

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"> - Sec06: Chain C (805 residues) - Sec08: Chain D (1065 residues) - Sec15: Chain F (910 residues) - Sec10: Chain E (871 residues) - Exo84: Chain H (753 residues) - Sec05: Chain B (971 residues) - Sec03: Chain A (1336 residues) - Exo70: Chain G (623 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Experimental model, PDB ID: 2PFT - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2D2S - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2A2F - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2FJI - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 3FHN - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 5H11 - Comparative model, template PDB ID: Not available - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2B1E - Experimental model, PDB ID: 1ZC3 - Comparative model, template PDB ID: Not available - Experimental model, PDB ID: 2D2S - Crosslinking-MS data, Linker name and number of cross-links: DSS, 256 cross-links - Crosslinking-MS data, Linker name and number of cross-links: EDC, 178 cross-links - 3DEM volume, EMDB: EMD-21226 - 3DEM volume, File: 10.5281/zenodo.3951752
2. Representation	
Resolution	Coarse-grained: 1, 2, 3, 4, 5, 7, 9, 10, 15 residue(s) per bead
Number of rigid bodies, flexible units	43, 48

<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: 731-884, 924-956, 991-1137, 1157-1223, 1242-1333 - B: 232-327, 350-371, 457-501, 529-556, 627-658, 686-786, 806-921, 945-957 - C: 411-805 - D: 159-230, 326-361, 393-420, 549-570, 588-610, 631-648, 660-672, 690-698, 745-772, 825-972 - E: 230-280, 319-399, 414-460, 568-624, 639-864 - F: 474-525, 566-639, 663-685, 703-769 - G: 67-116, 121-221, 234-295, 301-414, 419-623 - H: 344-451, 525-570, 578-647, 650-711, 715-753
<i>Flexible units</i>	<ul style="list-style-type: none"> - A: 1-730, 885-923, 957-990, 1138-1156, 1224-1241, 1334-1336 - B: 1-231, 328-349, 372-456, 502-528, 557-626, 659-685, 787-805, 922-944, 958-971 - C: 1-410 - D: 1-158, 231-325, 362-392, 421-548, 571-587, 611-630, 649-659, 673-689, 699-744, 773-824, 973-1065 - E: 1-229, 281-318, 400-413, 461-567, 625-638, 865-871 - F: 1-473, 526-565, 640-662, 686-702, 770-910 - G: 1-66, 117-120, 222-233, 296-300, 415-418 - H: 1-343, 452-524, 571-577, 648-649, 712-714
<i>Structural coverage (rigid bodies)</i>	45%
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 cross-links - 1 unique CrossLinkRestraint: EDC, 178 cross-links - 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>	38.0, Å
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of excluded volume</i>	Satisfaction: 99.84-99.84%
<i>Fit to data used for modeling</i>	Fit of model to information used to compute it has not been determined
<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	
<i>1. Method</i>	Sampling
<i>Name</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)