



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:17 PM BST

PDB ID : 1DE3
Title : SOLUTION STRUCTURE OF THE CYTOTOXIC RIBONUCLEASE
ALPHA-SARCIN
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Deposited on : 1999-11-12

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.
We welcome your comments at 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.

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

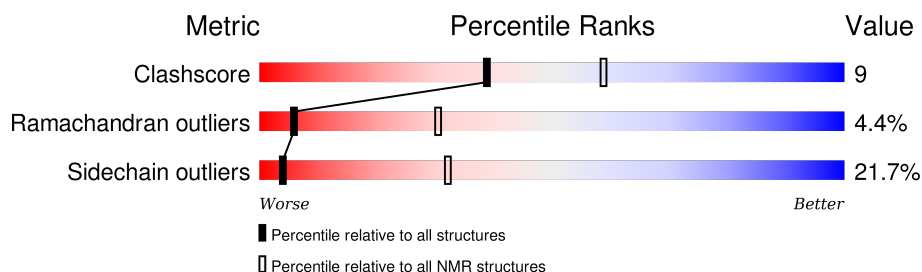
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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

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 ≥ 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	150	 58% 32% • 6%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 4 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	A:2-A:58, A:67-A:150 (141)	0.35	4

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2355 atoms, of which 1155 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RIBONUCLEASE ALPHA-SARCIN.

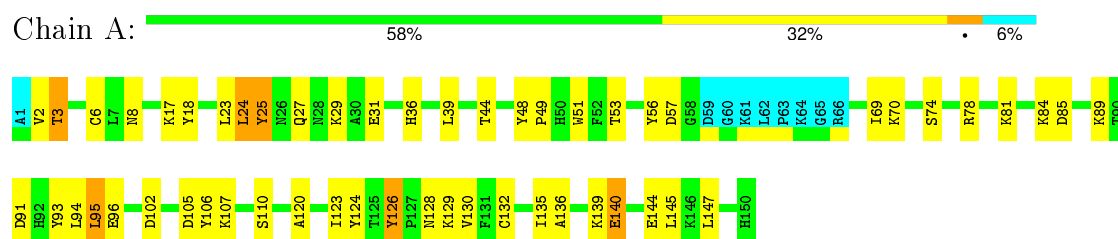
Mol	Chain	Residues	Atoms						Trace
1	A	150	Total	C	H	N	O	S	0
			2355	755	1155	214	227	4	

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: RIBONUCLEASE ALPHA-SARCIN

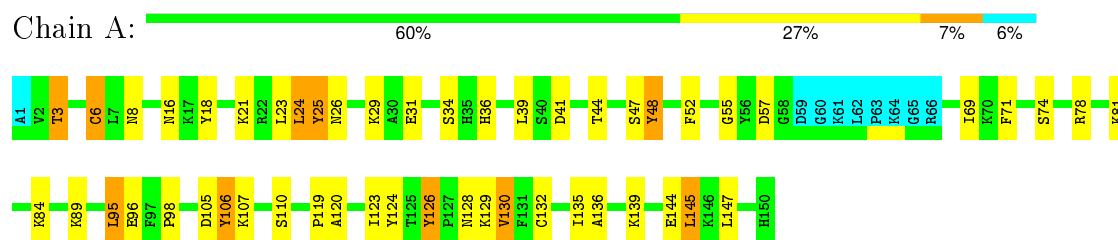


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

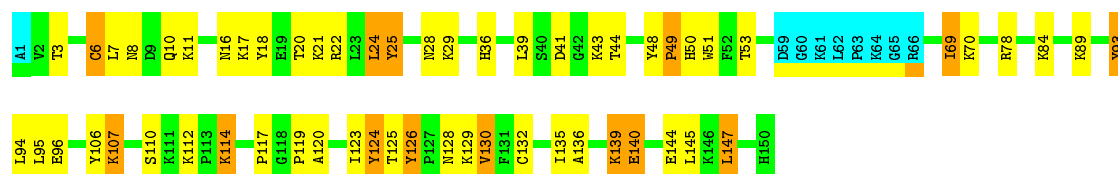
- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



