



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 12:05 AM BST

PDB ID : 2L14
Title : Structure of CBP nuclear coactivator binding domain in complex with p53 TAD
Authors : Lee, C.; Martinez-Yamout, M.A.; Dyson, H.J.; Wright, P.E.
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
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

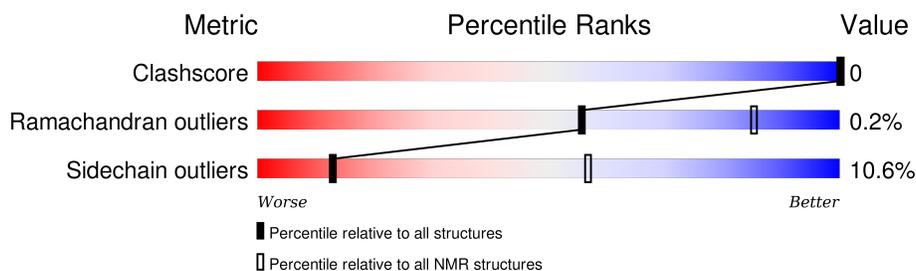
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	A	59	 73% 5% 22%
2	B	49	 35% 8% 57%

2 Ensemble composition and analysis

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)	0.47	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	
			Total	C	H	N	O		S
1	A	59	941	286	482	86	85	2	0

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

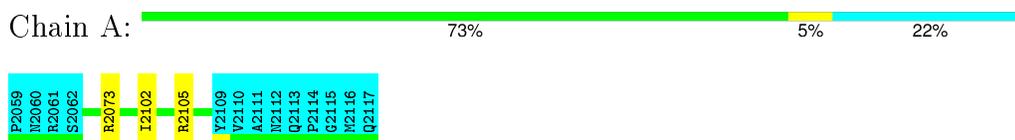
Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
2	B	49	752	249	361	57	83	2	0

4 Residue-property plots

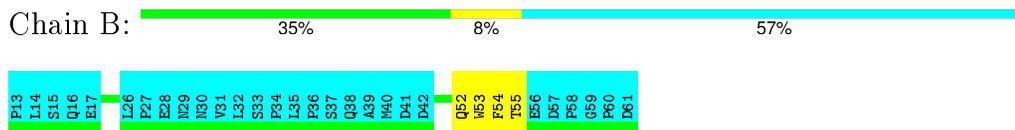
4.1 Average score per residue in the NMR ensemble

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



- Molecule 2: Cellular tumor antigen p53

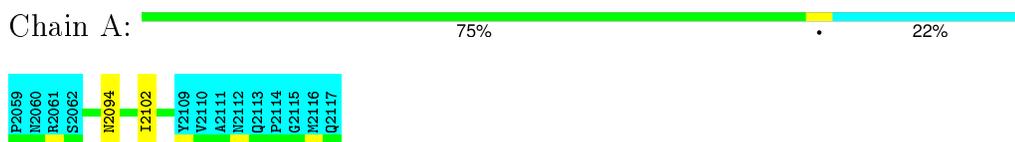


4.2 Scores per residue for each member of the ensemble

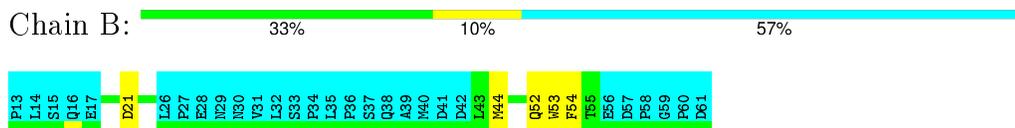
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: CREB-binding protein

