

Summary of integrative structure determination of USP7 UBL 1-2 domains in complex with DNA polymerase iota peptide 438-448 (PDB ID: 9A0X, PDB-Dev ID: PDBDEV_00000069)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - DNA polymerase iota peptide 438-448: chain(s) A (11 residues) - USP7 UBL 1-2 domains: chain(s) B (214 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - Comparative model, Not available - Comparative model, Not available - Experimental model, PDB: 5gg4 - NMR data, BMRB: 26782 - Mutagenesis data, Not available: 10.1016/j.jmb.2020.166733
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	2, 0
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 176 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	20
Model precision (uncertainty of models)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 7.83-12.87 - Ramachandran outliers: 1-4 - Sidechain outliers: 12-29
Fit to data used for modeling	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>Method</i>	docking
<i>Number of computed models</i>	?
<i>Software</i>	<ul style="list-style-type: none">- MODELLER (version Not available)- HADDOCK (version Not available)- PYMOL (version Not available)