

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

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

<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: - - B: - - C: - - D: - - E: - - F: - - G: - - H: 37-127:Comparative model/None. - I: 12-84:Experimental model/None, 112-206:Experimental model/None. - J: 65-149:Comparative model/None. - K: 19-110:Experimental model/None. - L: 2-128:Experimental model/None. - M: - - N: - - O: - - P: - - Q: - - R: - - S: - - T: - - 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.
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-60, 61-82, 83-192, 193-295. - B: 1-22, 23-173, 174-181, 182-214, 215-223. - C: 1-3, 4-115. - D: 123-181, 182-371, 372-377, 378-661, 662-669, 670-687, 1-122. - E: 1-1, 2-110, 111-157, 158-301, 302-307. - F: 1-1, 2-210. - G: 1-121. - H: 1-36, 128-284. - I: 1-11, 85-111, 207-222. - J: 1-64. - K: 1-18, 111-127. - L: 1-1, 129-140. - M: 1-157. - N: 1-566. - O: 1-1082. - P: 1-220. - Q: 1-436. - R: 1-401. - S: 1-1146. - T: 1-1094. - U: 50-93, 151-164, 175-230, 407-436, 477-502, 539-986.
<u>Resolution</u>	<ul style="list-style-type: none"> - Rigid bodies: 1 residue per bead. - Flexible regions: N/A
3. Restraints	
<u>Physical principles</u>	Excluded volume and Sequence connectivity.
<u>Experimental data</u>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 359 cross-links - 1 unique EM3DRestraint: Gaussian mixture models, 29 - 1 unique EM3DRestraint: Gaussian mixture models, 49
4. Validation	

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