

Summary of integrative structure determination of Tomaymycin NRPS system: complex of the substrate-loaded peptidyl-carrier-protein domain from the A module (APCP-load) with the adaptor (BN91) and condensation (BC) domains of the B module (PDB ID: 9A82, PDB-Dev ID: PDBDEV_00000367)

1. Model Composition	
Entry composition	<ul style="list-style-type: none"> - Adaptor (BN91) and condensation (BC) domains of Tomaymycin B module : chain(s) A (508 residues) - Substrate-loaded peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module: chain(s) B (75 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, Not available - Predicted contacts, Not available - NMR data, Not available - Predicted contacts, Not available - Experimental model, PDB: 8QSX - Experimental model, PDB: 8QNF - Experimental model, PDB: 8QRX
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 3
3. Restraints	
Physical principles	Information about physical principles was not provided
	<ul style="list-style-type: none"> - 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.2 - 3 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.3 - 7 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.4 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.0 - 6 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.6 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.6 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.1 - 3 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.3 - 3 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.5 - 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.6 - 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-21.9

Experimental data

- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.5
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-21.7
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.1
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.8
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-21.8
- 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.4
- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.8
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.0
- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.9
- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.2
- 4 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.7
- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.9
- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.1
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-24.8
- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-23.7
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-20.9
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.7
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-25.8
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-27.0
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-29.2
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-26.6
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 14.0-16.5
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-8.0
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.3
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-26.0
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-27.6
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-22.0
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-26.5
- 2 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-21.6
- 1 unique DerivedDistanceRestraint: Lower Upper Bound Distance: 0.0-59.5

4. Validation

<i>Number of ensembles</i>	1
<i>Number of models in ensembles</i>	4
<i>Number of deposited models</i>	4
<i>Model precision (uncertainty of models)</i>	Not available
<i>Data quality</i>	Data quality has not been assessed
<i>Model quality: assessment of atomic segments</i>	<ul style="list-style-type: none"> - Clashscore: 10.52-12.62 - Ramachandran outliers: 2-5 - Sidechain outliers: 44-55
<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>Name</i>	None
<i>Description</i>	Step 1: docking of BC domain and APCP to form a binary BC-APCP complex (representing the starting models for step 2).
2. <i>Name</i>	None
<i>Description</i>	Step 2: docking of BN91 domain to binary BC-APCP complex generated in step 1.
<i>Software</i>	HADDOCK (version 2.4)