

Table S1: Summary of Integrative Structure Determination of Yeast Exocyst Complex (PDBDEV_000000XX)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Sec03: Chain A (1336 residues) - Sec05: Chain B (971 residues) - Sec06: Chain C (805 residues) - Sec08: Chain D (1065 residues) - Sec10: Chain E (871 residues) - Sec15: Chain F (910 residues) - Exo70: Chain G (623 residues) - Exo84: Chain H (753 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Comparative model, template PDB ID: 2PFT - Comparative model, template PDB ID: 2D2S - Comparative model, template PDB ID: 2A2F - Experimental model, PDB ID: 2FJI - Comparative model, template PDB ID: 3FHN - Comparative model, template PDB ID: 2D2S - Comparative model, template PDB ID: 5H11 - Comparative model, template PDB ID: 3FHN - Experimental model, PDB ID: 2D2S - Comparative model, template PDB ID: 1ZC3 - Experimental model, PDB ID: 2B1E - CX-MS data, Linker name: DSS, Number of cross-links: 256 cross-links - CX-MS data, Linker name: BS3, Number of cross-links: 178 cross-links - 3DEM volume, EMDB ID: EMD-XXX
2. Representation	
Atomic structural coverage	51 %
Number of rigid bodies , flexible units	11, 48
<i>Rigid bodies</i>	<ul style="list-style-type: none"> - A: 731-1333:Comparative model/2PFT. - B: 232-555:Comparative model/2D2S, 627-957:Comparative model/2D2S. - C: 411-805:Comparative model/2A2F. - D: 159-419:Experimental model/2FJI, 549-971:Experimental model/2FJI. - E: 230-864:Comparative model/3FHN. - F: 474-512:Comparative model/2D2S, 513-768:Comparative model/2D2S. - G: 67-623:Comparative model/5H11. - H: 344-753:Comparative model/3FHN.
<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, 556-626, 659-685, 787-805, 922-944, 958-971. - C: 1-410. - D: 1-158, 231-325, 362-392, 420-548, 571-587, 611-630, 649-659, 673-689, 699-744, 773-824, 972-1065. - E: 1-229, 281-318, 400-413, 461-567, 625-638, 865-871.

	<ul style="list-style-type: none"> - F: 1-473, 526-565, 640-662, 686-702, 769-910. - G: 1-66, 117-120, 222-233, 296-300, 415-418. - H: 1-343, 452-524, 571-577, 648-649, 712-714.
Resolution	Rigid bodies: 1 residue per bead. Flexible regions: 50 residues per bead.
3. Restraints	
Physical principles	Excluded volume and Sequence connectivity.
Experimental data	<ul style="list-style-type: none"> - EM3DRestraint: 200, Gaussian mixture models - CrossLinkRestraint: 256 cross-links, DSS - CrossLinkRestraint: 178 cross-links, BS3
4. Validation	
Sampling validation	1. Sampling precision : 51 Å 2. p-value and D-statistic of non-parametric Kolmogorov-Smirnov two-sample test : p-value=0.1 (threshold p-value > 0.05), D-statistic=0.1 (threshold D-statistic < 0.3) 3. Homogeneity of proportions χ^2 test : 0.0/0.098 (threshold p-value > 0.05 or Cramer's V < 0.1)
Clustering algorithm ,clustering feature	distance threshold-based clustering,
Number of ensembles	1
Number of models in ensembles	9668
Model precision (uncertainty of models)	38 Å (average RMSF of the solution ensemble with respect to the centroid structure)
Quality of data	-
Assessment of atomic segments	-
Fit of the model to information used to compute it	1. Cross-links satisfaction: 98 % 2. 3D-EM satisfaction/average cross-correlation between model and map densities: 0.82 3. Satisfaction of physical principles: 99 % sequence connectivity and 98 % excluded volume
Fit of the model to information not used to compute it	1. 3D-EM satisfaction with previously published cryo-EM map (EMDB:6827)/average cross-correlation between model and map densities: 0.78 2. Cross-links satisfaction with previously published data (PMID: 29335562): 98 % 3. <i>In vivo</i> inter subunit distance satisfaction (PMID: 28129539): 100 %
5. Methodology and Software	
Method	Sampling
Name	Replica exchange Monte Carlo

Details

- Replica exchange temperature range used: 1.0-5.0
- Number of replicas: 8
- Number of runs: 100
- Number of structures generated: 2,000,000
- Movers for rigid bodies: Random translation up to 4 Å, rotation up to 1.0 Å
- Movers for flexible units: Random translation up to 4 Å

Software

- IMP PMI module (version 2.11.1)
- Integrative Modeling Platform (IMP) (version 2.11.1)
- HHpred (version 2.0.16)
- MODELLER (version 9.12)
- Scripts and data: <https://salilab.org/exocyst>
- Output files: <https://zenodo.org/record/XXX>