4.2.2 Score per residue for model 2

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN

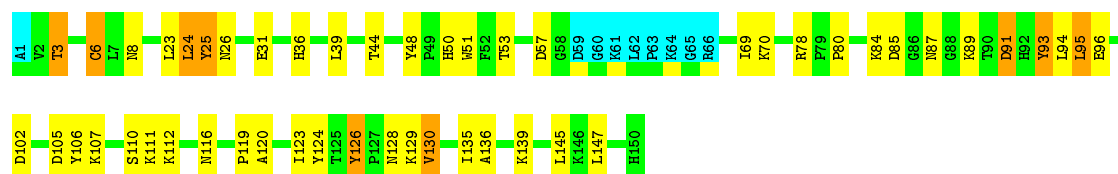




4.2.3 Score per residue for model 3

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN

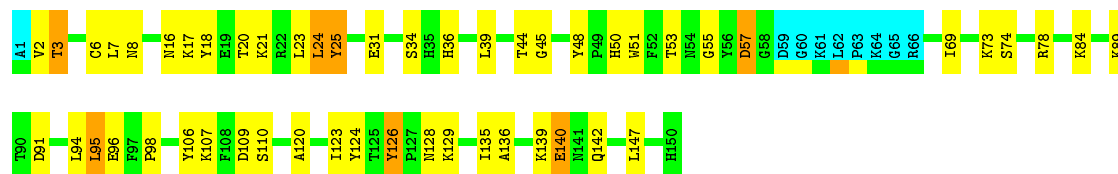
Chain A: 61% 27% 6% 6%



4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN

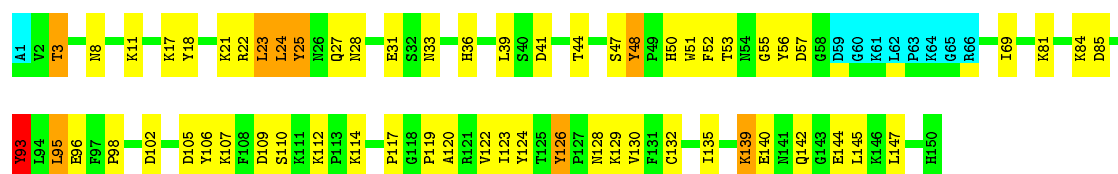
Chain A: 59% 30% 5% 6%



4.2.5 Score per residue for model 5

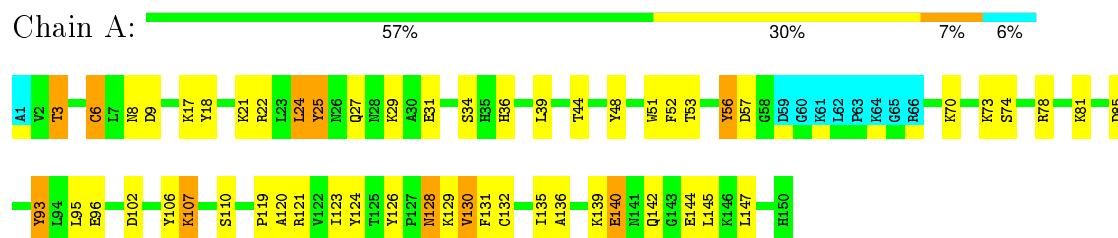
- Molecule 1: RIBONUCLEASE ALPHA-SARCIN

Chain A: 53% 35% 5% 6%



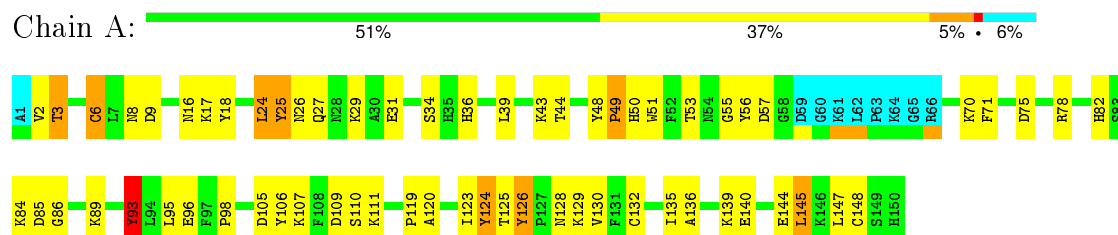
4.2.6 Score per residue for model 6

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



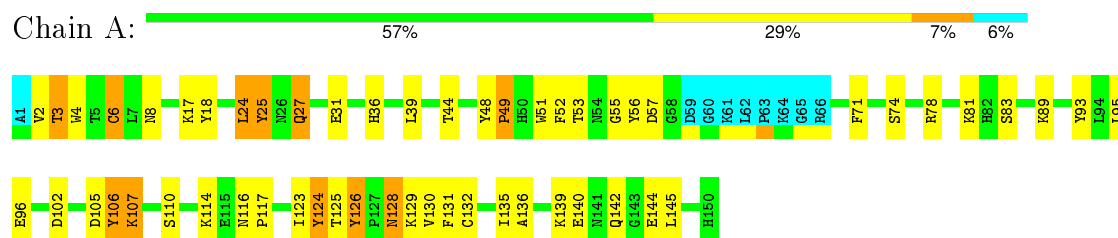
4.2.7 Score per residue for model 7

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



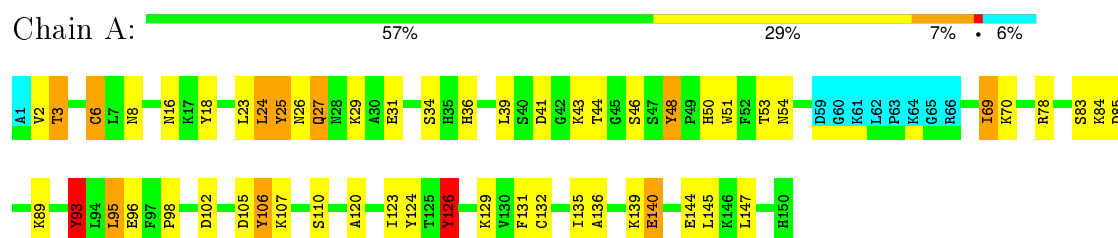
4.2.8 Score per residue for model 8

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



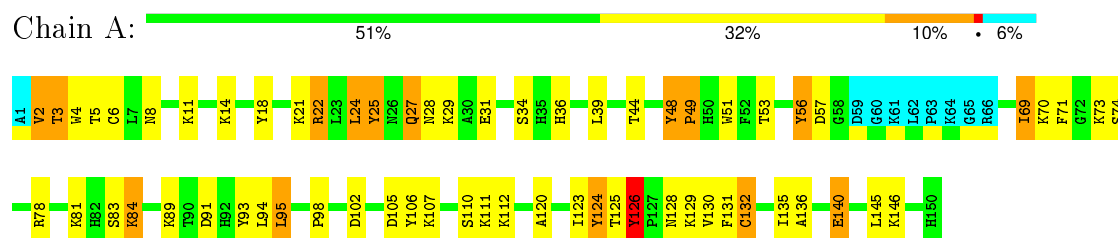
4.2.9 Score per residue for model 9

