



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 04:33 am BST

PDB ID : 4BS2
Title : NMR structure of human TDP-43 tandem RRM_s in complex with UG-rich RNA
Authors : Lukavsky, P.J.; Daujotyte, D.; Tollervey, J.R.; Ule, J.; Stuani, C.; Buratti, E.; Baralle, F.E.; Damberger, F.F.; Allain, F.H.T.
Deposited on : 2013-06-06

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

<https://www.wwpdb.org/validation/2017/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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

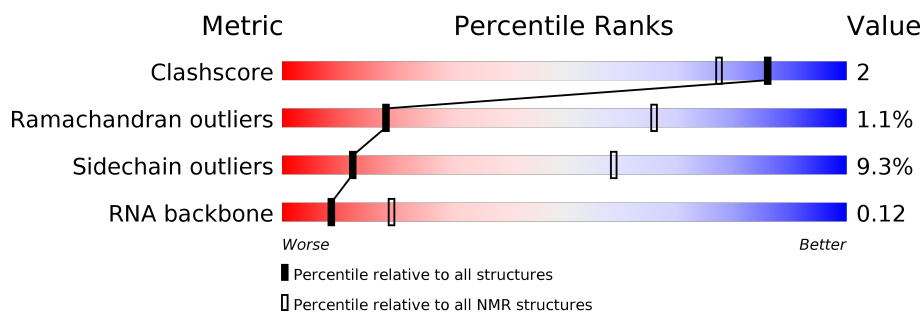
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 90%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428
RNA backbone	4643	676

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	174	
2	B	12	

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.

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:101-A:138, A:145-A:261 (155)	0.25	4

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 4 clusters and 7 single-model clusters were found.

Cluster number	Models
1	1, 4, 13, 14, 15, 19
2	2, 3, 20
3	16, 17
4	7, 9
Single-model clusters	5; 6; 8; 10; 11; 12; 18

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3143 atoms, of which 1485 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TAR DNA-BINDING PROTEIN 43.

Mol	Chain	Residues	Atoms						Trace
1	A	174	Total	C	H	N	O	S	0
			2774	885	1373	241	265	10	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	GLY	-	expression tag	UNP Q13148
A	97	SER	-	expression tag	UNP Q13148
A	98	HIS	-	expression tag	UNP Q13148
A	99	MET	-	expression tag	UNP Q13148
A	100	ALA	-	expression tag	UNP Q13148
A	101	SER	-	expression tag	UNP Q13148

- Molecule 2 is a RNA chain called 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'.

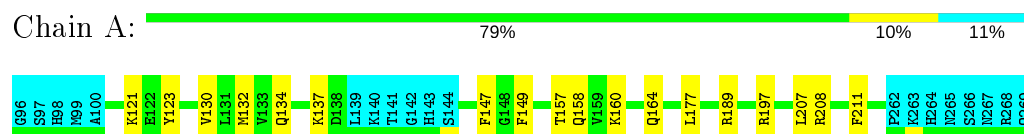
Mol	Chain	Residues	Atoms						Trace
2	B	12	Total	C	H	N	O	P	0
			369	116	112	48	82	11	

4 Residue-property plots [i](#)

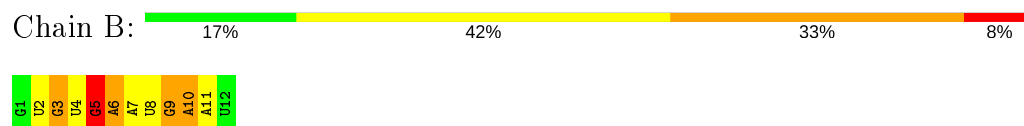
4.1 Average score per residue in the NMR ensemble

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: TAR DNA-BINDING PROTEIN 43



