulin	C	451	1-37, 47-435	-	94.46 / 100.00	Coarse-grained: 1 residue(s) per bead
				D					
				E					
				F					
				G					
				H					
				I					
				J					
				K					
		3	Beta-Tubulin	L	445	1-37, 38-429	-	96.40 / 100.00	Coarse-grained: 1 residue(s) per bead
				M					
				N					

ID	Model(s)	Entity ID	Molecule name	Chain(s) [auth]	Total residues	Rigid segments	Flexible segments	Model coverage/ Starting model coverage (%)	Scale
				O					
				P					
				Q					
				R					
				S					
				T					

Datasets used for modeling ?

There are 4 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
1	Experimental model	PDB	4ATU
2	Experimental model	PDB	6FNZ
3	Experimental model	PDB	6EVZ
4	Crosslinking-MS data	Zenodo	10.5281/zenodo.4526498

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	240000	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	32389176	19061	99.94

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 7452 crosslinking restraints combined in 414 restraint groups.

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
LCSDA	LYS	coarse-grained	PRO	coarse-grained	upper bound	30.0	72
LCSDA	GLU	coarse-grained	LYS	coarse-grained	upper bound	30.0	810
LCSDA	GLN	coarse-grained	LYS	coarse-grained	upper bound	30.0	126
LCSDA	LEU	coarse-grained	LYS	coarse-grained	upper bound	30.0	198
LCSDA	ILE	coarse-grained	LYS	coarse-grained	upper bound	30.0	180

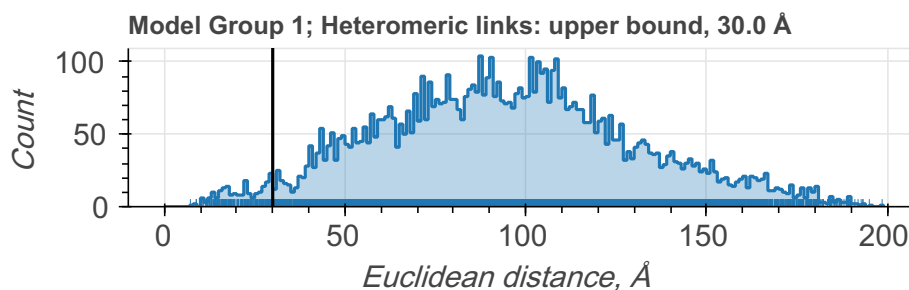
Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
LCSDA	GLU	CA	LYS	CA	upper bound	30.0	342
LCSDA	LYS	CA	TYR	CA	upper bound	30.0	126
LCSDA	ASP	CA	LYS	CA	upper bound	30.0	90
LCSDA	LYS	CA	THR	CA	upper bound	30.0	90
LCSDA	GLY	CA	LYS	CA	upper bound	30.0	216
LCSDA	HIS	CA	LYS	CA	upper bound	30.0	108
LCSDA	ALA	CA	LYS	CA	upper bound	30.0	126
LCSDA	LEU	CA	LYS	CA	upper bound	30.0	162
LCSDA	LYS	CA	SER	CA	upper bound	30.0	72
LCSDA	ALA	coarse-grained	TYR	coarse-grained	upper bound	30.0	36
LCSDA	ALA	coarse-grained	THR	coarse-grained	upper bound	30.0	72
LCSDA	THR	coarse-grained	TYR	coarse-grained	upper bound	30.0	18
LCSDA	SER	coarse-grained	TYR	coarse-grained	upper bound	30.0	36
LCSDA	THR	coarse-grained	THR	coarse-grained	upper bound	30.0	18
LCSDA	SER	coarse-grained	THR	coarse-grained	upper bound	30.0	18
LCSDA	GLU	coarse-grained	THR	coarse-grained	upper bound	30.0	36
LCSDA	GLU	coarse-grained	SER	coarse-grained	upper bound	30.0	72
LCSDA	GLY	coarse-grained	THR	coarse-grained	upper bound	30.0	18
LCSDA	GLY	coarse-grained	SER	coarse-grained	upper bound	30.0	18
LCSDA	ALA	coarse-grained	SER	coarse-grained	upper bound	30.0	36
LCSDA	ASP	coarse-grained	LYS	coarse-grained	upper bound	30.0	324
LCSDA	LYS	coarse-grained	TYR	coarse-grained	upper bound	30.0	270
LCSDA	LYS	coarse-grained	THR	coarse-grained	upper bound	30.0	126
LCSDA	GLY	coarse-grained	LYS	coarse-grained	upper bound	30.0	198
LCSDA	HIS	coarse-grained	LYS	coarse-grained	upper bound	30.0	252
LCSDA	ALA	coarse-grained	LYS	coarse-grained	upper bound	30.0	216
LCSDA	THR	CA	THR	CA	upper bound	30.0	36
LCSDA	GLY	CA	THR	CA	upper bound	30.0	144
LCSDA	SER	CA	THR	CA	upper bound	30.0	72
LCSDA	GLY	CA	SER	CA	upper bound	30.0	72
LCSDA	GLU	CA	THR	CA	upper bound	30.0	36
LCSDA	CYS	CA	THR	CA	upper bound	30.0	54
LCSDA	ASP	CA	THR	CA	upper bound	30.0	90
LCSDA	LEU	CA	THR	CA	upper bound	30.0	144
LCSDA	GLN	CA	THR	CA	upper bound	30.0	54

