



# wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 2LUP  
Title : RDC refined solution structure of double-stranded RNA binding domain of  
S. cerevisiae RNase III (rnt1p) in complex with the terminal RNA hairpin of  
snr47 precursor  
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Deposited on : 2012-06-19

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20027457  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

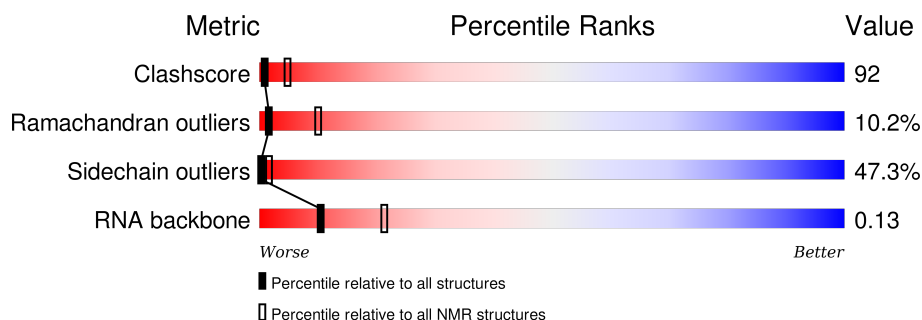
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 76%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958
RNA backbone	3027	600

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	32	
2	B	90	

## 2 Ensemble composition and analysis

This entry contains 16 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	B:366-B:447 (82)	0.50	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 9, 14
2	4, 7
3	6, 13
4	3, 8
5	10, 11
Single-model clusters	12; 15; 16

### 3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2437 atoms, of which 1067 are hydrogens and 0 are deuteriums.

- Molecule 1 is a RNA chain called RNA (32-MER).

Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	P	0
			1028	306	346	124	221	31	

- Molecule 2 is a protein called Ribonuclease 3.

Mol	Chain	Residues	Atoms						Trace
2	B	90	Total	C	H	N	O	S	0
			1409	429	721	129	127	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	364	GLY	-	EXPRESSION TAG	UNP Q02555
B	365	SER	-	EXPRESSION TAG	UNP Q02555

## 4 Residue-property plots

### 4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

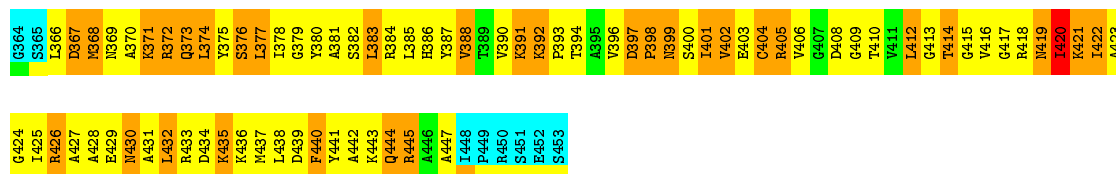
- Molecule 1: RNA (32-MER)

Chain A: 



- Molecule 2: Ribonuclease 3

Chain B: 



### 4.2 Residue scores for the representative (medoid) model from the NMR ensemble


The representative model is number 5. Colouring as in section 4.1 above.

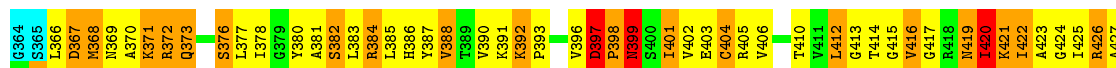
- Molecule 1: RNA (32-MER)

Chain A: 



- Molecule 2: Ribonuclease 3

Chain B: 



K428	K429	N430	L431	L432	R433	D434	K435	K436	N437	L438	D439	F440	Y441	A442	K443	Q444	R445	K446	A447	I448	P449	R450	S451	P452	S453
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## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 16 were deposited, based on the following criterion: *structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR NIH	structure solution	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2lup_cs.str
Number of chemical shift lists	1
Total number of shifts	1317
Number of shifts mapped to atoms	1317
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.13±0.01	0±0/763 (0.0±0.0%)	1.99±0.01	43±1/1188 (3.7±0.1%)
2	B	0.27±0.02	0±0/638 (0.0±0.0%)	0.45±0.02	0±0/859 (0.0±0.0%)
All	All	0.85	0/22416 (0.0%)	1.55	695/32752 (2.1%)

There are no bond-length outliers.

