

Summary of integrative structure determination of Integrative structure and function of the yeast exocyst complex (PDB ID: 9A05, PDB-Dev ID: PDBDEV_00000041)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Sec03: chain(s) A (1336 residues) - Sec05: chain(s) B (971 residues) - Sec06: chain(s) C (805 residues) - Sec08: chain(s) D (1065 residues) - Sec10: chain(s) E (871 residues) - Sec15: chain(s) F (910 residues) - Exo70: chain(s) G (623 residues) - Exo84: chain(s) H (753 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB: 2PFT - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Experimental model, PDB: 2D2S - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Experimental model, PDB: 2A2F - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Experimental model, PDB: 2FJI - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Experimental model, PDB: 3FHN - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Experimental model, PDB: 5H11 - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Experimental model, PDB: 2B1E - Experimental model, PDB: 1ZC3 - Comparative model, Zenodo: 10.5281/zenodo.3951752 - Experimental model, PDB: 2D2S - Crosslinking-MS data, Zenodo: 10.5281/zenodo.3951752 - Crosslinking-MS data, Zenodo: 10.5281/zenodo.3951752 - 3DEM volume, EMDB: EMD-21226 - 3DEM volume, Zenodo: 10.5281/zenodo.3951752
2. Representation	
Number of representations	1
Scale	Multiscale: Coarse-grained: 1 - 50 residue(s) per bead
Number of rigid and flexible segments	43, 48
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, 256 crosslinks - 1 unique CrossLinkRestraint: EDC, 178 crosslinks - 1 unique EM3DRestraint: Gaussian mixture models
4. Validation	
<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	9669
<i>Number of deposited models</i>	1
<i>Model precision (uncertainty of models)</i>	38.00, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.84%
<i>Fit to data used for modeling</i>	Satisfaction of crosslinks: 71.89%
<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>	200000
<i>Software</i>	<ul style="list-style-type: none"> - IMP PMI module (version 2.13.0) - Integrative Modeling Platform (IMP) (version 2.13.0) - MODELLER (version SVN)