Table 9: Summary of the Pom34-Pom152 tetramer integrative structure modeling

1) Gathering information	
Prior models	2-fold symmetry derived from cryo-EM structure
Physical principles and statistical preferences	Excluded volume Sequence connectivity
Experimental data	14 DSS0 Atomic structure prediction from Alphafold2 (AF_Q12445, AF_P39685)
2) Representing the system	
Composition (number of copies)	4
Atomic (structured) components	Pom152: 105-130, 144-167, 176-192, 200-212, 105-130, 144-167, 176-192, 200-212 Pom34: 44-86, 89-110, 122-150, 222-237, 44-86, 89-110, 122-150, 222-237
Unstructured components	Pom152: 1-104, 131-143, 168-175, 193-199, 213-250, 1-104, 131-143, 168-175, 193-199, 213-250 Pom34: 1-43, 87-88, 111-121, 151-221, 238-250, 1-43, 87-88, 111-121, 151-221, 238-250
Resolution of structured components	1 [R1] residue per bead
Resolution of unstructured components	2 [R2] residues per bead
Structural coverage	37.76 %
Rigid body (RB) definitions	RB1: $Pom152_{105-130}$ RB2: $Pom152_{144-167}$ RB3: $Pom152_{176-192}$ RB4: $Pom152_{200-212}$ RB5: $Pom34_{44-86}$ RB6: $Pom34_{89-110}$
Resolution of disordered regions	2 [R2] residues per bead
Spatial restraints encoded into scoring function	Excluded volume; applied to the R1 representation Sequence connectivity; applied to the R1 representation Cross-link restraints; applied to the R1 representation
3) Structural Sampling	
Sampling method	Replica Exchange Gibbs sampling, based on Metropolis Monte Carlo
Replica exchange temperature range	1.0 - 4.0
Number of replicas	6
Number of runs	80
Number of structures generated	6400000

Movers for flexible string of bead	Random translation up to 4.0 Å
CPU time	22 hours on 80 processors
4) Validating the Pom34-Pom152 models	
Models selected for validation	
Number of models after equilibration	6400000
Number of models that satisfy the input information	7089
Number of structures in samples A/B	2378/4711
p-value of non-parametric Kolmogorov-Smirnov two-sample test	0.539 (threshold p-value > 0.05)
Kolmogorov-Smirnov two-sample test statistic, D	0.0
Thoroughness of the structural sampling	
Sampling precision	14.08 Å
Homogeneity of proportions χ^2 test (p-value)/Cramers V value	1.000/0.000 (thresholds: p-value>0.05 OR Cramer's V<0.1)
Number of clusters	1
Cluster populations	cluster 1 : 100.0 %
Cluster precisions	cluster 1 : 9.52 Å
Average cross-correlation between localization probability densities of samples A and B	cluster 1: 0.78
Validation by information used for modeling	
Percent of sequence connectivity restraints satisfied per structure	99 %
Percent cross-link restraints satisfied by ensemble	99 %
Percent of excluded volume restraints satisfied per structure	99 %
5) Software and data availability	
Software	
Modeling programs	IMP PMI module, version develop-1350fc67f7 Integrative Modeling Platform (IMP), version develop-1350fc67f7
Modeling scripts	https://github.com/integrativemodeling/NPC_TMD
Structure prediction	AlphaFold2
Visualization and plotting	UCSF Chimera
Data	
PDB-dev accesion code	TBD