

Integrative Structure Validation Report ?

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

Python-IHM Version 1.3
Integrative Modeling Validation Version 1.2

PDB ID	9A2A
PDB-Dev ID	PDBDEV_00000152
Structure Title	Integrative structure of the human MHM complex
Structure Authors	Arvindekar S; Jackman MJ; Low JKK; Landsberg MJ; Mackay JP; Viswanath S

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

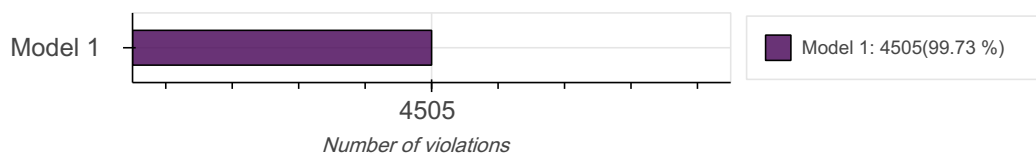
A user guide is available at https://pdb-dev.wwpdb.org/validation_help.html with specific help available everywhere you see the ? symbol.

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 8 subunits in each model. A total of 17 datasets or restraints were used to build this entry. Each model is represented by 16 rigid bodies and 14 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	MTA1	A	A	431
1	2	1	MTA1	B	B	431
1	3	2	HDAC1	C	C	482
1	4	2	HDAC1	D	D	482
1	5	3	MBD3	E	E	291
1	6	3	MBD3	F	F	291
1	7	4	P66A	G	G	633
1	8	4	P66A	H	H	633

Datasets used for modeling

There are 17 unique datasets used to build the models in this entry.

ID	Dataset type	Database name	Data access code
14	Crosslinking-MS data	PRIDE	PXD010111

ID	Dataset type	Database name	Data access code
15	Crosslinking-MS data	PRIDE	PXD010111
2	Comparative model	File	10.5281/zenodo.6674232
4	De Novo model	File	10.5281/zenodo.6674232
6	Comparative model	File	10.5281/zenodo.6674232
7	Comparative model	File	10.5281/zenodo.6674232
8	De Novo model	File	10.5281/zenodo.6674232
9	Comparative model	File	10.5281/zenodo.6674232
12	Experimental model	PDB	2L2L
13	Experimental model	PDB	2L2L
17	3DEM volume	File	10.5281/zenodo.6674232
1	Experimental model	PDB	2FVU
3	Experimental model	PDB	4BKX
10	Experimental model	PDB	6CC8
5	Experimental model	PDB	2GAT
11	Experimental model	PDB	2L2L
16	3DEM volume	EMDB	EMD-21382

Representation

This entry has only one representation and includes 16 rigid bodies and 14 flexible units

Chain ID	Rigid bodies	Non-rigid segments
F	1-71, 221-249	72-220, 250-291
E	1-71, 221-249	72-220, 250-291
B	1-164, 165-333, 334-353, 389-431	229-236, 354-388

Chain ID	Rigid bodies	Non-rigid segments
A	1-164, 165-333, 334-353, 389-431	229-236, 354-388
D	8-376	1-7, 377-482
C	8-376	1-7, 377-482
H	137-178	136-136
G	137-178	136-136

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	600000	False	True

There are 2 software packages reported in this entry.

ID	Software name	Software version	Software classification	Software location
1	IMP PMI module	2.16.0	integrative model building	https://integrativemodeling.org
2	Integrative Modeling Platform (IMP)	2.16.0	integrative model building	https://integrativemodeling.org

Data quality ?

3DEM volume

Validation for this section is under development.

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	99.73	4505.0

Fit of model to data used for modeling ?

3DEM volume

Validation for this section is under development.

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

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