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



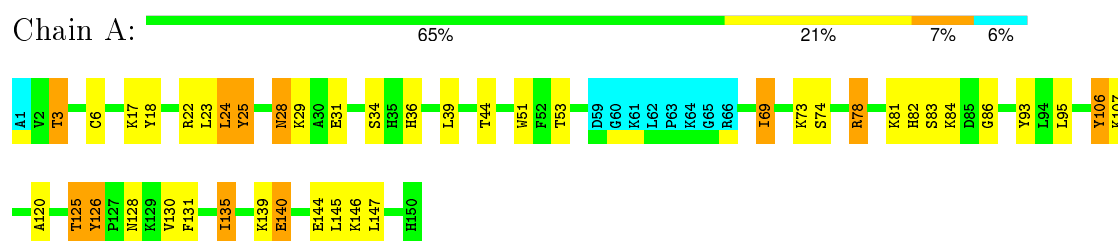
4.2.10 Score per residue for model 10

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



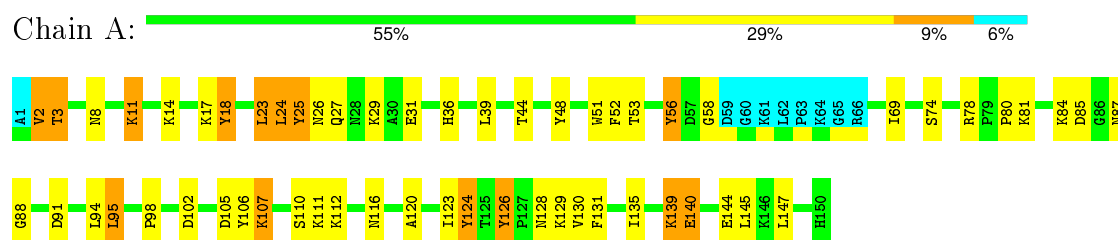
4.2.11 Score per residue for model 11

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



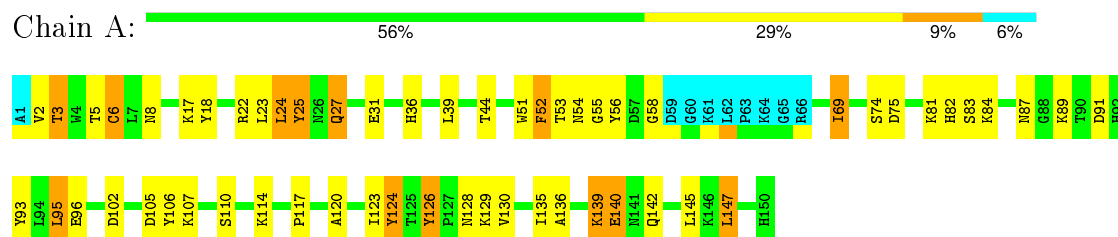
4.2.12 Score per residue for model 12

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



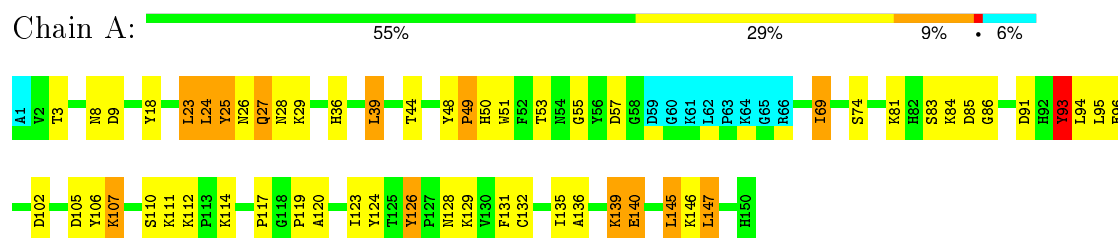
4.2.13 Score per residue for model 13

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



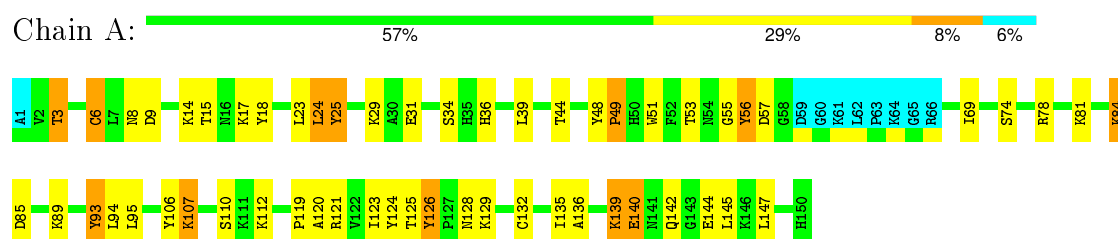
4.2.14 Score per residue for model 14

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



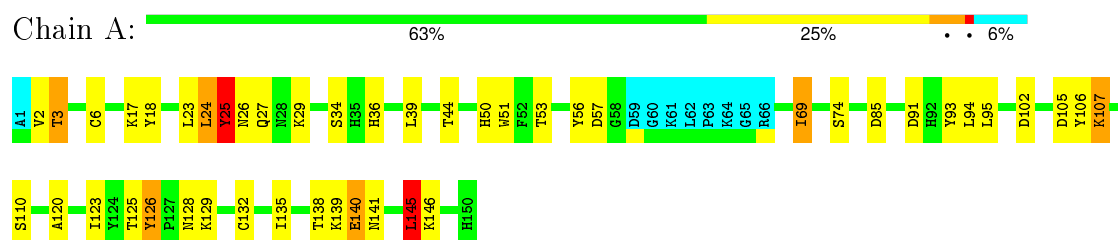
4.2.15 Score per residue for model 15

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



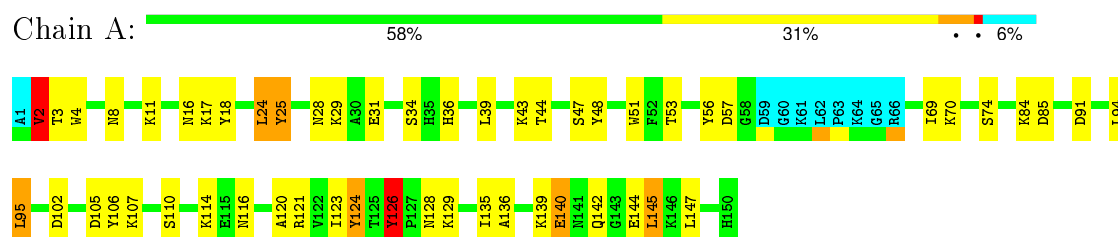
4.2.16 Score per residue for model 16

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



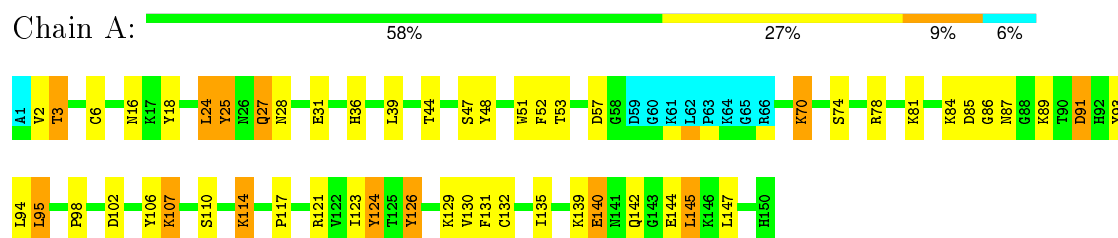
4.2.17 Score per residue for model 17

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



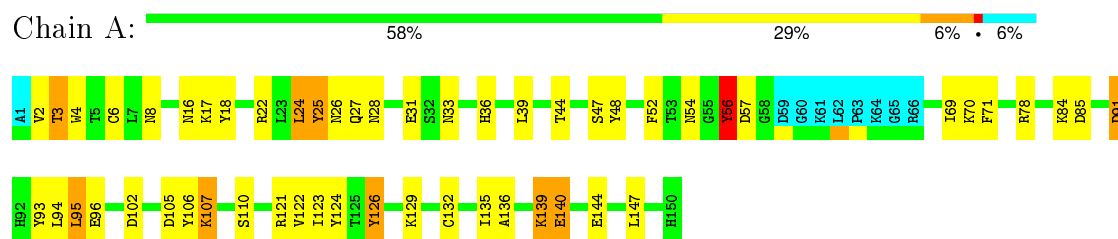
4.2.18 Score per residue for model 18

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



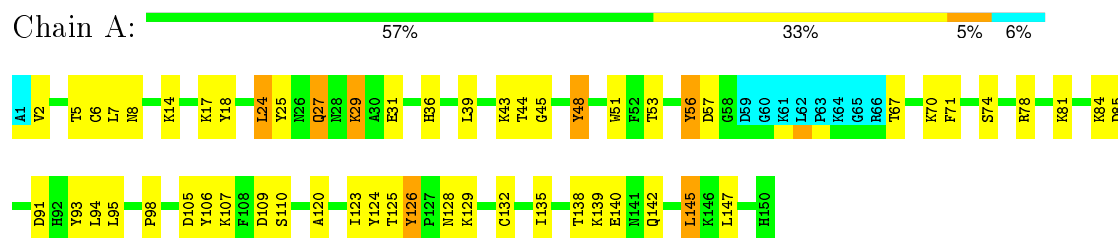
4.2.19 Score per residue for model 19

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



4.2.20 Score per residue for model 20

- Molecule 1: RIBONUCLEASE ALPHA-SARCIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *TORSION ANGLE DYNAMICS*.

Of the 47 calculated structures, 20 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
DYANA	structure solution	1.5
GROMOS	structure solution	97
GROMOS	refinement	97

No chemical shift data was provided. 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	0.83±0.01	0±0/1172 (0.0±0.0%)	1.16±0.02	5±1/1585 (0.3±0.1%)
All	All	0.83	0/23440 (0.0%)	1.16	109/31700 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.8±1.0
All	All	0	35

There are no bond-length outliers.

All 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	48	TYR	CB-CG-CD2	-9.00	115.60	121.00	19	13
