

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(s) A (73 residues) - Substrate-loaded form of the peptidyl-carrier-protein (APCP) domain of the Tomaymycin A module: chain(s) B (72 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, Not available - Experimental model, PDB: 8QSX - Experimental model, PDB: 8QRX
2. Representation	
Number of representations	1
Scale	Atomic
Number of rigid and flexible segments	0, 2
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)	Not available
Data quality	Data quality has not been assessed
Model quality: assessment of atomic segments	<ul style="list-style-type: none"> - Clashscore: 14.29-19.82 - Ramachandran outliers: 0-2 - Sidechain outliers: 15-23
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	None
Description	Data-driven docking using CSP-derived distance restraints within HADDOCK.
Software	HADDOCK (version 2.4)