

Summary of integrative structure determination of Structure of *Saccharomyces cerevisiae* exosome determined with CX-MS (PDB ID: 8ZZ2, PDB-Dev ID: PDBDEV_00000002)

1. Model Composition	
<u>Entry composition</u>	<ul style="list-style-type: none"> - Mtr3: Chain E (250 residues) - Rrp46_gfp: Chain I (475 residues) - Csl4: Chain D (292 residues) - Rrp45: Chain B (305 residues) - Rrp40: Chain F (240 residues) - Rrp42: Chain G (265 residues) - Lrp1: Chain K (184 residues) - Rrp6: Chain L (733 residues) - Dis3: Chain A (1001 residues) - Rrp4: Chain C (359 residues) - Ski6: Chain H (265 residues) - MPP6: Chain M (186 residues) - Ski7: Chain N (747 residues) - Rrp43: Chain J (394 residues)
<u>Datasets used for modeling</u>	<ul style="list-style-type: none"> - Experimental model, PDB ID: 4IFD - Experimental model, PDB ID: 1GFL - Experimental model, PDB ID: 2HBJ - Comparative model, template PDB ID: Not available - Crosslinking-MS data, Linker name and number of cross-links: DSS, 218 cross-links
2. Representation	
<u>Resolution</u>	Coarse-grained: 1, 2, 3, 4, 5, 6, 7, 23, 26, 37, 38, 52 residue(s) per bead
<u>Number of rigid bodies, flexible units</u>	30, 31
<u>Rigid bodies</u>	<ul style="list-style-type: none"> - A: 9-237, 249-329, 364-471, 472-1001 - B: 2-301 - C: 2-17, 50-102, 103-245, 275-357 - D: 1-71, 99-113, 126-162, 185-291 - E: 4-22, 42-149, 163-248 - F: 1-60, 61-236 - G: 1-265 - H: 1-242 - I: 1-223, 247-475 - J: 7-99, 121-193, 206-309, 327-394 - K: - - L: 127-516, 532-557, 565-619 - M: - - N: 259-747

<i>Flexible units</i>	- 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
<i>Structural coverage (rigid bodies)</i>	79%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	- 1 unique CrossLinkRestraint: DSS, 218 cross-links
4. Validation	
<i>Number of ensembles</i>	4
<i>Number of models in ensembles</i>	69, 131, 159, 41
<i>Number of deposited models</i>	4
<i>Model precision (uncertainty of models)</i>	24.374, Å, 19.258, Å, 9.798, Å, 11.517, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.89-99.89%
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<i>Fit to data used for validation</i>	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
<i>1. Method</i>	Sampling
<i>Name</i>	Replica exchange monte carlo
<i>Number of computed models</i>	50000
<i>2. Method</i>	Sampling
<i>Name</i>	Replica exchange monte carlo

<u>Number of computed models</u>	50000
<u>Software</u>	<ul style="list-style-type: none">- Integrative Modeling Platform (IMP) (version develop-0a5706e202)- IMP PMI module (version 67456c0)- Phyre2 (version 2.0)