

Summary of integrative structure determination of Implications of a multiscale structure of the yeast Nuclear Pore Complex (PDB ID: 9A3S, PDB-Dev ID: PDBDEV_00000213)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Nucleoporin POM34: Chain C (299 residues) - Nucleoporin POM152: Chain A (1337 residues) - Nucleoporin POM152: Chain B (1337 residues) - Nucleoporin POM34: Chain D (299 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - 3DEM volume, File: 10.5281/zenodo.8226857 - Crosslinking-MS data, Linker name and number of cross-links: DSSO, 36 cross-links - De Novo model, AlphaFoldDB: AF-P39685-F1 - De Novo model, AlphaFoldDB: AF-Q12445-F1 - 3DEM volume, EMDB: EMD-41117
2. Representation	
Resolution	Coarse-grained: 1, 4, 6, 7, 19, 22, 36, 52 residue(s) per bead
Number of rigid bodies, flexible units	16, 20
Rigid bodies	<ul style="list-style-type: none"> - A: 105-130, 144-167, 176-192, 200-212 - B: 105-130, 144-167, 176-192, 200-212 - C: 44-86, 89-110, 122-150, 222-237 - D: 44-86, 89-110, 122-150, 222-237
Flexible units	<ul style="list-style-type: none"> - A: 1-104, 131-143, 168-175, 193-199, 213-250 - B: 1-104, 131-143, 168-175, 193-199, 213-250 - C: 1-43, 87-88, 111-121, 151-221, 238-250 - D: 1-43, 87-88, 111-121, 151-221, 238-250
Structural coverage (rigid bodies)	38%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	<ul style="list-style-type: none"> - 1 unique EM3DRestraint: DSSO, 36 cross-links - 1 unique GeometricRestraint: Gaussian mixture models
4. Validation	
Number of ensembles	1
Number of models in ensembles	11
Number of deposited models	11
Model precision (uncertainty of models)	9.52, Å

Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.53-99.54%
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	6400000
Software	<ul style="list-style-type: none"> - AlphaFold2 (version Not available) - IMP PMI module (version 20230908.develop.a93cf91143) - Integrative Modeling Platform (IMP) (version 20230908.develop.a93cf91143)