

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	<ul style="list-style-type: none"> - med6: chain(s) A (295 residues) - med8: chain(s) B (223 residues) - med11: chain(s) C (115 residues) - med17: chain(s) D (687 residues) - med18: chain(s) E (307 residues) - med20: chain(s) F (210 residues) - med22: chain(s) G (121 residues) - med4: chain(s) H (284 residues) - med7: chain(s) I (222 residues) - med9: chain(s) J (149 residues) - med31: chain(s) K (127 residues) - med21: chain(s) L (140 residues) - med10: chain(s) M (157 residues) - med1: chain(s) N (566 residues) - med14: chain(s) O (1082 residues) - med19: chain(s) P (220 residues) - med2: chain(s) Q (436 residues) - med3: chain(s) R (401 residues) - med5: chain(s) S (1146 residues) - med15: chain(s) T (1094 residues) - med16: chain(s) U (986 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 4GWP - Comparative model, Not available: 10.1093/nar/gkt704 - Comparative model, Zenodo: 10.5281/zenodo.802915 - Experimental model, PDB: 3FBI - Experimental model, Zenodo: 10.5281/zenodo.802915 - Experimental model, PDB: 1YKH - Experimental model, Zenodo: 10.5281/zenodo.802915 - Experimental model, PDB: 4BZK - Comparative model, Zenodo: 10.5281/zenodo.802915 - Mass Spectrometry data, MASSIVE: MSV000079237 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.802915 - 3DEM volume, EMDB: EMD-2634 - 3DEM volume, Zenodo: 10.5281/zenodo.802915 - 3DEM volume, Zenodo: 10.5281/zenodo.802915 - 3DEM volume, Zenodo: 10.5281/zenodo.802915 - 3DEM volume, Zenodo: 10.5281/zenodo.802915
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 40 residue(s) per bead
Number of rigid and flexible segments	12, 50

3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	<ul style="list-style-type: none"> - 1 unique CrossLinkRestraint: DSS, 359 crosslinks - 2 unique EM3DRestraint: Gaussian mixture models
4. Validation	
<i>Number of ensembles</i>	4
<i>Number of models in ensembles</i>	142, 192, 39, 126
<i>Number of deposited models</i>	4
<i>Model precision (uncertainty of models)</i>	<ul style="list-style-type: none"> - 19.52, Å - 21.83, Å - 25.29, Å - 21.06, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.83-99.83%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 84.64-86.31%
<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	
1. <i>Name</i>	Sampling
<i>Method</i>	Replica exchange monte carlo
<i>Number of computed models</i>	20000
<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)