



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 1IV6
Title : Solution Structure of the DNA Complex of Human TRF1
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This is a wwPDB NMR Structure Validation Summary 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

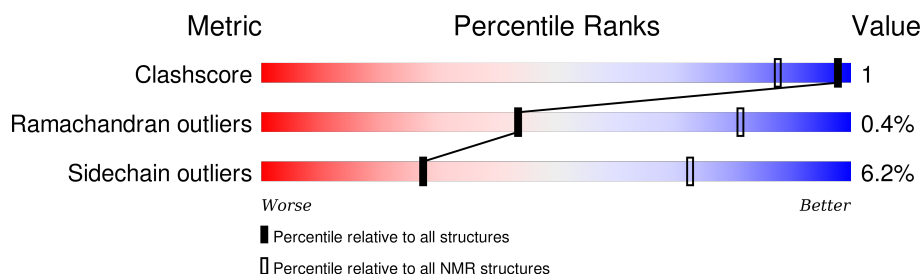
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 56%.

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	B	13	
2	C	13	
3	A	70	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 16 is the overall representative, medoid model (most similar to other models). The authors have identified model 2 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:381-A:429 (49)	0.35	16

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 are 3 unique types of molecules in this entry. The entry contains 1846 atoms, of which 819 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*GP*TP*TP*AP*GP*GP*GP*TP*TP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms						Trace
1	B	13	Total	C	H	N	O	P	0
			422	130	149	53	78	12	

- Molecule 2 is a DNA chain called 5'-D(*CP*CP*CP*TP*AP*AP*CP*CP*CP*TP*AP*AP*C)-3'.

Mol	Chain	Residues	Atoms						Trace
2	C	13	Total	C	H	N	O	P	0
			401	123	147	45	74	12	

- Molecule 3 is a protein called TELOMERIC REPEAT BINDING FACTOR 1.

Mol	Chain	Residues	Atoms						Trace
3	A	57	Total	C	H	N	O	S	0
			1023	320	523	98	80	2	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	MET	-	SEE REMARK 999	UNP P54274

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.

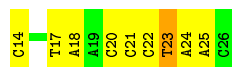
- Molecule 1: 5'-D(*GP*TP*TP*AP*GP*GP*GP*TP*TP*AP*GP*GP*G)-3'

Chain B: 



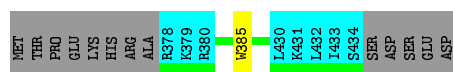
- Molecule 2: 5'-D(*CP*CP*CP*TP*AP*AP*CP*CP*CP*TP*AP*AP*C)-3'

Chain C: 



- Molecule 3: TELOMERIC REPEAT BINDING FACTOR 1

Chain A: 

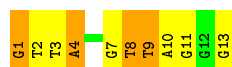


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 16. Colouring as in section 4.1 above.

- Molecule 1: 5'-D(*GP*TP*TP*AP*GP*GP*GP*TP*TP*AP*GP*GP*G)-3'

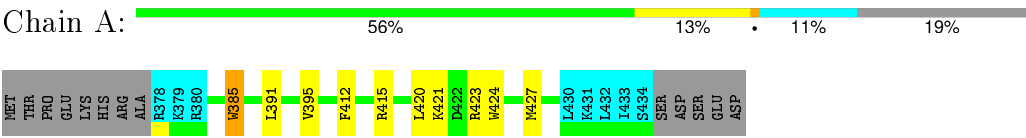
Chain B: 



- Molecule 2: 5'-D(*CP*CP*CP*TP*AP*AP*CP*CP*CP*TP*AP*AP*C)-3'



● Molecule 3: TELOMERIC REPEAT BINDING FACTOR 1



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
EMBOSS	refinement	5.0
EMBOSS	structure solution	5.0

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)	BMRB entry 5361
Number of chemical shift lists	3
Total number of shifts	908
Number of shifts mapped to atoms	908
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	56%

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

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	B	1.24±0.02	0±0/307 (0.0±0.0%)	2.33±0.03	21±1/475 (4.4±0.2%)
2	C	1.26±0.01	0±0/283 (0.0±0.0%)	1.93±0.04	11±2/432 (2.5±0.5%)
3	A	0.62±0.01	0±0/442 (0.0±0.0%)	0.95±0.04	1±1/592 (0.1±0.1%)
All	All	1.03	0/20640 (0.0%)	1.77	645/29980 (2.2%)

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	B	0.0±0.0	2.2±0.9
2	C	0.0±0.0	3.0±1.2
3	A	0.0±0.0	0.3±0.5
All	All	0	110

There are no bond-length outliers.

5 of 63 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	B	3	DT	C6-C5-C7	-12.79	115.22	122.90	8	20
1	B	4	DA	O4'-C1'-N9	12.64	116.85	108.00	3	20
1	B	9	DT	C6-C5-C7	-12.20	115.58	122.90	4	20
2	C	17	DT	C6-C5-C7	-11.97	115.72	122.90	20	20
1	B	8	DT	C6-C5-C7	-11.47	116.02	122.90	6	20

There are no chirality outliers.

5 of 21 unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
2	C	22	DC	Sidechain	14
2	C	23	DT	Sidechain	13
1	B	4	DA	Sidechain	13
2	C	21	DC	Sidechain	9
1	B	9	DT	Sidechain	6

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	B	273	149	149	1±1
2	C	254	147	147	1±1
3	A	430	433	433	1±1
All	All	19140	14580	14580	25

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 1.

5 of 8 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
3:A:385:TRP:CG	3:A:386:GLU:N	0.51	2.79	19	5
1:B:4:DA:C2	2:C:24:DA:C2	0.46	3.03	5	7
3:A:412:PHE:CE2	3:A:420:LEU:HD21	0.46	2.45	16	2
3:A:395:VAL:HG11	3:A:424:TRP:CZ2	0.43	2.49	11	2
3:A:385:TRP:CD1	3:A:386:GLU:N	0.43	2.87	15	1

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
3	A	49/70 (70%)	46±1 (93±2%)	3±1 (7±2%)	0±0 (0±1%)	43 81
All	All	980/1400 (70%)	910 (93%)	66 (7%)	4 (0%)	43 81

All 3 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
3	A	414	ASN	2
3	A	385	TRP	1
3	A	400	GLU	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
3	A	45/65 (69%)	42±1 (94±3%)	3±1 (6±3%)	27 73
All	All	900/1300 (69%)	844 (94%)	56 (6%)	27 73

5 of 18 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)
3	A	385	TRP	8
3	A	421	LYS	7
3	A	423	ARG	7
3	A	427	MET	6
3	A	411	LYS	4

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 [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 [i](#)

The completeness of assignment taking into account all chemical shift lists is 56% for the well-defined parts and 57% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5361

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 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	702
Number of shifts mapped to atoms	702
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	67	1.85 ± 0.16	Should be applied
$^{13}\text{C}_\beta$	54	2.78 ± 0.21	Should be applied
$^{13}\text{C}'$	65	2.11 ± 0.11	Should be applied
^{15}N	67	0.19 ± 0.32	None needed (< 0.5 ppm)

7.1.3 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 41%, i.e. 493 atoms were assigned a chemical shift out of a possible 1213. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	245/245 (100%)	98/98 (100%)	98/98 (100%)	49/49 (100%)
Sidechain	209/373 (56%)	169/222 (76%)	40/124 (32%)	0/27 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	39/80 (49%)	39/41 (95%)	0/34 (0%)	0/5 (0%)
Overall	493/1213 (41%)	306/668 (46%)	138/431 (32%)	49/114 (43%)

7.1.4 Statistically unusual chemical shifts ⓘ

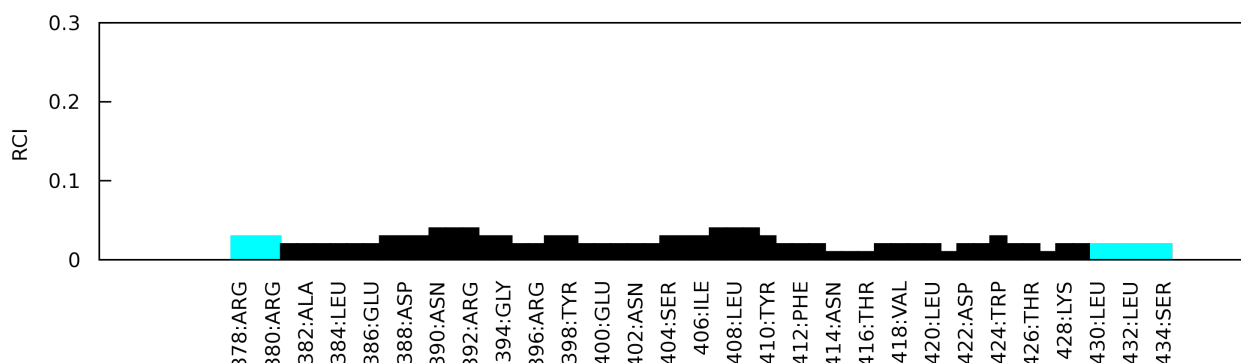
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	423	ARG	HD2	1.65	4.27 – 1.97	-6.4
1	A	423	ARG	HB2	0.08	3.15 – 0.45	-6.4
1	A	421	LYS	HB2	0.22	3.03 – 0.53	-6.2
1	A	421	LYS	HA	1.70	6.46 – 2.06	-5.8
1	A	401	GLY	H	4.83	11.63 – 5.03	-5.3

7.1.5 Random Coil Index (RCI) plots ⓘ

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:



7.2 Chemical shift list 2

File name: BMRB entry 5361

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	107
Number of shifts mapped to atoms	107
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.2.2 Chemical shift referencing [i](#)

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

7.2.3 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 8%, i.e. 95 atoms were assigned a chemical shift out of a possible 1213. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/245 (0%)	0/98 (0%)	0/98 (0%)	0/49 (0%)
Sidechain	0/373 (0%)	0/222 (0%)	0/124 (0%)	0/27 (0%)
Aromatic	0/80 (0%)	0/41 (0%)	0/34 (0%)	0/5 (0%)
Overall	95/1213 (8%)	95/668 (14%)	0/431 (0%)	0/114 (0%)

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_2). RCI is only applicable to proteins.

7.3 Chemical shift list 3

File name: BMRB entry 5361

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	99
Number of shifts mapped to atoms	99
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.3.2 Chemical shift referencing [i](#)

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

7.3.3 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 8%, i.e. 93 atoms were assigned a chemical shift out of a possible 1213. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	0/245 (0%)	0/98 (0%)	0/98 (0%)	0/49 (0%)
Sidechain	0/373 (0%)	0/222 (0%)	0/124 (0%)	0/27 (0%)
Aromatic	0/80 (0%)	0/41 (0%)	0/34 (0%)	0/5 (0%)
Overall	93/1213 (8%)	93/668 (14%)	0/431 (0%)	0/114 (0%)

7.3.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_3). RCI is only applicable to proteins.