1	A	106	TYR	CB-CG-CD2	-8.92	115.65	121.00	12	20
1	A	56	TYR	CB-CG-CD2	-8.35	115.99	121.00	12	6
1	A	126	TYR	CB-CG-CD2	-8.14	116.12	121.00	19	15
1	A	126	TYR	CB-CG-CD1	-8.05	116.17	121.00	9	3
1	A	124	TYR	CB-CG-CD2	-7.93	116.24	121.00	17	9
1	A	25	TYR	CB-CG-CD2	-7.64	116.42	121.00	2	17
1	A	56	TYR	CB-CG-CD1	-7.52	116.49	121.00	15	3
1	A	93	TYR	CB-CG-CD2	-7.24	116.65	121.00	14	8
1	A	25	TYR	CB-CG-CD1	-7.19	116.68	121.00	19	1
1	A	93	TYR	CB-CG-CD1	-6.77	116.94	121.00	9	3
1	A	91	ASP	CB-CG-OD1	-5.77	113.11	118.30	19	1
1	A	52	PHE	CB-CG-CD2	-5.75	116.78	120.80	13	4
1	A	2	VAL	CG1-CB-CG2	-5.64	101.88	110.90	4	4
1	A	18	TYR	CB-CG-CD1	-5.41	117.75	121.00	16	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	2	VAL	CA-CB-CG1	5.32	118.88	110.90	17	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	34	SER	Mainchain	8
1	A	93	TYR	Sidechain	7
1	A	49	PRO	Mainchain	6
1	A	28	ASN	Mainchain	4
1	A	56	TYR	Sidechain	3
1	A	29	LYS	Mainchain	2
1	A	25	TYR	Sidechain	2
1	A	131	PHE	Sidechain	1
1	A	81	LYS	Mainchain	1
1	A	124	TYR	Sidechain	1

