Summary of integrative structure determination of Integrative structure of the human NuDe complex (PDB ID: 9A2C, PDB-Dev ID: PDBDEV_00000155)

1. Model Composition	
Entry composition	- MTA1: Chain A (715 residues) - RBBP4: Chain G (425 residues) - HDAC1: Chain D (482 residues) - P66A: Chain J (633 residues) - MBD3: Chain I (291 residues) - RBBP4: Chain H (425 residues) - HDAC1: Chain C (482 residues) - RBBP4: Chain F (425 residues) - RBBP4: Chain E (425 residues) - MTA1: Chain B (715 residues)
Datasets used for modeling	- Crosslinking-MS data, Linker name and number of cross-links: ADH, 17 cross-links - Crosslinking-MS data, Linker name and number of cross-links: BS3, 280 cross-links - Crosslinking-MS data, Linker name and number of cross-links: Other, 35 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 - 3DEM volume, File: 10.5281/zenodo.6674232 - Experimental model, PDB ID: 4BKX - Experimental model, PDB ID: 5FXY - Experimental model, PDB ID: 4PBZ - Experimental model, PDB ID: 6CC8 - Experimental model, PDB ID: 2FVU - Experimental model, PDB ID: 2GAT - Experimental model, PDB ID: 2L2L - 3DEM volume, EMDB: EMD-22904
2. Representation	
Resolution	Coarse-grained: 1, 2, 3, 4, 5, 6 residue(s) per bead
Number of rigid bodies, flexible units	21, 37

Rigid bodies	- H: 10-411 - E: 2-411 - F: 2-411 - G: 10-411 - B: 1-164, 165-333, 334-353, 389-431, 468-546, 670-691 - A: 1-164, 165-333, 334-353, 389-431, 468-546, 670-691 - D: 8-376 - C: 8-376 - I: 1-71, 221-249 - J: 137-178
Flexible units	- H: 1-9, 90-102, 164-165, 176-179, 212-213, 412-425 - E: 1-1, 90-113, 412-425 - F: 1-1, 90-113, 412-425 - G: 1-9, 90-102, 164-165, 176-179, 212-213, 412-425 - B: 229-236, 354-388, 432-467, 519-528, 547-669, 692-715 - A: 229-236, 354-388, 432-467, 519-528, 547-669, 692-715 - D: 1-7, 377-482 - C: 1-7, 377-482 - I: 72-220, 250-291 - J: 136-136
Structural coverage (rigid bodies)	77%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: ADH, 17 cross-links - 1 unique CrossLinkRestraint: BS3, 280 cross-links - 1 unique CrossLinkRestraint: Other, 35 cross-links - 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
Number of ensembles	1
Number of models in ensembles	18239
Number of deposited models	1
Model precision (uncertainty of models)	34.0, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.86-99.86%
Fit to data used for modeling	Fit of model to information used to compute it has not been determined

Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	Sampling
Name	Replica exchange monte carlo
Number of computed models	1000000
Software	- IMP PMI module (version 2.16.0) - Integrative Modeling Platform (IMP) (version 2.16.0)