

Summary of integrative structure determination of Integrative structure of the human MHR complex (PDB ID: 9A2B, PDB-Dev ID: PDBDEV_00000154)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - MTA1: chain(s) A, B (715 residues) - HDAC1: chain(s) C, D (482 residues) - RBBP4: chain(s) E, F (425 residues) - RBBP4: chain(s) G, H (425 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Crosslinking-MS data, Zenodo: 10.5281/zenodo.6674232 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.6674232 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.6674232 - Comparative model, Zenodo: 10.5281/zenodo.6674232 - De Novo model, Zenodo: 10.5281/zenodo.6674232 - Comparative model, Zenodo: 10.5281/zenodo.6674232 - Comparative model, Zenodo: 10.5281/zenodo.6674232 - De Novo model, Zenodo: 10.5281/zenodo.6674232 - Comparative model, Zenodo: 10.5281/zenodo.6674232 - 3DEM volume, Zenodo: 10.5281/zenodo.6674232 - 3DEM volume, Zenodo: 10.5281/zenodo.6674232 - Experimental model, PDB: 2FVU - Experimental model, PDB: 4BKX - Experimental model, PDB: 5FXV - Experimental model, PDB: 4PBZ - Experimental model, PDB: 2GAT
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 30 residue(s) per bead
Number of rigid and flexible segments	18, 34
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: ADH, 17 crosslinks - 1 unique CrossLinkRestraint: BS3, 314 crosslinks - 1 unique CrossLinkRestraint: Other, 30 crosslinks - 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
Number of ensembles	1

<i>Number of models in ensembles</i>	12913
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	27.00, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.85%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 57.06%
<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	
1. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	500000
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version 2.16.0) - Integrative Modeling Platform (IMP) (version 2.16.0)