

Summary of integrative structure determination of Integrative structure of the human MHM complex (PDB ID: 9A2A, PDB-Dev ID: PDBDEV_00000152)

1. Model Composition	
<i>Entry composition</i>	<ul style="list-style-type: none"> - HDAC1: Chain C (482 residues) - P66A: Chain H (633 residues) - MTA1: Chain B (431 residues) - P66A: Chain G (633 residues) - MBD3: Chain E (291 residues) - MTA1: Chain A (431 residues) - HDAC1: Chain D (482 residues) - MBD3: Chain F (291 residues)
<i>Datasets used for modeling</i>	<ul style="list-style-type: none"> - Crosslinking-MS data, Linker name and number of cross-links: BS3, 283 cross-links - Crosslinking-MS data, Linker name and number of cross-links: BS3, 135 cross-links - Comparative model, template PDB ID: Not available - De Novo model, File: 10.5281/zenodo.6674232 - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - De Novo model, File: 10.5281/zenodo.6674232 - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2L2L - Experimental model, PDB ID: 2L2L - 3DEM volume, File: 10.5281/zenodo.6674232 - Experimental model, PDB ID: 2FVU - Experimental model, PDB ID: 4BKX - Experimental model, PDB ID: 6CC8 - Experimental model, PDB ID: 2GAT - Experimental model, PDB ID: 2L2L - 3DEM volume, EMDB: EMD-21382
2. Representation	
<i>Resolution</i>	Coarse-grained: 1, 2, 4, 6 residue(s) per bead
<i>Number of rigid bodies, flexible units</i>	16, 14
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - F: 1-71, 221-249 - E: 1-71, 221-249 - B: 1-164, 165-333, 334-353, 389-431 - A: 1-164, 165-333, 334-353, 389-431 - D: 8-376 - C: 8-376 - H: 137-178 - G: 137-178

<i>Flexible units</i>	<ul style="list-style-type: none"> - F: 72-220, 250-291 - E: 72-220, 250-291 - B: 229-236, 354-388 - A: 229-236, 354-388 - D: 1-7, 377-482 - C: 1-7, 377-482 - H: 136-136 - G: 136-136
<i>Structural coverage (rigid bodies)</i>	72%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: BS3, 283 cross-links - 1 unique CrossLinkRestraint: BS3, 135 cross-links - 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	28451
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	28.0, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.73-99.73%
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>1. Method</i>	Sampling
<i>Name</i>	Replica exchange monte carlo
<i>Number of computed models</i>	600000
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version 2.16.0) - Integrative Modeling Platform (IMP) (version 2.16.0)