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

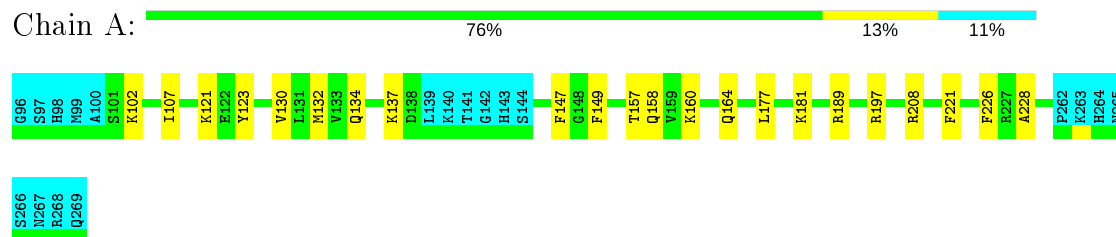


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: TAR DNA-BINDING PROTEIN 43



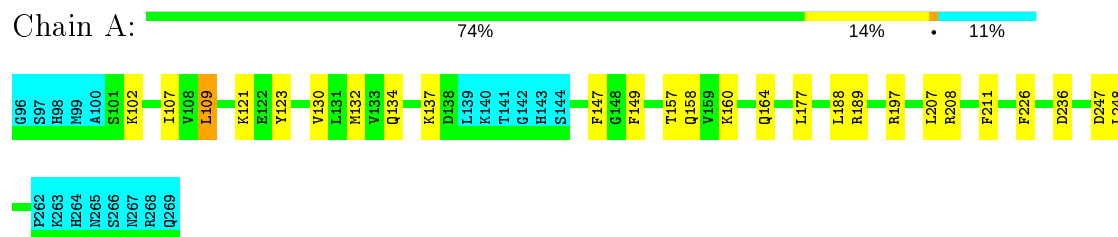
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'



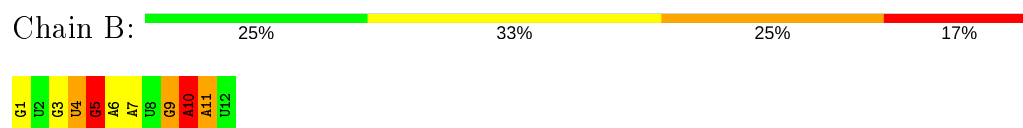


4.2.2 Score per residue for model 2

- Molecule 1: TAR DNA-BINDING PROTEIN 43

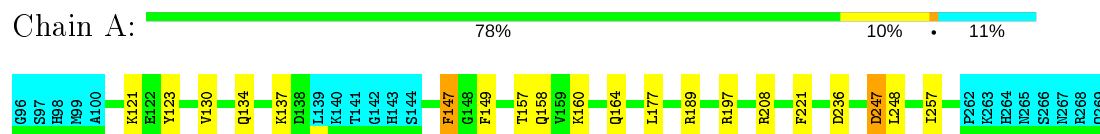


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

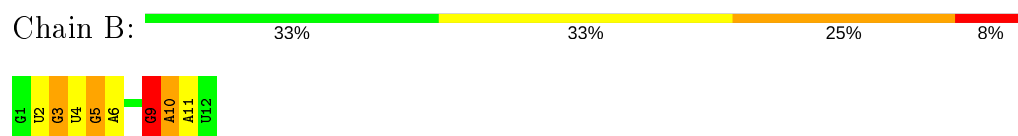


4.2.3 Score per residue for model 3

- Molecule 1: TAR DNA-BINDING PROTEIN 43

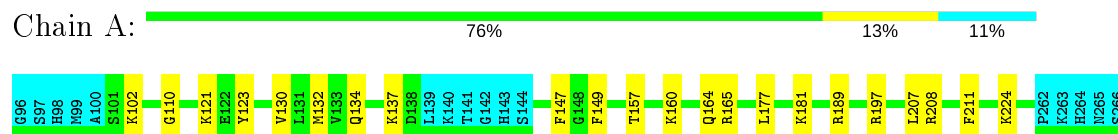


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'



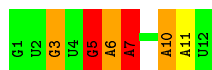
4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: TAR DNA-BINDING PROTEIN 43





- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

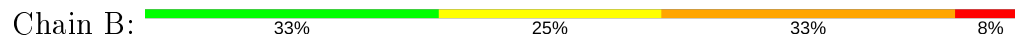


4.2.5 Score per residue for model 5

- Molecule 1: TAR DNA-BINDING PROTEIN 43

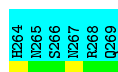
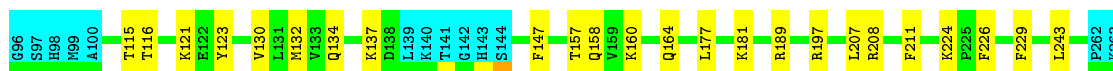