5 of 45 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	25	G	N7-C8-N9	9.54	117.87	113.10	10	16
1	A	11	G	N7-C8-N9	9.40	117.80	113.10	16	16
1	A	16	G	N7-C8-N9	9.33	117.77	113.10	6	16
1	A	19	G	N7-C8-N9	9.30	117.75	113.10	10	16
1	A	1	G	N7-C8-N9	9.29	117.74	113.10	16	16

There are no chirality outliers.

There are no planarity outliers.

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	682	346	346	94±10
2	B	630	664	663	126±9
All	All	20992	16160	16144	3434

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



hydrogen atoms). The all-atom clashscore for this structure is 92.

5 of 1059 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:370:ALA:HB3	2:B:428:ALA:HB1	1.03	1.25	15	2
2:B:374:LEU:HD11	2:B:428:ALA:HB2	1.01	1.32	16	4
2:B:370:ALA:HB1	2:B:428:ALA:HB1	1.00	1.28	14	14
2:B:380:TYR:CB	2:B:383:LEU:HD22	0.98	1.88	13	1
2:B:374:LEU:HD11	2:B:428:ALA:CB	0.97	1.88	16	5

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	82/90 (91%)	56±2 (68±3%)	18±3 (22±3%)	8±2 (10±2%)	1	10
All	All	1312/1440 (91%)	889 (68%)	289 (22%)	134 (10%)	1	10

5 of 23 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	420	ILE	16
2	B	397	ASP	16
2	B	392	LYS	15
2	B	399	ASN	13
2	B	391	LYS	10

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	65/72 (90%)	34±3 (53±4%)	31±3 (47±4%)	<b>0</b> <b>1</b>
All	All	1040/1152 (90%)	548 (53%)	492 (47%)	<b>0</b> <b>1</b>

5 of 58 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	388	VAL	16
2	B	432	LEU	16
2	B	376	SER	16
2	B	412	LEU	16
2	B	421	LYS	16

### 6.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	A	31/32 (97%)	4±2 (14±5%)	2±1 (5±3%)	0.13±0.02
All	All	497/512 (97%)	67 (13%)	24 (5%)	0.13

The overall RNA backbone suiteness is 0.13.

5 of 13 unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	17	A	16
1	A	18	A	15
1	A	15	A	13
1	A	13	U	6
1	A	16	G	5

5 of 7 unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	A	17	A	13
1	A	16	G	5
1	A	3	G	2
1	A	18	A	1
1	A	7	C	1

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 76% for the well-defined parts and 76% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2lup\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1317
Number of shifts mapped to atoms	1317
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	89	$2.17 \pm 0.32$	Should be applied
$^{13}\text{C}_\beta$	82	$2.66 \pm 0.15$	Should be applied
$^{13}\text{C}'$	0	—	—
$^{15}\text{N}$	84	$0.51 \pm 0.29$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 76%, i.e. 1223 atoms were assigned a chemical shift out of a possible 1614. 14 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	322/406 (79%)	161/162 (99%)	82/164 (50%)	79/80 (99%)
Sidechain	426/558 (76%)	256/325 (79%)	164/199 (82%)	6/34 (18%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	13/49 (27%)	13/25 (52%)	0/22 (0%)	0/2 (0%)
Overall	1223/1614 (76%)	685/857 (80%)	453/600 (76%)	85/157 (54%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	391	LYS	CG	33.40	30.67 – 19.17	7.4
2	B	444	GLN	CG	26.40	39.38 – 28.18	-6.6
2	B	421	LYS	CD	22.42	34.86 – 23.06	-5.5
2	B	392	LYS	CD	22.50	34.86 – 23.06	-5.5
1	A	29	U	H4'	3.69	5.04 – 3.74	-5.4
2	B	420	ILE	CD1	22.46	21.91 – 5.01	5.3
2	B	451	SER	CB	55.96	71.24 – 56.34	-5.3

#### 7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain B:

