

**Summary of integrative structure determination of N4BP1 CUE domain in complex with ubiquitin (PDB ID: 9A1L, PDB-Dev ID: PDBDEV\_00000093)**

<b>1. Model Composition</b>	
<a href="#"><u>Entry composition</u></a>	- N4BP1 CUE domain: Chain A (47 residues) - Ubiquitin: Chain B (76 residues)
<a href="#"><u>Datasets used for modeling</u></a>	- Integrative model, PDB-Dev: PDBDEV_00000076 - Experimental model, PDB ID: 1UBQ - Other, Not available
<b>2. Representation</b>	
<a href="#"><u>Resolution</u></a>	Atomic
<a href="#"><u>Number of rigid bodies, flexible units</u></a>	2, 9
<a href="#"><u>Rigid bodies</u></a>	- A: 1-47 - B: 1-76
<a href="#"><u>Flexible units</u></a>	- A: 7-25, 27-28, 37-47 - B: 4-13, 27-27, 34-34, 36-36, 39-51, 66-76
<a href="#"><u>Structural coverage (rigid bodies)</u></a>	100%
<b>3. Restraints</b>	
<a href="#"><u>Physical principles</u></a>	Information about physical principles was not provided
<a href="#"><u>Experimental data</u></a>	- 1890 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
<b>4. Validation</b>	
<a href="#"><u>Number of ensembles</u></a>	0
<a href="#"><u>Number of models in ensembles</u></a>	Not applicable
<a href="#"><u>Number of deposited models</u></a>	1
<a href="#"><u>Model precision (uncertainty of models)</u></a>	Model precision can not be calculated with one structure
<a href="#"><u>Data quality</u></a>	Data quality has not been assessed
<a href="#"><u>Model quality: assessment of atomic segments</u></a>	Model-1: Clashscore = 0.0, Number of Ramachandran outliers = 0, Number of sidechain outliers = 13
<a href="#"><u>Model quality: assessment of excluded volume</u></a>	Not applicable

<u>Fit to data used for modeling</u>	Fit of model to information used to compute it has not been determined
<u>Fit to data used for validation</u>	Fit of model to information not used to compute it has not been determined
<b>5. Methodology and Software</b>	
1. <u>Method</u>	Rigid-body minimization
<u>Name</u>	Rigid-body minimization in HADDOCK (it0)
<u>Number of computed models</u>	1000
2. <u>Method</u>	Simulated annealing
<u>Name</u>	Semi-flexible SA in HADDOCK (it1)
<u>Number of computed models</u>	200
3. <u>Method</u>	Refinement
<u>Name</u>	Water refinement in HADDOCK (itw)
<u>Number of computed models</u>	200
<u>Software</u>	<a href="#">HADDOCK</a> (version Not available)