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
LCSDA	PHE	CA	THR	CA	upper bound	30.0	36
LCSDA	HIS	CA	THR	CA	upper bound	30.0	18
LCSDA	ALA	CA	THR	CA	upper bound	30.0	54
LCSDA	ALA	CA	TYR	CA	upper bound	30.0	90
LCSDA	GLN	coarse-grained	SER	coarse-grained	upper bound	30.0	36
LCSDA	SER	coarse-grained	SER	coarse-grained	upper bound	30.0	18
LCSDA	GLN	coarse-grained	TYR	coarse-grained	upper bound	30.0	18
LCSDA	PHE	coarse-grained	SER	coarse-grained	upper bound	30.0	18
LCSDA	LYS	coarse-grained	SER	coarse-grained	upper bound	30.0	198
LCSDA	LYS	coarse-grained	PHE	coarse-grained	upper bound	30.0	216
LCSDA	LYS	coarse-grained	TRP	coarse-grained	upper bound	30.0	18
LCSDA	ILE	CA	LYS	CA	upper bound	30.0	36
LCSDA	ARG	coarse-grained	LYS	coarse-grained	upper bound	30.0	54
LCSDA	HIS	coarse-grained	SER	coarse-grained	upper bound	30.0	36
LCSDA	ILE	CA	THR	CA	upper bound	30.0	36
LCSDA	ARG	CA	THR	CA	upper bound	30.0	36
LCSDA	THR	CA	TYR	CA	upper bound	30.0	18
LCSDA	MET	CA	THR	CA	upper bound	30.0	18
LCSDA	GLN	CA	TYR	CA	upper bound	30.0	72
LCSDA	CYS	CA	TYR	CA	upper bound	30.0	54
LCSDA	LEU	CA	TYR	CA	upper bound	30.0	90
LCSDA	HIS	CA	TYR	CA	upper bound	30.0	36
LCSDA	ASP	CA	TYR	CA	upper bound	30.0	108
LCSDA	PHE	CA	TYR	CA	upper bound	30.0	36
LCSDA	GLY	CA	TYR	CA	upper bound	30.0	90
LCSDA	LYS	coarse-grained	MET	coarse-grained	upper bound	30.0	198
LCSDA	LYS	coarse-grained	LYS	coarse-grained	upper bound	30.0	18
LCSDA	MET	coarse-grained	SER	coarse-grained	upper bound	30.0	18
LCSDA	PRO	CA	THR	CA	upper bound	30.0	18
LCSDA	ASN	CA	THR	CA	upper bound	30.0	18
LCSDA	ASN	coarse-grained	LYS	coarse-grained	upper bound	30.0	108
LCSDA	LYS	CA	PRO	CA	upper bound	30.0	18
LCSDA	TYR	CA	TYR	CA	upper bound	30.0	18
LCSDA	ILE	CA	TYR	CA	upper bound	30.0	36
LCSDA	ASN	CA	TYR	CA	upper bound	30.0	18

Linker	Residue 1	Atom 1	Residue 2	Atom 2	Restraint type	Distance, Å	Count
LCSDA	TRP	CA	TYR	CA	upper bound	30.0	18
LCSDA	GLU	CA	TYR	CA	upper bound	30.0	36
LCSDA	ARG	coarse-grained	THR	coarse-grained	upper bound	30.0	18
LCSDA	CYS	coarse-grained	LYS	coarse-grained	upper bound	30.0	36
LCSDA	THR	coarse-grained	TRP	coarse-grained	upper bound	30.0	18
LCSDA	SER	coarse-grained	TRP	coarse-grained	upper bound	30.0	18
LCSDA	CYS	coarse-grained	THR	coarse-grained	upper bound	30.0	18
LCSDA	CYS	coarse-grained	SER	coarse-grained	upper bound	30.0	18
LCSDA	GLU	coarse-grained	TYR	coarse-grained	upper bound	30.0	18
LCSDA	ASN	coarse-grained	TYR	coarse-grained	upper bound	30.0	18
LCSDA	GLU	CA	SER	CA	upper bound	30.0	18
LCSDA	MET	CA	SER	CA	upper bound	30.0	18
LCSDA	LYS	CA	MET	CA	upper bound	30.0	18
LCSDA	LYS	CA	PHE	CA	upper bound	30.0	18
LCSDA	ALA	CA	ASP	CA	upper bound	30.0	18
LCSDA	ALA	CA	ALA	CA	upper bound	30.0	18
LCSDA	ALA	CA	LEU	CA	upper bound	30.0	18
LCSDA	ASN	CA	LYS	CA	upper bound	30.0	18

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.



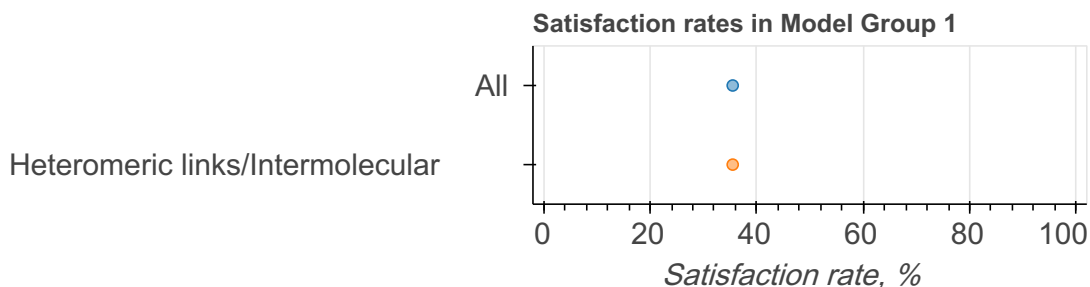
Satisfaction of restraints

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=414)
1	1	1	1/30000	All	35.51	64.49	414
				Heteromeric links/Intermolecular	35.51	64.49	414

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

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