

Summary of integrative structure determination of Encounter complex in the cross-modular condensation step of the Tomaymycin NRPS system: complex of the substrate-loaded peptidyl-carrier-protein domain from the TomA module (APCP-load) with the adaptor (BN91) of the TomB module (PDB ID: 9A83, PDB-Dev ID: PDBDEV_00000368)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Adaptor BN91 domain of Tomaymycin B module : Chain A (73 residues) - Substrate-loaded form of the peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module: Chain B (72 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, Not available - Experimental model, PDB ID: 8Q SX - Experimental model, PDB ID: 8QRX
2. Representation	
Resolution	Atomic
Number of rigid bodies , flexible units	0, 2
Flexible units	<ul style="list-style-type: none"> - B: 1-72 - A: 1-73
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 171 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-2.0
4. Validation	
Number of ensembles	1
Number of models in ensembles	10
Number of deposited models	10
Model precision (uncertainty of models)	None, Å
Data quality	Data quality has not been assessed

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 14.79, Number of Ramachandran outliers = 1, Number of sidechain outliers = 18 - Model-2: Clashscore = 14.79, Number of Ramachandran outliers = 2, Number of sidechain outliers = 17 - Model-3: Clashscore = 16.64, Number of Ramachandran outliers = 1, Number of sidechain outliers = 18 - Model-4: Clashscore = 18.02, Number of Ramachandran outliers = 1, Number of sidechain outliers = 23 - Model-5: Clashscore = 15.71, Number of Ramachandran outliers = 1, Number of sidechain outliers = 16 - Model-6: Clashscore = 19.87, Number of Ramachandran outliers = 1, Number of sidechain outliers = 18 - Model-7: Clashscore = 16.64, Number of Ramachandran outliers = 1, Number of sidechain outliers = 22 - Model-8: Clashscore = 14.33, Number of Ramachandran outliers = 0, Number of sidechain outliers = 17 - Model-9: Clashscore = 16.64, Number of Ramachandran outliers = 0, Number of sidechain outliers = 15 - Model-10: Clashscore = 16.17, Number of Ramachandran outliers = 2, Number of sidechain outliers = 17
<p><i>Model quality: assessment of excluded volume</i></p>	<p>Not applicable</p>
<p><i>Fit to data used for modeling</i></p>	<p>Fit of model to information used to compute it has not been determined</p>
<p><i>Fit to data used for validation</i></p>	<p>Fit of model to information not used to compute it has not been determined</p>
<p>5. Methodology and Software</p>	
<p>1. <i>Method</i></p>	<p>None</p>
<p><i>Name</i></p>	<p>Data-driven docking using CSP-derived distance restraints within HADDOCK.</p>
<p><i>Description</i></p>	<p>Data-driven docking using CSP-derived distance restraints within HADDOCK.</p>
<p><i>Software</i></p>	<p>HADDOCK (version 2.4)</p>