



Full wwPDB NMR Structure Validation Report ⓘ

Sep 12, 2017 – 05:46 PM EDT

PDB ID : 5HOU
Title : Solution Structure of p53TAD-TAZ1
Authors : Krois, A.S.; Ferreon, J.C.; Martinez-Yamout, M.A.; Dyson, H.J.; Wright, P.E.
Deposited on : unknown

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20029824
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

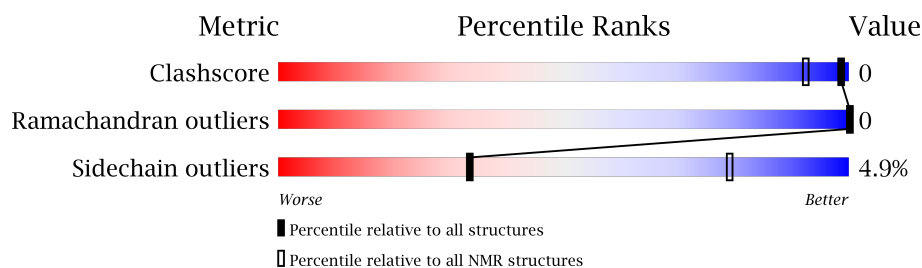
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	171	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 10 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:1018-A:1026, A:1043-A:1053, A:3349-A:3367, A:3383-A:3435 (92)	0.22	10

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 6 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2613 atoms, of which 1281 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cellular tumor antigen p53,CREB-binding protein fusion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	171	Total	C	H	N	O	S	0
			2610	814	1281	245	255	15	

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P04637
A	2	SER	-	expression tag	UNP P04637
A	3	HIS	-	expression tag	UNP P04637
A	2001	GLY	-	linker	UNP P04637
A	2002	SER	-	linker	UNP P04637
A	2003	CYS	-	linker	UNP P04637
A	2004	PHE	-	linker	UNP P04637
A	2005	ASN	-	linker	UNP P04637
A	2006	GLY	-	linker	UNP P04637
A	2007	THR	-	linker	UNP P04637

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

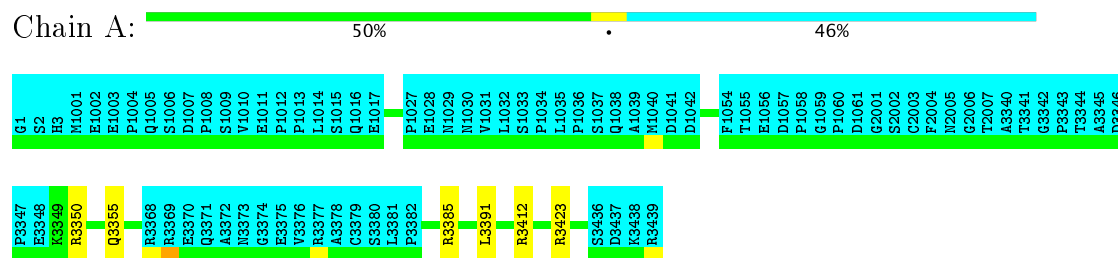
Mol	Chain	Residues	Atoms	
2	A	3	Total	Zn
			3	3

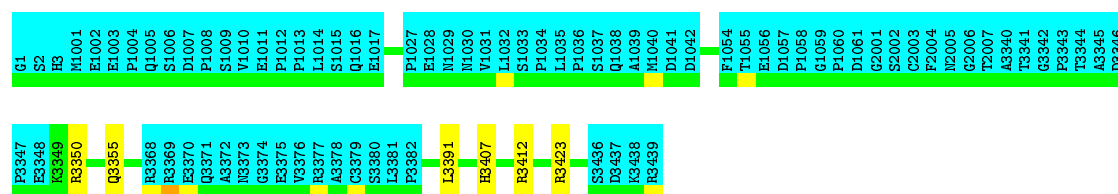
4 Residue-property plots

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.

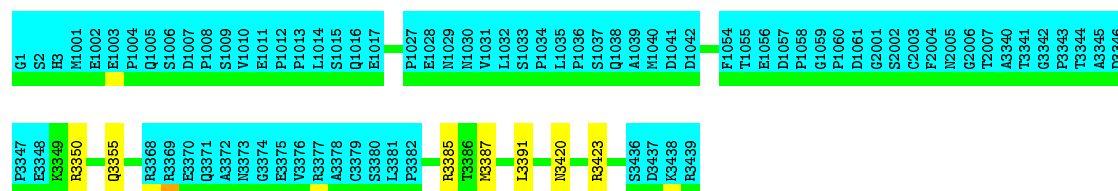
- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein





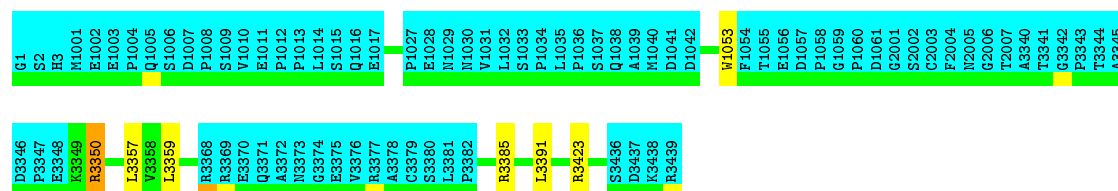
4.2.3 Score per residue for model 3

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



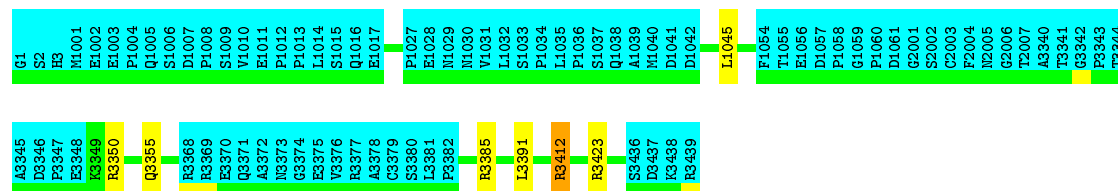
4.2.4 Score per residue for model 4

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



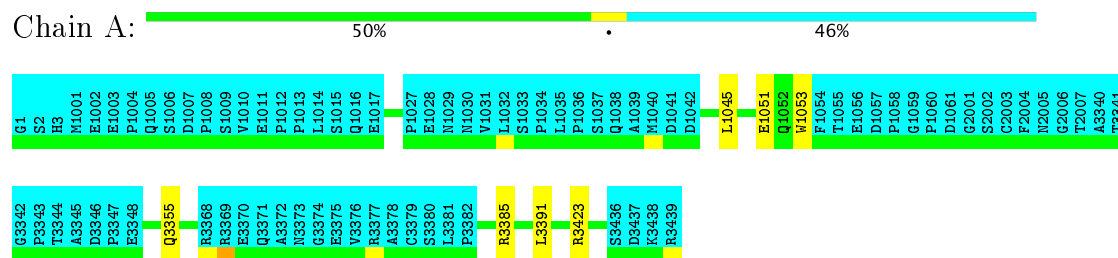
4.2.5 Score per residue for model 5

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



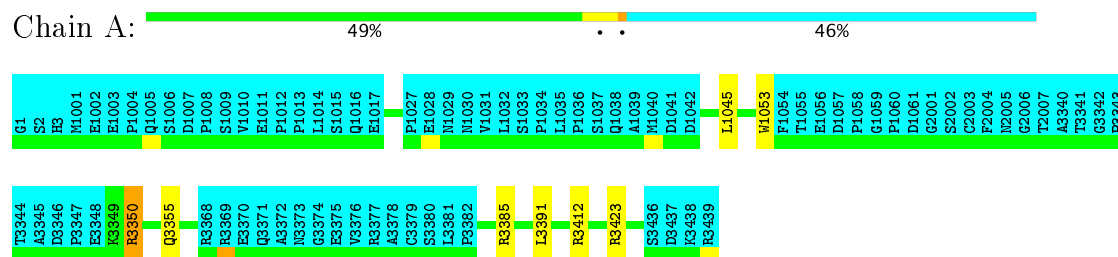
4.2.6 Score per residue for model 6

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



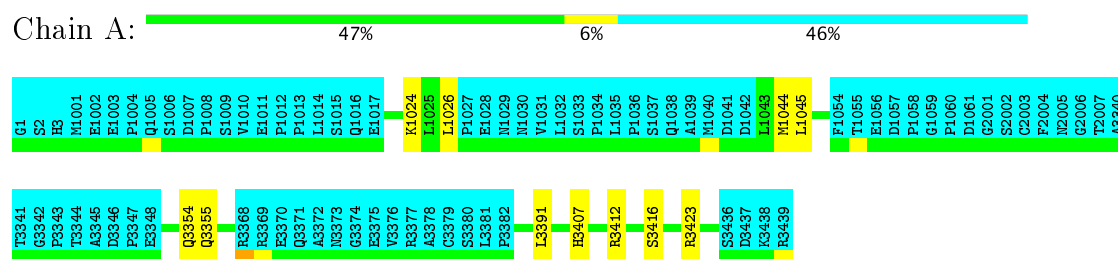
4.2.7 Score per residue for model 7

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



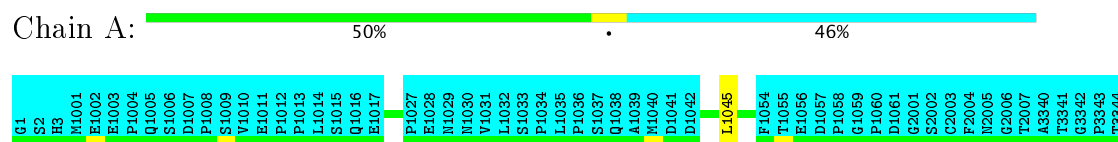
4.2.8 Score per residue for model 8

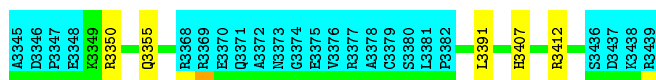
- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



4.2.9 Score per residue for model 9

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein

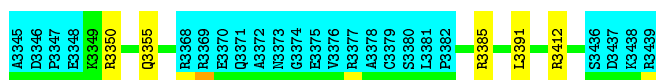
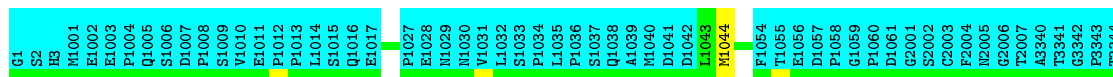




4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein

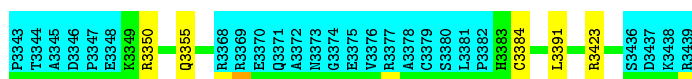
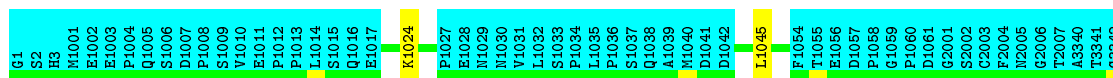
Chain A: 50% 46%



4.2.11 Score per residue for model 11

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein

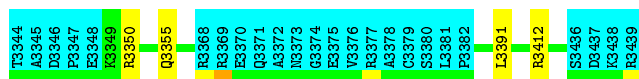
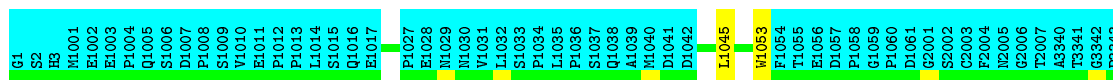
Chain A: 50% 46%



4.2.12 Score per residue for model 12

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein

Chain A: 50% 46%



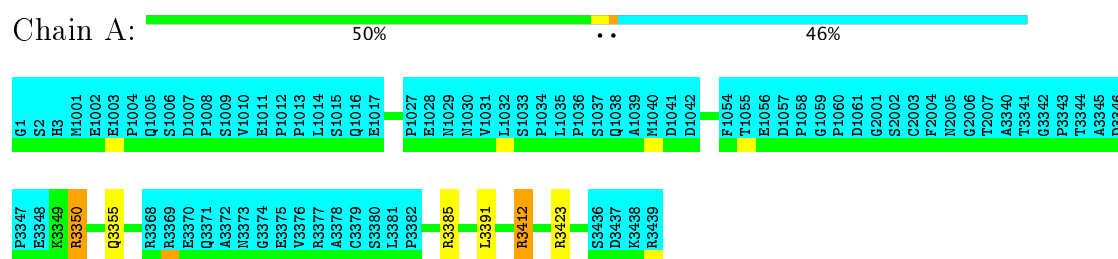
4.2.13 Score per residue for model 13

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



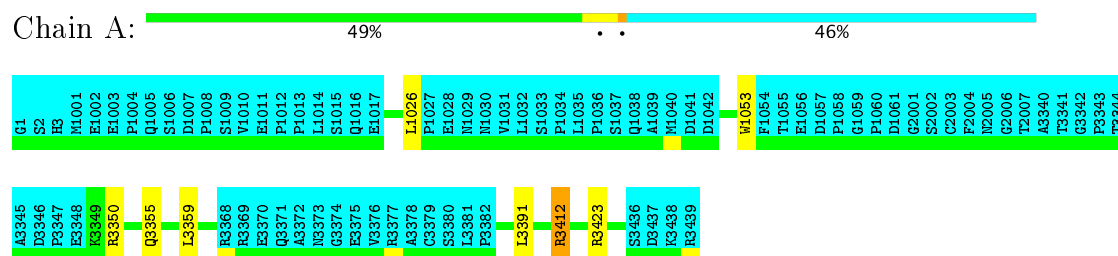
4.2.14 Score per residue for model 14

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



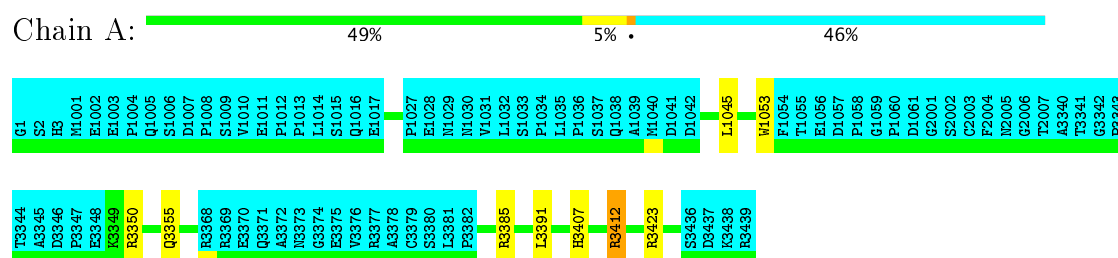
4.2.15 Score per residue for model 15

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



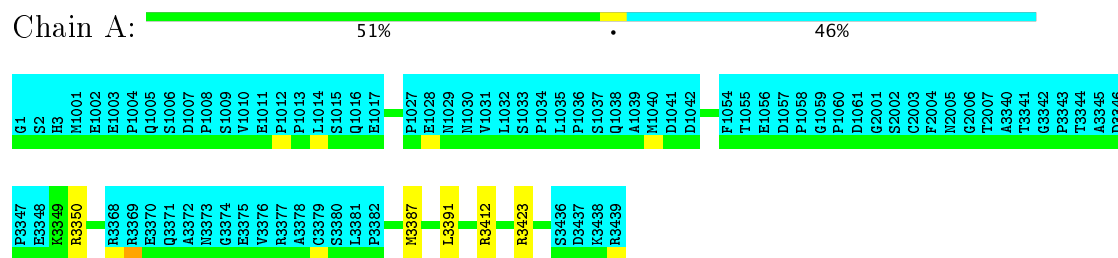
4.2.16 Score per residue for model 16

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



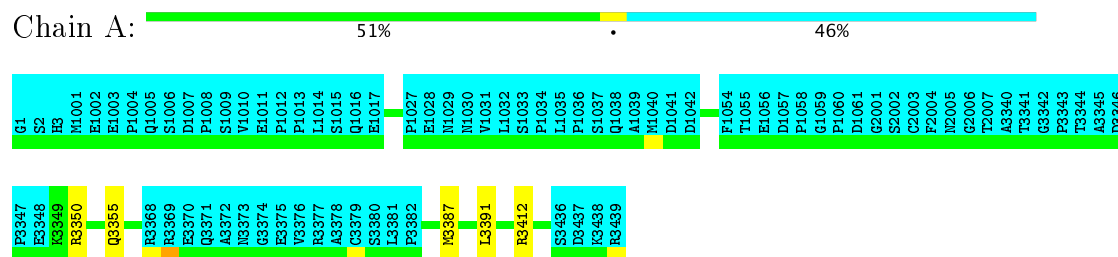
4.2.17 Score per residue for model 17

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



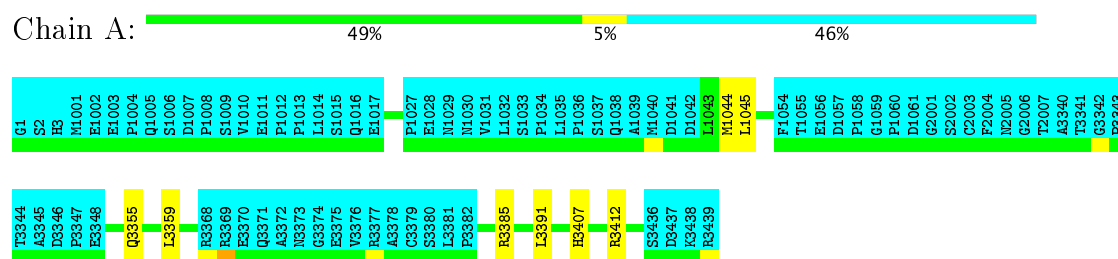
4.2.18 Score per residue for model 18

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



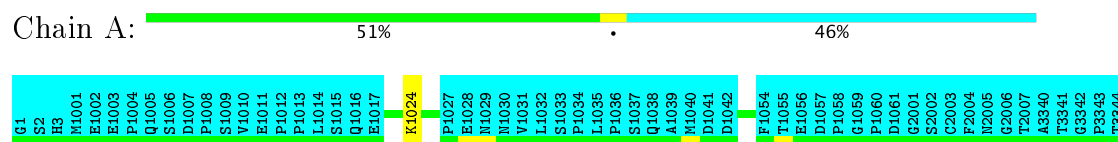
4.2.19 Score per residue for model 19

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



4.2.20 Score per residue for model 20

- Molecule 1: Cellular tumor antigen p53,CREB-binding protein fusion protein



A3345	D3346	P3347	E3348	R3349	R3350	Q3355	R3368	R3369	E3370	Q3371	A3372	I3373	G3374	E3375	V3376	R3377	A3378	C3379	S3380	L3381	P3382	R3385	L3391	S3436	D3437	K3438	R3439
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5 Refinement protocol and experimental data overview

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

Of the 200 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
AMBER	refinement	12

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)	5hou_cs.cif
Number of chemical shift lists	1
Total number of shifts	1842
Number of shifts mapped to atoms	1842
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.59±0.00	0±0/761 (0.0±0.0%)	1.03±0.02	3±1/1030 (0.3±0.1%)
All	All	0.59	0/15220 (0.0%)	1.03	55/20600 (0.3%)

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	3412	ARG	NE-CZ-NH2	7.09	123.85	120.30	16	10
1	A	3350	ARG	NE-CZ-NH2	6.95	123.77	120.30	16	9
1	A	3423	ARG	NE-CZ-NH1	6.51	123.55	120.30	4	6
1	A	3385	ARG	NE-CZ-NH2	6.46	123.53	120.30	19	10
1	A	3423	ARG	NE-CZ-NH2	6.13	123.37	120.30	6	8
1	A	3412	ARG	NE-CZ-NH1	6.06	123.33	120.30	10	3
1	A	3350	ARG	NE-CZ-NH1	5.89	123.24	120.30	17	8
1	A	3385	ARG	NE-CZ-NH1	5.16	122.88	120.30	14	1

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	743	755	750	0±0
All	All	14920	15100	15000	3

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1045:LEU:CD1	1:A:1053:TRP:HE1	0.45	2.24	16	3

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	
1	A	92/171 (54%)	90±1 (98±1%)	2±1 (2±1%)	0±0 (0±0%)	100	100
All	All	1840/3420 (54%)	1809 (98%)	31 (2%)	0 (0%)	100	100

There are no Ramachandran outliers.

6.3.2 Protein sidechains [i](#)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	85/153 (56%)	81±2 (95±2%)	4±2 (5±2%)	33	79
All	All	1700/3060 (56%)	1616 (95%)	84 (5%)	33	79

All 20 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	3391	LEU	20
1	A	3355	GLN	18
1	A	1045	LEU	6
1	A	1044	MET	5
1	A	3407	HIS	5
1	A	3412	ARG	4
1	A	3359	LEU	4
1	A	3350	ARG	3
1	A	1053	TRP	3
1	A	3387	MET	3
1	A	1024	LYS	3
1	A	1026	LEU	2
1	A	3384	CYS	1
1	A	1051	GLU	1
1	A	3416	SER	1
1	A	3357	LEU	1
1	A	3413	GLN	1
1	A	3354	GLN	1
1	A	3388	LYS	1
1	A	3420	ASN	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 ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 80% for the entire structure.

7.1 Chemical shift list 1

File name: 5hou_cs.cif

Chemical shift list name: *p53taz1_correct_assignments.str*

7.1.1 Bookkeeping

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

Total number of shifts	1842
Number of shifts mapped to atoms	1842
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	163	-0.29 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	154	0.19 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	141	-0.39 ± 0.24	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 978 atoms were assigned a chemical shift out of a possible 1198. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	346/454 (76%)	178/181 (98%)	89/184 (48%)	79/89 (89%)
Sidechain	549/638 (86%)	346/378 (92%)	192/228 (84%)	11/32 (34%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	83/106 (78%)	47/55 (85%)	33/35 (94%)	3/16 (19%)
Overall	978/1198 (82%)	571/614 (93%)	314/447 (70%)	93/137 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 1676 atoms were assigned a chemical shift out of a possible 2085. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	622/825 (75%)	318/327 (97%)	163/342 (48%)	141/156 (90%)
Sidechain	952/1128 (84%)	608/672 (90%)	326/403 (81%)	18/53 (34%)
Aromatic	102/132 (77%)	58/69 (84%)	41/45 (91%)	3/18 (17%)
Overall	1676/2085 (80%)	984/1068 (92%)	530/790 (67%)	162/227 (71%)

7.1.4 Statistically unusual chemical shifts [i](#)

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	3359	LEU	CB	31.83	51.69 – 32.89	-5.6

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

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

Random coil index (RCI) for chain A:

