

Summary of integrative structure determination of PTEN model. Model restrained with crosslinking-MS data from "eased" conformation and CTT. RoseTTAFold-generated initial structure (PDB ID: 9A96)

1. Model Composition	
Entry composition	Phosphatidylinositol 3,4,5-trisphosphate 3-phosphatase and dual-specificity protein phosphatase PTEN: chain(s) A (403 residues)
Datasets used for modeling	- Crosslinking-MS data, PRIDE: PXD059974 - De Novo model, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	0, 1
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1 unique CrossLinkRestraint: DSSO, 46 crosslinks - 1 unique CrossLinkRestraint: DHSO, 15 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: 1.07-1.99 - Ramachandran outliers: 2-3 - Sidechain outliers: 0-1
Fit to data used for modeling	Satisfaction of crosslinks: 77.55-79.59%
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. <u>Name</u>	Protein structure prediction
<u>Method</u>	RoseTTAFold
<u>Number of computed models</u>	1
2. <u>Name</u>	Rosetta pre-relaxation
<u>Method</u>	Rosetta relax protocol. Unrestrained. Lowest energy model of 200 used in next step
<u>Number of computed models</u>	200
3. <u>Name</u>	Restrained modeling
<u>Method</u>	Rosetta, crosslinking-MS distance restraints
<u>Description</u>	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.
<u>Number of computed models</u>	2000
<u>Software</u>	<ul style="list-style-type: none"> - RoseTTAFold (version Not available) - Rosetta (version 2020.08) - Rosetta (version 3.12)