Summary of integrative structure determination of PTX3 hybrid cryoEM and AlphaFold model (PDB ID: 9A24, PDB-Dev ID: PDBDEV_00000141)

1. Model Composition	
Entry composition	- BETA-D-MANNOSE: Chain P (Not available residues) - ALPHA-D-MANNOSE: Chain U (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain DA (Not available residues) - PTX3 (protein complex): Chain B (364 residues) - ALPHA-D-MANNOSE: Chain KA (Not available residues) - BETA-D-MANNOSE: Chain K (Not available residues) - ALPHA-D-MANNOSE: Chain QA (Not available residues) - ALPHA-D-MANNOSE: Chain AA (Not available residues) - PTX3 (protein complex): Chain G (364 residues) - PTX3 (protein complex): Chain E (364 residues) - N-ACETYL-D-GLUCOSAMINE: Chain N (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain NA (Not available residues) - BETA-D-MANNOSE: Chain T (Not available residues) - BETA-D-MANNOSE: Chain JA (Not available residues) - ALPHA-D-MANNOSE: Chain BA (Not available residues) - water: Chain WA (1 residues) - PTX3 (protein complex): Chain C (364 residues) - N-ACETYL-D-GLUCOSAMINE: Chain MA (Not available residues) - ALPHA-D-MANNOSE: Chain GA (Not available residues) - ALPHA-D-MANNOSE: Chain M (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain Y (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain O (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain W (Not available residues) - ALPHA-D-MANNOSE: Chain Q (Not available residues) - ALPHA-D-MANNOSE: Chain PA (Not available residues) - ALPHA-D-MANNOSE: Chain L (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain HA (Not available residues) - PTX3 (protein complex): Chain A (364 residues) - BETA-D-MANNOSE: Chain OA (Not available residues) - ALPHA-D-MANNOSE: Chain UA (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain X (Not available residues)

	- water: Chain YA (1 residues) - N-ACETYL-D-GLUCOSAMINE: Chain RA (Not available residues) - ALPHA-D-MANNOSE: Chain VA (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain J (Not available residues) - BETA-D-MANNOSE: Chain Z (Not available residues) - ALPHA-D-MANNOSE: Chain V (Not available residues) - ALPHA-D-MANNOSE: Chain R (Not available residues) - water: Chain XA (1 residues) - ALPHA-D-MANNOSE: Chain LA (Not available residues) - BETA-D-MANNOSE: Chain TA (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain CA (Not available residues) - ALPHA-D-MANNOSE: Chain FA (Not available residues) - PTX3 (protein complex): Chain D (364 residues) - PTX3 (protein complex): Chain H (364 residues) - N-ACETYL-D-GLUCOSAMINE: Chain SA (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain IA (Not available residues) - BETA-D-MANNOSE: Chain EA (Not available residues) - PTX3 (protein complex): Chain F (364 residues) - N-ACETYL-D-GLUCOSAMINE: Chain I (Not available residues) - N-ACETYL-D-GLUCOSAMINE: Chain S (Not available residues)
Datasets used for modeling	- De Novo model, Not available - 3DEM volume, EMDB: EMD-14774 - Mass Spectrometry data, PRIDE: PXD034602 - 2DEM class average, Not available - Other, Not available - Experimental model, PDB ID: 7ZL1
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 59

Flexible units	- A: 1-147, 136-364 - B: 1-147, 136-364 - C: 1-147, 136-364 - D: 1-147, 136-364 - E: 1-147, 136-364 - F: 1-147, 136-364 - G: 1-147, 136-364 - H: 1-147, 136-364 - I: None-None - J: None-None - N: None-None - O: None-None - S: None-None - W: None-None - X: None-None - Y: None-None - CA: None-None - DA: None-None - HA: None-None - IA: None-None - MA: None-None - NA: None-None - RA: None-None - SA: None-None - K: None-None - P: None-None - T: None-None - Z: None-None - EA: None-None - JA: None-None - OA: None-None - TA: None-None - L: None-None - M: None-None - Q: None-None - R: None-None - U: None-None - V: None-None - AA: None-None - BA: None-None - FA: None-None - GA: None-None - KA: None-None - LA: None-None - PA: None-None - QA: None-None - UA: None-None - VA: None-None - WA: 1-1 - XA: 1-1 - YA: 1-1
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique EM3DRestraint: None

4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	1
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	Model-1: Clashscore = 5.64, Number of Ramachandran outliers = 33, Number of sidechain outliers = 8
Model quality: assessment of excluded volume	Not applicable
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	None
Name	None
Software	- EMAN2 (version Not available) - IMOD (version Not available) - Relion (version Not available) - AlphaFold (version Not available)