

Summary of integrative structure determination of INTEGRATIVE STRUCTURE OF BTG2 IN COMPLEX WITH RRM1-2 OF PABPC1 (PDB ID: 9A1R, PDB-Dev ID: PDBDEV_00000099)

1. Model Composition	
<i>Entry composition</i>	- POLY(A) BINDING PROTEIN CYTOPLASMIC 1: Chain A (175 residues) - PROTEIN BTG2: Chain B (121 residues)
<i>Datasets used for modeling</i>	- Experimental model, PDB ID: 4F02 - Experimental model, PDB ID: 3DJU - NMR data, BMRB: 50526
2. Representation	
<i>Resolution</i>	Atomic
<i>Number of rigid bodies, flexible units</i>	0, 2
<i>Flexible units</i>	- A: 1-175 - B: 1-121
<i>Structural coverage (rigid bodies)</i>	100%
3. Restraints	
<i>Physical principles</i>	Information about physical principles was not provided
<i>Experimental data</i>	- 1066 unique DerivedDistanceRestraint: Upper Bound Distance: 2.0
4. Validation	
<i>Number of ensembles</i>	0
<i>Number of models in ensembles</i>	Not applicable
<i>Number of deposited models</i>	4
<i>Model precision (uncertainty of models)</i>	Model precision can not be calculated with one structure
<i>Data quality</i>	Data quality has not been assessed

<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Model-1: Clashscore = 13.45, Number of Ramachandran outliers = 1, Number of sidechain outliers = 21 - Model-2: Clashscore = 12.81, Number of Ramachandran outliers = 1, Number of sidechain outliers = 19 - Model-3: Clashscore = 11.96, Number of Ramachandran outliers = 1, Number of sidechain outliers = 21 - Model-4: Clashscore = 10.67, Number of Ramachandran outliers = 1, Number of sidechain outliers = 19
<i>Model quality: assessment of excluded volume</i>	Not applicable
<i>Fit to data used for modeling</i>	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>Method</i>	Rigid-body minimization
<i>Name</i>	Rigid-body minimization in HADDOCK (it0)
<i>Number of computed models</i>	1000
2. <i>Method</i>	Simulated annealing
<i>Name</i>	Semi-flexible SA in HADDOCK (it1)
<i>Number of computed models</i>	200
3. <i>Method</i>	Refinement
<i>Name</i>	Water refinement in HADDOCK (itw)
<i>Number of computed models</i>	200
<i>Software</i>	HADDOCK (version 2.4)