



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:20 pm BST

PDB ID : 2J11  
Title : p53 tetramerization domain mutant Y327S T329G Q331G  
Authors : Carbajo, R.J.; Mora, P.; Sanchez del Pino, M.M.; Perez-Paya, E.; Pineda-Lucena, A.  
Deposited on : 2006-08-08

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)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 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

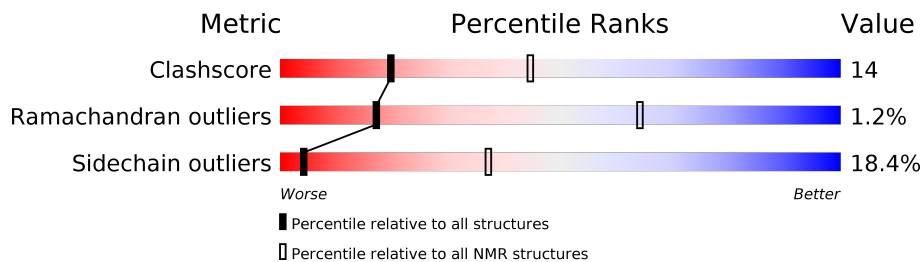
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment 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	31	
1	B	31	
1	C	31	
1	D	31	

## 2 Ensemble composition and analysis i

This entry contains 29 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 17 as representative.

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:327-A:354, B:327-B:354, C:327-C:354, D:327-D:354 (112)	0.48	20

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 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 5, 6, 8, 9, 11, 12, 13, 16, 19, 20, 21, 22, 23, 29
2	18, 25, 28
3	7, 17, 26
4	3, 4, 27
5	15, 24
Single-model clusters	10; 14

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1980 atoms, of which 976 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	31	495	155	244	46	49	1	0
1	B	31	495	155	244	46	49	1	0
1	C	31	495	155	244	46	49	1	0
1	D	31	495	155	244	46	49	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	SER	TYR	engineered mutation	UNP P04637
A	329	GLY	THR	engineered mutation	UNP P04637
A	331	GLY	GLN	engineered mutation	UNP P04637
B	327	SER	TYR	engineered mutation	UNP P04637
B	329	GLY	THR	engineered mutation	UNP P04637
B	331	GLY	GLN	engineered mutation	UNP P04637
C	327	SER	TYR	engineered mutation	UNP P04637
C	329	GLY	THR	engineered mutation	UNP P04637
C	331	GLY	GLN	engineered mutation	UNP P04637
D	327	SER	TYR	engineered mutation	UNP P04637
D	329	GLY	THR	engineered mutation	UNP P04637
D	331	GLY	GLN	engineered mutation	UNP P04637

## 4 Residue-property plots [i](#)

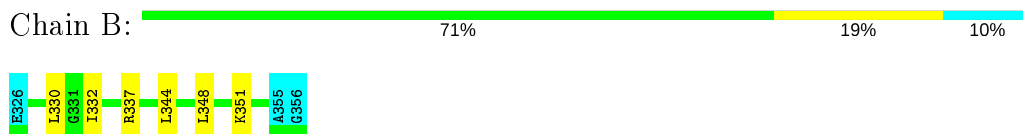
### 4.1 Average score per residue in the NMR ensemble

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.

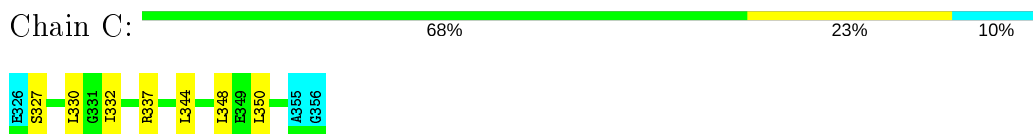
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



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

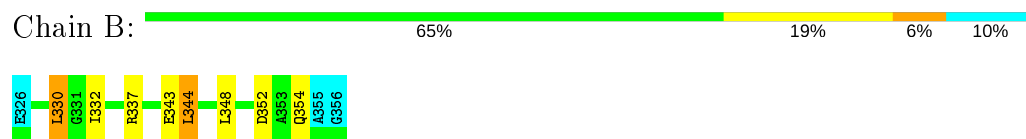
Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

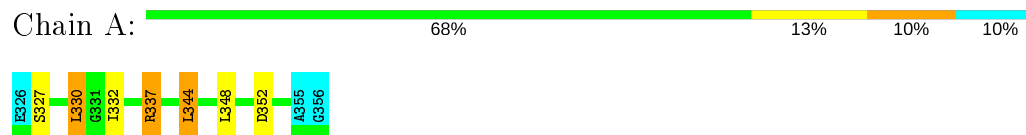


- Molecule 1: CELLULAR TUMOR ANTIGEN P53

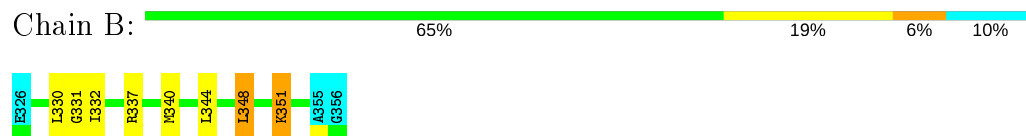


#### 4.2.2 Score per residue for model 2

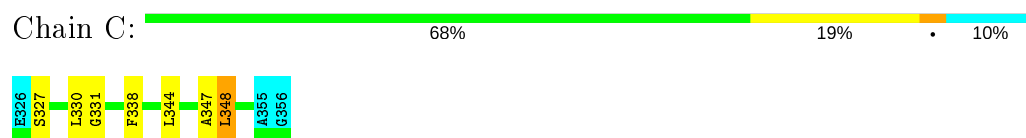
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### 4.2.3 Score per residue for model 3

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



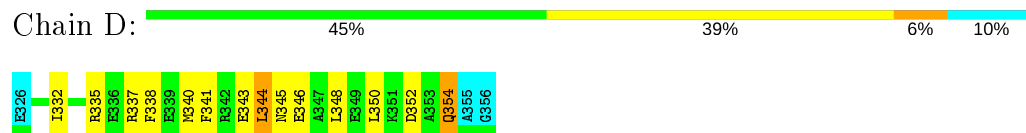
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



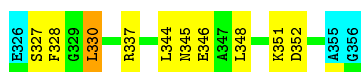
#### 4.2.4 Score per residue for model 4

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### 4.2.5 Score per residue for model 5

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



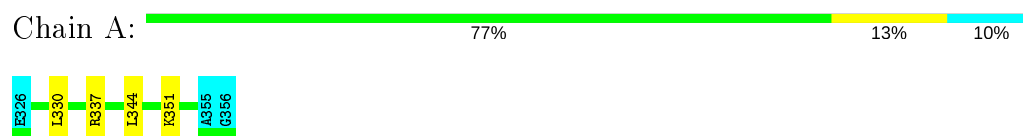
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



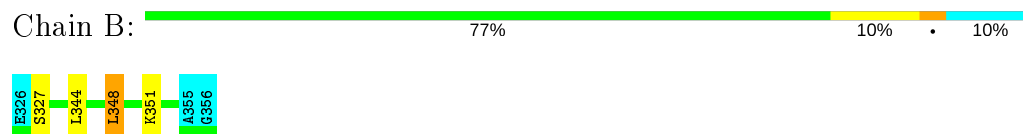


### 4.2.6 Score per residue for model 6

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



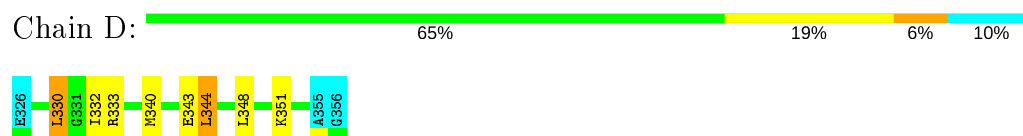
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

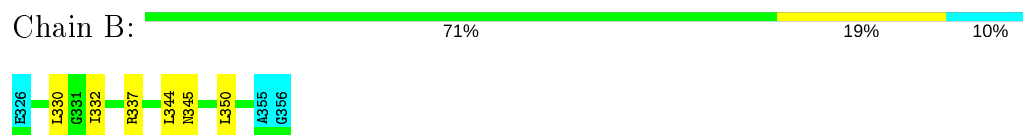


### 4.2.7 Score per residue for model 7

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

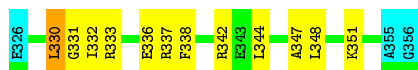


- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- Molecule 1: CELLULAR TUMOR ANTIGEN P53

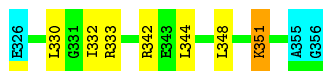


#### 4.2.8 Score per residue for model 8

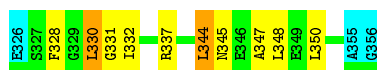
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



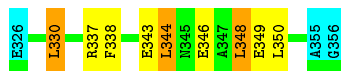
#### 4.2.9 Score per residue for model 9

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B: 



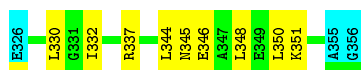
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C: 



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D: 



#### 4.2.10 Score per residue for model 10

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A: 



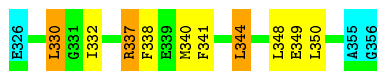
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B: 



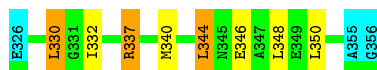
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C: 



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D: 



### 4.2.11 Score per residue for model 11

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



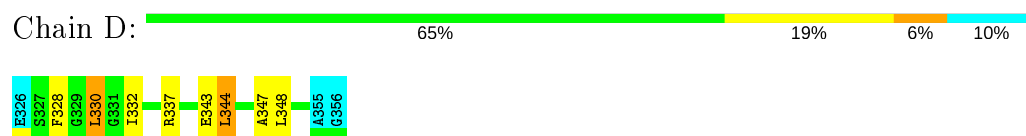
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



### 4.2.12 Score per residue for model 12

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- Molecule 1: CELLULAR TUMOR ANTIGEN P53

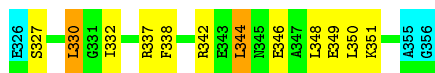


#### 4.2.13 Score per residue for model 13

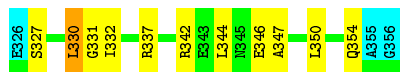
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

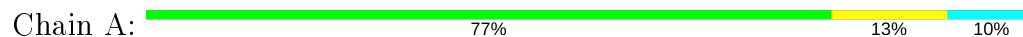


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### 4.2.14 Score per residue for model 14

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  61% 26% 10%



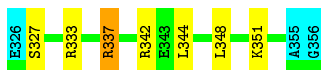
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  52% 39% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  68% 19% 10%



#### 4.2.15 Score per residue for model 15

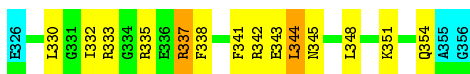
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  55% 32% 10%



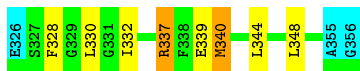
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  45% 39% 6% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  65% 19% 6% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  61% 29% 10%



#### 4.2.16 Score per residue for model 16

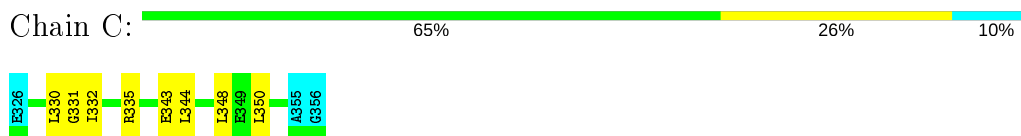
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

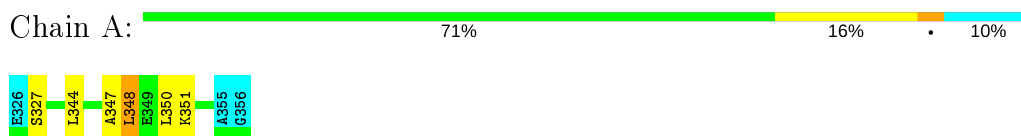


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### 4.2.17 Score per residue for model 17

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### 4.2.18 Score per residue for model 18

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### 4.2.19 Score per residue for model 19

- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  58% 26% 6% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  68% 23% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  55% 32% 10%



#### 4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  65% 23% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  48% 35% 6% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  68% 19% 10%



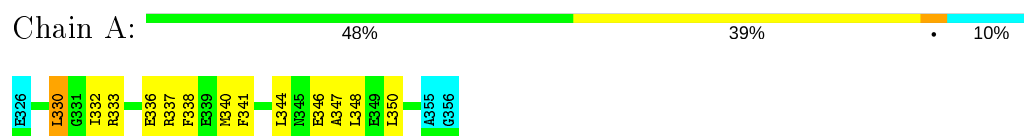
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  55% 32% 10%



### 4.2.21 Score per residue for model 21

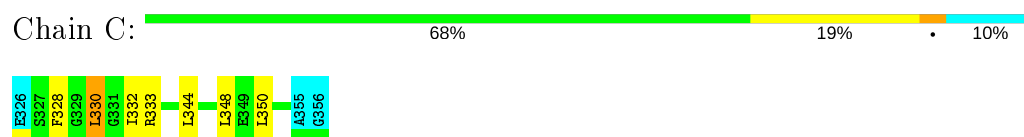
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

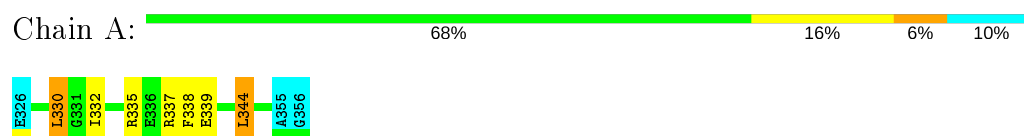


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



### 4.2.22 Score per residue for model 22

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

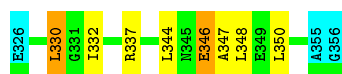


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



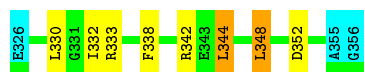


- Molecule 1: CELLULAR TUMOR ANTIGEN P53

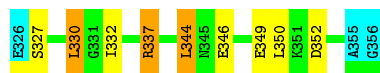


#### 4.2.23 Score per residue for model 23

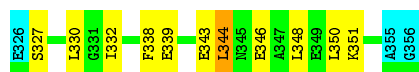
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

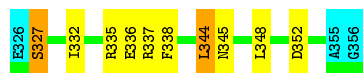


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### 4.2.24 Score per residue for model 24

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



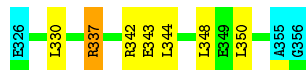
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  52% 35% 10%



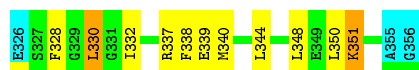
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  68% 19% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  55% 29% 6% 10%



#### 4.2.25 Score per residue for model 25

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  61% 23% 6% 10%




- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  55% 35% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  81% 6% 10%



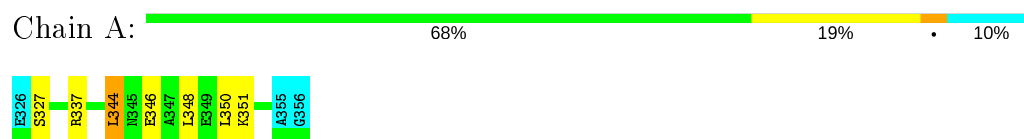
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  68% 13% 10% 10%



#### 4.2.26 Score per residue for model 26

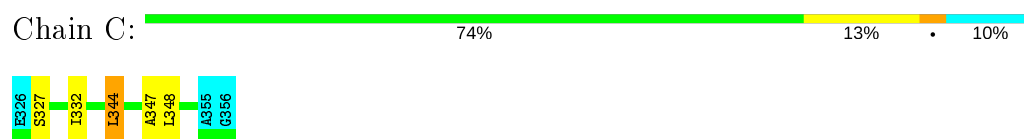
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



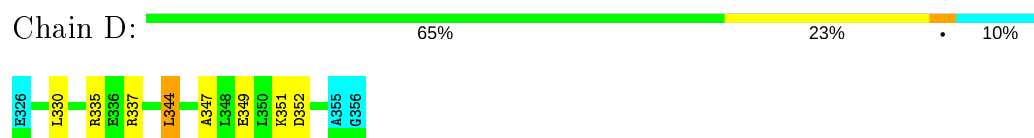
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

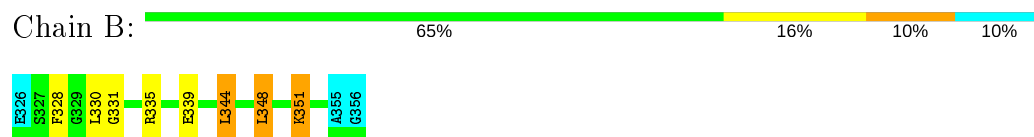


#### 4.2.27 Score per residue for model 27

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

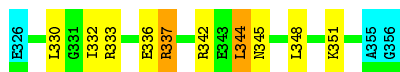


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



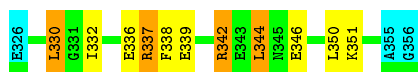


- Molecule 1: CELLULAR TUMOR ANTIGEN P53

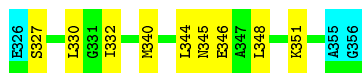


#### 4.2.28 Score per residue for model 28

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

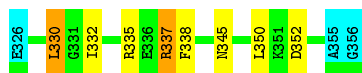


- Molecule 1: CELLULAR TUMOR ANTIGEN P53

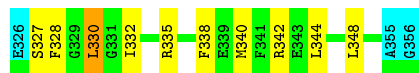


#### 4.2.29 Score per residue for model 29

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



## • Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  58% 29% 10%

## • Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  65% 23% 10%

## • Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  68% 16% 6% 10%

## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *CNS*.

Of the 30 calculated structures, 29 were deposited, based on the following criterion: *TOTAL ENERGY*.

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

Software name	Classification	Version
CNS	refinement	
SPARKY	structure solution	

No chemical shift data was provided. 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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

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	232	228	228	10±3
1	B	232	228	228	10±3
1	C	232	228	228	9±4
1	D	232	228	228	10±4
All	All	26912	26448	26448	740

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:344:LEU:HD22	1:C:344:LEU:HD11	1.04	1.30	12	3
1:A:344:LEU:HD21	1:D:344:LEU:HD22	1.00	1.31	20	1
1:B:330:LEU:HD22	1:B:332:ILE:HD11	0.95	1.37	20	5
1:B:344:LEU:HD11	1:C:344:LEU:HD22	0.93	1.35	6	2
1:C:330:LEU:HD23	1:C:332:ILE:HD11	0.92	1.40	29	4
1:B:330:LEU:HD23	1:B:332:ILE:HD11	0.92	1.41	10	4
1:A:344:LEU:HD21	1:D:344:LEU:HD21	0.91	1.42	24	12
1:D:330:LEU:HD23	1:D:332:ILE:HD11	0.90	1.39	19	3
1:A:330:LEU:HD23	1:A:332:ILE:HD11	0.89	1.44	4	3
1:A:344:LEU:HD22	1:D:344:LEU:HD11	0.87	1.45	11	2
1:A:344:LEU:HD21	1:D:344:LEU:HD11	0.84	1.50	6	6

