

**Summary of integrative structure determination of Structure of Saccharomyces cerevisiae exosome determined with CX-MS (PDB ID: 8ZZZ, PDB-Dev ID: PDBDEV\_00000002)**

<b>1. Model Composition</b>	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- Dis3: chain(s) A (1001 residues)</li> <li>- Rrp45: chain(s) B (305 residues)</li> <li>- Rrp4: chain(s) C (359 residues)</li> <li>- Csl4: chain(s) D (292 residues)</li> <li>- Mtr3: chain(s) E (250 residues)</li> <li>- Rrp40: chain(s) F (240 residues)</li> <li>- Rrp42: chain(s) G (265 residues)</li> <li>- Ski6: chain(s) H (265 residues)</li> <li>- Rrp46_gfp: chain(s) I (475 residues)</li> <li>- Rrp43: chain(s) J (394 residues)</li> <li>- Lrp1: chain(s) K (184 residues)</li> <li>- Rrp6: chain(s) L (733 residues)</li> <li>- MPP6: chain(s) M (186 residues)</li> <li>- Ski7: chain(s) N (747 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB: <a href="#">4IFD</a></li> <li>- Experimental model, PDB: <a href="#">1GFL</a></li> <li>- Experimental model, PDB: <a href="#">2HBJ</a></li> <li>- Comparative model, Zenodo: <a href="#">10.5281/zenodo.583313</a></li> <li>- Crosslinking-MS data, Zenodo: <a href="#">10.5281/zenodo.583313</a></li> </ul>
<b>2. Representation</b>	
<a href="#">Number of representations</a>	1
<a href="#">Scale</a>	Multiscale: Coarse-grained: 1 - 5 residue(s) per bead
<a href="#">Number of <i>rigid</i> and <i>flexible</i> segments</a>	30, 31
<b>3. Restraints</b>	
<a href="#">Physical principles</a>	Information about physical principles was not provided
<a href="#">Experimental data</a>	- 1 unique CrossLinkRestraint: DSS, 218 crosslinks
<b>4. Validation</b>	
<a href="#">Number of ensembles</a>	4
<a href="#">Number of models in ensembles</a>	69, 131, 159, 41
<a href="#">Number of deposited models</a>	4

<a href="#"><i>Model precision (uncertainty of models)</i></a>	<ul style="list-style-type: none"> <li>- 24.37, Å</li> <li>- 19.26, Å</li> <li>- 9.80, Å</li> <li>- 11.52, Å</li> </ul>
<a href="#"><i>Data quality</i></a>	Data quality has not been assessed
<a href="#"><i>Model quality: assessment of excluded volume</i></a>	Satisfaction: 99.89-99.89%
<a href="#"><i>Fit to data used for modeling</i></a>	Satisfaction of crosslinks: 75.17-81.66%
<a href="#"><i>Fit to data used for validation</i></a>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <a href="#"><i>Name</i></a>	Sampling
<a href="#"><i>Method</i></a>	Replica exchange monte carlo
<a href="#"><i>Number of computed models</i></a>	50000
2. <a href="#"><i>Name</i></a>	Sampling
<a href="#"><i>Method</i></a>	Replica exchange monte carlo
<a href="#"><i>Number of computed models</i></a>	50000
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"> <li>- <a href="#">Integrative Modeling Platform (IMP)</a> (version develop-0a5706e202)</li> <li>- <a href="#">IMP PMI module</a> (version 67456c0)</li> <li>- <a href="#">Phyre2</a> (version 2.0)</li> </ul>