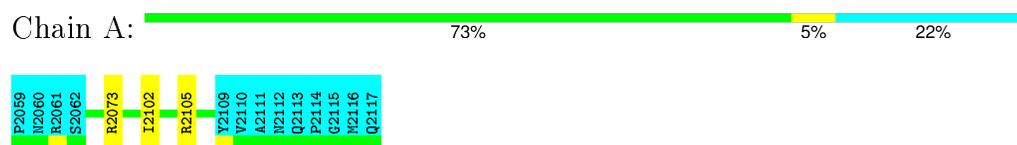


- Molecule 2: Cellular tumor antigen p53

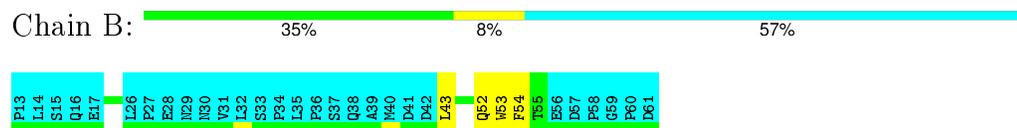


4.2.2 Score per residue for model 2

- Molecule 1: CREB-binding protein

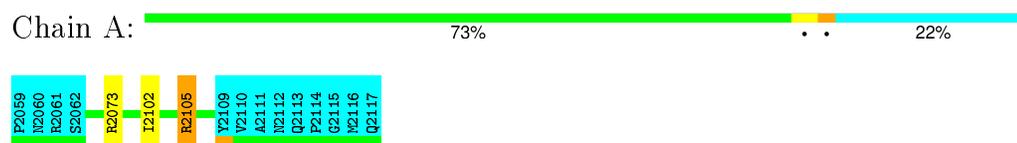


- Molecule 2: Cellular tumor antigen p53

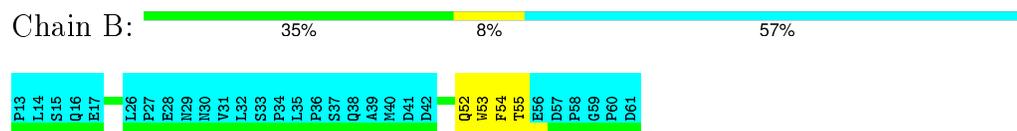


4.2.3 Score per residue for model 3

- Molecule 1: CREB-binding protein

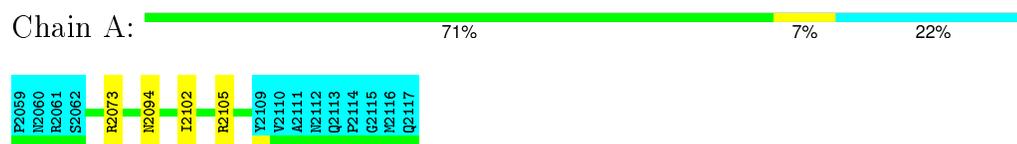


- Molecule 2: Cellular tumor antigen p53

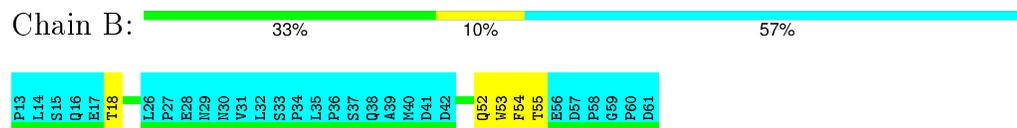


4.2.4 Score per residue for model 4

- Molecule 1: CREB-binding protein

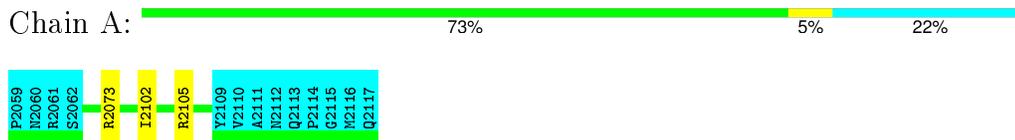


- Molecule 2: Cellular tumor antigen p53

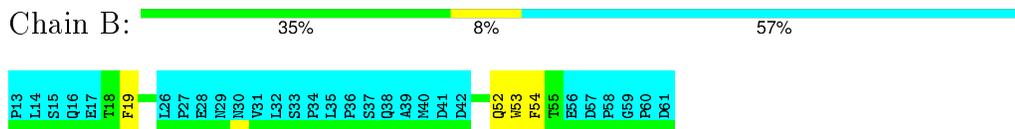


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: CREB-binding protein

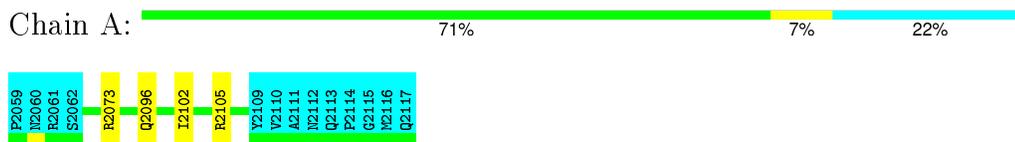


- Molecule 2: Cellular tumor antigen p53

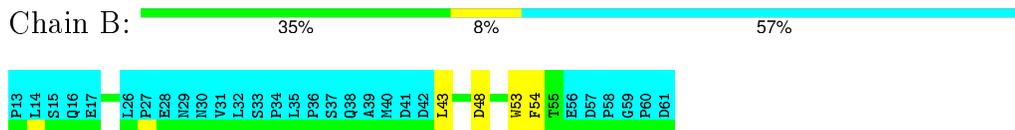


4.2.6 Score per residue for model 6

- Molecule 1: CREB-binding protein

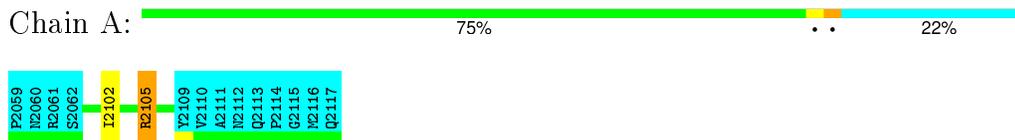


