

**Summary of integrative structure determination of PTEN-4A model.
Model restrained with crosslinking-MS data from "eased" conformation
and CTT. AlphaFold2-generated initial structure (PDB ID: 9A9A)**

1. Model Composition	
Entry composition	Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN, PTEN-4A variant: chain(s) A (403 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD060469 - De Novo model, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 52 crosslinks - 1 unique CrossLinkRestraint: DHSO, 10 crosslinks
4. Validation	
Number of ensembles	1
Number of models in ensembles	17
Number of deposited models	17
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	- Clashscore: 0.15-1.07 - Ramachandran outliers: 0-1 - Sidechain outliers: 0-0
Fit to data used for modeling	Satisfaction of crosslinks: 69.57-73.91%
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. <i>Name</i>	Protein structure prediction and 4A mutation (S380A/T382A/T383A/S385A)
<i>Method</i>	AlphaFold2, PyMOL
<i>Number of computed models</i>	1
2. <i>Name</i>	Rosetta pre-relaxation
<i>Method</i>	Rosetta relax protocol. Unrestrained. Lowest energy model of 200 used in next step
<i>Number of computed models</i>	200
3. <i>Name</i>	Restrained modeling
<i>Method</i>	Rosetta, crosslinking-MS distance restraints
<i>Description</i>	The individual models were restrained with subsets of experimental crosslink data in order to parse out specific restraints that correspond to a particular model. The crosslink list table provides the full set of experimental data obtained and the crosslink restraint table identifies the subset of crosslink restraints used in the modeling.
<i>Number of computed models</i>	2000
<i>Software</i>	<ul style="list-style-type: none"> - AlphaFold 2 (version ColabFold v1.5.0) - Rosetta (version 2020.08) - Rosetta (version 3.12)