

Summary of integrative structure determination of N4BP1 CUE domain in complex with ubiquitin (PDB ID: 9A1L, PDB-Dev ID: PDBDEV_00000093)

1. Model Composition	
Entry composition	- N4BP1 CUE domain: chain(s) A (47 residues) - Ubiquitin: chain(s) B (76 residues)
Datasets used for modeling	- Integrative model, PDB: 9A14 - Experimental model, PDB: 1UBQ - Other, Not available
2. Representation	
Number of representations	1
Scale	Atomic
Number of <i>rigid</i> and <i>flexible</i> segments	2, 9
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 1890 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
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
Model quality: assessment of atomic segments	- Clashscore: 0.00 - Ramachandran outliers: 0 - Sidechain outliers: 13
Fit to data used for modeling	Fit of model to information used to compute it has not been determined
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. Name	Rigid-body minimization

<i>Method</i>	Rigid-body minimization in HADDOCK (it0)
<i>Number of computed models</i>	1000
2. <i>Name</i>	Simulated annealing
<i>Method</i>	Semi-flexible SA in HADDOCK (it1)
<i>Number of computed models</i>	200
3. <i>Name</i>	Refinement
<i>Method</i>	Water refinement in HADDOCK (itw)
<i>Number of computed models</i>	200
<i>Software</i>	HADDOCK (version Not available)