Summary of integrative structure determination of structure of saccharomyces cerevisiae exosome determined with cx-ms (PDBDEV00000002)

1. Model Composition	
Entry composition	- Dis3: Chain A (1001 residues) - Rrp6: Chain L (733 residues) - Rrp46_gfp: Chain I (475 residues) - Rrp45: Chain B (305 residues) - Rrp42: Chain G (265 residues) - Ski7: Chain N (747 residues) - Lrp1: Chain K (184 residues) - Rrp43: Chain J (394 residues) - Csl4: Chain D (292 residues) - Mtr3: Chain E (250 residues) - Ski6: Chain H (265 residues) - MPP6: Chain M (186 residues) - Rrp4: Chain C (359 residues) - Rrp40: Chain F (240 residues)
Datasets used for modeling	- Experimental model, PDB ID: 4IFD - Experimental model, PDB ID: 1GFL - Experimental model, PDB ID: 2HBJ - Comparative model, template PDB ID: Not listed - CX-MS data, Linker name and number of cross-links: DSS, 218 cross-links
2. Representation	
Atomic structural coverage	79%
Number of rigid bodies, flexible units	30, 31
Rigid bodies	- A: 9-237:Experimental model/4IFD, 249-329:Experimental model/4IFD, 364-471:Experimental model/4IFD, 472-1001:Experimental model/4IFD. - B: 2-301:Experimental model/4IFD. - C: 2-17:Experimental model/4IFD, 50-102:Experimental model/4IFD, 103-245:Experimental model/4IFD, 275-357:Experimental model/4IFD. - D: 1-71:Experimental model/4IFD, 99-113:Experimental model/4IFD, 126-162:Experimental model/4IFD, 185-291:Experimental model/4IFD. - E: 4-22:Experimental model/4IFD, 42-149:Experimental model/4IFD, 163-248:Experimental model/4IFD. - F: 1-60:Experimental model/4IFD, 61-236:Experimental model/4IFD. - G: 1-265:Experimental model/4IFD. - H: 1-242:Experimental model/4IFD. - I: 1-223:Experimental model/4IFD, 247-475:Experimental model/1GFL. - J: 7-99:Experimental model/4IFD, 121-193:Experimental model/4IFD, 206-309:Experimental model/4IFD, 327-394:Experimental model/4IFD. - K: - - L: 127-516:Experimental model/2HBJ, 532-557:Experimental model/4IFD, 565-619:Experimental model/4IFD. - M: - - N: 259-747:Comparative model/None.

Flexible units	- A: 1-8, 238-248, 330-363. - B: 1-1, 302-305. - C: 1-1, 18-49, 246-274, 358-359. - D: 72-98, 114-125, 163-184, 292-292. - E: 1-3, 23-41, 150-162, 249-250. - F: 237-240. - G: - - H: 243-265. - I: 224-246. - J: 1-6, 100-120, 194-205, 310-326. - K: 1-184. - L: 1-126, 517-531, 558-564, 620-733. - M: 1-186. - N: 1-258.
Resolution	- Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSS, 218 cross-links
4. Validation	
Sampling validation	- Information related to sampling validation has not been provided
Clustering algorithm ,*clustering feature*	Distance threshold-based clustering used if ensembles are deposited, RMSD
Number of ensembles	4
Number of models in ensembles	69, 131, 159, 41
Model precision (uncertainty of models)	24.374Å, 19.258Å, 9.798Å, 11.517Å
Quality of data	- Quality of input data has not be assessed
Model quality: assessment of atomic segments	Not applicable
Model quality: assessment of excluded volume	- Model-1: Number of violations-9530.0 - Model-2: Number of violations-9561.0 - Model-3: Number of violations-9595.0 - Model-4: Number of violations-9583.0
Fit of the model to information used to compute it	- Fit of model to information used to compute it has not been determined
Fit of the model to information not used to compute it	- Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
Method	Sampling
Name	Replica exchange Monte Carlo

Details	- Method details unspecified
Software	- Integrative Modeling Platform (IMP) (version develop-0a5706e202) - IMP PMI module (version 67456c0) - Phyre2 (version 2.0) - No location specified