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:330:LEU:HD22	1:A:332:ILE:HD11	0.83	1.48	29	4
1:D:330:LEU:HD22	1:D:332:ILE:HD11	0.82	1.51	29	5
1:C:344:LEU:HD12	1:C:348:LEU:HD11	0.82	1.48	23	1
1:B:344:LEU:HD11	1:C:344:LEU:HD21	0.80	1.53	28	5
1:A:348:LEU:HD13	1:B:337:ARG:CG	0.77	2.09	13	7
1:A:344:LEU:CD1	1:D:344:LEU:HD21	0.77	2.09	2	3
1:A:344:LEU:HD11	1:D:344:LEU:HD21	0.77	1.56	5	5
1:B:344:LEU:HD11	1:C:344:LEU:HD11	0.76	1.57	15	2
1:D:348:LEU:HD12	1:D:349:GLU:N	0.76	1.95	21	1
1:B:344:LEU:HD21	1:C:344:LEU:HD21	0.75	1.58	5	11
1:D:330:LEU:CD2	1:D:332:ILE:HD11	0.74	2.12	19	3
1:B:344:LEU:CD1	1:C:344:LEU:HD21	0.74	2.12	27	3
1:A:338:PHE:CZ	1:B:330:LEU:HD13	0.74	2.18	8	1
1:B:344:LEU:CD1	1:C:344:LEU:HD11	0.74	2.12	23	2
1:A:330:LEU:CD1	1:A:332:ILE:HD11	0.74	2.12	20	2
1:A:344:LEU:HD21	1:D:344:LEU:CD1	0.73	2.13	6	4
1:B:344:LEU:O	1:B:348:LEU:HD12	0.73	1.84	29	12
1:D:330:LEU:HD12	1:D:332:ILE:HD11	0.72	1.59	18	1
1:A:348:LEU:HD23	1:B:337:ARG:HD2	0.72	1.61	16	1
1:B:344:LEU:O	1:B:348:LEU:HD23	0.72	1.85	11	5
1:C:330:LEU:HD22	1:D:338:PHE:CE2	0.72	2.20	24	2
1:D:344:LEU:O	1:D:348:LEU:HD23	0.71	1.85	20	9
1:A:330:LEU:HD22	1:A:332:ILE:CD1	0.71	2.14	23	8
1:A:344:LEU:HD21	1:D:344:LEU:CD2	0.71	2.12	20	7
1:C:330:LEU:HD22	1:C:332:ILE:CD1	0.71	2.15	16	6
1:B:344:LEU:HD21	1:C:344:LEU:CD2	0.70	2.15	5	6
1:C:344:LEU:O	1:C:348:LEU:HD23	0.70	1.87	4	6
1:D:330:LEU:HD22	1:D:332:ILE:CD1	0.70	2.16	29	7
1:A:344:LEU:O	1:A:348:LEU:HD23	0.70	1.86	27	5
1:B:344:LEU:O	1:B:348:LEU:HD13	0.70	1.87	18	1
1:A:332:ILE:HG23	1:B:345:ASN:OD1	0.70	1.86	28	4
1:A:338:PHE:CE2	1:B:330:LEU:HD12	0.70	2.20	23	4
1:B:348:LEU:HD13	1:B:351:LYS:NZ	0.69	2.01	8	1
1:D:344:LEU:O	1:D:348:LEU:HD13	0.69	1.87	24	3
1:A:344:LEU:O	1:A:348:LEU:HD12	0.69	1.88	25	11
1:C:344:LEU:O	1:C:348:LEU:HD12	0.69	1.87	5	8
1:A:338:PHE:CE1	1:B:330:LEU:HD23	0.69	2.21	28	2
1:A:344:LEU:CG	1:D:344:LEU:HD21	0.68	2.18	3	4
1:C:348:LEU:HD13	1:D:337:ARG:NE	0.68	2.03	16	3
1:A:338:PHE:CE2	1:B:330:LEU:HD22	0.68	2.23	15	2
1:C:344:LEU:HD12	1:C:348:LEU:CD1	0.68	2.19	23	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:348:LEU:HD23	1:D:337:ARG:HG3	0.68	1.64	14	1
1:B:330:LEU:CD2	1:B:332:ILE:HD11	0.68	2.15	10	4
1:A:337:ARG:HG2	1:B:348:LEU:HD22	0.68	1.65	10	1
1:A:344:LEU:CD2	1:D:344:LEU:HD11	0.68	2.19	11	2
1:C:348:LEU:HD22	1:D:337:ARG:CZ	0.67	2.19	15	1
1:C:348:LEU:HD13	1:D:337:ARG:CG	0.67	2.19	2	7
1:B:330:LEU:HD22	1:B:332:ILE:CD1	0.67	2.19	3	5
1:B:346:GLU:O	1:B:350:LEU:HD23	0.67	1.90	19	3
1:B:350:LEU:HD12	1:B:351:LYS:N	0.67	2.04	13	1
1:A:344:LEU:CD2	1:D:344:LEU:HD21	0.67	2.20	24	7
1:D:350:LEU:HD12	1:D:351:LYS:N	0.67	2.04	24	2
1:A:348:LEU:HD13	1:B:337:ARG:HD3	0.67	1.66	2	4
1:A:330:LEU:HD22	1:A:332:ILE:HD13	0.67	1.65	23	5
1:C:330:LEU:HD13	1:D:338:PHE:CZ	0.66	2.26	29	2
1:A:337:ARG:HG3	1:B:348:LEU:HD13	0.66	1.68	9	4
1:D:346:GLU:O	1:D:350:LEU:HD23	0.65	1.91	3	3
1:B:351:LYS:NZ	1:C:347:ALA:HB2	0.65	2.06	28	1
1:B:344:LEU:HD21	1:C:344:LEU:HG	0.65	1.68	25	5
1:C:338:PHE:CZ	1:D:330:LEU:HD12	0.65	2.26	10	2
1:C:332:ILE:HG23	1:D:345:ASN:OD1	0.65	1.91	17	2
1:A:330:LEU:HD22	1:B:338:PHE:CE1	0.65	2.27	25	1
1:D:348:LEU:HD13	1:D:351:LYS:HD3	0.65	1.68	6	3
1:C:348:LEU:HD22	1:D:337:ARG:HG2	0.64	1.68	7	2
1:A:344:LEU:HD23	1:D:344:LEU:HD11	0.64	1.68	17	1
1:A:344:LEU:HD21	1:D:344:LEU:CG	0.64	2.23	23	4
1:B:344:LEU:HD21	1:C:344:LEU:CG	0.64	2.22	18	6
1:A:347:ALA:HB2	1:D:351:LYS:HE3	0.64	1.70	17	2
1:C:348:LEU:HD13	1:D:337:ARG:HG3	0.63	1.68	2	1
1:D:344:LEU:O	1:D:348:LEU:HD12	0.63	1.94	10	6
1:A:344:LEU:HD22	1:D:344:LEU:HD22	0.63	1.71	18	1
1:C:350:LEU:HD12	1:C:351:LYS:N	0.63	2.08	3	1
1:C:348:LEU:HD22	1:D:337:ARG:CD	0.63	2.23	28	2
1:C:337:ARG:HG2	1:D:348:LEU:HD22	0.63	1.69	28	1
1:A:337:ARG:HD2	1:B:348:LEU:HD13	0.62	1.71	2	1
1:A:346:GLU:O	1:A:350:LEU:HD23	0.62	1.94	13	4
1:C:337:ARG:CG	1:D:348:LEU:HD13	0.62	2.24	11	4
1:B:348:LEU:HD13	1:B:351:LYS:HD3	0.62	1.72	5	2
1:B:330:LEU:HD22	1:B:332:ILE:CG1	0.62	2.25	1	3
1:B:344:LEU:CG	1:C:344:LEU:HD21	0.62	2.24	10	3
1:B:344:LEU:HD11	1:C:344:LEU:CD2	0.62	2.23	28	3
1:B:344:LEU:HD23	1:B:348:LEU:HD23	0.62	1.69	27	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:337:ARG:NE	1:B:348:LEU:HD22	0.61	2.09	2	1
1:B:351:LYS:CE	1:C:347:ALA:HB2	0.61	2.24	28	5
1:A:344:LEU:HG	1:D:344:LEU:HD11	0.61	1.72	12	1
1:C:348:LEU:HD13	1:D:337:ARG:HG2	0.61	1.70	3	3
1:C:348:LEU:HD13	1:D:337:ARG:HD2	0.60	1.74	11	3
1:A:346:GLU:O	1:A:350:LEU:HD12	0.60	1.96	3	3
1:A:338:PHE:CE1	1:B:330:LEU:HD13	0.60	2.31	8	1
1:A:330:LEU:HD22	1:B:338:PHE:CE2	0.60	2.31	20	1
1:C:348:LEU:HD13	1:D:337:ARG:CZ	0.60	2.25	7	1
1:C:330:LEU:HD22	1:C:332:ILE:HD11	0.60	1.71	12	6
1:C:330:LEU:HD12	1:D:338:PHE:CZ	0.60	2.31	17	1
1:C:332:ILE:HG21	1:C:338:PHE:HB2	0.59	1.73	3	2
1:D:330:LEU:HD22	1:D:332:ILE:HG13	0.59	1.75	23	6
1:A:344:LEU:HD11	1:D:344:LEU:CD2	0.59	2.28	19	4
1:C:337:ARG:HG3	1:D:348:LEU:HD13	0.58	1.75	4	5
1:A:344:LEU:HD21	1:D:344:LEU:HG	0.58	1.75	23	2
1:C:344:LEU:HD23	1:D:337:ARG:NH1	0.58	2.13	27	1
1:D:330:LEU:HD22	1:D:332:ILE:CG1	0.57	2.29	10	4
1:A:330:LEU:HD12	1:B:338:PHE:CE2	0.57	2.33	12	2
1:C:330:LEU:HD22	1:C:332:ILE:CG1	0.57	2.29	12	2
1:A:337:ARG:CG	1:B:348:LEU:HD13	0.57	2.29	12	4
1:C:337:ARG:CD	1:D:348:LEU:HD13	0.57	2.29	10	1
1:A:344:LEU:HD11	1:D:344:LEU:HD11	0.57	1.73	28	2
1:A:348:LEU:HD13	1:A:351:LYS:HD3	0.57	1.76	17	1
1:C:348:LEU:HD22	1:D:337:ARG:HD2	0.57	1.76	28	1
1:A:332:ILE:HD13	1:B:330:LEU:CD2	0.57	2.30	24	1
1:B:344:LEU:CD2	1:C:344:LEU:HD11	0.57	2.28	8	2
1:C:330:LEU:HD22	1:C:332:ILE:HG13	0.57	1.76	22	8
1:C:340:MET:O	1:C:344:LEU:HD23	0.56	1.99	15	2
1:A:351:LYS:HD2	1:D:347:ALA:HB2	0.56	1.77	16	3
1:A:350:LEU:HD23	1:D:354:GLN:OE1	0.56	2.01	19	2
1:A:330:LEU:HD23	1:A:332:ILE:CD1	0.56	2.27	4	1
1:A:330:LEU:HD11	1:B:342:ARG:HA	0.56	1.78	10	2
1:B:344:LEU:HG	1:C:344:LEU:HD21	0.56	1.78	10	2
1:D:348:LEU:HD13	1:D:351:LYS:HD2	0.56	1.76	27	1
1:D:332:ILE:HD12	1:D:332:ILE:N	0.55	2.16	20	2
1:A:330:LEU:HD13	1:B:338:PHE:CE1	0.55	2.36	16	2
1:A:341:PHE:HB2	1:B:330:LEU:HD11	0.55	1.77	3	2
1:B:351:LYS:HE3	1:C:347:ALA:HB2	0.55	1.78	8	1
1:A:337:ARG:CG	1:B:348:LEU:HD22	0.55	2.32	10	1
1:B:330:LEU:HD13	1:B:332:ILE:HD11	0.55	1.78	28	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:332:ILE:N	1:C:332:ILE:HD12	0.55	2.16	26	2
1:A:345:ASN:ND2	1:B:332:ILE:HD12	0.55	2.15	29	1
1:B:332:ILE:HD12	1:B:332:ILE:N	0.54	2.18	13	1
1:A:348:LEU:HD13	1:B:337:ARG:HD2	0.54	1.79	1	3
1:B:344:LEU:HD11	1:C:344:LEU:CD1	0.54	2.32	23	2
1:A:350:LEU:HD23	1:D:354:GLN:CD	0.54	2.22	19	1
1:A:348:LEU:HD13	1:B:337:ARG:HG3	0.54	1.76	13	4
1:B:344:LEU:HD22	1:C:344:LEU:HD22	0.54	1.79	21	1
1:C:348:LEU:HD13	1:D:337:ARG:CD	0.54	2.33	19	3
1:C:345:ASN:HD21	1:D:332:ILE:HD12	0.54	1.62	3	1
1:A:340:MET:O	1:A:344:LEU:HD13	0.54	2.03	1	2
1:C:338:PHE:CE2	1:D:330:LEU:HD12	0.54	2.37	10	4
1:B:344:LEU:CD2	1:C:344:LEU:HD21	0.54	2.31	5	5
1:D:330:LEU:CG	1:D:332:ILE:HD11	0.54	2.33	28	2
1:C:340:MET:O	1:C:344:LEU:HD13	0.54	2.02	14	1
1:C:338:PHE:CE2	1:D:330:LEU:HD13	0.54	2.38	19	1
1:A:330:LEU:HD22	1:A:332:ILE:HG13	0.54	1.79	1	4
1:A:344:LEU:HG	1:D:344:LEU:HD21	0.53	1.79	3	4
1:A:332:ILE:HG23	1:B:345:ASN:HD21	0.53	1.64	20	1
1:B:348:LEU:HD12	1:B:349:GLU:N	0.53	2.18	16	1
1:B:330:LEU:HD22	1:B:332:ILE:HG13	0.53	1.81	1	5
1:A:341:PHE:CB	1:B:330:LEU:HD11	0.53	2.33	3	1
1:C:344:LEU:HD23	1:D:337:ARG:HH12	0.53	1.63	27	1
1:B:344:LEU:HD22	1:C:344:LEU:CD1	0.53	2.21	12	1
1:C:330:LEU:HD22	1:D:338:PHE:CE1	0.53	2.38	19	1
1:A:344:LEU:CD2	1:D:344:LEU:HD22	0.53	2.33	18	2
1:B:351:LYS:HE2	1:C:347:ALA:HB2	0.52	1.79	6	3
1:A:348:LEU:HD13	1:B:337:ARG:CD	0.52	2.33	7	3
1:C:346:GLU:O	1:C:350:LEU:HD23	0.52	2.03	9	3
1:B:330:LEU:HD23	1:B:331:GLY:N	0.52	2.20	19	5
1:C:341:PHE:HB2	1:D:330:LEU:HD11	0.52	1.80	20	1
1:A:338:PHE:CD2	1:B:330:LEU:HD22	0.52	2.39	15	1
1:A:330:LEU:HD22	1:A:332:ILE:CG1	0.52	2.34	1	1
1:A:337:ARG:HG2	1:B:348:LEU:HD13	0.52	1.82	25	2
1:D:330:LEU:HD23	1:D:331:GLY:N	0.52	2.20	2	4
1:C:345:ASN:ND2	1:D:330:LEU:HD21	0.52	2.20	8	1
1:A:330:LEU:HD13	1:B:338:PHE:CZ	0.52	2.40	11	2
1:A:330:LEU:HD12	1:A:332:ILE:HD11	0.52	1.82	20	2
1:C:348:LEU:HD13	1:D:337:ARG:HD3	0.52	1.82	25	3
1:B:332:ILE:N	1:B:332:ILE:HD12	0.51	2.19	10	2
1:B:330:LEU:O	1:B:332:ILE:HD12	0.51	2.06	21	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:332:ILE:HG21	1:D:338:PHE:N	0.51	2.20	8	1
1:A:344:LEU:CG	1:D:344:LEU:HD11	0.51	2.35	12	1
1:D:348:LEU:HD23	1:D:351:LYS:HD3	0.51	1.83	2	1
1:A:330:LEU:HD12	1:B:338:PHE:CZ	0.51	2.41	9	2
1:C:348:LEU:HD23	1:C:351:LYS:NZ	0.50	2.21	3	1
1:A:348:LEU:HD13	1:B:337:ARG:HG2	0.50	1.82	13	3
1:D:330:LEU:HD23	1:D:330:LEU:N	0.50	2.21	18	1
1:B:332:ILE:HG21	1:B:337:ARG:HD2	0.50	1.84	24	1
1:A:347:ALA:HB2	1:D:351:LYS:CE	0.50	2.37	17	5
1:C:348:LEU:HD22	1:D:337:ARG:HG3	0.50	1.83	27	1
1:A:344:LEU:HD11	1:D:344:LEU:CD1	0.50	2.37	28	1
1:A:330:LEU:HD23	1:A:331:GLY:N	0.50	2.22	18	1
1:D:330:LEU:HD13	1:D:332:ILE:HD11	0.50	1.83	24	1
1:C:346:GLU:O	1:C:350:LEU:HD12	0.49	2.07	20	3
1:A:330:LEU:HD22	1:B:338:PHE:CD1	0.49	2.41	25	1
1:B:348:LEU:HD23	1:B:351:LYS:HD3	0.49	1.84	3	1
1:B:350:LEU:C	1:B:350:LEU:HD12	0.49	2.28	13	1
1:A:337:ARG:HG3	1:B:348:LEU:HD22	0.49	1.83	1	2
1:C:330:LEU:HD22	1:C:332:ILE:HD13	0.49	1.84	11	3
1:B:340:MET:O	1:B:344:LEU:HD12	0.49	2.07	10	2
1:B:332:ILE:HD13	1:B:338:PHE:CD2	0.49	2.42	12	1
1:D:330:LEU:HD23	1:D:330:LEU:H	0.49	1.66	18	1
1:C:330:LEU:CD2	1:C:332:ILE:HD11	0.49	2.38	28	1
1:A:338:PHE:CE1	1:B:330:LEU:HD12	0.49	2.43	9	3
1:C:348:LEU:HD22	1:D:337:ARG:NH1	0.49	2.23	11	1
1:C:337:ARG:HD3	1:D:348:LEU:HD13	0.49	1.82	10	1
1:C:338:PHE:CZ	1:D:330:LEU:HD13	0.49	2.43	19	1
1:D:340:MET:O	1:D:344:LEU:HD12	0.49	2.08	24	2
1:A:351:LYS:HE3	1:D:347:ALA:HB2	0.49	1.85	11	1
1:B:340:MET:O	1:B:344:LEU:HD23	0.49	2.07	2	1
1:A:330:LEU:HD11	1:A:332:ILE:HD11	0.49	1.81	25	1
1:A:332:ILE:N	1:A:332:ILE:HD12	0.48	2.23	24	1
1:A:351:LYS:CE	1:D:347:ALA:HB2	0.48	2.38	25	2
1:B:330:LEU:HD23	1:B:332:ILE:CD1	0.48	2.28	10	1
1:C:330:LEU:HD23	1:C:331:GLY:N	0.48	2.24	8	5
1:A:344:LEU:HD23	1:A:348:LEU:CD2	0.48	2.38	24	1
1:B:344:LEU:CG	1:C:344:LEU:HD11	0.48	2.39	19	1
1:D:330:LEU:HB3	1:D:332:ILE:HD11	0.48	1.84	9	5
1:A:340:MET:O	1:A:344:LEU:HD23	0.48	2.08	13	1
1:C:350:LEU:C	1:C:350:LEU:HD12	0.48	2.29	3	1
1:A:330:LEU:CD2	1:A:332:ILE:HD11	0.48	2.39	7	2

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:LYS:HE2	1:D:347:ALA:HB2	0.48	1.86	7	1
1:A:332:ILE:HD13	1:A:338:PHE:CD1	0.48	2.44	12	1
1:C:330:LEU:HD22	1:D:338:PHE:CD2	0.48	2.42	24	1
1:C:348:LEU:HD22	1:D:337:ARG:NH2	0.48	2.24	15	1
1:D:330:LEU:CD1	1:D:332:ILE:HD11	0.48	2.34	18	1
1:B:344:LEU:CD2	1:C:344:LEU:HD22	0.48	2.39	21	2
1:B:330:LEU:HD22	1:B:332:ILE:HD13	0.48	1.86	2	1
1:A:332:ILE:HD13	1:A:338:PHE:CD2	0.48	2.44	19	1
1:A:332:ILE:HG23	1:B:345:ASN:ND2	0.47	2.23	20	2
1:B:348:LEU:HD13	1:B:351:LYS:HZ2	0.47	1.69	8	1
1:C:330:LEU:HB3	1:D:330:LEU:HD21	0.47	1.85	18	1
1:A:338:PHE:CD2	1:B:330:LEU:HD12	0.47	2.45	4	3
1:B:347:ALA:HB2	1:C:351:LYS:CE	0.47	2.39	3	1
1:D:350:LEU:C	1:D:350:LEU:HD12	0.47	2.30	19	1
1:C:342:ARG:HA	1:D:330:LEU:HD11	0.47	1.85	4	1
1:A:332:ILE:HD12	1:A:332:ILE:N	0.47	2.25	20	1
1:A:348:LEU:HD21	1:D:343:GLU:OE1	0.47	2.09	1	1
1:A:338:PHE:CZ	1:B:330:LEU:HD12	0.47	2.44	12	1
1:A:337:ARG:HB3	1:B:348:LEU:HD13	0.47	1.87	3	1
1:D:348:LEU:HD23	1:D:351:LYS:NZ	0.47	2.25	15	3
1:B:332:ILE:HD13	1:B:338:PHE:CD1	0.47	2.45	19	1
1:D:340:MET:CG	1:D:341:PHE:CE1	0.47	2.98	3	1
1:B:344:LEU:HD13	1:C:344:LEU:HD11	0.47	1.87	22	1
1:B:351:LYS:HD3	1:C:347:ALA:HB2	0.46	1.86	13	1
1:C:330:LEU:HD12	1:D:338:PHE:CD1	0.46	2.45	21	1
1:D:350:LEU:HD12	1:D:350:LEU:C	0.46	2.30	24	1
1:A:338:PHE:CD1	1:B:330:LEU:HD12	0.46	2.45	13	1
1:D:348:LEU:HD12	1:D:348:LEU:C	0.46	2.29	21	1
1:C:340:MET:O	1:C:344:LEU:HD12	0.46	2.11	28	1
1:B:354:GLN:HE22	1:C:350:LEU:HD13	0.46	1.70	24	1
1:D:332:ILE:HD13	1:D:338:PHE:HD1	0.46	1.71	8	2
1:B:330:LEU:CD1	1:B:332:ILE:HD11	0.46	2.41	25	1
1:B:347:ALA:HB2	1:C:351:LYS:HE2	0.45	1.88	5	1
1:A:344:LEU:HD11	1:D:344:LEU:HG	0.45	1.88	13	1
1:B:340:MET:CG	1:B:341:PHE:CE2	0.45	2.99	11	1
1:B:344:LEU:HD22	1:C:344:LEU:CD2	0.45	2.41	21	1
1:A:344:LEU:HD11	1:D:344:LEU:HD22	0.45	1.87	4	1
1:B:338:PHE:CE2	1:B:342:ARG:CD	0.45	3.00	14	1
1:C:341:PHE:CB	1:D:330:LEU:HD11	0.45	2.41	20	1
1:C:330:LEU:HD13	1:D:338:PHE:CE2	0.45	2.47	5	1
1:A:337:ARG:NE	1:B:348:LEU:HD12	0.45	2.27	14	1

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:328:PHE:CD2	1:B:328:PHE:N	0.45	2.85	17	3
1:A:348:LEU:HD12	1:B:337:ARG:HD3	0.45	1.89	20	1
1:C:330:LEU:CD2	1:D:338:PHE:CZ	0.45	3.00	20	1
1:A:330:LEU:CD1	1:B:338:PHE:CZ	0.45	3.00	19	2
1:B:330:LEU:N	1:B:330:LEU:HD23	0.45	2.26	24	1
1:C:330:LEU:HB3	1:C:332:ILE:HD11	0.45	1.89	6	4
1:C:338:PHE:CZ	1:D:330:LEU:CD1	0.45	3.00	19	1
1:C:330:LEU:HD23	1:C:332:ILE:CD1	0.45	2.30	29	1
1:C:337:ARG:HD2	1:D:348:LEU:HD13	0.45	1.88	28	1
1:A:345:ASN:HD22	1:B:330:LEU:HD21	0.44	1.72	12	1
1:A:330:LEU:CD1	1:B:332:ILE:HD12	0.44	2.42	15	1
1:A:347:ALA:HB2	1:D:351:LYS:HD2	0.44	1.88	18	1
1:A:330:LEU:CD2	1:B:338:PHE:CE1	0.44	3.00	25	1
1:A:338:PHE:CE2	1:A:342:ARG:CG	0.44	3.00	28	1
1:C:338:PHE:CE1	1:D:330:LEU:HD12	0.44	2.47	6	1
1:A:345:ASN:ND2	1:B:330:LEU:HD21	0.44	2.28	12	1
1:A:338:PHE:CD1	1:B:328:PHE:CB	0.44	3.00	24	1
1:C:344:LEU:HD22	1:D:341:PHE:HE2	0.44	1.72	28	1
1:A:330:LEU:CD1	1:B:338:PHE:CE1	0.44	3.00	16	1
1:B:332:ILE:HG23	1:B:337:ARG:HD2	0.44	1.88	19	1
1:B:344:LEU:HD21	1:C:344:LEU:HD11	0.44	1.89	10	1
1:D:330:LEU:HD22	1:D:332:ILE:HD13	0.44	1.88	7	1
1:D:328:PHE:CD2	1:D:328:PHE:N	0.44	2.85	8	1
1:D:332:ILE:HD13	1:D:338:PHE:CD1	0.44	2.48	8	2
1:A:338:PHE:CE2	1:B:330:LEU:CD1	0.44	3.00	10	1
1:B:344:LEU:HG	1:C:344:LEU:HD11	0.44	1.89	19	1
1:C:345:ASN:ND2	1:D:332:ILE:HD12	0.44	2.27	3	1
1:B:328:PHE:N	1:B:328:PHE:CD1	0.44	2.85	4	1
1:B:344:LEU:HD11	1:C:344:LEU:CG	0.44	2.43	28	1
1:A:337:ARG:HD2	1:B:348:LEU:HD11	0.44	1.88	29	1
1:A:354:GLN:NE2	1:D:350:LEU:HD21	0.44	2.28	5	1
1:C:330:LEU:HD12	1:D:338:PHE:CE1	0.43	2.48	21	1
1:C:337:ARG:CG	1:D:348:LEU:HD23	0.43	2.42	24	1
1:A:330:LEU:HD11	1:B:342:ARG:CA	0.43	2.43	22	1
1:D:332:ILE:HG23	1:D:337:ARG:HG2	0.43	1.89	8	1
1:C:328:PHE:N	1:C:328:PHE:CD2	0.43	2.86	18	1
1:A:330:LEU:HD13	1:A:332:ILE:HD11	0.43	1.89	1	2
1:B:330:LEU:HD22	1:B:332:ILE:HG12	0.43	1.90	16	1
1:C:337:ARG:HG3	1:C:341:PHE:CE2	0.43	2.48	18	2
1:C:328:PHE:N	1:C:328:PHE:CD1	0.43	2.86	1	1
1:D:328:PHE:N	1:D:328:PHE:CD1	0.43	2.87	1	1

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:330:LEU:CD1	1:D:338:PHE:CZ	0.43	3.00	5	1
1:A:344:LEU:HD22	1:D:344:LEU:CD2	0.43	2.41	18	1
1:A:344:LEU:O	1:A:348:LEU:HD13	0.42	2.13	16	1
1:B:344:LEU:HD12	1:C:344:LEU:HD21	0.42	1.87	27	1
1:D:332:ILE:N	1:D:332:ILE:HD12	0.42	2.29	9	2
1:A:338:PHE:CD1	1:B:330:LEU:HD23	0.42	2.48	28	1
1:B:344:LEU:CD1	1:C:344:LEU:HD22	0.42	2.26	6	1
1:C:328:PHE:CD2	1:C:328:PHE:N	0.42	2.86	8	2
1:D:328:PHE:CD1	1:D:328:PHE:N	0.42	2.86	28	1
1:A:347:ALA:HB2	1:D:351:LYS:HE2	0.42	1.91	27	1
1:C:332:ILE:HG23	1:D:345:ASN:ND2	0.42	2.29	5	1
1:C:332:ILE:HG23	1:C:337:ARG:HG2	0.42	1.90	10	1
1:C:330:LEU:HD11	1:D:341:PHE:HB2	0.42	1.92	3	1
1:A:338:PHE:CZ	1:B:330:LEU:CD1	0.42	3.00	8	1
1:A:348:LEU:HD12	1:B:337:ARG:CD	0.42	2.45	20	1
1:C:344:LEU:HD22	1:D:340:MET:HE1	0.42	1.92	1	1
1:C:337:ARG:NE	1:D:348:LEU:HD23	0.41	2.30	13	1
1:A:330:LEU:HD11	1:B:338:PHE:CD2	0.41	2.50	15	1
1:B:344:LEU:HD23	1:C:344:LEU:HD11	0.41	1.92	16	1
1:A:348:LEU:HD22	1:B:337:ARG:NE	0.41	2.30	23	1
1:A:351:LYS:NZ	1:D:347:ALA:HB2	0.41	2.29	11	1
1:A:337:ARG:CD	1:A:341:PHE:CZ	0.41	3.03	1	1
1:C:338:PHE:CE2	1:D:330:LEU:CD1	0.41	3.03	19	1
1:A:344:LEU:HD22	1:B:341:PHE:HE1	0.41	1.73	22	1
1:A:345:ASN:ND2	1:B:332:ILE:HG23	0.41	2.30	1	1
1:C:348:LEU:HD22	1:D:337:ARG:HD3	0.41	1.92	28	1
1:A:341:PHE:CD2	1:B:341:PHE:CD2	0.41	3.09	21	1
1:B:332:ILE:HG21	1:B:338:PHE:HB2	0.41	1.92	11	1
1:A:344:LEU:HD11	1:D:344:LEU:CG	0.41	2.45	13	1
1:B:337:ARG:HG3	1:B:341:PHE:CE1	0.41	2.50	15	1
1:B:330:LEU:HD23	1:B:331:GLY:H	0.41	1.76	3	1
1:A:345:ASN:OD1	1:B:341:PHE:CE1	0.41	2.74	24	1
1:A:345:ASN:OD1	1:B:341:PHE:CE2	0.41	2.74	25	1
1:A:338:PHE:CE2	1:A:342:ARG:HG3	0.41	2.51	28	1
1:D:330:LEU:HG	1:D:332:ILE:HD11	0.41	1.93	28	1
1:A:337:ARG:HG3	1:A:341:PHE:CE1	0.41	2.51	11	1
1:D:338:PHE:O	1:D:338:PHE:CD1	0.41	2.74	3	1
1:A:332:ILE:HD13	1:A:338:PHE:HD2	0.41	1.75	19	1
1:A:337:ARG:CD	1:B:348:LEU:HD13	0.41	2.46	22	1
1:C:345:ASN:HD21	1:D:332:ILE:HG23	0.40	1.75	29	1
1:A:341:PHE:CE1	1:B:345:ASN:OD1	0.40	2.75	4	1

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:330:LEU:HD23	1:D:338:PHE:CZ	0.40	2.50	20	1
1:B:332:ILE:H	1:B:332:ILE:HD12	0.40	1.77	23	1
1:A:337:ARG:NE	1:B:348:LEU:HD23	0.40	2.31	26	1
1:B:330:LEU:HD12	1:B:332:ILE:HD11	0.40	1.94	15	1
1:B:338:PHE:CD1	1:B:338:PHE:O	0.40	2.74	11	1
1:A:345:ASN:OD1	1:B:341:PHE:CZ	0.40	2.74	24	1
1:B:340:MET:HG2	1:B:341:PHE:CD2	0.40	2.52	11	1
1:C:332:ILE:HD13	1:C:338:PHE:CD1	0.40	2.52	7	1
1:D:332:ILE:CG2	1:D:337:ARG:CD	0.40	3.00	13	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	28/31 (90%)	26±1 (93±4%)	2±1 (6±4%)	0±0 (1±1%)	29	74
1	B	28/31 (90%)	26±1 (94±3%)	1±1 (4±3%)	0±0 (1±2%)	14	59
1	C	28/31 (90%)	26±1 (94±3%)	1±1 (5±3%)	0±0 (1±2%)	15	61
1	D	28/31 (90%)	26±1 (94±4%)	1±1 (5±4%)	0±0 (1±2%)	14	59
All	All	3248/3596 (90%)	3044 (94%)	164 (5%)	40 (1%)	17	64

All 4 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	D	327	SER	12
1	B	327	SER	12
1	C	327	SER	11
1	A	327	SER	5

### 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	23/24 (96%)	19±2 (81±8%)	4±2 (19±8%)	4	36
1	B	23/24 (96%)	19±2 (82±8%)	4±2 (18±8%)	4	38
1	C	23/24 (96%)	19±2 (83±9%)	4±2 (17±9%)	5	39
1	D	23/24 (96%)	18±2 (80±8%)	5±2 (20±8%)	4	34
All	All	2668/2784 (96%)	2176 (82%)	492 (18%)	4	37

All 75 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	344	LEU	15
1	D	333	ARG	15
1	D	344	LEU	14
1	C	330	LEU	14
1	D	330	LEU	14
1	B	330	LEU	13
1	B	344	LEU	13
1	C	344	LEU	12
1	C	337	ARG	12
1	A	335	ARG	11
1	A	337	ARG	10
1	A	330	LEU	10
1	D	337	ARG	9
1	D	335	ARG	9
1	D	351	LYS	9
1	A	350	LEU	9
1	A	333	ARG	9
1	B	349	GLU	9
1	B	351	LYS	8
1	A	351	LYS	8
1	B	348	LEU	8
1	C	350	LEU	7
1	B	342	ARG	7
1	D	342	ARG	7
1	D	354	GLN	7
1	C	327	SER	7
1	B	350	LEU	7
1	C	343	GLU	7
1	A	348	LEU	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	A	327	SER	7
1	B	346	GLU	7
1	B	352	ASP	7
1	C	354	GLN	6
1	D	340	MET	6
1	C	333	ARG	6
1	A	336	GLU	6
1	C	348	LEU	6
1	D	343	GLU	6
1	B	335	ARG	6
1	B	333	ARG	6
1	A	352	ASP	6
1	A	342	ARG	6
1	C	351	LYS	6
1	D	352	ASP	5
1	C	342	ARG	5
1	D	336	GLU	5
1	C	352	ASP	5
1	A	354	GLN	5
1	D	346	GLU	5
1	C	340	MET	5
1	D	345	ASN	5
1	D	350	LEU	5
1	D	349	GLU	5
1	B	337	ARG	5
1	C	339	GLU	5
1	B	340	MET	4
1	A	340	MET	4
1	B	336	GLU	4
1	A	343	GLU	4
1	A	345	ASN	4
1	B	343	GLU	4
1	B	354	GLN	4
1	A	339	GLU	3
1	D	327	SER	3
1	C	335	ARG	3
1	B	339	GLU	3
1	D	339	GLU	3
1	B	345	ASN	3
1	C	336	GLU	3
1	C	349	GLU	2
1	C	346	GLU	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Models (Total)
1	C	345	ASN	2
1	B	327	SER	1
1	D	348	LEU	1
1	A	346	GLU	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 [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided