

## Summary of integrative structure determination of molecular architecture of the yeast mediator complex (PDBDEV00000003)

1. Model Composition	
<a href="#">Entry composition</a>	<ul style="list-style-type: none"> <li>- med3: Chain R (401 residues)</li> <li>- med9: Chain J (149 residues)</li> <li>- med7: Chain I (222 residues)</li> <li>- med22: Chain G (121 residues)</li> <li>- med5: Chain S (1146 residues)</li> <li>- med11: Chain C (115 residues)</li> <li>- med2: Chain Q (436 residues)</li> <li>- med15: Chain T (1094 residues)</li> <li>- med21: Chain L (140 residues)</li> <li>- med31: Chain K (127 residues)</li> <li>- med10: Chain M (157 residues)</li> <li>- med16: Chain U (986 residues)</li> <li>- med18: Chain E (307 residues)</li> <li>- med6: Chain A (295 residues)</li> <li>- med14: Chain O (1082 residues)</li> <li>- med20: Chain F (210 residues)</li> <li>- med4: Chain H (284 residues)</li> <li>- med8: Chain B (223 residues)</li> <li>- med19: Chain P (220 residues)</li> <li>- med1: Chain N (566 residues)</li> <li>- med17: Chain D (687 residues)</li> </ul>
<a href="#">Datasets used for modeling</a>	<ul style="list-style-type: none"> <li>- Experimental model, PDB ID: 4GWP</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Experimental model, PDB ID: 3FBI</li> <li>- Experimental model, PDB ID: Not listed</li> <li>- Experimental model, PDB ID: 1YKH</li> <li>- Experimental model, PDB ID: Not listed</li> <li>- Experimental model, PDB ID: 4BZK</li> <li>- Comparative model, template PDB ID: Not listed</li> <li>- Mass Spectrometry data, MSV000079237</li> <li>- CX-MS data, Linker name and number of cross-links: DSS, 359 cross-links</li> <li>- 3DEM volume, EMDB ID: EMD-2634</li> <li>- 3DEM volume, EMDB ID: Not listed</li> <li>- 3DEM volume, EMDB ID: Not listed</li> <li>- 3DEM volume, EMDB ID: Not listed</li> <li>- 3DEM volume, EMDB ID: Not listed</li> </ul>
2. Representation	
<a href="#">Atomic structural coverage</a>	10%
Number of <a href="#">rigid bodies</a> , <a href="#">flexible units</a>	12, 50

<i>Rigid bodies</i>	<ul style="list-style-type: none"> <li>- A: -</li> <li>- B: -</li> <li>- C: -</li> <li>- D: -</li> <li>- E: -</li> <li>- F: -</li> <li>- G: -</li> <li>- H: 37-127:Comparative model/None.</li> <li>- I: 12-84:Experimental model/None, 112-206:Experimental model/None.</li> <li>- J: 65-149:Comparative model/None.</li> <li>- K: 19-110:Experimental model/None.</li> <li>- L: 2-128:Experimental model/None.</li> <li>- M: -</li> <li>- N: -</li> <li>- O: -</li> <li>- P: -</li> <li>- Q: -</li> <li>- R: -</li> <li>- S: -</li> <li>- T: -</li> <li>- U: 8-49:Comparative model/None, 94-150:Comparative model/None, 165-174:Comparative model/None, 231-406:Comparative model/None, 437-476:Comparative model/None, 503-538:Comparative model/None.</li> </ul>
<i>Flexible units</i>	<ul style="list-style-type: none"> <li>- A: 1-60, 61-82, 83-192, 193-295.</li> <li>- B: 1-22, 23-173, 174-181, 182-214, 215-223.</li> <li>- C: 1-3, 4-115.</li> <li>- D: 123-181, 182-371, 372-377, 378-661, 662-669, 670-687, 1-122.</li> <li>- E: 1-1, 2-110, 111-157, 158-301, 302-307.</li> <li>- F: 1-1, 2-210.</li> <li>- G: 1-121.</li> <li>- H: 1-36, 128-284.</li> <li>- I: 1-11, 85-111, 207-222.</li> <li>- J: 1-64.</li> <li>- K: 1-18, 111-127.</li> <li>- L: 1-1, 129-140.</li> <li>- M: 1-157.</li> <li>- N: 1-566.</li> <li>- O: 1-1082.</li> <li>- P: 1-220.</li> <li>- Q: 1-436.</li> <li>- R: 1-401.</li> <li>- S: 1-1146.</li> <li>- T: 1-1094.</li> <li>- U: 50-93, 151-164, 175-230, 407-436, 477-502, 539-986.</li> </ul>
<a href="#"><u>Resolution</u></a>	<ul style="list-style-type: none"> <li>- Rigid bodies: 1 residue per bead.</li> <li>- Flexible regions: N/A</li> </ul>
<b>3. Restraints</b>	
<a href="#"><u>Physical principles</u></a>	Information about physical principles was not provided
<a href="#"><u>Experimental data</u></a>	<ul style="list-style-type: none"> <li>- 1 unique CrossLinkRestraint: DSS, 359 cross-links</li> <li>- 1 unique EM3DRestraint: Gaussian mixture models, 29</li> <li>- 1 unique EM3DRestraint: Gaussian mixture models, 49</li> </ul>
<b>4. Validation</b>	

<a href="#"><i>Sampling validation</i></a>	- Information related to sampling validation has not been provided
<a href="#"><i>Clustering algorithm ,clustering feature</i></a>	Distance threshold-based clustering used if ensembles are deposited, RMSD
<a href="#"><i>Number of ensembles</i></a>	4
<a href="#"><i>Number of models in ensembles</i></a>	142, 192, 39, 126
<a href="#"><i>Model precision (uncertainty of models)</i></a>	19.519Å, 21.833Å, 25.289Å, 21.061Å
<a href="#"><i>Quality of data</i></a>	- Quality of input data has not be assessed
<a href="#"><i>Model quality: assessment of atomic segments</i></a>	Not applicable
<a href="#"><i>Model quality: assessment of excluded volume</i></a>	<ul style="list-style-type: none"> <li>- Model-1: Number of violations-6332.0</li> <li>- Model-2: Number of violations-6318.0</li> <li>- Model-3: Number of violations-6347.0</li> <li>- Model-4: Number of violations-6337.0</li> </ul>
<a href="#"><i>Fit of the model to information used to compute it</i></a>	<ul style="list-style-type: none"> <li>- CX-MS Fit of mediod: model # 1, percentage satisfied 88.86%</li> <li>- CX-MS Fit of mediod: model # 2, percentage satisfied 90.53%</li> <li>- CX-MS Fit of mediod: model # 3, percentage satisfied 88.3%</li> <li>- CX-MS Fit of mediod: model # 4, percentage satisfied 88.86%</li> </ul>
<a href="#"><i>Fit of the model to information not used to compute it</i></a>	- Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
<a href="#"><i>Method</i></a>	Sampling
<a href="#"><i>Name</i></a>	Replica exchange Monte Carlo
<a href="#"><i>Details</i></a>	- Method details unspecified
<a href="#"><i>Software</i></a>	<ul style="list-style-type: none"> <li>- Integrative Modeling Platform (IMP) (version develop-0a5706e202)</li> <li>- IMP PMI module (version 67456c0)</li> <li>- Protein Prospector (version 5.13.1)</li> <li>- Situs (version 2.7)</li> <li>- Phyre2 (version 2.0)</li> <li>- No location specified</li> </ul>