Summary of integrative structure determination of Modeling of Yeast NPC basket (PDB ID: 9A8M, PDB-Dev ID: PDBDEV_00000386)

1. Model Composition	
Entry composition	- Unknown MLP Protein: chain(s) A, B (1875 residues) - Nucleoporin NUP1: chain(s) C (1076 residues) - Nucleoporin NUP2: chain(s) D, E (720 residues) - Nucleoporin NUP60: chain(s) F, G (539 residues) - Nucleoporin NUP120: chain(s) H, I (1037 residues) - Nucleoporin NUP85: chain(s) J (744 residues) - Nucleoporin NUP85: chain(s) K, L (744 residues) - Nucleoporin NUP145C: chain(s) M, N (712 residues) - Protein transport protein SEC13: chain(s) O, P (297 residues) - Nucleoporin SEH1: chain(s) Q, R (349 residues) - Nucleoporin NUP84: chain(s) S, T (726 residues) - Nucleoporin NUP133: chain(s) U (1157 residues) - Nucleoporin NUP133: chain(s) V (1157 residues)
Datasets used for modeling	- 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.13131753 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - De Novo model, Zenodo: 10.5281/zenodo.13131753 - Experimental model, Zenodo: 10.5281/zenodo.13131753 - 3DEM volume, Zenodo: 10.5281/zenodo.13131753 - Experimental model, PDB: 7N84 - 3DEM volume, EMDB: EMD-44377
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead

Number of rigid and flexible segments	118, 128
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique EM3DRestraint: Bayesian EM restraint on Gaussian mixture models - 1 unique GeometricRestraint: DSS, 164 crosslinks - 1 unique CrossLinkRestraint: DSS, 539 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	21
Number of deposited models	22
Model precision (uncertainty of models)	57.20, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.96-99.96%
Fit to data used for modeling	Satisfaction of crosslinks: 62.84-70.81%
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. Name	Sampling
Method	Replica exchange monte carlo
Number of computed models	1000
2. Name	Sampling
Method	Replica exchange monte carlo
Number of computed models	15467933
Software	- IMP PMI module (version 2.19.0) - COCONUT (version 1.0.0) - Integrative Modeling Platform (IMP) (version 2.19.0)