6.2 Too-close contacts

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	1135	1083	1075	21±4
All	All	22700	21660	21500	419

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 9.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:49:PRO:HB2	1:A:95:LEU:HD13	0.87	1.44	10	6
1:A:3:THR:HG23	1:A:24:LEU:HD23	0.82	1.51	17	19
1:A:95:LEU:HD11	1:A:124:TYR:CZ	0.75	2.16	8	6
1:A:8:ASN:HD21	1:A:136:ALA:HB1	0.69	1.48	2	11
1:A:135:ILE:HD12	1:A:145:LEU:HD22	0.69	1.64	8	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ILE:HD13	1:A:145:LEU:HD22	0.66	1.67	5	4
1:A:135:ILE:HG22	1:A:147:LEU:HA	0.65	1.69	11	14
1:A:51:TRP:CZ3	1:A:53:THR:HG22	0.64	2.28	13	7
1:A:39:LEU:HD11	1:A:129:LYS:HD2	0.61	1.71	8	19
1:A:70:LYS:O	1:A:147:LEU:HD22	0.61	1.95	20	5
1:A:25:TYR:CZ	1:A:120:ALA:HB3	0.61	2.30	11	17
1:A:95:LEU:HD11	1:A:124:TYR:OH	0.61	1.94	7	6
1:A:95:LEU:HD12	1:A:124:TYR:O	0.61	1.95	9	8
1:A:123:ILE:HD11	1:A:135:ILE:HD11	0.60	1.72	17	5
1:A:24:LEU:HD22	1:A:25:TYR:N	0.60	2.12	19	19
1:A:69:ILE:HG21	1:A:135:ILE:HG21	0.59	1.74	11	4
1:A:95:LEU:HD13	1:A:124:TYR:CE2	0.58	2.33	12	10
1:A:2:VAL:HG12	1:A:4:TRP:CD1	0.58	2.34	17	1
1:A:78:ARG:HH21	1:A:125:THR:HG21	0.57	1.60	11	1
1:A:69:ILE:HD11	1:A:145:LEU:O	0.56	2.00	9	10
1:A:48:TYR:CD2	1:A:98:PRO:HD3	0.56	2.35	12	1
1:A:96:GLU:OE2	1:A:123:ILE:HD11	0.56	2.00	1	7
1:A:51:TRP:CH2	1:A:53:THR:HG22	0.56	2.36	7	14
1:A:95:LEU:HD12	1:A:95:LEU:C	0.56	2.21	10	4
1:A:39:LEU:HB3	1:A:126:TYR:CD2	0.55	2.36	8	3
1:A:94:LEU:HD22	1:A:123:ILE:HG22	0.55	1.78	15	11
1:A:124:TYR:CD2	1:A:129:LYS:HG2	0.55	2.36	7	2
1:A:114:LYS:NZ	1:A:117:PRO:HD3	0.55	2.17	18	6
1:A:39:LEU:HD22	1:A:126:TYR:HD1	0.54	1.62	20	6
1:A:6:CYS:SG	1:A:136:ALA:HB3	0.54	2.43	13	9
1:A:48:TYR:CD1	1:A:98:PRO:HD3	0.53	2.39	18	5
1:A:39:LEU:HD22	1:A:126:TYR:CD1	0.52	2.39	19	17
1:A:27:GLN:HG3	1:A:131:PHE:CZ	0.52	2.39	8	2
1:A:82:HIS:CD2	1:A:86:GLY:HA2	0.52	2.40	11	1
1:A:4:TRP:CD1	1:A:27:GLN:HB2	0.52	2.40	19	3
1:A:52:PHE:HB2	1:A:96:GLU:HB2	0.52	1.79	5	5
1:A:39:LEU:HD22	1:A:126:TYR:CD2	0.52	2.39	9	2
1:A:95:LEU:H	1:A:95:LEU:HD12	0.51	1.65	19	3
1:A:95:LEU:HD12	1:A:95:LEU:H	0.51	1.65	17	7
1:A:95:LEU:C	1:A:95:LEU:HD12	0.51	2.26	7	2
1:A:128:ASN:HB3	1:A:130:VAL:HG23	0.51	1.82	6	7
1:A:123:ILE:HD11	1:A:135:ILE:HG12	0.50	1.84	10	4
1:A:87:ASN:O	1:A:91:ASP:HB2	0.50	2.07	18	3
1:A:5:THR:HG21	1:A:22:ARG:HD2	0.50	1.83	10	1
1:A:69:ILE:HG21	1:A:135:ILE:CG2	0.49	2.37	17	2
1:A:3:THR:HG23	1:A:24:LEU:CD2	0.49	2.33	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LEU:HB3	1:A:126:TYR:CD1	0.49	2.42	13	15
1:A:93:TYR:CE2	1:A:95:LEU:HB3	0.49	2.42	2	1
1:A:25:TYR:CE1	1:A:120:ALA:HB3	0.48	2.43	2	3
1:A:8:ASN:OD1	1:A:23:LEU:HD22	0.48	2.08	5	3
1:A:71:PHE:CD2	1:A:147:LEU:HD13	0.48	2.44	7	1
1:A:39:LEU:HD23	1:A:95:LEU:HD21	0.48	1.84	15	3
1:A:7:LEU:HB3	1:A:20:THR:HG22	0.47	1.86	2	2
1:A:95:LEU:HD11	1:A:126:TYR:CB	0.47	2.40	19	1
1:A:27:GLN:HG3	1:A:131:PHE:CE2	0.47	2.44	10	5
1:A:124:TYR:HD2	1:A:129:LYS:HG2	0.47	1.70	13	1
1:A:53:THR:O	1:A:56:TYR:CD2	0.46	2.67	10	4
1:A:122:VAL:O	1:A:123:ILE:HD13	0.46	2.10	5	2
1:A:93:TYR:CE1	1:A:95:LEU:HG	0.45	2.47	9	2
1:A:135:ILE:HD12	1:A:135:ILE:O	0.45	2.10	19	1
1:A:135:ILE:HD12	1:A:145:LEU:HB3	0.45	1.87	1	1
1:A:48:TYR:CD2	1:A:98:PRO:HG3	0.45	2.46	20	3
1:A:41:ASP:HB2	1:A:93:TYR:CZ	0.45	2.46	9	2
1:A:93:TYR:CE1	1:A:95:LEU:HB3	0.45	2.47	8	1
1:A:71:PHE:CD1	1:A:147:LEU:HD13	0.45	2.47	20	2
1:A:96:GLU:OE2	1:A:135:ILE:HD11	0.45	2.11	8	4
1:A:69:ILE:HG23	1:A:147:LEU:HB2	0.44	1.88	11	1
1:A:120:ALA:HB2	1:A:136:ALA:HB2	0.44	1.89	2	1
1:A:5:THR:HG23	1:A:24:LEU:HB3	0.44	1.88	20	1
1:A:39:LEU:HD21	1:A:129:LYS:HE3	0.44	1.88	7	1
1:A:39:LEU:HD22	1:A:126:TYR:HD2	0.44	1.72	9	2
1:A:34:SER:HB2	1:A:124:TYR:CZ	0.44	2.46	7	2
1:A:71:PHE:HA	1:A:147:LEU:HD22	0.44	1.89	7	1
1:A:52:PHE:CE2	1:A:54:ASN:ND2	0.44	2.85	13	1
1:A:49:PRO:CB	1:A:95:LEU:HD13	0.44	2.35	2	1
1:A:95:LEU:HD11	1:A:126:TYR:HB2	0.44	1.89	19	3
1:A:39:LEU:HB3	1:A:126:TYR:CE1	0.44	2.47	11	4
1:A:71:PHE:CZ	1:A:123:ILE:HG21	0.44	2.48	10	4
1:A:93:TYR:OH	1:A:95:LEU:HD23	0.43	2.13	9	2
1:A:45:GLY:HA3	1:A:109:ASP:O	0.43	2.13	4	2
1:A:94:LEU:HD21	1:A:132:CYS:SG	0.43	2.54	20	1
1:A:7:LEU:O	1:A:138:THR:HG22	0.43	2.14	20	1
1:A:95:LEU:HD13	1:A:124:TYR:CD2	0.43	2.49	9	1
1:A:80:PRO:HB2	1:A:93:TYR:HA	0.42	1.91	3	1
1:A:69:ILE:HD13	1:A:135:ILE:HG21	0.42	1.91	4	1
1:A:27:GLN:HE21	1:A:28:ASN:N	0.42	2.12	18	1
1:A:56:TYR:CE2	1:A:80:PRO:HD2	0.42	2.49	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:93:TYR:CE2	1:A:95:LEU:HG	0.42	2.49	19	2
1:A:71:PHE:CD1	1:A:132:CYS:HB3	0.42	2.49	10	1
1:A:124:TYR:CE2	1:A:129:LYS:HE2	0.42	2.50	8	1
1:A:96:GLU:OE1	1:A:135:ILE:HD11	0.42	2.15	7	1
1:A:11:LYS:HD3	1:A:18:TYR:CD2	0.41	2.50	12	1
1:A:138:THR:HG23	1:A:146:LYS:HB2	0.41	1.91	16	1
1:A:6:CYS:HB3	1:A:136:ALA:HB3	0.41	1.90	10	1
1:A:7:LEU:HD23	1:A:21:LYS:O	0.41	2.15	4	1
1:A:5:THR:HG21	1:A:22:ARG:HD3	0.41	1.90	13	1
1:A:82:HIS:CD2	1:A:86:GLY:HA3	0.41	2.50	7	1
1:A:54:ASN:ND2	1:A:94:LEU:HD12	0.41	2.30	19	1
1:A:9:ASP:HB3	1:A:139:LYS:HA	0.41	1.92	14	1
1:A:3:THR:CG2	1:A:24:LEU:HD23	0.41	2.45	16	1
1:A:96:GLU:CB	1:A:123:ILE:HD13	0.41	2.45	7	1
1:A:96:GLU:CG	1:A:121:ARG:HD2	0.41	2.46	6	1
1:A:71:PHE:CG	1:A:132:CYS:HB3	0.40	2.51	20	1
1:A:93:TYR:CZ	1:A:95:LEU:HB3	0.40	2.52	7	1
1:A:51:TRP:CZ2	1:A:53:THR:HA	0.40	2.52	7	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	
1	A	140/150 (93%)	105±3 (75±2%)	29±4 (21±3%)	6±2 (4±1%)	6	30
All	All	2800/3000 (93%)	2101 (75%)	576 (21%)	123 (4%)	6	30

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

Mol	Chain	Res	Type	Models (Total)
1	A	140	GLU	18
1	A	139	LYS	15
1	A	107	LYS	12
1	A	2	VAL	10

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Mol	Chain	Res	Type	Models (Total)
1	A	130	VAL	9
1	A	119	PRO	8
1	A	125	THR	8
1	A	69	ILE	7
1	A	47	SER	5
1	A	147	LEU	4
1	A	106	TYR	4
1	A	83	SER	4
1	A	105	ASP	4
1	A	84	LYS	3
1	A	58	GLY	2
1	A	86	GLY	2
1	A	145	LEU	2
1	A	91	ASP	1
1	A	131	PHE	1
1	A	148	CYS	1
1	A	88	GLY	1
1	A	87	ASN	1
1	A	39	LEU	1

6.3.2 Protein sidechains ⓘ

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	
1	A	126/132 (95%)	99±3 (78±2%)	27±3 (22±2%)	4	32
All	All	2520/2640 (95%)	1974 (78%)	546 (22%)	4	32

All 64 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)
1	A	24	LEU	20
1	A	36	HIS	20
1	A	44	THR	20
1	A	110	SER	19
1	A	18	TYR	18
1	A	31	GLU	17

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Mol	Chain	Res	Type	Models (Total)
1	A	107	LYS	17
1	A	84	LYS	16
1	A	3	THR	16
1	A	78	ARG	15
1	A	57	ASP	15
1	A	6	CYS	15
1	A	95	LEU	15
1	A	140	GLU	14
1	A	74	SER	14
1	A	17	LYS	14
1	A	102	ASP	13
1	A	144	GLU	13
1	A	85	ASP	13
1	A	132	CYS	13
1	A	128	ASN	12
1	A	29	LYS	12
1	A	89	LYS	11
1	A	81	LYS	11
1	A	23	LEU	11
1	A	27	GLN	10
1	A	105	ASP	10
1	A	139	LYS	10
1	A	91	ASP	9
1	A	142	GLN	9
1	A	16	ASN	8
1	A	26	ASN	8
1	A	50	HIS	8
1	A	112	LYS	7
1	A	70	LYS	6
1	A	22	ARG	6
1	A	145	LEU	6
1	A	21	LYS	5
1	A	11	LYS	5
1	A	43	LYS	5
1	A	111	LYS	5
1	A	73	LYS	4
1	A	121	ARG	4
1	A	126	TYR	4
1	A	14	LYS	4
1	A	8	ASN	4
1	A	116	ASN	4
1	A	9	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	114	LYS	3
1	A	146	LYS	3
1	A	93	TYR	3
1	A	33	ASN	2
1	A	28	ASN	2
1	A	41	ASP	2
1	A	83	SER	2
1	A	75	ASP	2
1	A	109	ASP	2
1	A	15	THR	1
1	A	10	GLN	1
1	A	54	ASN	1
1	A	141	ASN	1
1	A	46	SER	1
1	A	135	ILE	1
1	A	82	HIS	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided