Summary of integrative structure determination of Molecular architecture of the yeast Mediator complex (PDB ID: 8ZZ3, PDB-Dev ID: PDBDEV_00000003)

1. Model Composition	
Entry composition	- med17: Chain D (687 residues) - med11: Chain C (115 residues) - med3: Chain R (401 residues) - med21: Chain L (140 residues) - med8: Chain B (223 residues) - med14: Chain O (1082 residues) - med16: Chain U (986 residues) - med5: Chain S (1146 residues) - med7: Chain I (222 residues) - med6: Chain A (295 residues) - med19: Chain P (220 residues) - med20: Chain F (210 residues) - med31: Chain K (127 residues) - med1: Chain N (566 residues) - med22: Chain G (121 residues) - med15: Chain T (1094 residues) - med2: Chain Q (436 residues) - med9: Chain J (149 residues) - med10: Chain M (157 residues) - med4: Chain H (284 residues) - med18: Chain E (307 residues)
Datasets used for modeling	- Experimental model, PDB ID: 4GWP - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3FBI - Experimental model, PDB ID: Not available - Experimental model, PDB ID: 1YKH - Experimental model, PDB ID: Not available - Experimental model, PDB ID: 4BZK - Comparative model, template PDB ID: Not available - Mass Spectrometry data, MASSIVE: MSV000079237 - Crosslinking-MS data, Linker name and number of cross-links: DSS, 359 cross-links - 3DEM volume, EMDB: EMD-2634 - 3DEM volume, File: 10.5281/zenodo.802915 - 3DEM volume, File: 10.5281/zenodo.802915 - 3DEM volume, File: 10.5281/zenodo.802915 - 3DEM volume, File: 10.5281/zenodo.802915
2. Representation	
Resolution	Coarse-grained: 1, 2, 3, 4, 6, 7, 8, 9, 11, 12, 28, 29, 46 residue(s) per bead
Number of rigid bodies, flexible units	12, 50

Rigid bodies	- A: - - B: - - C: - - D: - - E: - - F: - - G: - - H: 37-127 - I: 12-84, 112-206 - J: 65-149 - K: 19-110 - L: 2-128 - M: - - N: - - O: - - P: - - Q: - - R: - - S: - - T: - - U: 8-49, 94-150, 165-174, 231-406, 437-476, 503-538
Flexible units	- 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
Structural coverage (rigid bodies)	10%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSS, 359 cross-links - 2 unique EM3DRestraint: Gaussian mixture models
4. Validation	

Number of ensembles	4
Number of models in ensembles	142, 192, 39, 126
Number of deposited models	4
Model precision (uncertainty of models)	19.519, Å, 21.833, Å, 25.289, Å, 21.061, Å
Data quality	Data quality has not been assessed
Model quality: assessment of excluded volume	Satisfaction: 99.83-99.83%
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
Fit to data used for validation	Fit of model to information not used to compute it has not been determined
5. Methodology and Software	
1. Method	Sampling
Name	Replica exchange monte carlo
Number of computed models	20000
Software	- 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)