

Integrative Structure Validation Report ?

July 22, 2024 - 04:20 PM PDT

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

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

This is a PDB-Dev IM Structure Validation Report for a publicly released PDB-Dev entry.

We welcome your comments at pdb-dev@mail.wwpdb.org

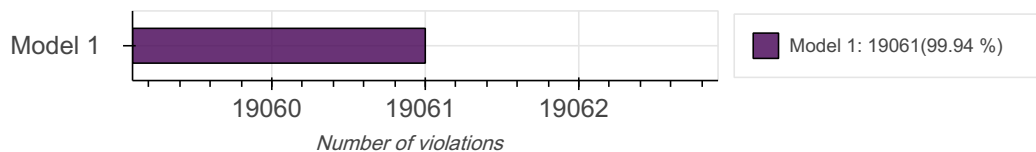
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 assessment for SAS datasets and fit to model assessments for SAS 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 unique models, with 20 subunits in each model. A total of 4 datasets or restraints were used to build this entry. Each model is represented by 40 rigid bodies and 4 flexible or non-rigid units.

Entry composition

There is 1 unique type of models in this entry. This model is titled Cluster 0/None.

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	1	1	Doublecortin	A	A	365
1	2	1	Doublecortin	B	B	365
1	3	2	Alpha-Tubulin	C	C	451
1	4	2	Alpha-Tubulin	D	D	451
1	5	2	Alpha-Tubulin	E	E	451
1	6	2	Alpha-Tubulin	F	F	451
1	7	2	Alpha-Tubulin	G	G	451
1	8	2	Alpha-Tubulin	H	H	451
1	9	2	Alpha-Tubulin	I	I	451
1	10	2	Alpha-Tubulin	J	J	451
1	11	2	Alpha-Tubulin	K	K	451
1	12	3	Beta-Tubulin	L	L	445
1	13	3	Beta-Tubulin	M	M	445
1	14	3	Beta-Tubulin	N	N	445

Model ID	Subunit number	Subunit ID	Subunit name	Chain ID	Chain ID [auth]	Total residues
1	15	3	Beta-Tubulin	O	O	445
1	16	3	Beta-Tubulin	P	P	445
1	17	3	Beta-Tubulin	Q	Q	445
1	18	3	Beta-Tubulin	R	R	445
1	19	3	Beta-Tubulin	S	S	445
1	20	3	Beta-Tubulin	T	T	445

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	PRIDE	PXD033167

Representation

This entry has only one representation and includes 40 rigid bodies and 4 flexible units

Chain ID	Rigid bodies	Non-rigid segments
A	51-140, 177-251	141-176, 252-330
B	51-140, 177-251	141-176, 252-330
C	1-37, 47-435	-
D	1-37, 47-435	-

Chain ID	Rigid bodies	Non-rigid segments
E	1-37, 47-435	-
F	1-37, 47-435	-
G	1-37, 47-435	-
H	1-37, 47-435	-
I	1-37, 47-435	-
J	1-37, 47-435	-
K	1-37, 47-435	-
L	1-37, 38-429	-
M	1-37, 38-429	-
N	1-37, 38-429	-
O	1-37, 38-429	-
P	1-37, 38-429	-
Q	1-37, 38-429	-
R	1-37, 38-429	-
S	1-37, 38-429	-
T	1-37, 38-429	-

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	Replica exchange monte carlo	Sampling	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

Validation for this section is under development.

Model quality ?

For models with atomic structures, molprobability 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.

Models	Excluded Volume Satisfaction (%)	Number of violations
1	99.94	19061.0

Fit of model to data used for modeling ?

Crosslinking-MS

Validation for this section is under development.

Fit of model to data used for validation ?

Validation for this section is under development.

Acknowledgements

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 ABI awards (DBI-1756248, DBI-2112966, DBI-2112967, DBI-2112968, and DBI-1756250). The [PDB-Dev team](#) and members of [Sali lab](#) contributed model validation metrics and software packages.

Implementation of validation methods for SAS data and SAS-based models are funded by [RCSB PDB](#) (grant number DBI-1832184). Dr. Stephen Burley, Dr. John Westbrook, and Dr. Jasmine Young from [RCSB PDB](#), Dr. Jill Trehwella, Dr. Dina Schneidman, and members of the [SASBDB](#) repository are acknowledged for their advice and support in implementing SAS validation methods.

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