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

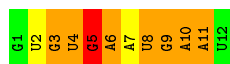


4.2.6 Score per residue for model 6

- Molecule 1: TAR DNA-BINDING PROTEIN 43

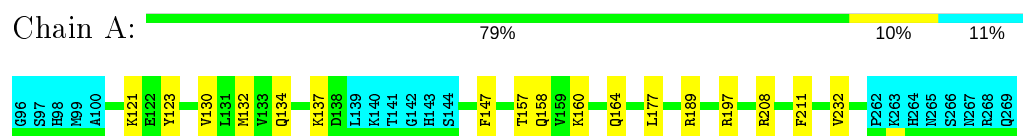


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'



4.2.7 Score per residue for model 7

- Molecule 1: TAR DNA-BINDING PROTEIN 43

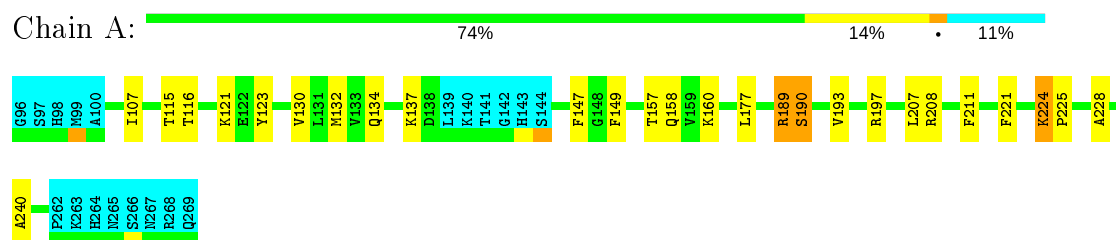


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

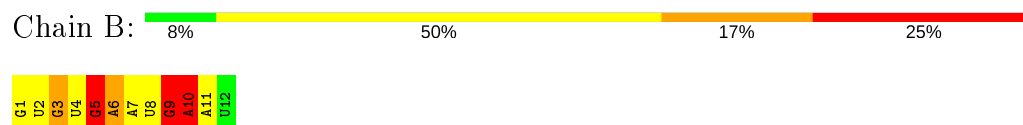


4.2.8 Score per residue for model 8

- Molecule 1: TAR DNA-BINDING PROTEIN 43

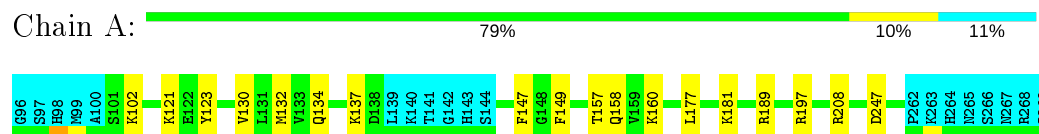


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

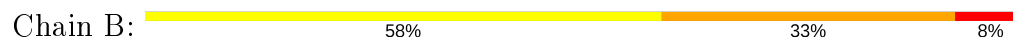


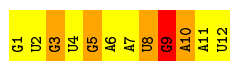
4.2.9 Score per residue for model 9

- Molecule 1: TAR DNA-BINDING PROTEIN 43



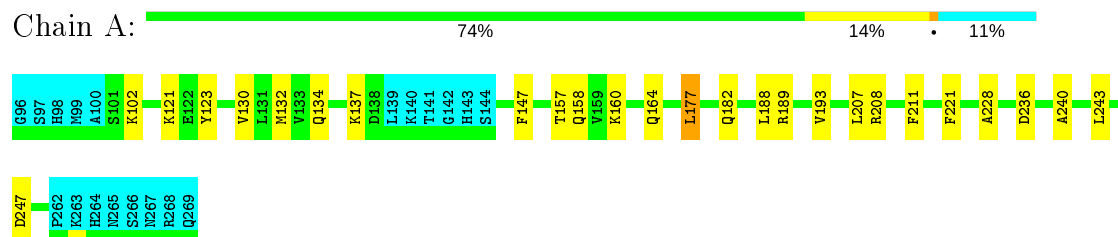
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'