- Molecule 2: Cellular tumor antigen p53

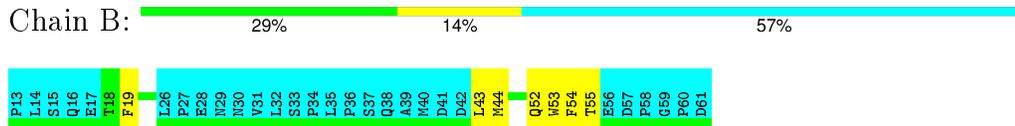


4.2.7 Score per residue for model 7

- Molecule 1: CREB-binding protein

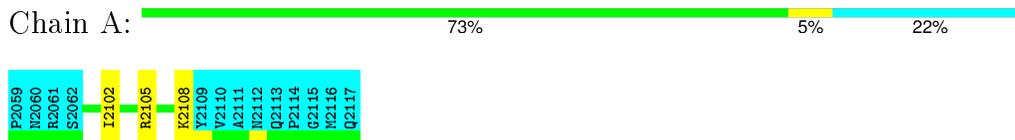


- Molecule 2: Cellular tumor antigen p53

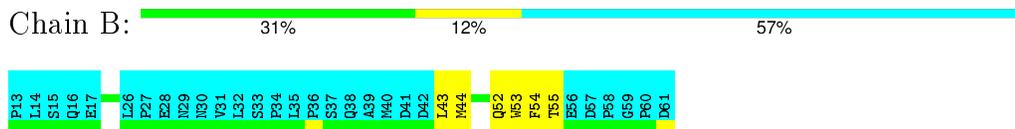


4.2.8 Score per residue for model 8

- Molecule 1: CREB-binding protein

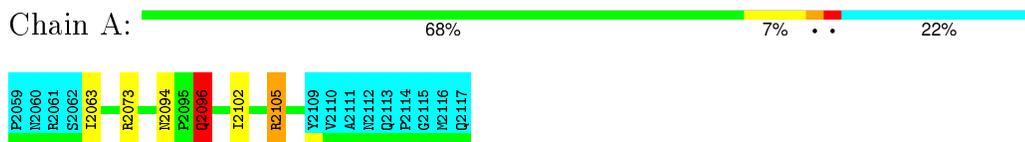


- Molecule 2: Cellular tumor antigen p53

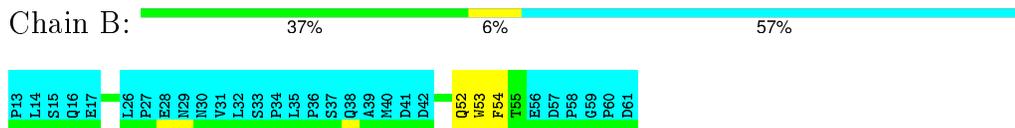


4.2.9 Score per residue for model 9

- Molecule 1: CREB-binding protein

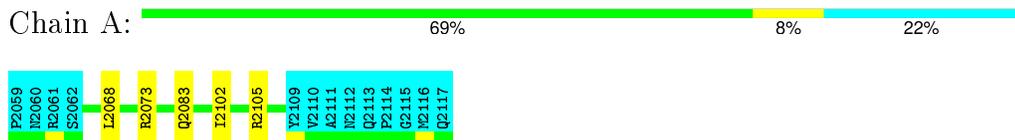


- Molecule 2: Cellular tumor antigen p53

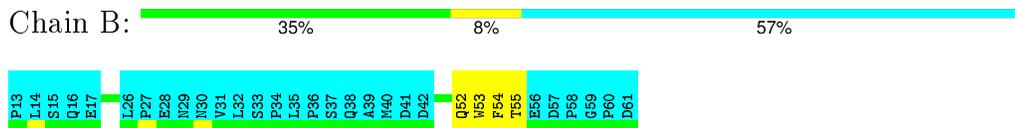


4.2.10 Score per residue for model 10

- Molecule 1: CREB-binding protein

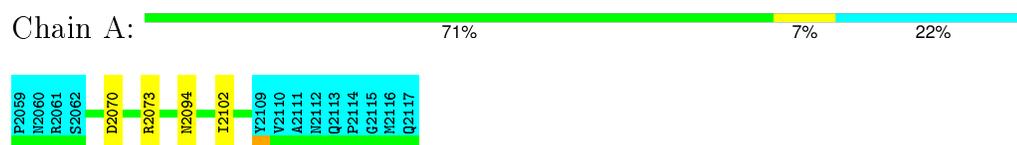


- Molecule 2: Cellular tumor antigen p53

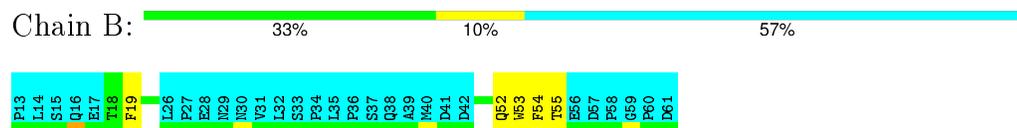


4.2.11 Score per residue for model 11

- Molecule 1: CREB-binding protein

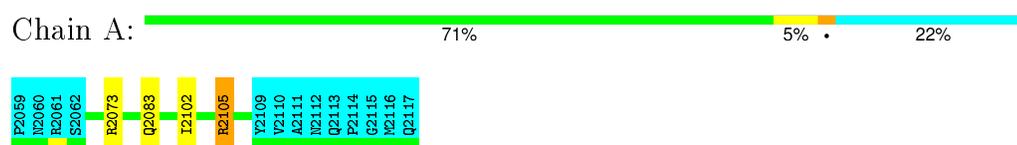


- Molecule 2: Cellular tumor antigen p53

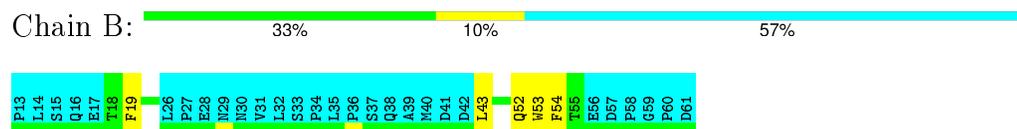


4.2.12 Score per residue for model 12

- Molecule 1: CREB-binding protein

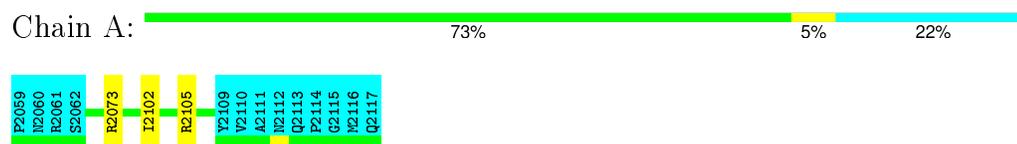


- Molecule 2: Cellular tumor antigen p53

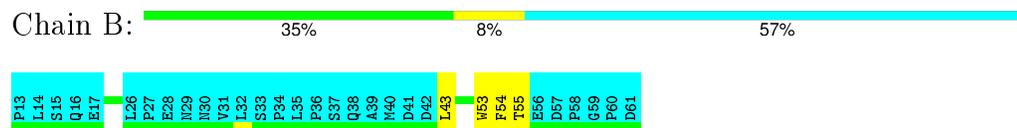


4.2.13 Score per residue for model 13

- Molecule 1: CREB-binding protein

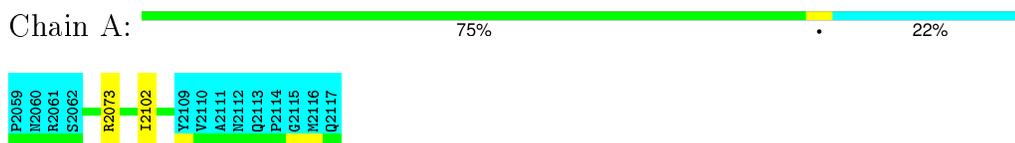


- Molecule 2: Cellular tumor antigen p53

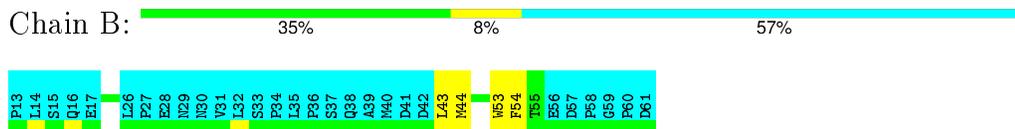


4.2.14 Score per residue for model 14

- Molecule 1: CREB-binding protein

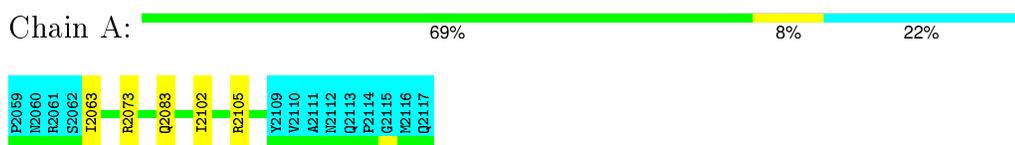


- Molecule 2: Cellular tumor antigen p53

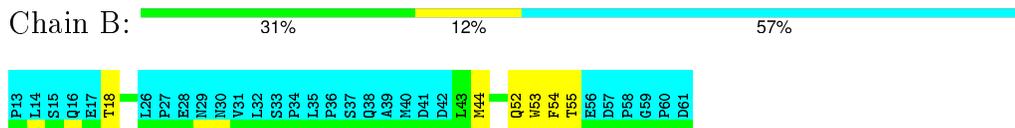


4.2.15 Score per residue for model 15

- Molecule 1: CREB-binding protein

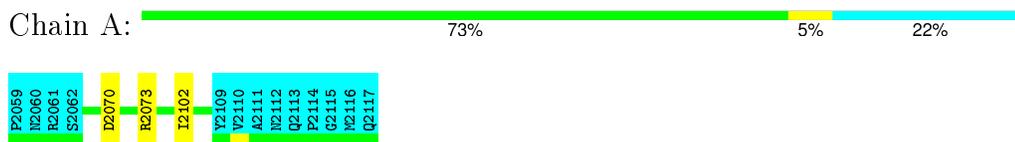


- Molecule 2: Cellular tumor antigen p53

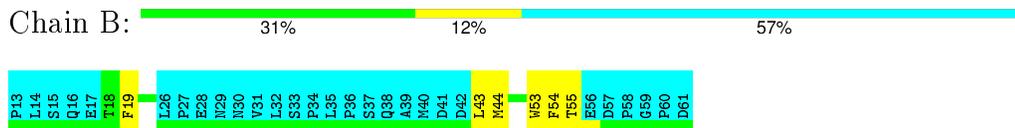


4.2.16 Score per residue for model 16

- Molecule 1: CREB-binding protein

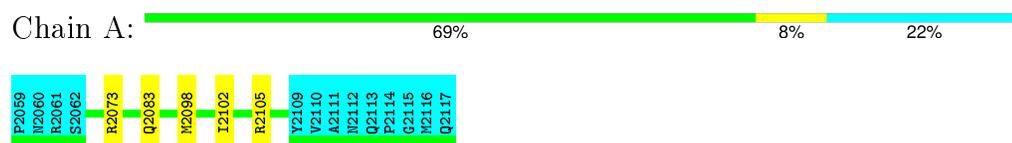


- Molecule 2: Cellular tumor antigen p53

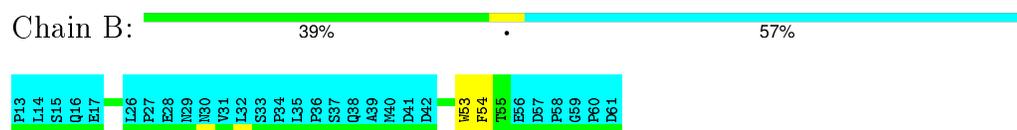


4.2.17 Score per residue for model 17

- Molecule 1: CREB-binding protein

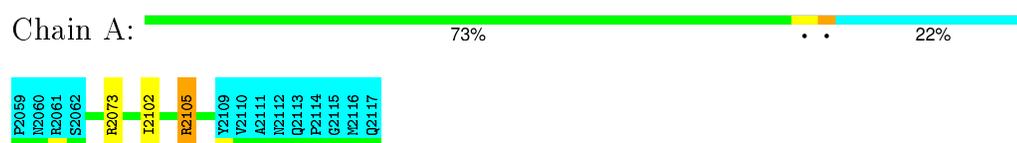


- Molecule 2: Cellular tumor antigen p53

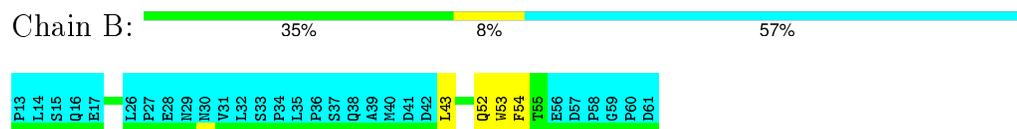


4.2.18 Score per residue for model 18

- Molecule 1: CREB-binding protein

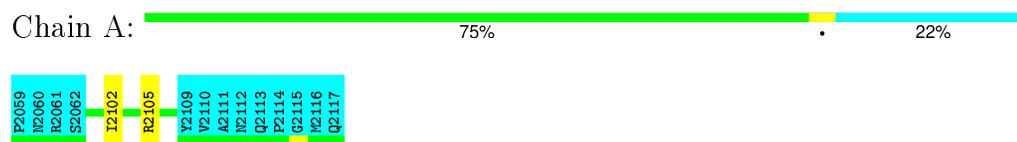


- Molecule 2: Cellular tumor antigen p53

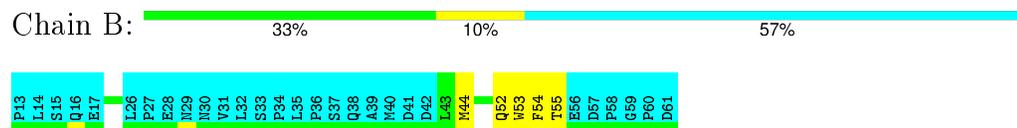


4.2.19 Score per residue for model 19

- Molecule 1: CREB-binding protein

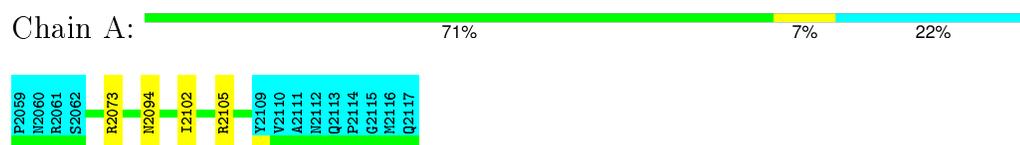


- Molecule 2: Cellular tumor antigen p53

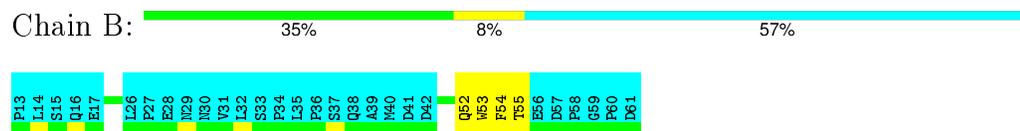


4.2.20 Score per residue for model 20

- Molecule 1: CREB-binding protein



- Molecule 2: Cellular tumor antigen p53



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

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 17073
Number of chemical shift lists	1
Total number of shifts	1362
Number of shifts mapped to atoms	1362
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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

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%)	59	88
2	B	21/49 (43%)	20±1 (97±3%)	1±1 (2±3%)	0±0 (0±1%)	38	79
All	All	1340/2160 (62%)	1315 (98%)	22 (2%)	3 (0%)	56	85

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%)	32	77
2	B	21/47 (45%)	17±1 (79±5%)	4±1 (21±5%)	4	33
All	All	1260/2000 (63%)	1126 (89%)	134 (11%)	13	57

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)
2	B	53	TRP	20
2	B	54	PHE	20
1	A	2102	ILE	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
2	B	19	PHE	5
1	A	2094	ASN	5
1	A	2083	GLN	4
1	A	2096	GLN	2
1	A	2070	ASP	2
2	B	48	ASP	1
1	A	2098	MET	1
1	A	2063	ILE	1
1	A	2068	LEU	1
1	A	2108	LYS	1
2	B	21	ASP	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 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

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 93% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17073

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	1362
Number of shifts mapped to atoms	1362
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	22

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
$^{13}\text{C}_\alpha$	107	0.65 ± 0.09	Should be applied
$^{13}\text{C}_\beta$	105	0.78 ± 0.04	Should be applied
$^{13}\text{C}'$	89	0.21 ± 0.08	None needed (< 0.5 ppm)
^{15}N	94	-0.12 ± 0.18	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 93%, i.e. 811 atoms were assigned a chemical shift out of a possible 869. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	316/325 (97%)	129/129 (100%)	125/134 (93%)	62/62 (100%)
Sidechain	446/493 (90%)	278/292 (95%)	157/179 (88%)	11/22 (50%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	49/51 (96%)	25/27 (93%)	22/22 (100%)	2/2 (100%)
Overall	811/869 (93%)	432/448 (96%)	304/335 (91%)	75/86 (87%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1247 atoms were assigned a chemical shift out of a possible 1344. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	492/514 (96%)	202/203 (100%)	196/216 (91%)	94/95 (99%)
Sidechain	698/771 (91%)	440/459 (96%)	239/279 (86%)	19/33 (58%)
Aromatic	57/59 (97%)	29/31 (94%)	26/26 (100%)	2/2 (100%)
Overall	1247/1344 (93%)	671/693 (97%)	461/521 (88%)	115/130 (88%)

7.1.4 Statistically unusual chemical shifts

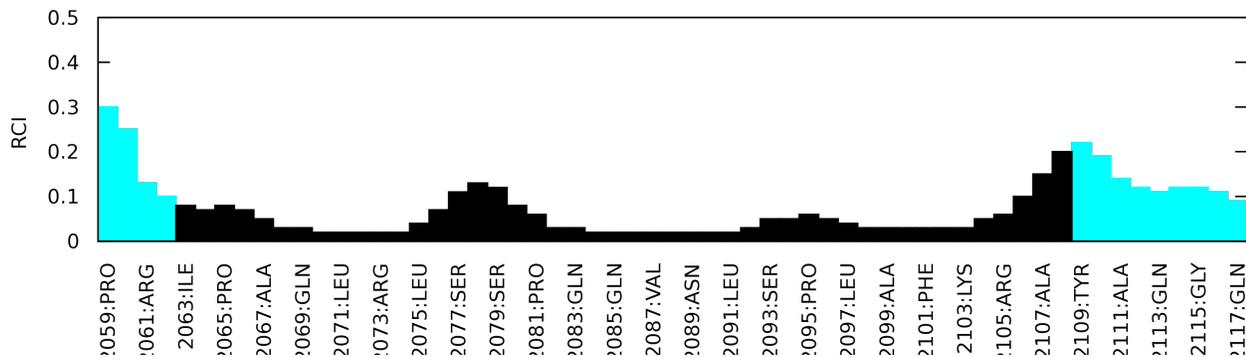
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	19	PHE	CD2	69.90	137.34 – 125.84	-53.6
1	A	2101	PHE	CD2	70.12	137.34 – 125.84	-53.4
2	B	19	PHE	CD1	70.09	137.63 – 125.43	-50.4
1	A	2101	PHE	CD1	70.12	137.63 – 125.43	-50.3
2	B	54	PHE	CD1	70.41	137.63 – 125.43	-50.1
1	A	2109	TYR	CE1	56.82	124.14 – 111.74	-49.3
1	A	2109	TYR	CD1	71.40	139.11 – 126.41	-48.3
1	A	2101	PHE	CE1	69.00	137.92 – 123.42	-42.5
2	B	19	PHE	CE1	69.90	137.92 – 123.42	-41.9
2	B	54	PHE	CE1	69.93	137.92 – 123.42	-41.9
2	B	54	PHE	CZ	67.83	137.04 – 121.44	-39.4
2	B	53	TRP	CZ3	60.09	129.20 – 113.60	-39.3
2	B	23	TRP	CZ3	60.34	129.20 – 113.60	-39.1
2	B	53	TRP	CE3	59.25	129.06 – 111.96	-35.8
2	B	23	TRP	CE3	59.47	129.06 – 111.96	-35.7
2	B	53	TRP	CH2	62.67	133.06 – 114.56	-33.0
2	B	23	TRP	CH2	62.95	133.06 – 114.56	-32.9
2	B	53	TRP	CD1	64.62	136.18 – 116.78	-31.9
2	B	23	TRP	CD1	65.50	136.18 – 116.78	-31.4
2	B	53	TRP	CZ2	83.06	121.76 – 106.66	-20.6
2	B	23	TRP	CZ2	83.28	121.76 – 106.66	-20.5
1	A	2069	GLN	CG	27.53	39.38 – 28.18	-5.6

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

The images below report *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:



Random coil index (RCI) for chain B:

