

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	<ul style="list-style-type: none"> - PTX3 (protein complex): chain(s) A [B], B [A], C [D], D [C], E [F], F [E], G [H], H [G] (364 residues) - N-ACETYL-D-GLUCOSAMINE: chain(s) I [B], J [B], N [A], O [A], S [D], W [D], X [C], Y [C], CA [F], DA [F], HA [E], IA [E], MA [H], NA [H], RA [G], SA [G] - BETA-D-MANNOSE: chain(s) K [B], P [A], T [D], Z [C], EA [F], JA [E], OA [H], TA [G] - ALPHA-D-MANNOSE: chain(s) L [B], M [B], Q [A], R [A], U [D], V [D], AA [C], BA [C], FA [F], GA [F], KA [E], LA [E], PA [H], QA [H], UA [G], VA [G] - water: chain(s) WA [B], XA [F], YA [I]
Datasets used for modeling	<ul style="list-style-type: none"> - 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: 7ZL1
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 16
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)	Not available
Data quality	Data quality has not been assessed

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 5.64 - Ramachandran outliers: 33 - Sidechain outliers: 8
<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	
1. <i>Name</i>	None
<i>Software</i>	<ul style="list-style-type: none"> - EMAN2 (version Not available) - IMOD (version Not available) - Relion (version Not available) - AlphaFold (version Not available)