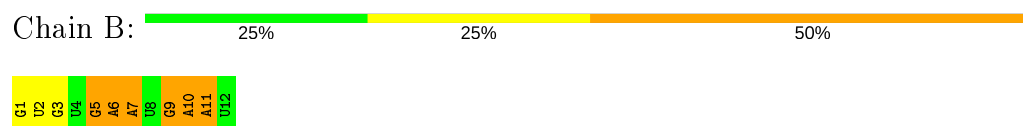


4.2.10 Score per residue for model 10

- Molecule 1: TAR DNA-BINDING PROTEIN 43

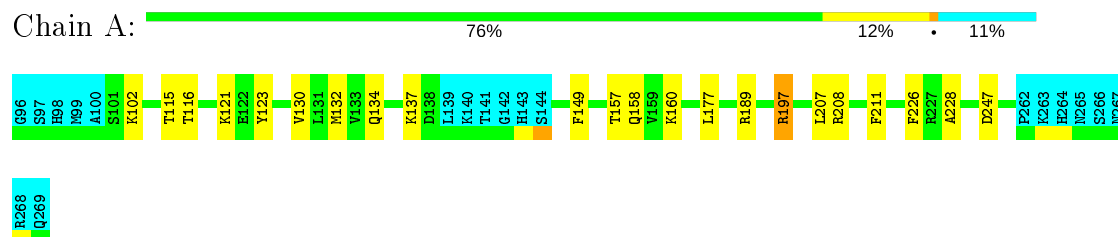


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

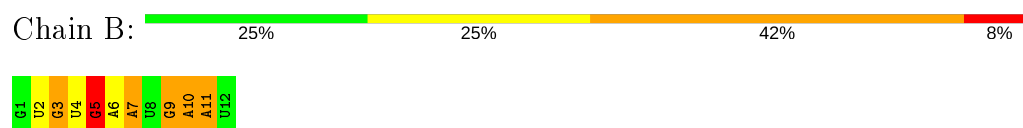


4.2.11 Score per residue for model 11

- Molecule 1: TAR DNA-BINDING PROTEIN 43

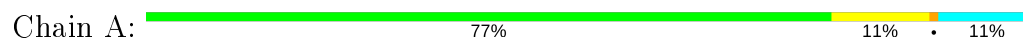


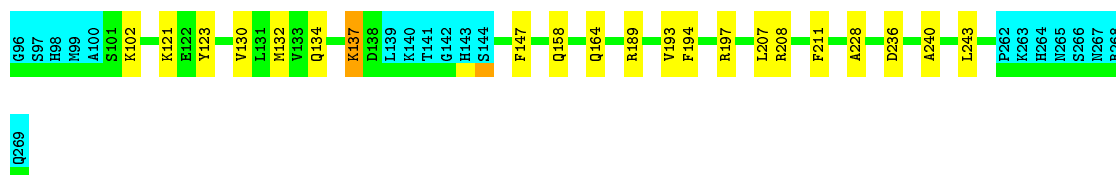
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'



4.2.12 Score per residue for model 12

- Molecule 1: TAR DNA-BINDING PROTEIN 43





- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

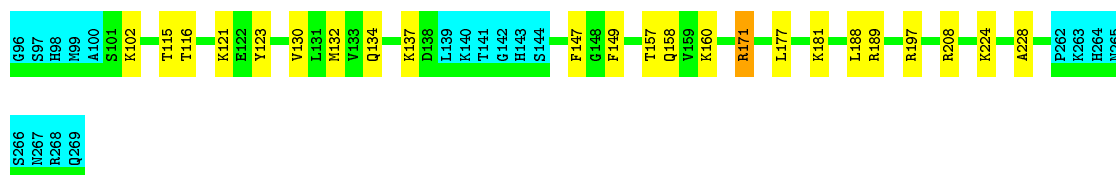
Chain B: 8% 58% 25% 8%



4.2.13 Score per residue for model 13

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 76% 13% 11%



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

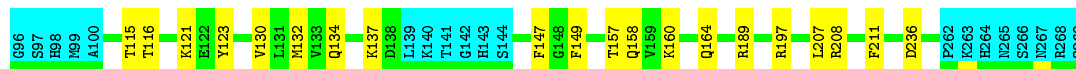
Chain B: 25% 50% 8% 17%



4.2.14 Score per residue for model 14

- Molecule 1: TAR DNA-BINDING PROTEIN 43

Chain A: 78% 11% 11%



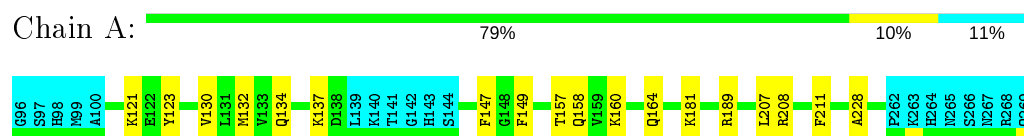
- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 33% 42% 17% 8%

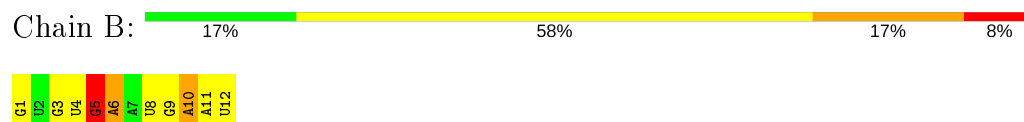


4.2.15 Score per residue for model 15

- Molecule 1: TAR DNA-BINDING PROTEIN 43

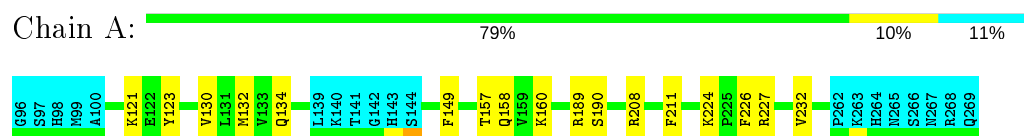


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

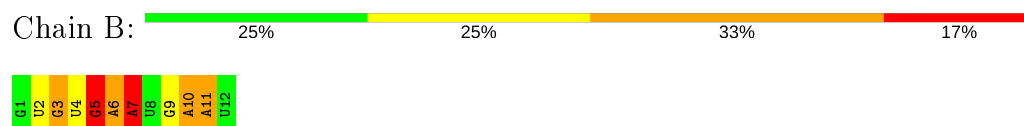


4.2.16 Score per residue for model 16

- Molecule 1: TAR DNA-BINDING PROTEIN 43

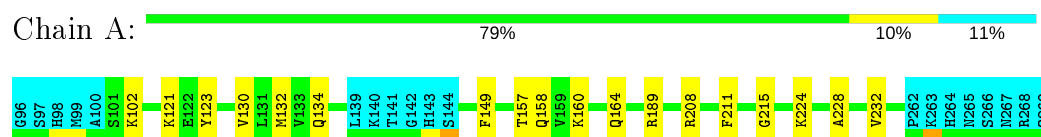


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

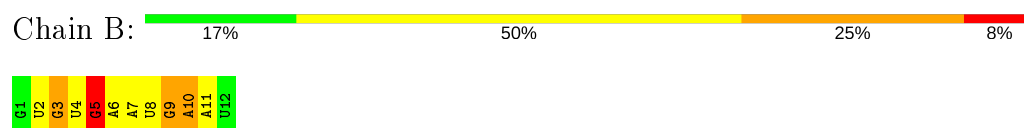


4.2.17 Score per residue for model 17

- Molecule 1: TAR DNA-BINDING PROTEIN 43

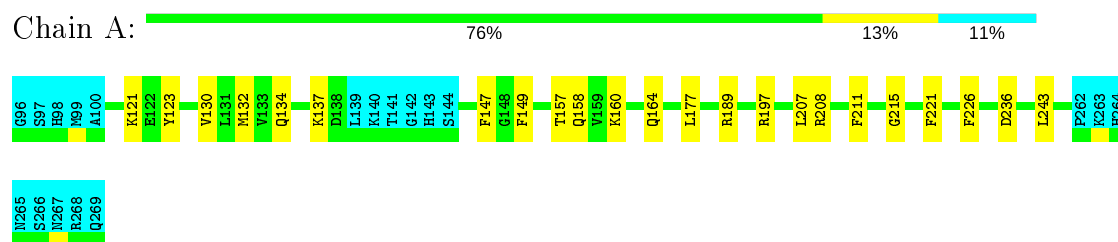


- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'



4.2.18 Score per residue for model 18

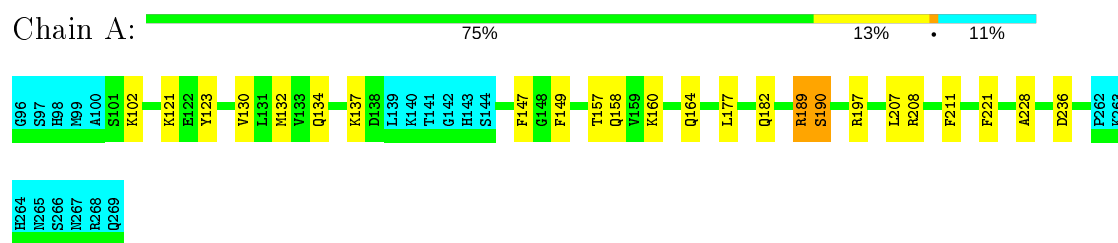
- Molecule 1: TAR DNA-BINDING PROTEIN 43



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

4.2.19 Score per residue for model 19

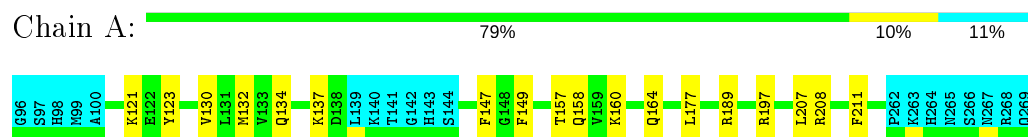
- Molecule 1: TAR DNA-BINDING PROTEIN 43



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

4.2.20 Score per residue for model 20

- Molecule 1: TAR DNA-BINDING PROTEIN 43



- Molecule 2: 5'-R(*GP*UP*GP*UP*GP*AP*AP*UP*GP*AP*AP*UP)-3'

Chain B: 33% 50% 17%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING COMBINED WITH MOLECULAR DYNAMICS IN TORSION ANGLE SPACE*.

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *LOWEST ENERGY AND RESTRAINT VIOLATION*.

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

Software name	Classification	Version
AMBER	refinement	
CYANA	structure solution	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	2
Total number of shifts	2382
Number of shifts mapped to atoms	2382
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	1256	1232	1231	5±2
2	B	257	112	130	3±1
All	All	30260	26880	27220	120

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 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:ALA:HB2	2:B:6:A:C4	0.64	2.27	12	2
1:A:247:ASP:C	1:A:248:LEU:HD12	0.57	2.19	3	1
2:B:6:A:H1'	2:B:7:A:C8	0.56	2.36	12	5
1:A:149:PHE:CZ	2:B:5:G:C4	0.53	2.97	20	15
1:A:207:LEU:HD22	1:A:211:PHE:CE1	0.48	2.42	19	6
2:B:10:A:H5''	2:B:10:A:C8	0.48	2.42	1	3
1:A:221:PHE:CE2	2:B:9:G:H1'	0.47	2.43	8	4
2:B:10:A:C8	2:B:10:A:H5''	0.47	2.45	4	3
1:A:207:LEU:HD22	1:A:211:PHE:CE2	0.46	2.44	14	7
1:A:243:LEU:C	1:A:243:LEU:HD12	0.46	2.31	5	3
2:B:6:A:H2'	2:B:7:A:C8	0.46	2.46	10	1
1:A:243:LEU:HD12	1:A:243:LEU:C	0.46	2.31	12	2
1:A:181:LYS:HE3	2:B:5:G:C5	0.45	2.45	6	1
2:B:10:A:C2	2:B:11:A:C4	0.45	3.04	6	2
1:A:221:PHE:CE1	2:B:9:G:H1'	0.45	2.46	19	2
1:A:157:THR:HA	1:A:160:LYS:HE2	0.45	1.89	15	19
2:B:10:A:N3	2:B:11:A:C8	0.44	2.86	2	2
2:B:9:G:N3	2:B:9:G:C5'	0.44	2.81	18	2
1:A:115:THR:HG22	1:A:116:THR:N	0.44	2.28	11	6
1:A:171:ARG:HD3	1:A:171:ARG:C	0.43	2.34	5	1
1:A:109:LEU:HD22	1:A:109:LEU:H	0.43	1.72	2	1
1:A:224:LYS:HA	1:A:225:PRO:C	0.43	2.34	8	1
1:A:228:ALA:HB2	2:B:6:A:C6	0.43	2.49	8	2
1:A:189:ARG:O	1:A:190:SER:CB	0.43	2.67	8	2
1:A:197:ARG:HD2	2:B:5:G:H1'	0.43	1.91	11	1
1:A:227:ARG:HG2	2:B:7:A:C2	0.42	2.50	16	1
1:A:107:ILE:HG22	1:A:149:PHE:CE2	0.42	2.50	1	1
1:A:147:PHE:CZ	2:B:5:G:C5'	0.42	3.02	3	1
1:A:229:PHE:CE2	2:B:8:U:H4'	0.42	2.50	6	1
1:A:211:PHE:CE1	1:A:232:VAL:HG21	0.41	2.50	7	3
1:A:193:VAL:CG1	1:A:240:ALA:HB1	0.41	2.44	8	2
2:B:10:A:C2	2:B:11:A:C8	0.41	3.08	11	2
1:A:107:ILE:CG2	1:A:149:PHE:CE2	0.41	3.04	2	1
1:A:177:LEU:CD2	1:A:182:GLN:NE2	0.41	2.84	10	1
1:A:181:LYS:HE2	1:A:181:LYS:HA	0.41	1.92	13	1
1:A:171:ARG:C	1:A:171:ARG:HD3	0.41	2.35	13	1
1:A:149:PHE:CE2	2:B:5:G:C5	0.41	3.09	1	2
1:A:248:LEU:HD13	1:A:257:ILE:HG12	0.41	1.93	3	1
1:A:107:ILE:HG22	1:A:149:PHE:CZ	0.41	2.50	8	1
1:A:194:PHE:CE2	2:B:8:U:C6	0.41	3.09	12	1
1:A:193:VAL:HG13	1:A:240:ALA:HB1	0.41	1.92	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:6:A:H2'	2:B:7:A:N7	0.41	2.30	7	1
1:A:110:GLY:HA2	2:B:3:G:C5	0.40	2.51	4	1
2:B:9:G:H5''	2:B:9:G:N3	0.40	2.32	18	1
2:B:10:A:N3	2:B:10:A:H2'	0.40	2.32	2	1
1:A:149:PHE:CZ	2:B:5:G:C5	0.40	3.09	8	1

5.2 Torsion angles [i](#)

5.2.1 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	
1	A	155/174 (89%)	138±1 (89±1%)	15±2 (10±1%)	2±1 (1±0%)	18	66
All	All	3100/3480 (89%)	2761 (89%)	304 (10%)	35 (1%)	18	66

All 5 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	130	VAL	20
1	A	228	ALA	5
1	A	247	ASP	5
1	A	190	SER	3
1	A	215	GLY	2

5.2.2 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	
1	A	141/157 (90%)	128±2 (91±1%)	13±2 (9±1%)	12	59
All	All	2820/3140 (90%)	2558 (91%)	262 (9%)	12	59

All 23 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	134	GLN	20
1	A	123	TYR	20
1	A	208	ARG	20
1	A	121	LYS	20
1	A	189	ARG	20
1	A	158	GLN	19
1	A	132	MET	19
1	A	137	LYS	18
1	A	147	PHE	17
1	A	197	ARG	16
1	A	177	LEU	14
1	A	164	GLN	14
1	A	102	LYS	10
1	A	236	ASP	8
1	A	226	PHE	7
1	A	224	LYS	7
1	A	181	LYS	4
1	A	188	LEU	3
1	A	171	ARG	2
1	A	248	LEU	1
1	A	165	ARG	1
1	A	182	GLN	1
1	A	109	LEU	1

5.2.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
2	B	11/12 (92%)	8±1 (72±12%)	3±1 (27±11%)	0.12±0.07
All	All	221/240 (92%)	159 (72%)	60 (27%)	0.11

The overall RNA backbone suiteness is 0.12.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	3	G	20
2	B	10	A	19
2	B	11	A	19
2	B	6	A	18
2	B	5	G	16

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Mol	Chain	Res	Type	Models (Total)
2	B	9	G	16
2	B	4	U	15
2	B	7	A	12
2	B	8	U	11
2	B	2	U	9
2	B	12	U	4

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
2	B	10	A	19
2	B	3	G	14
2	B	2	U	13
2	B	6	A	5
2	B	4	U	4
2	B	7	A	2
2	B	9	G	2
2	B	1	G	1

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.5 Ligand geometry [i](#)

There are no ligands in this entry.

5.6 Other polymers [i](#)

There are no such molecules in this entry.

5.7 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 89% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *YP597CN-aug12.1_withRNA2_RNA2.str.csh*

6.1.1 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	185
Number of shifts mapped to atoms	185
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

6.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

6.1.3 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 8%, i.e. 166 atoms were assigned a chemical shift out of a possible 2181. 0 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/765 (0%)	0/305 (0%)	0/310 (0%)	0/150 (0%)
Sidechain	0/1016 (0%)	0/597 (0%)	0/372 (0%)	0/47 (0%)
Aromatic	0/180 (0%)	0/97 (0%)	0/78 (0%)	0/5 (0%)
Overall	166/2181 (8%)	90/1127 (8%)	76/840 (9%)	0/214 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 166 atoms were assigned a chemical shift out of a possible 2414. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/858 (0%)	0/342 (0%)	0/348 (0%)	0/168 (0%)
Sidechain	0/1134 (0%)	0/669 (0%)	0/410 (0%)	0/55 (0%)
Aromatic	0/202 (0%)	0/109 (0%)	0/84 (0%)	0/9 (0%)
Overall	166/2414 (7%)	90/1248 (7%)	76/922 (8%)	0/244 (0%)

6.1.4 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	4	U	H4'	3.09	5.04 – 3.74	-10.0
2	B	9	G	H5'	5.42	5.20 – 3.30	6.2
2	B	4	U	H5''	3.01	5.21 – 3.21	-6.0
2	B	8	U	H4'	3.67	5.04 – 3.74	-5.6
2	B	9	G	H2'	5.68	5.66 – 3.46	5.1
2	B	8	U	H5''	3.20	5.21 – 3.21	-5.1

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (YP597CN-aug12.1_withRNA2_RNA2.str.csh). RCI is only applicable to proteins.

6.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: YP597CN-aug12.1_withRNA2_protein2.str.csh

6.2.1 Bookkeeping [i](#)

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	2197
Number of shifts mapped to atoms	2197
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

6.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	172	0.07 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	162	0.02 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}'$	158	0.25 ± 0.11	None needed (< 0.5 ppm)
^{15}N	159	0.24 ± 0.27	None needed (< 0.5 ppm)

6.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 83%, i.e. 1800 atoms were assigned a chemical shift out of a possible 2181. 22 out of 23 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	749/765 (98%)	302/305 (99%)	300/310 (97%)	147/150 (98%)
Sidechain	878/1016 (86%)	545/597 (91%)	315/372 (85%)	18/47 (38%)
Aromatic	173/180 (96%)	93/97 (96%)	78/78 (100%)	2/5 (40%)
Overall	1800/2181 (83%)	940/1127 (83%)	693/840 (82%)	167/214 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1982 atoms were assigned a chemical shift out of a possible 2414. 23 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	821/858 (96%)	332/342 (97%)	330/348 (95%)	159/168 (95%)
Sidechain	976/1134 (86%)	608/669 (91%)	347/410 (85%)	21/55 (38%)
Aromatic	185/202 (92%)	99/109 (91%)	84/84 (100%)	2/9 (22%)
Overall	1982/2414 (82%)	1039/1248 (83%)	761/922 (83%)	182/244 (75%)

6.2.4 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
1	A	250	ILE	HG13	-1.28	3.26 – -0.84	-6.1
1	A	167	MET	HB3	0.05	3.70 – 0.30	-5.7
1	A	168	ILE	HG13	-0.86	3.26 – -0.84	-5.1

6.2.5 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 A:

