



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 21, 2024 – 02:27 AM EDT

PDB ID : 2L14  
Title : Structure of CBP nuclear coactivator binding domain in complex with p53 TAD  
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Deposited on : 2010-07-22

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
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) : 2.36.2

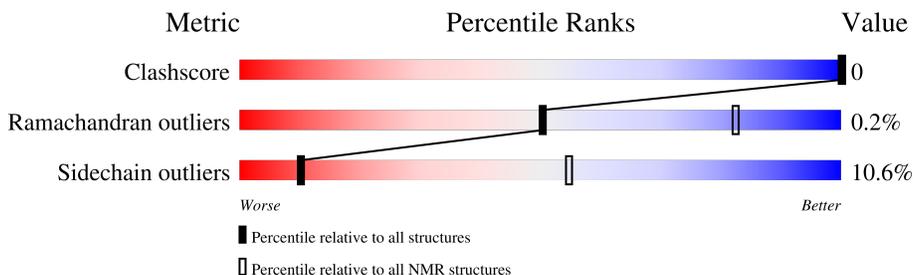
# 1 Overall quality at a glance

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	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  $\geq 3$ , 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	59	 73% 5% 22%
2	B	49	 35% 8% 57%

## 2 Ensemble composition and analysis i

This entry contains 20 models. Model 5 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:2063-A:2108, B:18-B:25, B:43-B:55 (67)	0.82	5

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 3 clusters and 2 single-model clusters were found.

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

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1693 atoms, of which 843 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CREB-binding protein.

Mol	Chain	Residues	Atoms					Trace	
1	A	59	Total	C	H	N	O	S	0
			941	286	482	86	85	2	

- Molecule 2 is a protein called Cellular tumor antigen p53.

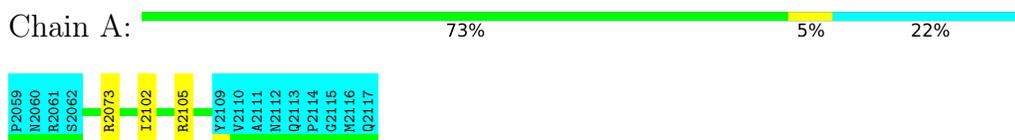
Mol	Chain	Residues	Atoms					Trace	
2	B	49	Total	C	H	N	O	S	0
			752	249	361	57	83	2	

## 4 Residue-property plots

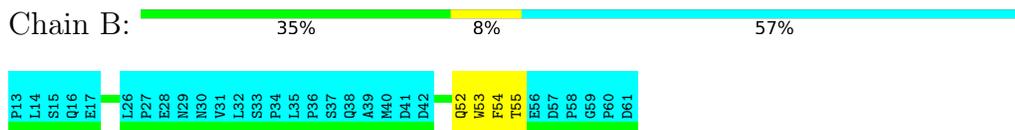
### 4.1 Average score per residue in the NMR ensemble

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: CREB-binding protein



- Molecule 2: Cellular tumor antigen p53

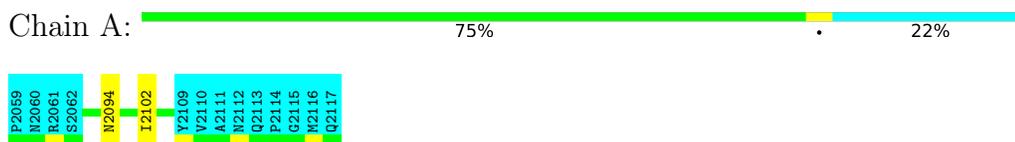


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: CREB-binding protein

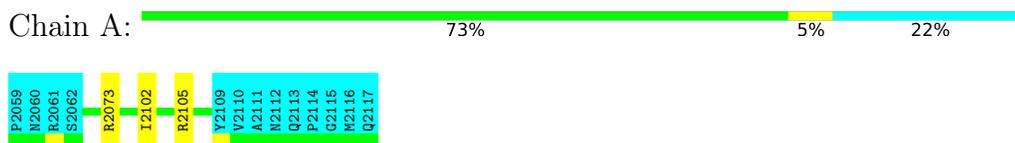


- Molecule 2: Cellular tumor antigen p53

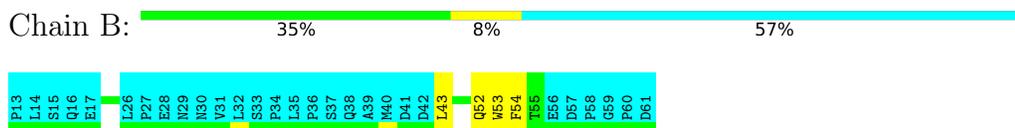


### 4.2.2 Score per residue for model 2

- Molecule 1: CREB-binding protein

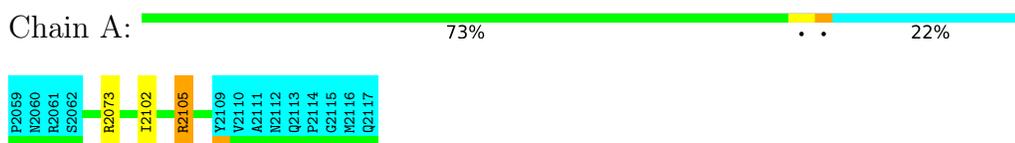


- Molecule 2: Cellular tumor antigen p53



### 4.2.3 Score per residue for model 3

- Molecule 1: CREB-binding protein

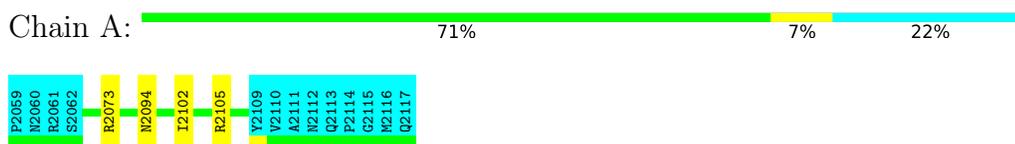


- Molecule 2: Cellular tumor antigen p53

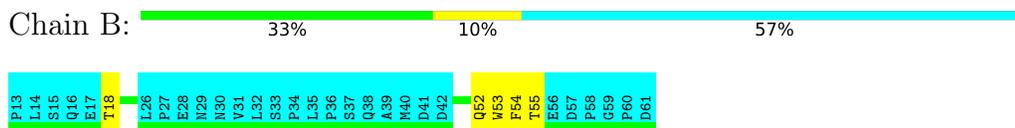


### 4.2.4 Score per residue for model 4

- Molecule 1: CREB-binding protein

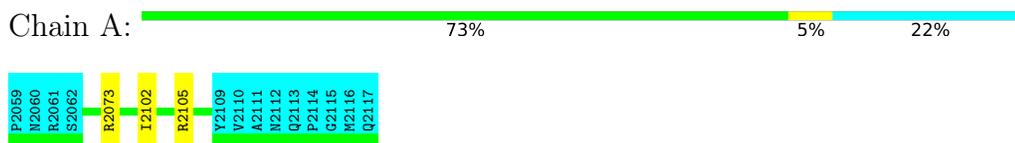


- Molecule 2: Cellular tumor antigen p53

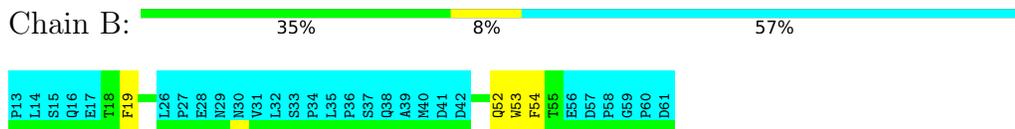


#### 4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: CREB-binding protein

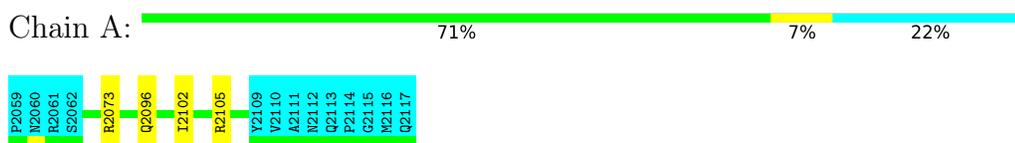


- Molecule 2: Cellular tumor antigen p53

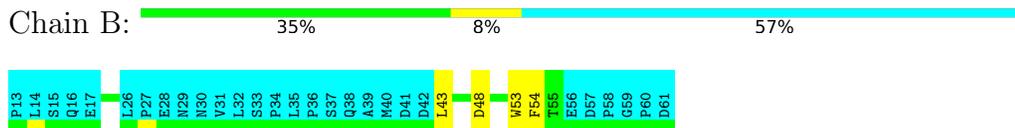


#### 4.2.6 Score per residue for model 6

- Molecule 1: CREB-binding protein

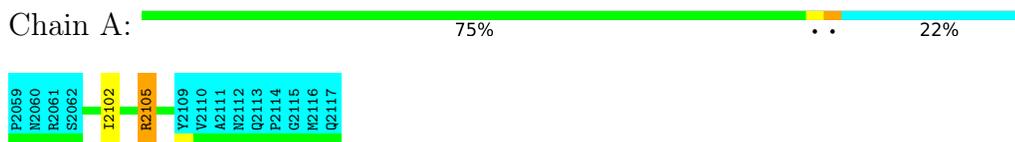


- Molecule 2: Cellular tumor antigen p53

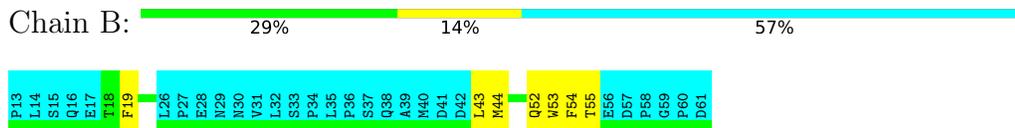


#### 4.2.7 Score per residue for model 7

- Molecule 1: CREB-binding protein

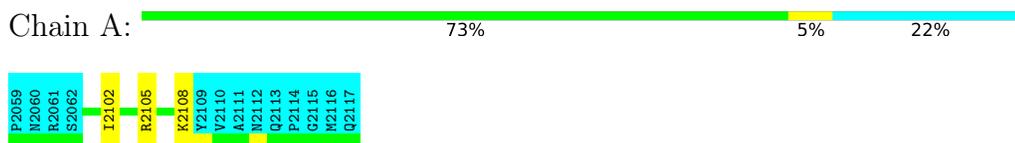


- Molecule 2: Cellular tumor antigen p53

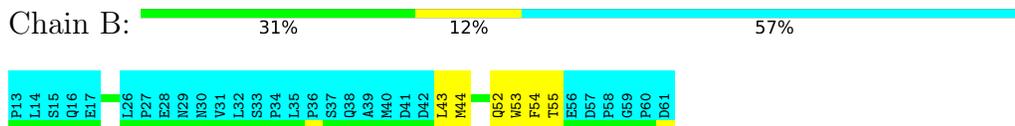


### 4.2.8 Score per residue for model 8

- Molecule 1: CREB-binding protein

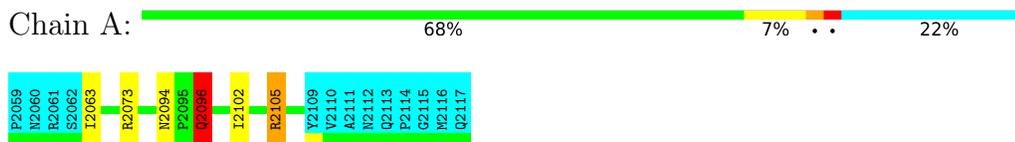


- Molecule 2: Cellular tumor antigen p53

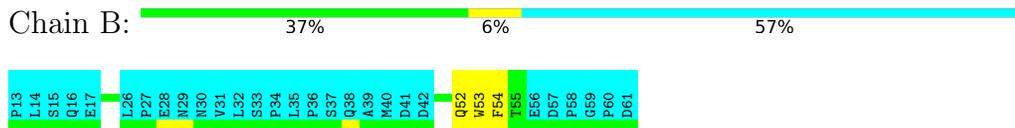


### 4.2.9 Score per residue for model 9

- Molecule 1: CREB-binding protein

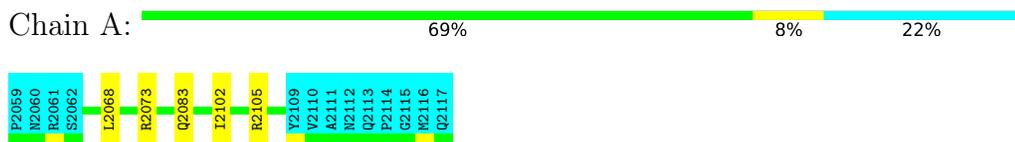


- Molecule 2: Cellular tumor antigen p53

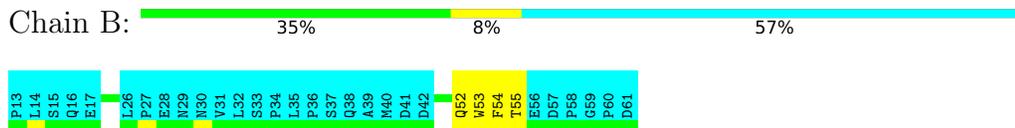


### 4.2.10 Score per residue for model 10

- Molecule 1: CREB-binding protein

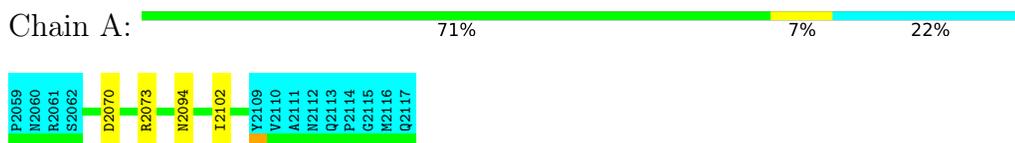


- Molecule 2: Cellular tumor antigen p53



### 4.2.11 Score per residue for model 11

- Molecule 1: CREB-binding protein

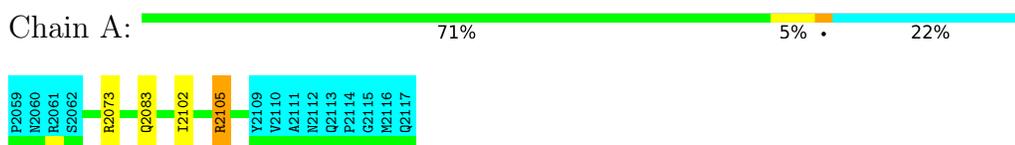


- Molecule 2: Cellular tumor antigen p53

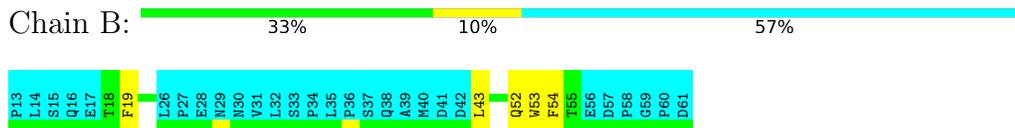


### 4.2.12 Score per residue for model 12

- Molecule 1: CREB-binding protein

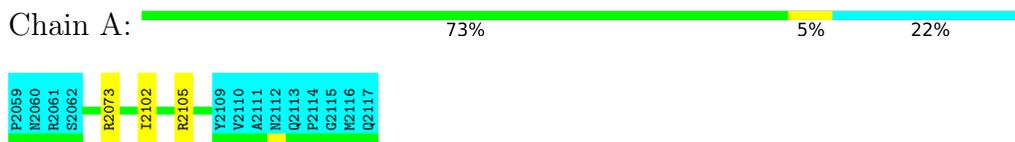


- Molecule 2: Cellular tumor antigen p53

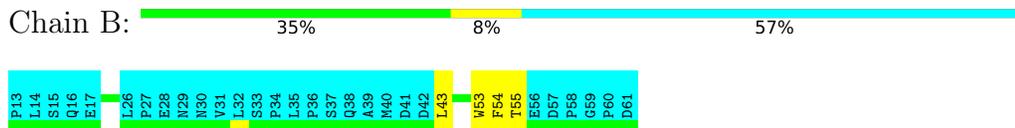


### 4.2.13 Score per residue for model 13

- Molecule 1: CREB-binding protein

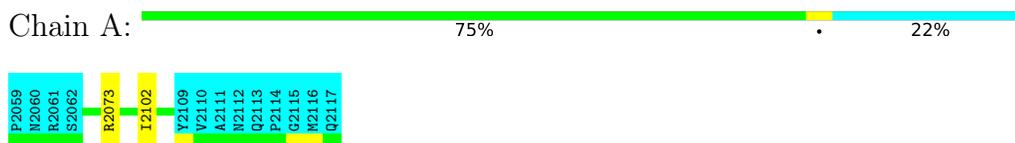


- Molecule 2: Cellular tumor antigen p53

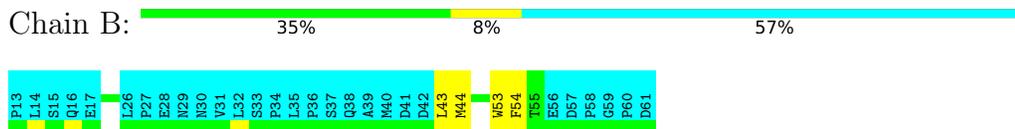


#### 4.2.14 Score per residue for model 14

- Molecule 1: CREB-binding protein

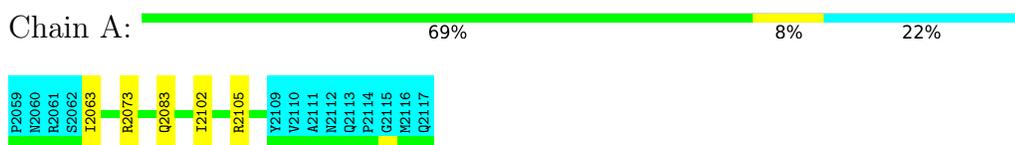


- Molecule 2: Cellular tumor antigen p53

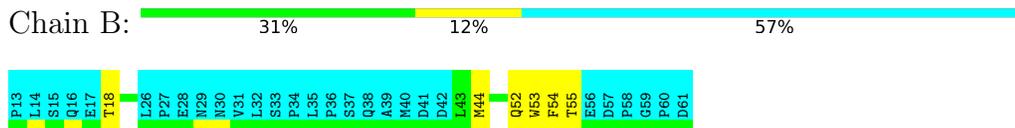


#### 4.2.15 Score per residue for model 15

- Molecule 1: CREB-binding protein

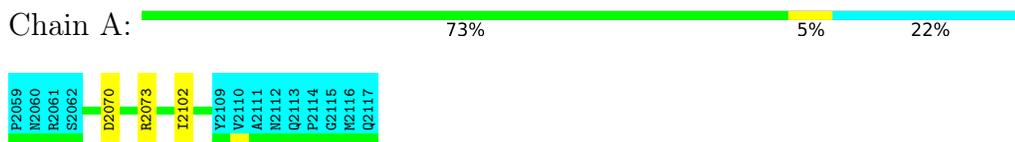


- Molecule 2: Cellular tumor antigen p53

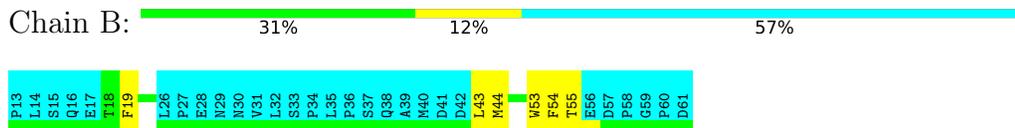


#### 4.2.16 Score per residue for model 16

- Molecule 1: CREB-binding protein

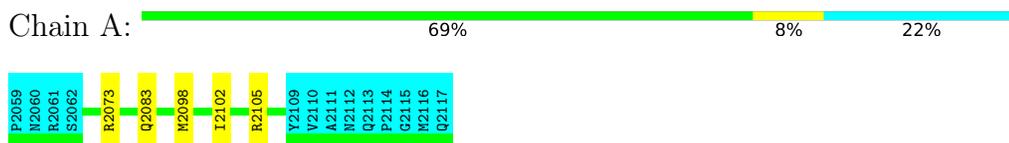


- Molecule 2: Cellular tumor antigen p53

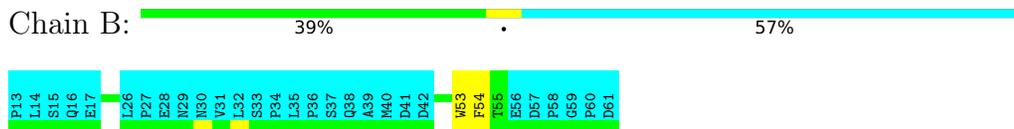


### 4.2.17 Score per residue for model 17

- Molecule 1: CREB-binding protein

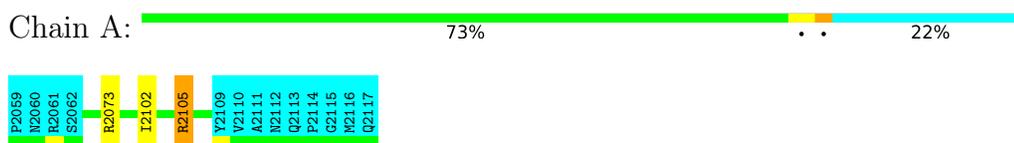


- Molecule 2: Cellular tumor antigen p53

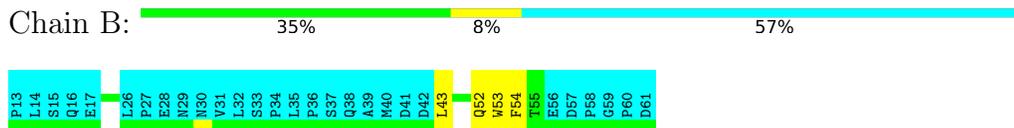


### 4.2.18 Score per residue for model 18

- Molecule 1: CREB-binding protein

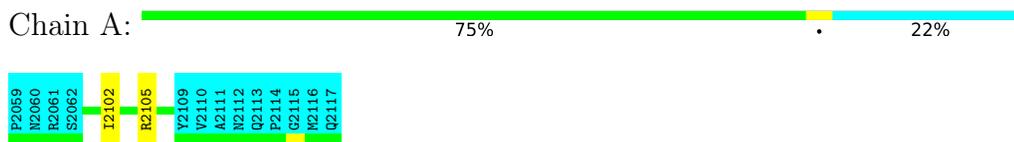


- Molecule 2: Cellular tumor antigen p53

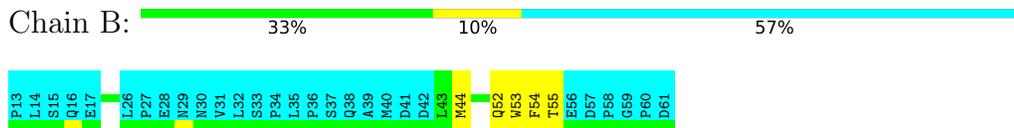


### 4.2.19 Score per residue for model 19

- Molecule 1: CREB-binding protein



- Molecule 2: Cellular tumor antigen p53



#### 4.2.20 Score per residue for model 20

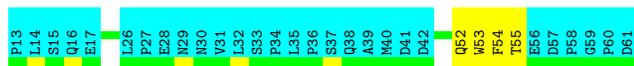
- Molecule 1: CREB-binding protein

Chain A:  71% 7% 22%



- Molecule 2: Cellular tumor antigen p53

Chain B:  35% 8% 57%



## 5 Refinement protocol and experimental data overview

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

Of the 100 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	9

No chemical shift data was provided.

## 6 Model quality i

### 6.1 Standard geometry i

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±0.01	0±0/363 ( 0.0± 0.0%)	0.97±0.04	2±1/491 ( 0.4± 0.3%)
2	B	0.75±0.01	0±0/189 ( 0.0± 0.0%)	1.03±0.04	0±0/259 ( 0.0± 0.0%)
All	All	0.65	0/11040 ( 0.0%)	0.99	42/15000 ( 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	2105	ARG	NE-CZ-NH1	7.62	124.11	120.30	17	13
1	A	2073	ARG	NE-CZ-NH1	6.85	123.72	120.30	12	16
1	A	2105	ARG	NE-CZ-NH2	-6.45	117.08	120.30	4	3
1	A	2073	ARG	NE-CZ-NH2	-5.67	117.47	120.30	3	9
1	A	2105	ARG	CD-NE-CZ	5.12	130.77	123.60	18	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	358	387	387	0±0
All	All	10800	11180	11180	1

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:2063:ILE:HG22	1:A:2096:GLN:CD	0.41	2.35	9	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	
1	A	46/59 (78%)	45±1 (99±2%)	1±1 (1±2%)	0±0 (0±0%)	54	85
2	B	21/49 (43%)	20±1 (97±3%)	0±1 (2±3%)	0±0 (0±1%)	32	76
All	All	1340/2160 (62%)	1315 (98%)	22 (2%)	3 (0%)	50	82

All 2 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	18	THR	2
1	A	2096	GLN	1

### 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	42/53 (79%)	40±1 (95±2%)	2±1 (5±2%)	26	75
2	B	21/47 (45%)	17±1 (79±5%)	4±1 (21±5%)	3	31
All	All	1260/2000 (63%)	1126 (89%)	134 (11%)	10	55

All 19 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	2102	ILE	20
2	B	53	TRP	20
2	B	54	PHE	20
2	B	52	GLN	15
2	B	55	THR	11
2	B	43	LEU	9
1	A	2105	ARG	8
2	B	44	MET	7
1	A	2094	ASN	5
2	B	19	PHE	5
1	A	2083	GLN	4
1	A	2096	GLN	2
1	A	2070	ASP	2
2	B	21	ASP	1
2	B	48	ASP	1
1	A	2108	LYS	1
1	A	2068	LEU	1
1	A	2063	ILE	1
1	A	2098	MET	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 6.5 Carbohydrates [i](#)

There are no monosaccharides 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

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided