



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 02:58 AM UTC

PDB ID : 2AAS / pdb_00002aas
Title : HIGH-RESOLUTION THREE-DIMENSIONAL STRUCTURE OF RIBONUCLEASE A IN SOLUTION BY NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY
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Deposited on : 1992-11-20

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We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

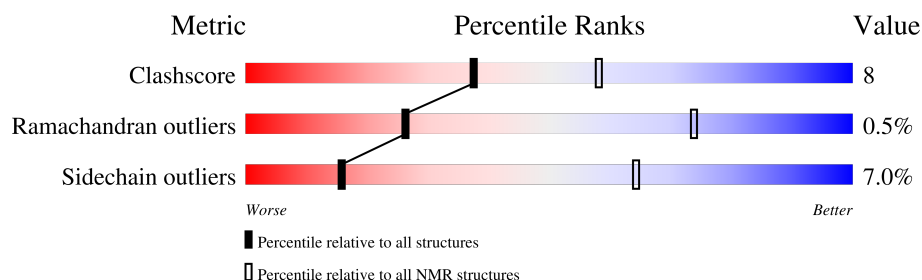
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	124	 75% 22% ..

2 Ensemble composition and analysis

This entry contains 32 models. Model 22 is the overall representative, medoid model (most similar to other models).

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:4-A:124 (121)	0.53	22

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 8 clusters and 2 single-model clusters were found.

Cluster number	Models
1	3, 4, 6, 8, 22, 24
2	17, 18, 19, 20, 21, 23
3	9, 25, 26, 29
4	2, 5, 7
5	14, 16, 30, 32
6	10, 11, 13
7	15, 31
8	12, 28
Single-model clusters	1; 27

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1196 atoms, of which 245 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RIBONUCLEASE A.

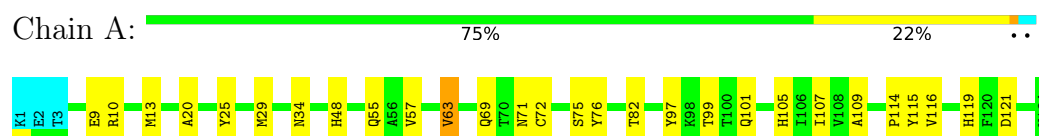
Mol	Chain	Residues	Atoms						Trace
1	A	124	Total	C	H	N	O	S	0
			1196	575	245	171	193	12	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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 A

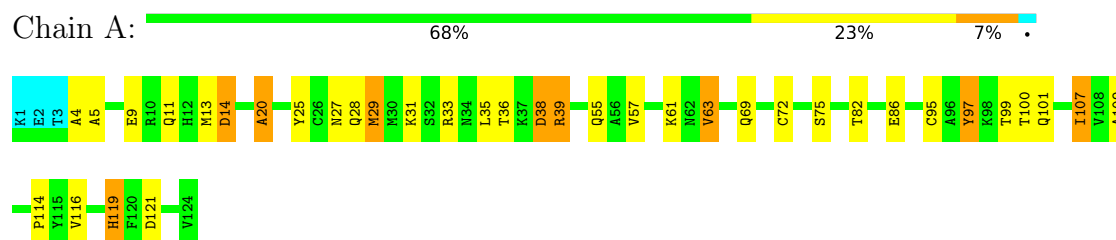


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

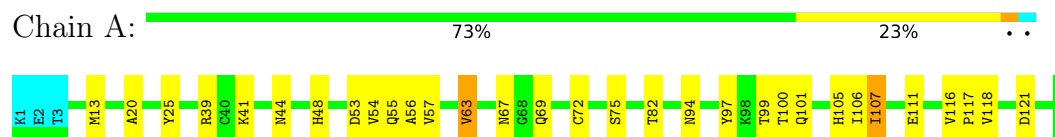
4.2.1 Score per residue for model 1

• Molecule 1: RIBONUCLEASE A



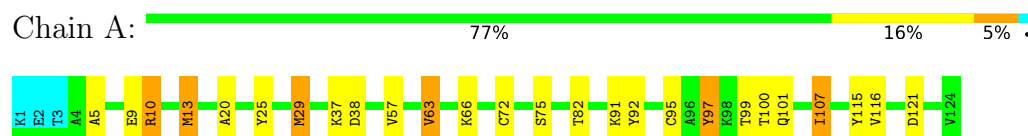
4.2.2 Score per residue for model 2

• Molecule 1: RIBONUCLEASE A



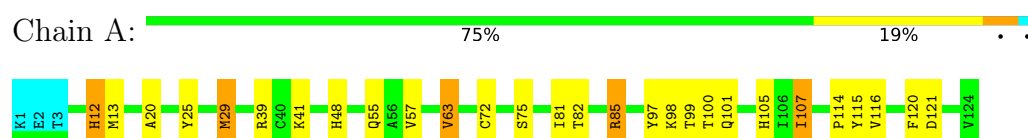
4.2.3 Score per residue for model 3

- Molecule 1: RIBONUCLEASE A



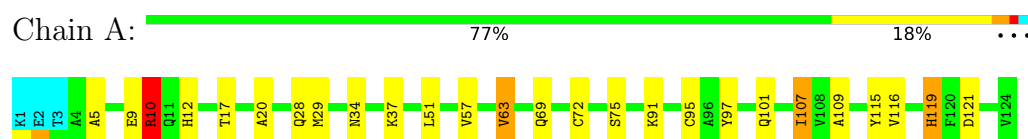
4.2.4 Score per residue for model 4

- Molecule 1: RIBONUCLEASE A



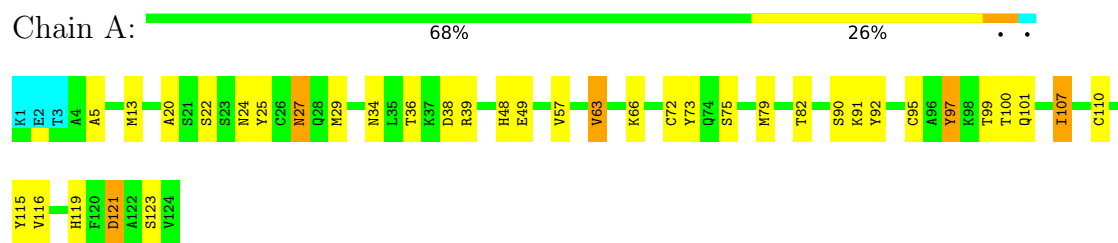
4.2.5 Score per residue for model 5

- Molecule 1: RIBONUCLEASE A



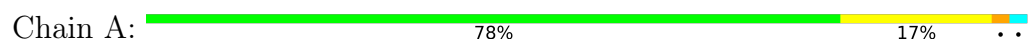
4.2.6 Score per residue for model 6

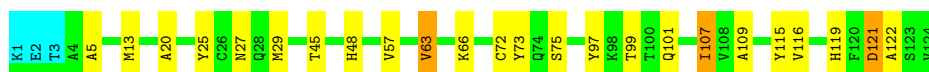
- Molecule 1: RIBONUCLEASE A



4.2.7 Score per residue for model 7

- Molecule 1: RIBONUCLEASE A





4.2.8 Score per residue for model 8

- Molecule 1: RIBONUCLEASE A

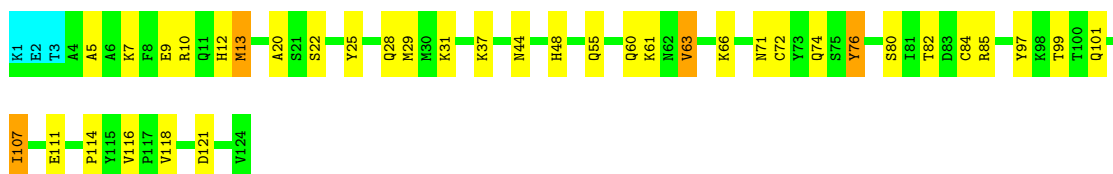
Chain A: 72% 21% 5%



4.2.9 Score per residue for model 9

- Molecule 1: RIBONUCLEASE A

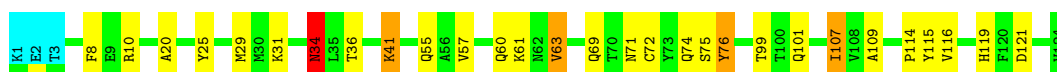
Chain A: 68% 27%



4.2.10 Score per residue for model 10

- Molecule 1: RIBONUCLEASE A

Chain A: 74% 19%



4.2.11 Score per residue for model 11

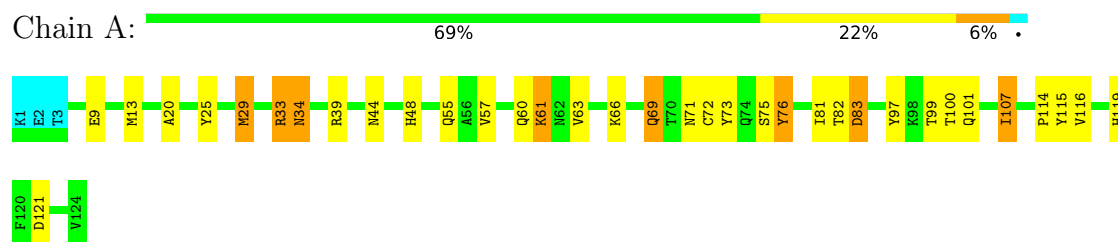
- Molecule 1: RIBONUCLEASE A

Chain A: 75% 19%



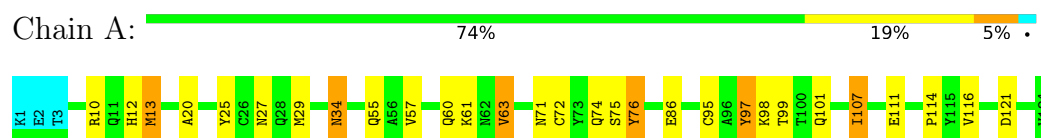
4.2.12 Score per residue for model 12

- Molecule 1: RIBONUCLEASE A



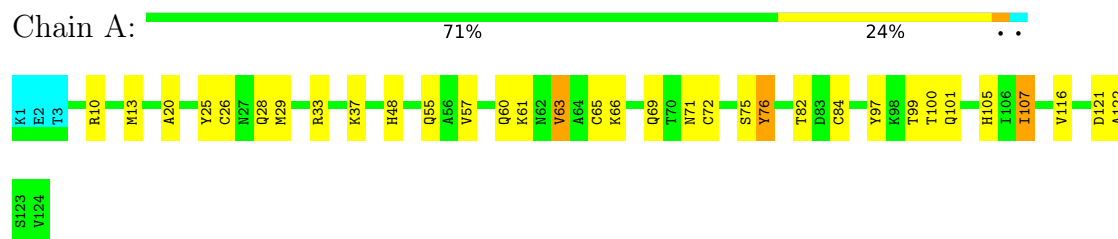
4.2.13 Score per residue for model 13

- Molecule 1: RIBONUCLEASE A



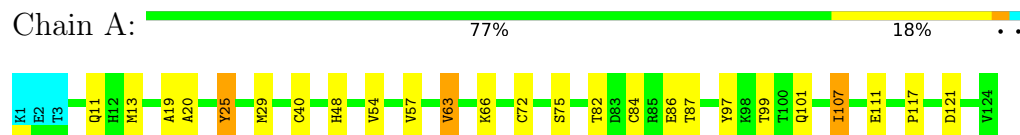
4.2.14 Score per residue for model 14

- Molecule 1: RIBONUCLEASE A



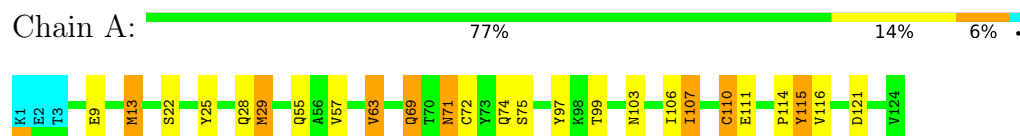
4.2.15 Score per residue for model 15

- Molecule 1: RIBONUCLEASE A



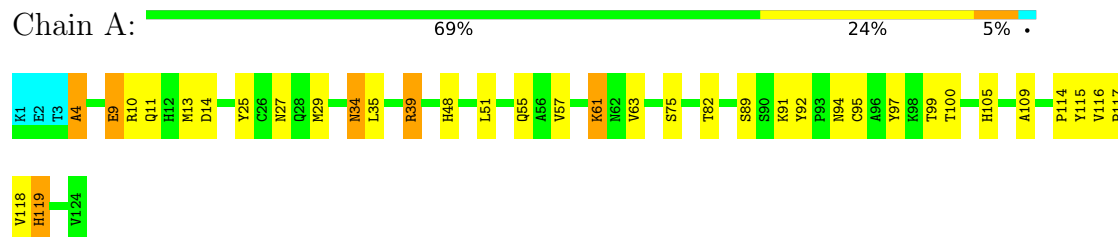
4.2.16 Score per residue for model 16

- Molecule 1: RIBONUCLEASE A



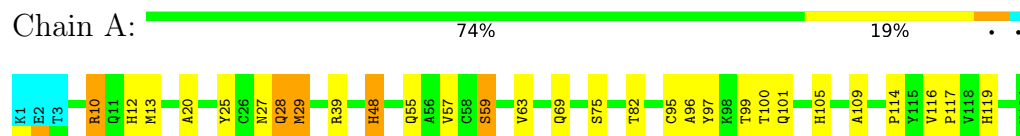
4.2.17 Score per residue for model 17

- Molecule 1: RIBONUCLEASE A



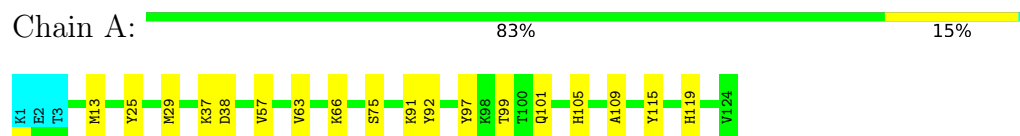
4.2.18 Score per residue for model 18

- Molecule 1: RIBONUCLEASE A



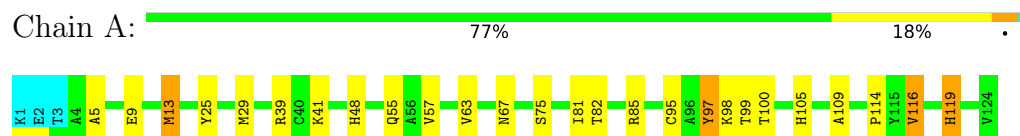
4.2.19 Score per residue for model 19

- Molecule 1: RIBONUCLEASE A



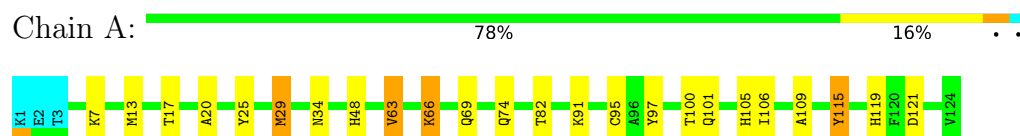
4.2.20 Score per residue for model 20

- Molecule 1: RIBONUCLEASE A



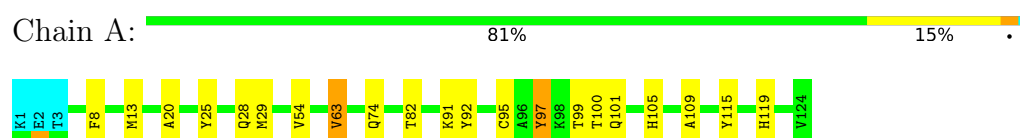
4.2.21 Score per residue for model 21

- Molecule 1: RIBONUCLEASE A



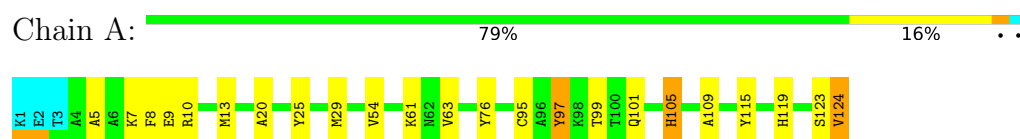
4.2.22 Score per residue for model 22 (medoid)

- Molecule 1: RIBONUCLEASE A



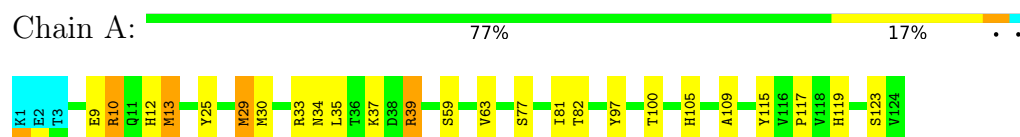
4.2.23 Score per residue for model 23

- Molecule 1: RIBONUCLEASE A



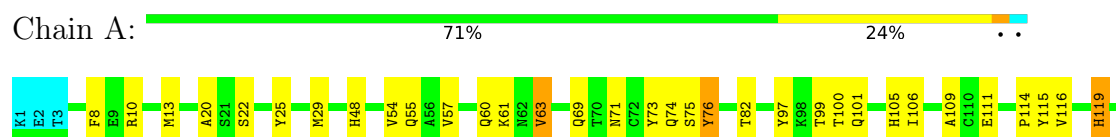
4.2.24 Score per residue for model 24

- Molecule 1: RIBONUCLEASE A



4.2.25 Score per residue for model 25

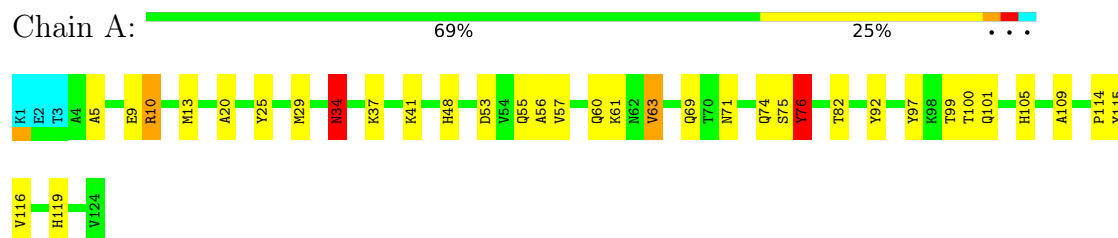
- Molecule 1: RIBONUCLEASE A



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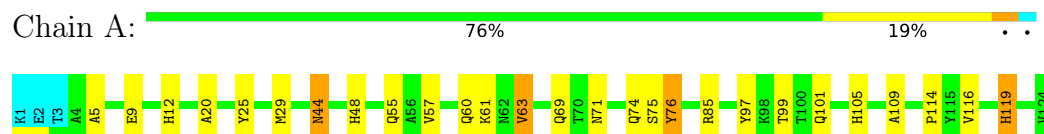
4.2.26 Score per residue for model 26

- Molecule 1: RIBONUCLEASE A



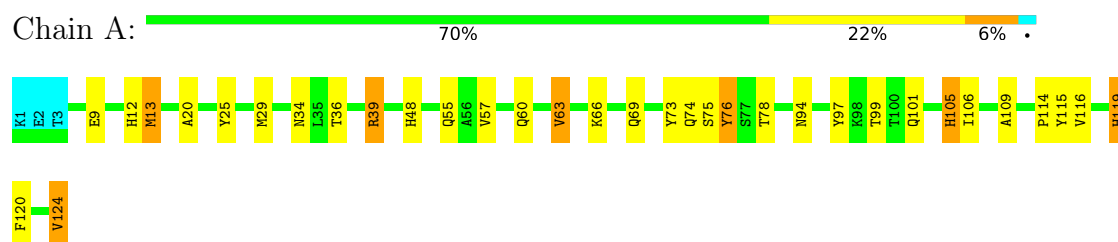
4.2.27 Score per residue for model 27

- Molecule 1: RIBONUCLEASE A



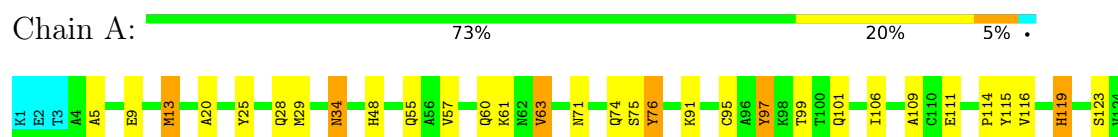
4.2.28 Score per residue for model 28

- Molecule 1: RIBONUCLEASE A



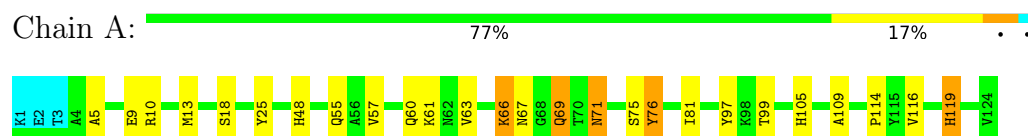
4.2.29 Score per residue for model 29

- Molecule 1: RIBONUCLEASE A



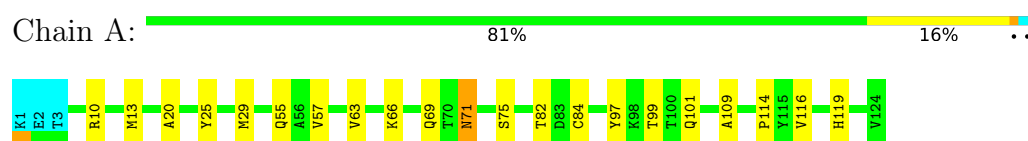
4.2.30 Score per residue for model 30

- Molecule 1: RIBONUCLEASE A



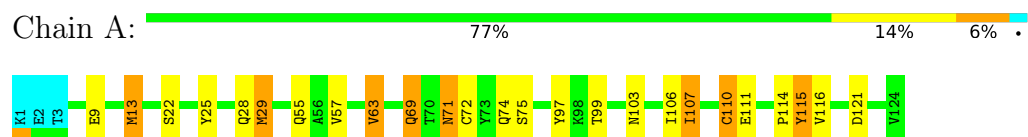
4.2.31 Score per residue for model 31

- Molecule 1: RIBONUCLEASE A



4.2.32 Score per residue for model 32

- Molecule 1: RIBONUCLEASE A



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 32 were deposited, based on the following criterion: ?.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	0.96±0.01	1±1/942 (0.1± 0.1%)	1.50±0.04	3±2/1271 (0.2± 0.2%)
All	All	0.96	45/30144 (0.1%)	1.50	96/40672 (0.2%)

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	3.0±1.6
All	All	0	95

All unique bond 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(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	10	ARG	NE-CZ	-6.86	1.25	1.33	5	1
1	A	48	HIS	CD2-NE2	-5.81	1.31	1.37	11	17
1	A	105	HIS	CG-ND1	-5.67	1.32	1.38	18	11
1	A	48	HIS	CG-ND1	-5.43	1.32	1.38	21	4
1	A	12	HIS	CG-ND1	-5.31	1.32	1.38	4	6
1	A	119	HIS	CG-ND1	-5.13	1.32	1.38	17	4
1	A	105	HIS	CD2-NE2	-5.09	1.32	1.37	4	2

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	10	ARG	NE-CZ-NH1	-17.28	104.22	121.50	3	2
1	A	44	ASN	OD1-CG-ND2	-16.21	106.39	122.60	27	2
1	A	10	ARG	NE-CZ-NH2	-16.18	104.64	119.20	5	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	34	ASN	CA-CB-CG	10.11	122.71	112.60	10	2
1	A	66	LYS	CD-CE-NZ	-8.65	84.22	111.90	21	3
1	A	66	LYS	CA-CB-CG	-8.39	97.32	114.10	12	2
1	A	44	ASN	CA-CB-CG	7.35	119.95	112.60	8	1
1	A	10	ARG	NH1-CZ-NH2	7.29	128.78	119.30	5	1
1	A	71	ASN	OD1-CG-ND2	-7.22	115.38	122.60	12	1
1	A	105	HIS	CA-CB-CG	6.85	120.65	113.80	17	11
1	A	34	ASN	N-CA-C	6.40	124.42	110.80	12	1
1	A	34	ASN	CA-C-N	6.13	128.96	120.63	12	2
1	A	34	ASN	C-N-CA	6.13	128.96	120.63	12	2
1	A	13	MET	N-CA-C	6.11	118.14	108.67	29	8
1	A	85	ARG	NE-CZ-NH2	6.05	124.64	119.20	20	2
1	A	24	ASN	N-CA-CB	-6.02	102.30	110.67	11	1
1	A	34	ASN	OD1-CG-ND2	-6.01	116.58	122.60	10	1
1	A	59	SER	CA-CB-OG	-5.96	99.19	111.10	18	1
1	A	77	SER	N-CA-C	5.95	116.95	108.74	24	1
1	A	28	GLN	CA-CB-CG	-5.82	102.47	114.10	8	1
1	A	7	LYS	CD-CE-NZ	-5.78	93.40	111.90	23	3
1	A	7	LYS	CA-CB-CG	-5.78	102.55	114.10	21	1
1	A	66	LYS	CG-CD-CE	-5.72	98.14	111.30	28	2
1	A	61	LYS	CB-CA-C	5.66	118.86	110.14	17	1
1	A	85	ARG	NH1-CZ-NH2	-5.63	111.98	119.30	4	1
1	A	10	ARG	N-CA-CB	-5.59	101.91	110.12	24	3
1	A	61	LYS	CD-CE-NZ	-5.52	94.22	111.90	12	1
1	A	7	LYS	CB-CG-CD	-5.50	98.65	111.30	23	1
1	A	47	VAL	N-CA-CB	-5.49	105.08	112.10	8	1
1	A	119	HIS	CB-CG-CD2	-5.47	124.08	131.20	29	9
1	A	37	LYS	N-CA-C	5.47	119.70	113.19	5	2
1	A	117	PRO	N-CA-CB	5.45	107.66	103.30	24	2
1	A	33	ARG	CA-C-O	-5.35	115.94	122.41	12	1
1	A	66	LYS	N-CA-C	5.32	117.76	111.33	12	1
1	A	66	LYS	N-CA-CB	-5.32	101.57	110.39	30	1
1	A	37	LYS	N-CA-CB	-5.29	101.13	110.39	26	1
1	A	28	GLN	N-CA-CB	-5.14	102.54	110.20	18	1
1	A	87	THR	CA-C-N	5.12	125.77	120.03	8	2
1	A	87	THR	C-N-CA	5.12	125.77	120.03	8	2
1	A	106	ILE	N-CA-C	5.12	115.85	108.48	2	1
1	A	69	GLN	OE1-CD-NE2	-5.12	117.48	122.60	30	1
1	A	37	LYS	CA-CB-CG	-5.12	103.87	114.10	14	1
1	A	41	LYS	CA-C-N	5.08	124.53	119.24	10	1
1	A	41	LYS	C-N-CA	5.08	124.53	119.24	10	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	66	LYS	CB-CA-C	5.08	120.92	110.31	30	1
1	A	67	ASN	CB-CG-ND2	-5.05	108.82	116.40	2	2
1	A	76	TYR	CB-CG-CD2	-5.04	113.24	120.80	26	1
1	A	105	HIS	N-CA-CB	5.03	117.36	109.97	22	1
1	A	11	GLN	N-CA-C	5.03	116.84	111.36	15	1
1	A	67	ASN	CA-CB-CG	5.02	117.62	112.60	30	1
1	A	116	VAL	CB-CA-C	5.00	114.98	110.13	20	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	97	TYR	Sidechain	27
1	A	115	TYR	Sidechain	17
1	A	76	TYR	Sidechain	13
1	A	92	TYR	Sidechain	7
1	A	73	TYR	Sidechain	6
1	A	69	GLN	Mainchain	3
1	A	10	ARG	Mainchain,Sidechain	2
1	A	37	LYS	Mainchain	2
1	A	12	HIS	Sidechain	2
1	A	13	MET	Mainchain	2
1	A	33	ARG	Mainchain	2
1	A	44	ASN	Mainchain,Sidechain	2
1	A	14	ASP	Mainchain	1
1	A	8	PHE	Sidechain	1
1	A	34	ASN	Mainchain	1
1	A	9	GLU	Mainchain	1
1	A	48	HIS	Sidechain	1
1	A	39	ARG	Sidechain	1
1	A	81	ILE	Mainchain	1
1	A	78	THR	Mainchain	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	926	236	877	14±5
All	All	29632	7552	28064	433

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:GLN:NE2	1:A:71:ASN:OD1	1.23	1.68	10	3
1:A:69:GLN:HE21	1:A:71:ASN:ND2	1.20	1.32	27	1
1:A:69:GLN:HE22	1:A:71:ASN:CG	1.18	1.44	26	1
1:A:114:PRO:O	1:A:116:VAL:HG13	1.17	1.40	17	19
1:A:69:GLN:HG2	1:A:71:ASN:OD1	1.13	1.41	27	2
1:A:69:GLN:NE2	1:A:71:ASN:HD21	1.13	1.39	27	1
1:A:69:GLN:CG	1:A:71:ASN:OD1	1.10	1.99	27	2
1:A:55:GLN:NE2	1:A:116:VAL:HG12	1.07	1.65	12	21
1:A:69:GLN:HE21	1:A:71:ASN:CG	1.04	1.61	27	1
1:A:69:GLN:CD	1:A:71:ASN:OD1	1.02	2.00	26	2
1:A:69:GLN:NE2	1:A:71:ASN:CG	0.91	2.24	26	2
1:A:71:ASN:OD1	1:A:71:ASN:O	0.91	1.88	16	4
1:A:69:GLN:NE2	1:A:71:ASN:ND2	0.89	2.07	27	2
1:A:69:GLN:OE1	1:A:71:ASN:OD1	0.84	1.95	26	1
1:A:55:GLN:NE2	1:A:116:VAL:CG1	0.82	2.43	9	11
1:A:63:VAL:HG21	1:A:107:ILE:HG12	0.75	1.56	8	16
1:A:69:GLN:HE22	1:A:71:ASN:ND2	0.75	1.79	26	1
1:A:61:LYS:HB2	1:A:76:TYR:CZ	0.70	2.21	27	9
1:A:107:ILE:HG22	1:A:121:ASP:HB3	0.69	1.64	1	12
1:A:60:GLN:HB3	1:A:76:TYR:HE2	0.69	1.47	26	11
1:A:5:ALA:HB2	1:A:116:VAL:HG21	0.67	1.64	3	5
1:A:71:ASN:ND2	1:A:71:ASN:O	0.67	2.28	27	3
1:A:20:ALA:HB3	1:A:101:GLN:HB2	0.66	1.67	3	24
1:A:55:GLN:HE21	1:A:116:VAL:HG12	0.66	1.50	1	7
1:A:41:LYS:HD3	1:A:44:ASN:HB2	0.66	1.68	2	1
1:A:10:ARG:HH11	1:A:34:ASN:HD21	0.66	1.31	10	1
1:A:109:ALA:HB3	1:A:119:HIS:HB3	0.66	1.66	31	15
1:A:61:LYS:HB3	1:A:76:TYR:CZ	0.63	2.28	30	2
1:A:71:ASN:O	1:A:71:ASN:CG	0.62	2.41	13	3
1:A:25:TYR:HB3	1:A:99:THR:HG21	0.62	1.70	10	29
1:A:65:CYS:SG	1:A:71:ASN:OD1	0.61	2.58	14	1
1:A:72:CYS:HB3	1:A:107:ILE:HG23	0.59	1.72	3	17
1:A:60:GLN:HB3	1:A:76:TYR:CE2	0.59	2.31	26	10
1:A:61:LYS:HB2	1:A:76:TYR:OH	0.58	1.98	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:PRO:O	1:A:116:VAL:CG1	0.58	2.36	12	2
1:A:95:CYS:HB3	1:A:97:TYR:HE1	0.58	1.59	17	12
1:A:71:ASN:HD22	1:A:71:ASN:C	0.58	2.07	30	1
1:A:57:VAL:HG22	1:A:75:SER:HB3	0.57	1.77	14	27
1:A:71:ASN:OD1	1:A:71:ASN:C	0.56	2.48	16	2
1:A:10:ARG:NH1	1:A:34:ASN:HD21	0.55	1.99	10	2
1:A:24:ASN:O	1:A:27:ASN:HB2	0.55	2.01	6	1
1:A:49:GLU:HG3	1:A:79:MET:HE2	0.55	1.78	6	1
1:A:107:ILE:HG22	1:A:121:ASP:HB2	0.53	1.77	15	4
1:A:10:ARG:HD2	1:A:34:ASN:HD21	0.53	1.63	13	1
1:A:19:ALA:HB1	1:A:101:GLN:HG2	0.53	1.81	15	1
1:A:63:VAL:HG11	1:A:74:GLN:HB2	0.52	1.82	9	11
1:A:55:GLN:CD	1:A:116:VAL:HG12	0.52	2.30	10	5
1:A:9:GLU:HA	1:A:13:MET:HG3	0.52	1.81	24	6
1:A:25:TYR:CZ	1:A:29:MET:HG3	0.51	2.40	8	10
1:A:69:GLN:HG2	1:A:71:ASN:CG	0.51	2.26	27	1
1:A:105:HIS:HB2	1:A:124:VAL:HG23	0.50	1.82	23	2
1:A:38:ASP:HB2	1:A:39:ARG:NH1	0.50	2.21	1	1
1:A:71:ASN:C	1:A:71:ASN:ND2	0.50	2.68	30	1
1:A:27:ASN:ND2	1:A:97:TYR:H	0.49	2.05	17	2
1:A:63:VAL:HG22	1:A:72:CYS:C	0.49	2.33	7	12
1:A:5:ALA:O	1:A:9:GLU:HG3	0.49	2.08	27	9
1:A:66:LYS:HE2	1:A:122:ALA:HB2	0.48	1.85	14	1
1:A:40:CYS:HB3	1:A:86:GLU:OE2	0.48	2.09	15	1
1:A:71:ASN:O	1:A:71:ASN:OD1	0.47	2.31	9	1
1:A:109:ALA:HB3	1:A:119:HIS:HB2	0.47	1.87	5	4
1:A:66:LYS:HE3	1:A:122:ALA:HB2	0.47	1.87	7	1
1:A:61:LYS:HB3	1:A:76:TYR:OH	0.47	2.09	14	2
1:A:82:THR:HA	1:A:100:THR:O	0.47	2.10	22	15
1:A:9:GLU:OE1	1:A:51:LEU:HD13	0.46	2.09	17	2
1:A:110:CYS:HB3	1:A:115:TYR:CE2	0.46	2.46	16	2
1:A:111:GLU:OE2	1:A:118:VAL:HG11	0.46	2.11	2	1
1:A:27:ASN:ND2	1:A:96:ALA:HA	0.46	2.26	18	1
1:A:60:GLN:HB3	1:A:76:TYR:OH	0.46	2.10	12	1
1:A:71:ASN:CG	1:A:71:ASN:O	0.46	2.59	29	1
1:A:55:GLN:HG2	1:A:117:PRO:HD2	0.45	1.88	18	1
1:A:27:ASN:HA	1:A:97:TYR:HD2	0.45	1.71	8	1
1:A:10:ARG:O	1:A:33:ARG:HG3	0.45	2.12	14	1
1:A:71:ASN:ND2	1:A:71:ASN:C	0.45	2.75	31	1
1:A:82:THR:HG22	1:A:84:CYS:SG	0.45	2.52	15	5
1:A:39:ARG:NE	1:A:39:ARG:H	0.44	2.10	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:GLN:O	1:A:31:LYS:HB2	0.44	2.12	9	1
1:A:91:LYS:HE2	1:A:94:ASN:HD21	0.44	1.72	17	1
1:A:31:LYS:HA	1:A:36:THR:OG1	0.44	2.12	1	1
1:A:66:LYS:HG2	1:A:121:ASP:OD1	0.43	2.13	21	1
1:A:111:GLU:HB2	1:A:118:VAL:HG11	0.43	1.90	9	1
1:A:4:ALA:HB1	1:A:118:VAL:HB	0.43	1.89	17	1
1:A:74:GLN:HA	1:A:106:ILE:O	0.42	2.14	8	3
1:A:61:LYS:HA	1:A:61:LYS:HD2	0.42	1.71	1	1
1:A:53:ASP:O	1:A:56:ALA:HB3	0.42	2.15	26	2
1:A:40:CYS:HB2	1:A:86:GLU:OE2	0.42	2.13	11	1
1:A:36:THR:HA	1:A:39:ARG:O	0.42	2.14	6	2
1:A:31:LYS:HB3	1:A:36:THR:OG1	0.42	2.15	10	1
1:A:74:GLN:OE1	1:A:124:VAL:HG21	0.42	2.14	28	1
1:A:12:HIS:CE1	1:A:120:PHE:HB3	0.42	2.49	4	2
1:A:73:TYR:CE1	1:A:110:CYS:HB2	0.41	2.50	6	1
1:A:81:ILE:HD13	1:A:83:ASP:OD1	0.41	2.15	12	1
1:A:39:ARG:H	1:A:39:ARG:NE	0.41	2.12	17	1
1:A:33:ARG:C	1:A:35:LEU:H	0.41	2.23	24	1
1:A:54:VAL:HG12	1:A:117:PRO:HG2	0.41	1.93	15	1
1:A:11:GLN:HG2	1:A:35:LEU:HD21	0.41	1.91	1	2
1:A:8:PHE:CZ	1:A:54:VAL:HG11	0.41	2.51	25	3
1:A:54:VAL:HG12	1:A:117:PRO:HG3	0.40	1.93	2	1
1:A:10:ARG:HD2	1:A:10:ARG:C	0.40	2.41	9	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	120/124 (97%)	111±2 (92±1%)	8±2 (7±1%)	1±1 (0±1%)	26	74
All	All	3840/3968 (97%)	3550 (92%)	272 (7%)	18 (0%)	26	74

All 7 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	34	ASN	9
1	A	4	ALA	2
1	A	38	ASP	2
1	A	22	SER	2
1	A	20	ALA	1
1	A	25	TYR	1
1	A	89	SER	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	106/109 (97%)	99±2 (93±2%)	7±2 (7±2%)	16	64
All	All	3392/3488 (97%)	3155 (93%)	237 (7%)	16	64

All 46 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	63	VAL	32
1	A	29	MET	30
1	A	13	MET	24
1	A	107	ILE	17
1	A	69	GLN	12
1	A	39	ARG	10
1	A	28	GLN	9
1	A	91	LYS	7
1	A	10	ARG	7
1	A	66	LYS	6
1	A	111	GLU	6
1	A	115	TYR	5
1	A	41	LYS	4
1	A	34	ASN	4
1	A	123	SER	4
1	A	71	ASN	4
1	A	106	ILE	4
1	A	81	ILE	3
1	A	85	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	98	LYS	3
1	A	22	SER	3
1	A	27	ASN	3
1	A	121	ASP	3
1	A	14	ASP	2
1	A	38	ASP	2
1	A	86	GLU	2
1	A	94	ASN	2
1	A	17	THR	2
1	A	30	MET	2
1	A	103	ASN	2
1	A	110	CYS	2
1	A	61	LYS	2
1	A	59	SER	2
1	A	124	VAL	2
1	A	33	ARG	1
1	A	90	SER	1
1	A	45	THR	1
1	A	108	VAL	1
1	A	37	LYS	1
1	A	80	SER	1
1	A	24	ASN	1
1	A	83	ASP	1
1	A	26	CYS	1
1	A	9	GLU	1
1	A	101	GLN	1
1	A	18	SER	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 oligosaccharides 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