

Summary of integrative structure determination of Hybrid NMR-SAXS structure of a trans-cleaving VS ribozyme (PDB ID: 9A0V, PDB-Dev ID: PDBDEV_0000067)

1. Model Composition	
Entry composition	Neurospora Varkud Satellite Ribozyme: Chain A (101 residues)
Datasets used for modeling	<ul style="list-style-type: none"> - NMR data, BMRB: 25654 - NMR data, BMRB: 25163 - NMR data, BMRB: 17292 - NMR data, BMRB: 50637 - SAS data, SASBDB: SASDKU3 - SAS data, SASBDB: SASDKV3 - SAS data, SASBDB: SASDKW3 - SAS data, SASBDB: SASDKY3 - Experimental model, PDB ID: 2N3Q - Experimental model, PDB ID: 2MTJ - Experimental model, PDB ID: 2L5Z - Experimental model, PDB ID: 1YN1
2. Representation	
Resolution	Atomic
Number of rigid bodies, flexible units	0, 15
Flexible units	A: 1-13, 14-18, 19-20, 21-22, 23-27, 28-31, 32-42, 43-46, 47-54, 55-65, 66-70, 71-80, 81-87, 88-100, 101-101
Structural coverage (rigid bodies)	100%
3. Restraints	
Physical principles	Information about physical principles was not provided
Experimental data	- 4 unique SASRestraint: Assembly name: Complete assembly Fitting method: Crysol Multi-state: False
4. Validation	
Number of ensembles	0
Number of models in ensembles	Not applicable
Number of deposited models	10
Model precision (uncertainty of models)	Model precision can not be calculated with one structure
Data quality	

<p><i>Model quality: assessment of atomic segments</i></p>	<ul style="list-style-type: none"> - Model-1: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-2: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-3: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-4: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-5: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-6: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-7: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-8: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-9: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0 - Model-10: Clashscore = 0.62, Number of Ramachandran outliers = 0, Number of sidechain outliers = 0
<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>?</p>
<p><i>Name</i></p>	<p>fragment assembly</p>
<p><i>Description</i></p>	<p>?</p>
<p><i>Number of computed models</i></p>	<p>?</p>
<p>2. <i>Method</i></p>	<p>?</p>
<p><i>Name</i></p>	<p>refinement</p>
<p><i>Description</i></p>	<p>?</p>
<p><i>Number of computed models</i></p>	<p>?</p>

Software

- [QRNAS](#) (version Not available)
- [Pymol](#) (version Not available)
- [Crysol](#) (version Not available)