Full wwPDB NMR Structure Validation Report (i)

May 29, 2020 – 07:08 am BST

PDB ID	:	5HPD
Title	:	Solution Structure of TAZ2-p53TAD
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Deposited on	:	2016-01-20

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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

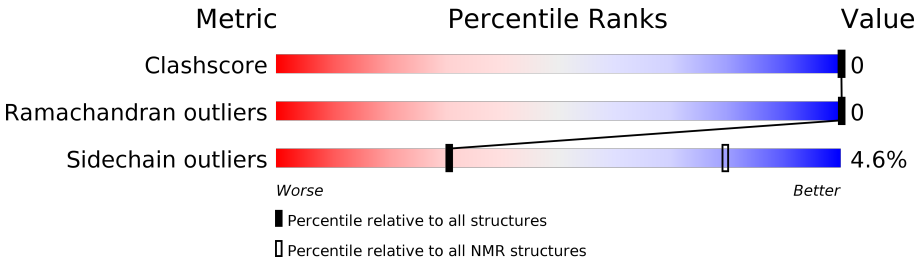
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	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 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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	158	63% 6% 31%

2 Ensemble composition and analysis

This entry contains 20 models. Model 8 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:1767-A:1853, A:3020-A:3026, A:3041-A:3055 (109)	0.20	8

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2431 atoms, of which 1200 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	158	Total	C	H	N	O	S	0
			2428	753	1200	224	235	16	

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2001	GLY	-	linker	UNP P45481
A	2002	SER	-	linker	UNP P45481
A	2003	GLY	-	linker	UNP P45481
A	2004	SER	-	linker	UNP P45481
A	2005	GLY	-	linker	UNP P45481
A	2006	SER	-	linker	UNP P45481

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

Mol	Chain	Residues	Atoms	
2	A	3	Total	Zn
			3	3

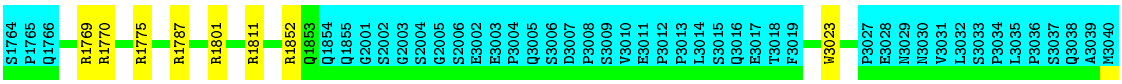
4 Residue-property plots

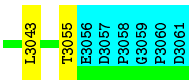
4.1 Average score per residue in the NMR ensemble

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

Chain A:





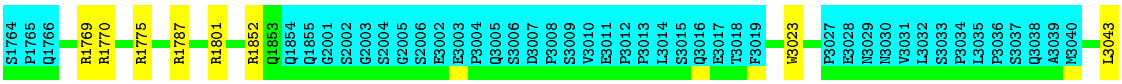
4.2 Scores per residue for each member of the ensemble

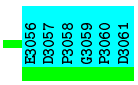
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

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

Chain A:

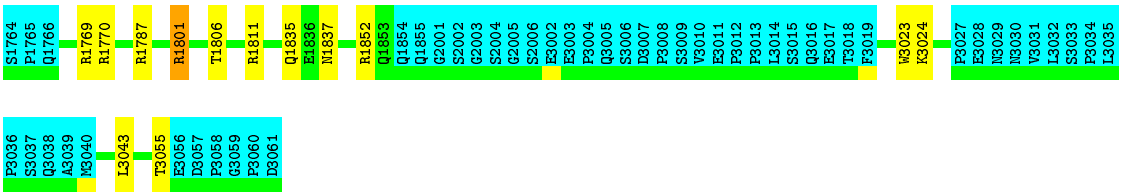




4.2.2 Score per residue for model 2

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

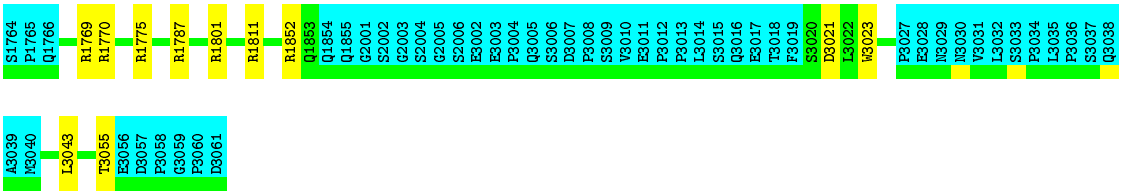
Chain A:



4.2.3 Score per residue for model 3

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

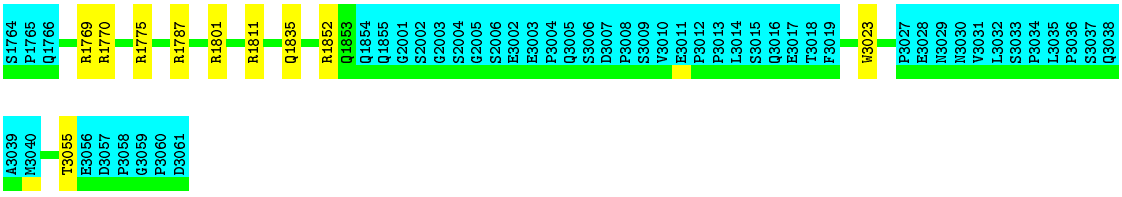
Chain A:



4.2.4 Score per residue for model 4

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

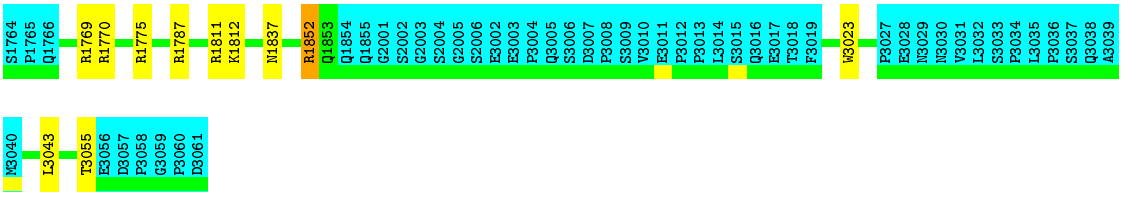
Chain A:



4.2.5 Score per residue for model 5

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

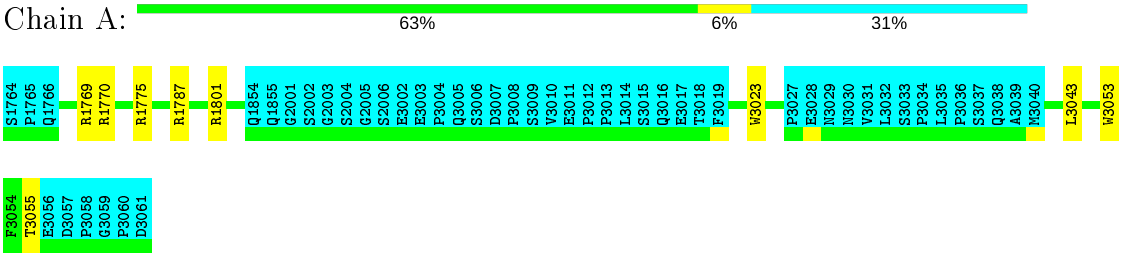
Chain A:



4.2.6 Score per residue for model 6

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

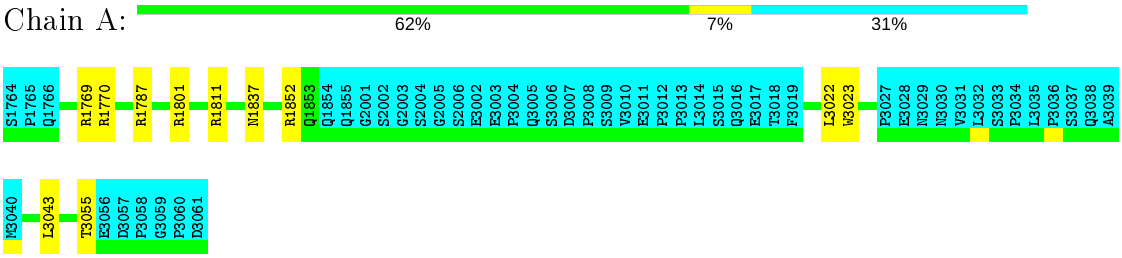
Chain A:



4.2.7 Score per residue for model 7

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

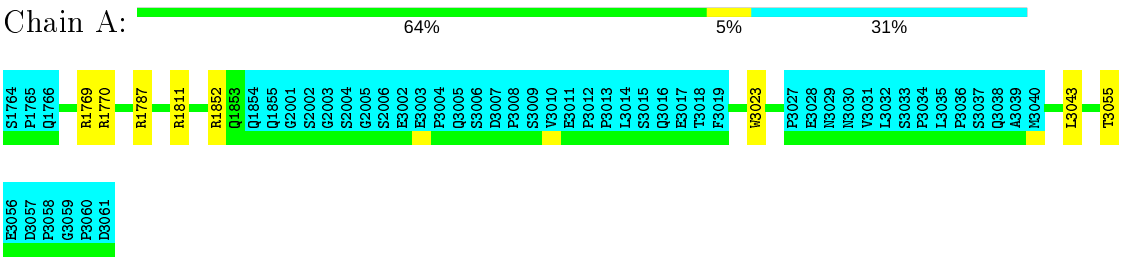
Chain A:



4.2.8 Score per residue for model 8 (medoid)

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

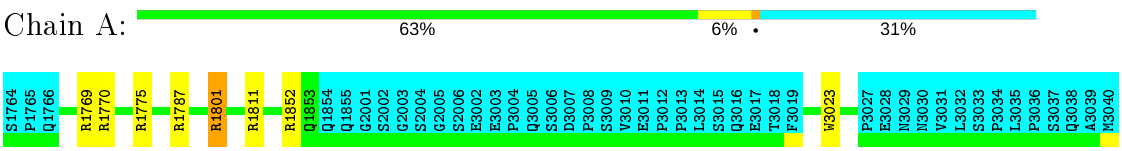
Chain A:

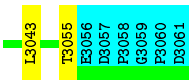


4.2.9 Score per residue for model 9

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

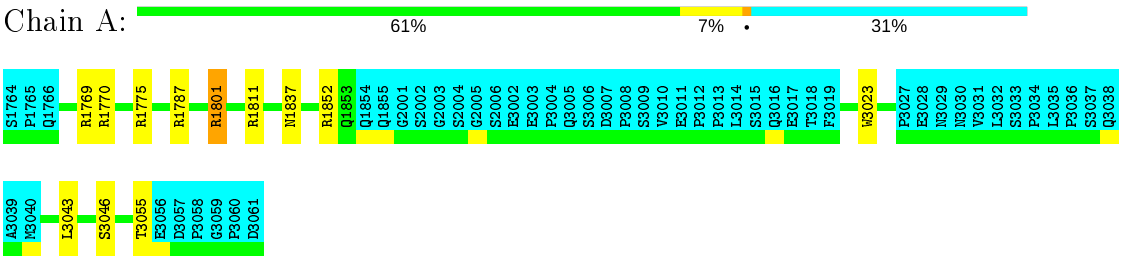
Chain A:





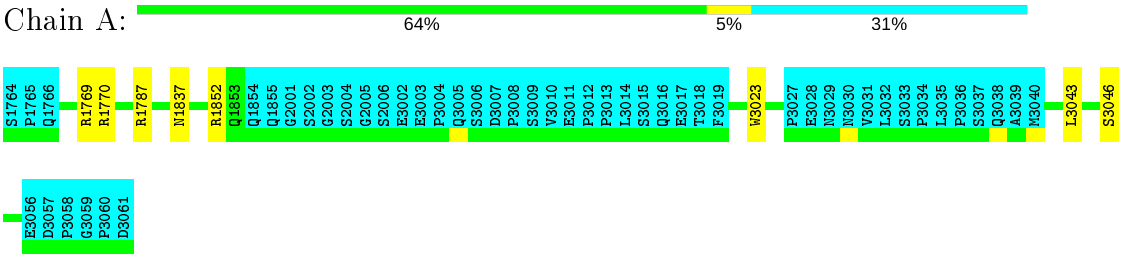
4.2.10 Score per residue for model 10

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



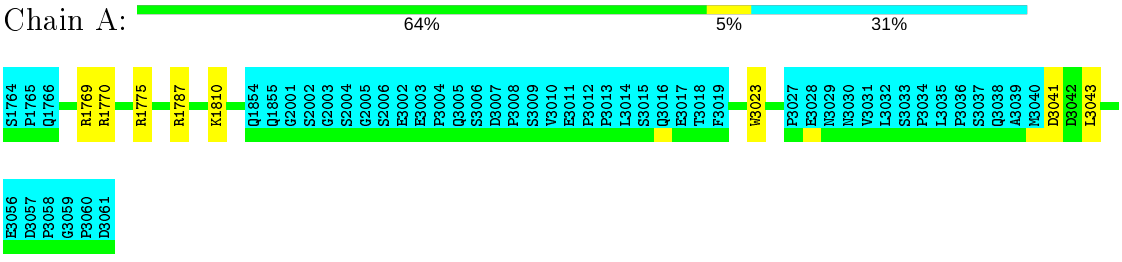
4.2.11 Score per residue for model 11

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



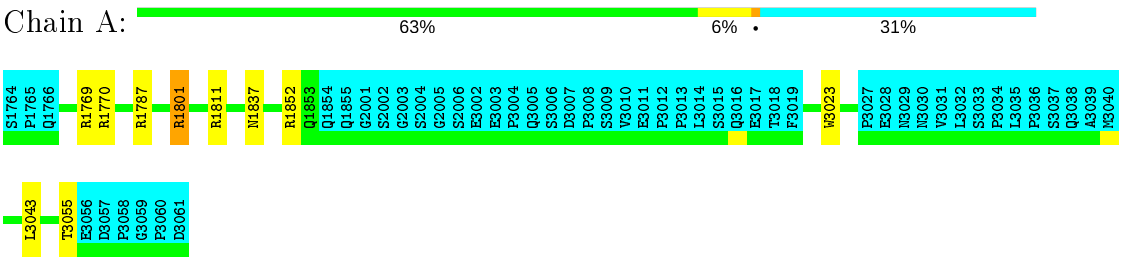
4.2.12 Score per residue for model 12

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



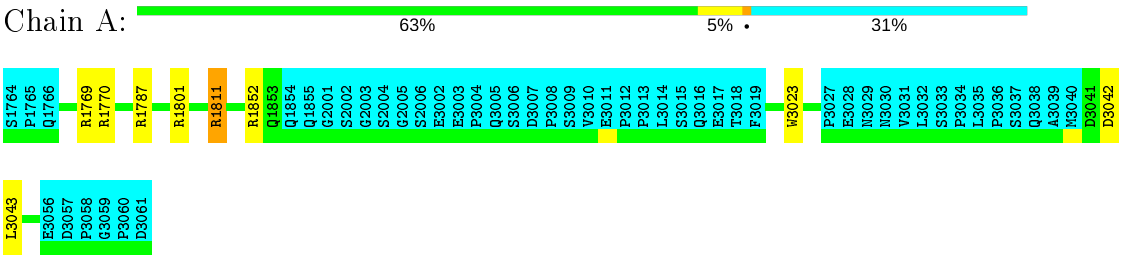
4.2.13 Score per residue for model 13

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



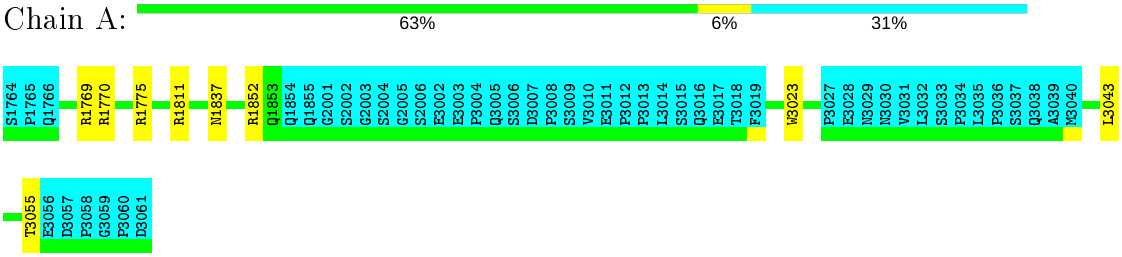
4.2.14 Score per residue for model 14

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



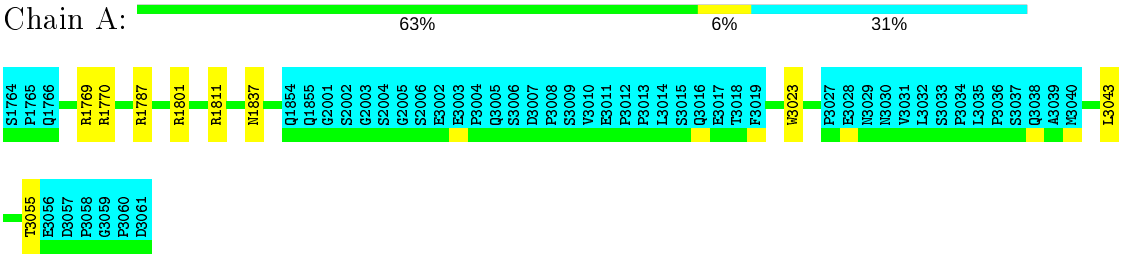
4.2.15 Score per residue for model 15

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



4.2.16 Score per residue for model 16

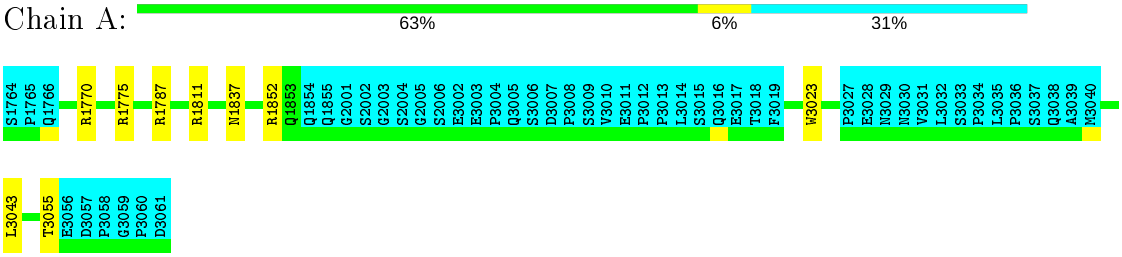
- Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein



4.2.17 Score per residue for model 17

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

Chain A:



4.2.18 Score per residue for model 18

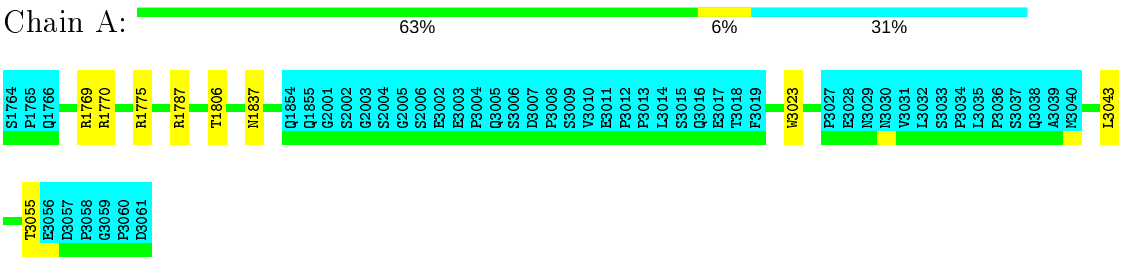
• Molecule 1: CREB-binding protein,Cellular tumor antigen p53 fusion protein

Chain A:

4.2.19 Score per residue for model 19

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

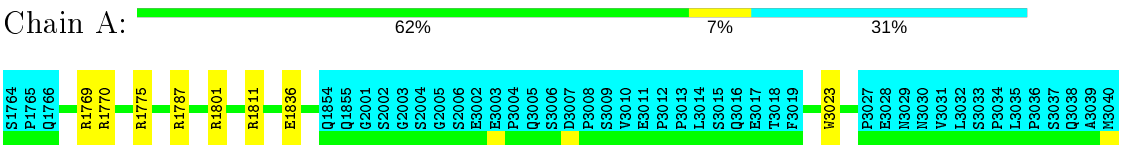
Chain A:

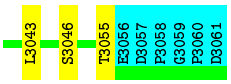


4.2.20 Score per residue for model 20

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

Chain A:




L3043
S3046
T3055
E3056
D3057
P3058
G3059
P3060
D3061

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
CYANA	structure calculation	2.1
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 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1735
Number of shifts mapped to atoms	1735
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.

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
All	All	17480	17680	17640	-

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 -.

There are no clashes.

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	109/158 (69%)	105±1 (96±1%)	4±1 (4±1%)	0±0 (0±0%)	100	100
All	All	2180/3160 (69%)	2099 (96%)	81 (4%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	102/146 (70%)	97±1 (95±1%)	5±1 (5±1%)	31	79
All	All	2040/2920 (70%)	1946 (95%)	94 (5%)	31	79

All 21 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	3023	TRP	20
1	A	3043	LEU	18
1	A	3055	THR	16
1	A	1837	ASN	10
1	A	1801	ARG	7
1	A	1835	GLN	3
1	A	3046	SER	3
1	A	1806	THR	2
1	A	1852	ARG	2
1	A	3042	ASP	2
1	A	1775	ARG	1
1	A	1811	ARG	1
1	A	3041	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	3022	LEU	1
1	A	3021	ASP	1
1	A	1812	LYS	1
1	A	1839	CYS	1
1	A	1836	GLU	1
1	A	1838	LYS	1
1	A	1810	LYS	1
1	A	3024	LYS	1

5.2.3 RNA

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains

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

5.4 Carbohydrates

There are no carbohydrates in this entry.

5.5 Ligand geometry

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

5.6 Other polymers

There are no such molecules in this entry.

5.7 Polymer linkage issues

There are no chain breaks in this entry.

6 Chemical shift validation

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

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *taz2p53_corrected_assignments.str*

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	1735
Number of shifts mapped to atoms	1735
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

6.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	152	-0.26 ± 0.08	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	145	0.28 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	130	-0.48 ± 0.23	None needed (< 0.5 ppm)

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 82%, i.e. 1152 atoms were assigned a chemical shift out of a possible 1411. 0 out of 17 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	401/535 (75%)	202/213 (95%)	106/218 (49%)	93/104 (89%)
Sidechain	676/789 (86%)	428/471 (91%)	235/272 (86%)	13/46 (28%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	75/87 (86%)	41/46 (89%)	32/32 (100%)	2/9 (22%)
Overall	1152/1411 (82%)	671/730 (92%)	373/522 (71%)	108/159 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1605 atoms were assigned a chemical shift out of a possible 1946. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	569/760 (75%)	287/301 (95%)	152/316 (48%)	130/143 (91%)
Sidechain	952/1090 (87%)	607/654 (93%)	324/382 (85%)	21/54 (39%)
Aromatic	84/96 (88%)	46/51 (90%)	36/36 (100%)	2/9 (22%)
Overall	1605/1946 (82%)	940/1006 (93%)	512/734 (70%)	153/206 (74%)

6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.1.5 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: