



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 09:32 PM BST

PDB ID : 2J10
Title : P53 TETRAMERIZATION DOMAIN MUTANT T329F Q331K
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
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

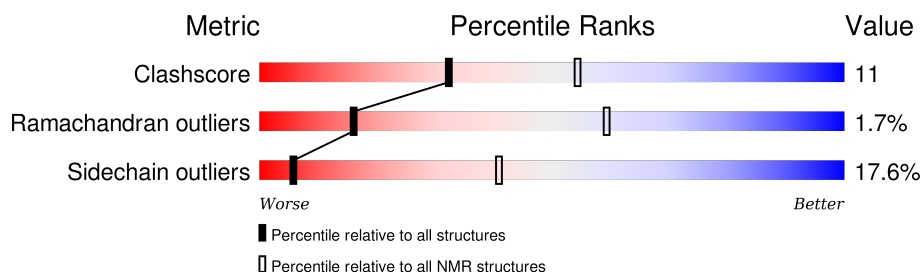
1 Overall quality at a glance

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	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	31	<div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	B	31	<div> <div>77%</div> <div>23%</div> </div>
1	C	31	<div> <div>81%</div> <div>19%</div> </div>
1	D	31	<div> <div>77%</div> <div>19%</div> <div>.</div> </div>

2 Ensemble composition and analysis

This entry contains 30 models. Model 20 is the overall representative, medoid model (most similar to other models). The authors have identified model 5 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:356, B:326-B:356, C:326-C:356, D:326-D:356 (123)	0.58	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 7 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 4, 5, 6, 9, 10, 25
2	12, 13, 24, 27, 28
3	7, 15, 17, 20, 29
4	21, 30
5	19, 23
6	11, 26
7	3, 22
Single-model clusters	2; 8; 14; 16; 18

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2132 atoms, of which 1056 are hydrogens and 0 are deuteriums.

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

Mol	Chain	Residues	Atoms						Trace
1	A	31	Total	C	H	N	O	S	0
			533	172	264	47	49	1	
1	B	31	Total	C	H	N	O	S	0
			533	172	264	47	49	1	
1	C	31	Total	C	H	N	O	S	0
			533	172	264	47	49	1	
1	D	31	Total	C	H	N	O	S	0
			533	172	264	47	49	1	

There are 8 discrepancies between the modelled and reference sequences:

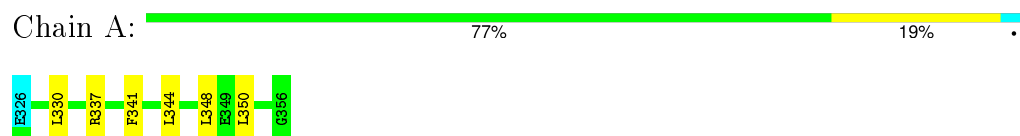
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	PHE	THR	ENGINEERED MUTATION	UNP P04637
A	331	LYS	GLN	ENGINEERED MUTATION	UNP P04637
B	329	PHE	THR	ENGINEERED MUTATION	UNP P04637
B	331	LYS	GLN	ENGINEERED MUTATION	UNP P04637
C	329	PHE	THR	ENGINEERED MUTATION	UNP P04637
C	331	LYS	GLN	ENGINEERED MUTATION	UNP P04637
D	329	PHE	THR	ENGINEERED MUTATION	UNP P04637
D	331	LYS	GLN	ENGINEERED MUTATION	UNP P04637

4 Residue-property plots

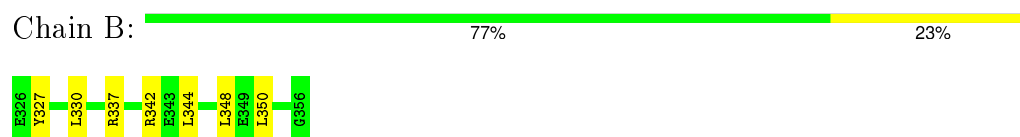
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

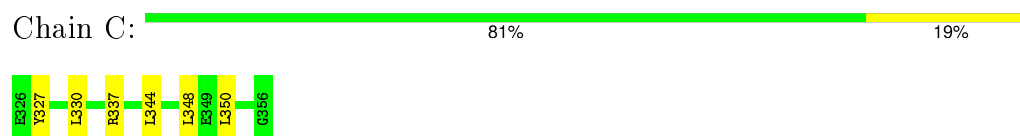
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



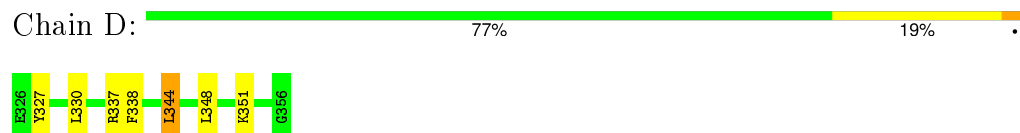
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- 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

Chain A:  68% 23% 6% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  52% 45% .



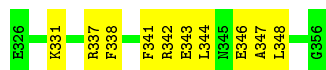
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  58% 39% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  68% 32% .



4.2.2 Score per residue for model 2

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  58% 39% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  71% 26% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  65% 32% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



4.2.3 Score per residue for model 3

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



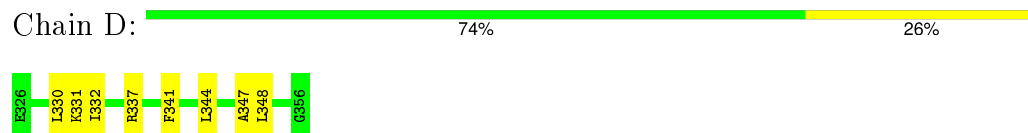
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

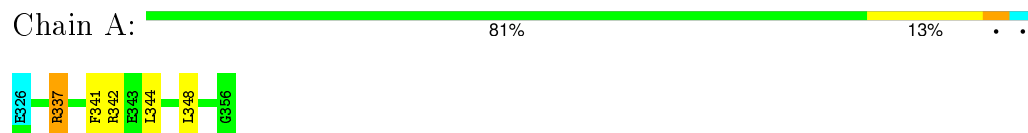


- Molecule 1: CELLULAR TUMOR ANTIGEN P53

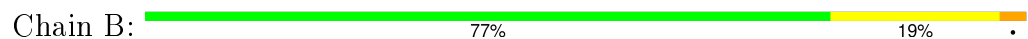


4.2.4 Score per residue for model 4

- 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

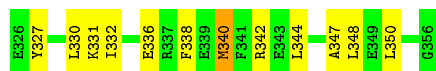
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

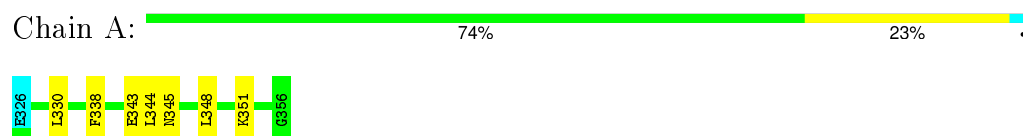


- Molecule 1: CELLULAR TUMOR ANTIGEN P53

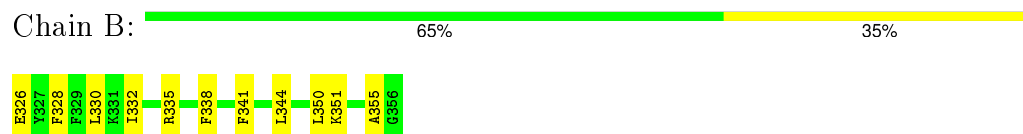


4.2.6 Score per residue for model 6

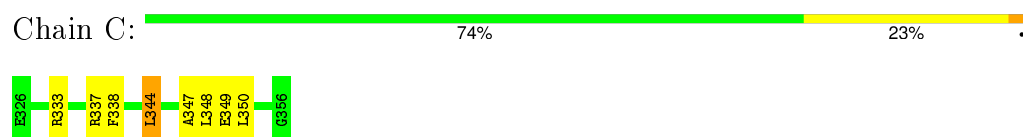
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



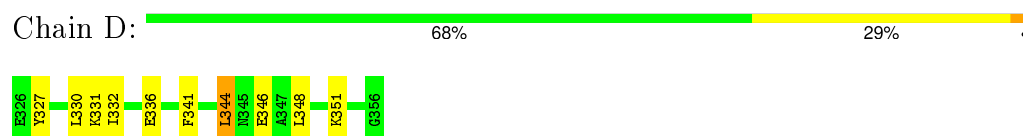
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

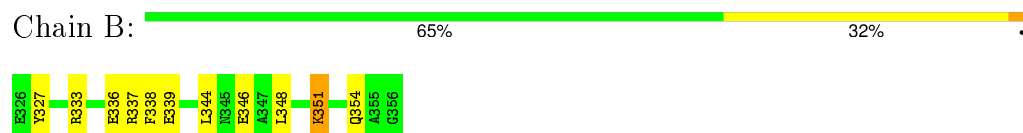


4.2.7 Score per residue for model 7

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

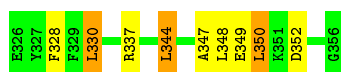


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- Molecule 1: CELLULAR TUMOR ANTIGEN P53

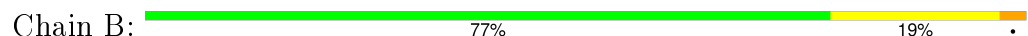


4.2.8 Score per residue for model 8

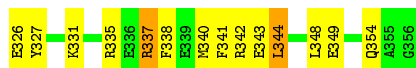
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



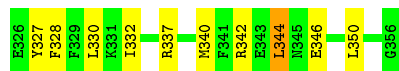
4.2.9 Score per residue for model 9

- Molecule 1: CELLULAR TUMOR ANTIGEN P53




- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  68% 29% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  77% 23%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

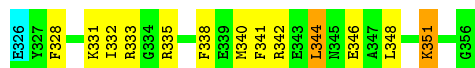
Chain D:  68% 29% .



4.2.10 Score per residue for model 10

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  55% 35% 6% .




- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  74% 23% .



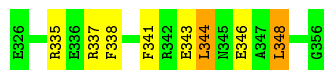
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  81% 13% 6%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  74% 19% 6%

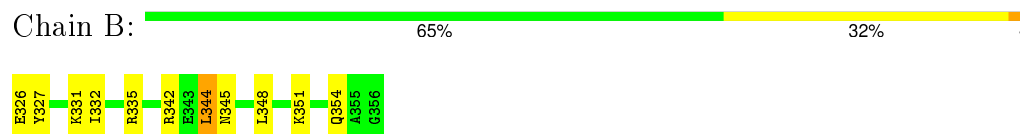


4.2.11 Score per residue for model 11

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



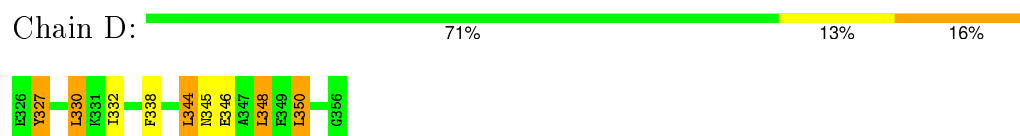
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

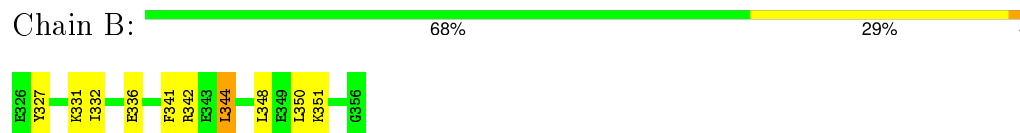


4.2.12 Score per residue for model 12

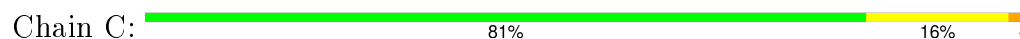
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- Molecule 1: CELLULAR TUMOR ANTIGEN P53

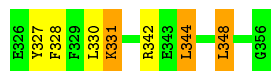


4.2.13 Score per residue for model 13

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53



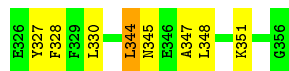
4.2.14 Score per residue for model 14

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



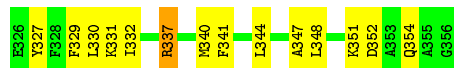
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  74% 23% .




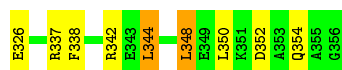
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  55% 42% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  71% 23% 6% .



4.2.15 Score per residue for model 15

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  65% 29% . .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  65% 32% .




- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  71% 23% 6% .



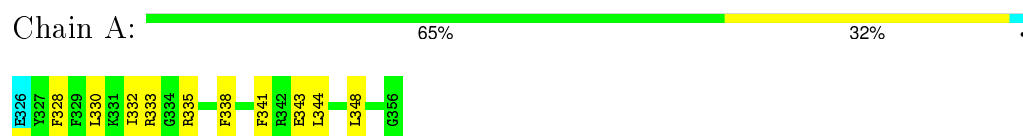
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  77% 16% 6% .

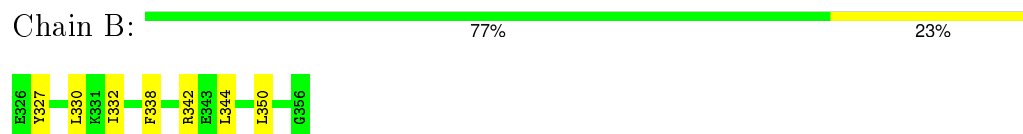


4.2.16 Score per residue for model 16

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



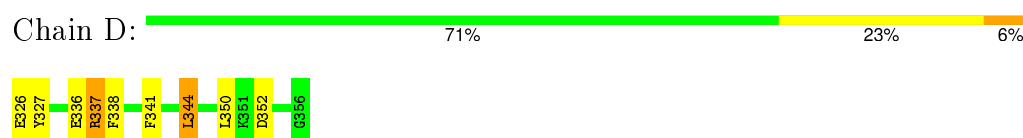
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

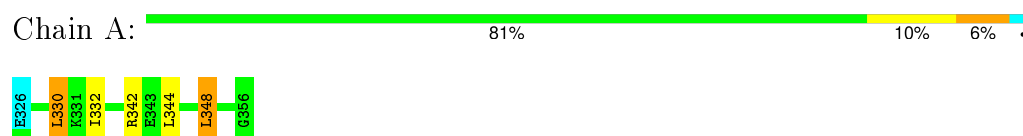


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



4.2.17 Score per residue for model 17

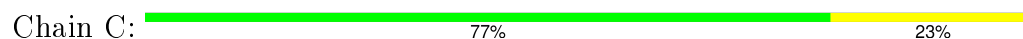
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

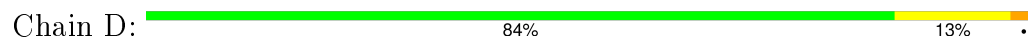


- Molecule 1: CELLULAR TUMOR ANTIGEN P53





- 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



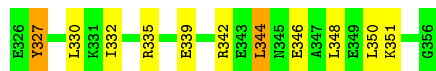
4.2.19 Score per residue for model 19

- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  65% 29% 6%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  55% 39% 6%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  68% 29% 3%



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  68% 19% 10% 3%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  68% 26% 6%




- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  71% 23% 6%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  77% 19% 4%



4.2.21 Score per residue for model 21

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  58% 26% 13% .



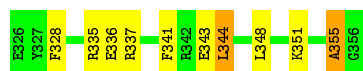
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  68% 29% .




- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  68% 26% 6%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  81% 16% .




4.2.22 Score per residue for model 22

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  61% 35% .



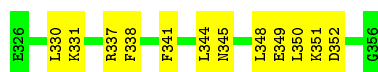
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  81% 19%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  61% 39%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D: 71% 23% 6%



4.2.23 Score per residue for model 23

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A: 55% 39% . .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B: 84% 13% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C: 61% 29% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D: 68% 29% .




4.2.24 Score per residue for model 24

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A: 71% 19% 6% .




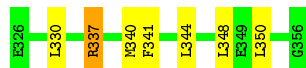
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  77% 19%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  77% 19%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  52% 42% 6%



4.2.25 Score per residue for model 25

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  68% 26%



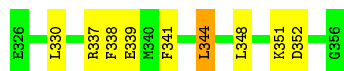
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  65% 32%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  71% 26%



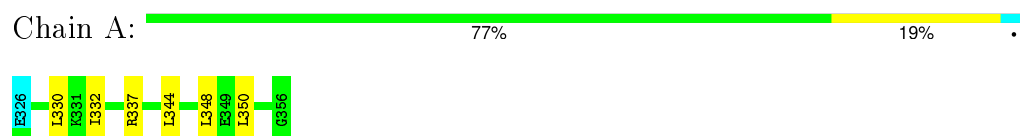
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  45% 52%

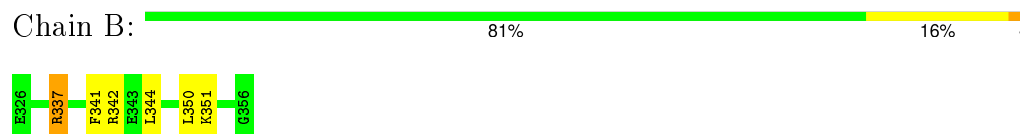


4.2.26 Score per residue for model 26

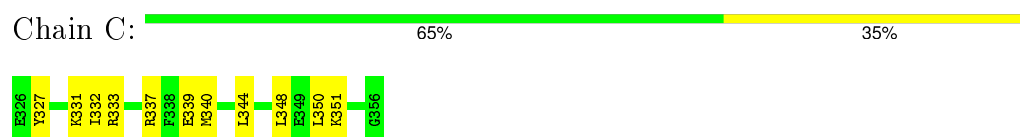
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



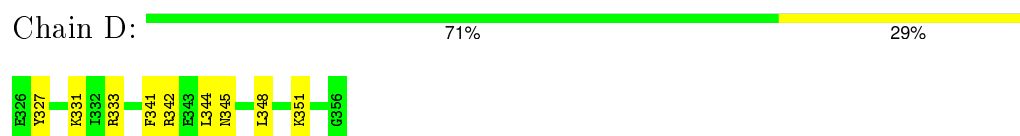
- Molecule 1: CELLULAR TUMOR ANTIGEN P53



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

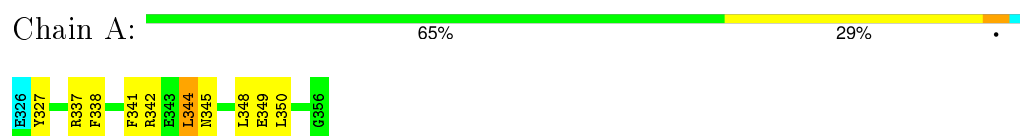


- Molecule 1: CELLULAR TUMOR ANTIGEN P53



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

Chain D: 81% 16%



4.2.28 Score per residue for model 28

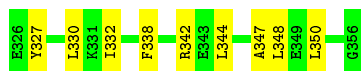
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A: 68% 19% 10%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B: 71% 29%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C: 74% 26%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D: 84% 13%



4.2.29 Score per residue for model 29

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A: 65% 19% 13%



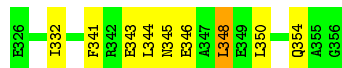
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  65% 35%



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  71% 26% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

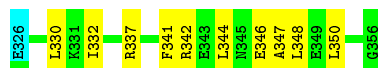
Chain D:  52% 39% 10%




4.2.30 Score per residue for model 30

- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain A:  65% 32% .



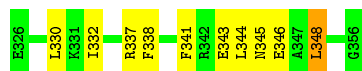
- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain B:  84% 13% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain C:  68% 29% .



- Molecule 1: CELLULAR TUMOR ANTIGEN P53

Chain D:  65% 29% 6%



5 Refinement protocol and experimental data overview

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

Of the 30 calculated structures, 30 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

6.1 Standard geometry

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

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	260	256	256	9±3
1	B	269	264	261	9±2
1	C	269	264	261	10±3
1	D	269	264	261	10±3
All	All	32010	31440	31170	709

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:330:LEU:HD23	1:D:332:ILE:HD11	0.94	1.35	29	6
1:B:344:LEU:HD22	1:C:344:LEU:HD11	0.91	1.41	7	2
1:B:344:LEU:HD22	1:C:344:LEU:HD22	0.89	1.44	28	3
1:A:344:LEU:HD22	1:D:344:LEU:HD21	0.85	1.44	16	1
1:A:344:LEU:HD11	1:D:344:LEU:HD21	0.85	1.48	5	5
1:A:330:LEU:HD23	1:A:332:ILE:HD11	0.83	1.50	30	9
1:C:330:LEU:HD23	1:C:332:ILE:HD11	0.81	1.51	5	6
1:A:344:LEU:HD22	1:D:344:LEU:HD11	0.81	1.49	6	3
1:A:344:LEU:HD11	1:D:344:LEU:HD23	0.81	1.53	23	1
1:D:330:LEU:CD1	1:D:332:ILE:HD11	0.80	2.06	11	2
1:C:338:PHE:CE1	1:D:330:LEU:HD13	0.80	2.12	19	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:330:LEU:HD12	1:D:332:ILE:HD11	0.79	1.51	11	1
1:C:338:PHE:CE2	1:D:330:LEU:HD22	0.79	2.13	13	2
1:C:330:LEU:HD13	1:D:338:PHE:CE1	0.78	2.12	13	9
1:A:330:LEU:HD13	1:B:338:PHE:CE1	0.78	2.12	16	6
1:A:330:LEU:HD12	1:B:338:PHE:CE1	0.76	2.15	15	1
1:B:344:LEU:HD11	1:C:344:LEU:HD21	0.76	1.56	12	7
1:C:330:LEU:HD21	1:C:332:ILE:HD11	0.75	1.56	30	1
1:A:330:LEU:HD22	1:B:338:PHE:CE1	0.75	2.16	17	2
1:C:344:LEU:O	1:C:348:LEU:HD13	0.74	1.82	28	2
1:A:344:LEU:HD11	1:D:344:LEU:CD2	0.74	2.12	18	2
1:C:348:LEU:HD22	1:D:337:ARG:NE	0.74	1.97	18	1
1:A:338:PHE:CE2	1:B:330:LEU:HD13	0.74	2.17	19	5
1:A:337:ARG:CG	1:B:348:LEU:HD13	0.73	2.13	27	5
1:B:344:LEU:O	1:B:348:LEU:HD23	0.72	1.84	20	9
1:A:344:LEU:O	1:A:348:LEU:HD23	0.72	1.85	22	11
1:A:338:PHE:CE1	1:B:330:LEU:HD13	0.72	2.20	14	3
1:A:344:LEU:HD21	1:D:344:LEU:HD11	0.71	1.62	10	8
1:C:348:LEU:HD22	1:D:337:ARG:HG2	0.71	1.62	14	2
1:C:344:LEU:O	1:C:348:LEU:HD23	0.71	1.84	5	7
1:A:337:ARG:HG2	1:B:348:LEU:HD13	0.71	1.61	13	4
1:D:344:LEU:O	1:D:348:LEU:HD23	0.71	1.86	27	4
1:C:337:ARG:CG	1:D:348:LEU:HD13	0.71	2.16	21	9
1:B:344:LEU:O	1:B:348:LEU:HD13	0.71	1.85	18	1
1:D:330:LEU:CD2	1:D:332:ILE:HD11	0.70	2.15	4	3
1:A:345:ASN:OD1	1:B:332:ILE:HG23	0.70	1.85	6	2
1:D:344:LEU:O	1:D:348:LEU:HD12	0.69	1.87	10	16
1:A:344:LEU:O	1:A:348:LEU:HD13	0.69	1.86	2	1
1:C:344:LEU:O	1:C:348:LEU:HD12	0.69	1.87	30	7
1:A:346:GLU:O	1:A:350:LEU:HD23	0.69	1.87	12	4
1:A:348:LEU:HD13	1:B:337:ARG:HG3	0.69	1.62	18	6
1:B:344:LEU:CD1	1:C:344:LEU:HD21	0.69	2.17	19	2
1:A:344:LEU:HD21	1:D:344:LEU:HD21	0.69	1.65	11	15
1:B:348:LEU:HD21	1:C:343:GLU:OE1	0.69	1.88	8	1
1:A:344:LEU:O	1:A:348:LEU:HD12	0.69	1.87	17	10
1:B:344:LEU:HD21	1:C:344:LEU:HD21	0.68	1.65	9	9
1:A:348:LEU:HD13	1:B:337:ARG:CG	0.68	2.19	15	6
1:A:344:LEU:CG	1:D:344:LEU:HD21	0.68	2.18	25	7
1:A:332:ILE:HG23	1:B:345:ASN:OD1	0.68	1.87	2	2
1:C:348:LEU:HD13	1:D:337:ARG:HG3	0.68	1.66	23	4
1:B:344:LEU:O	1:B:348:LEU:HD12	0.68	1.88	13	10
1:B:344:LEU:CD2	1:C:344:LEU:HD11	0.68	2.17	20	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:330:LEU:HD23	1:B:332:ILE:HD11	0.67	1.66	6	6
1:A:344:LEU:CD2	1:D:344:LEU:HD21	0.67	2.19	16	11
1:A:348:LEU:HD13	1:B:337:ARG:NE	0.67	2.04	25	2
1:C:345:ASN:OD1	1:D:332:ILE:HG23	0.67	1.90	30	4
1:C:348:LEU:HD22	1:D:337:ARG:CD	0.67	2.19	18	2
1:A:344:LEU:CD2	1:D:344:LEU:HD11	0.67	2.20	6	6
1:A:344:LEU:HD21	1:D:344:LEU:CD2	0.67	2.20	20	7
1:D:348:LEU:HD23	1:D:351:LYS:HE3	0.66	1.65	22	1
1:C:348:LEU:HD13	1:D:337:ARG:CG	0.66	2.21	1	6
1:C:346:GLU:O	1:C:350:LEU:HD23	0.66	1.91	3	2
1:C:337:ARG:HD3	1:D:348:LEU:HD13	0.66	1.68	4	3
1:C:337:ARG:HD2	1:D:348:LEU:HD13	0.65	1.67	12	3
1:A:340:MET:O	1:A:344:LEU:HD12	0.65	1.91	10	4
1:B:344:LEU:HD22	1:C:344:LEU:HD21	0.65	1.67	6	1
1:A:337:ARG:HD3	1:B:348:LEU:HD13	0.65	1.68	1	4
1:C:337:ARG:HG2	1:D:348:LEU:HD22	0.65	1.67	26	2
1:C:337:ARG:HG3	1:D:348:LEU:HD13	0.64	1.69	14	7
1:B:350:LEU:HD12	1:B:351:LYS:N	0.64	2.07	17	2
1:A:344:LEU:HG	1:D:344:LEU:HD21	0.64	1.70	10	5
1:C:330:LEU:HD13	1:D:338:PHE:CZ	0.63	2.29	13	4
1:A:354:GLN:OE1	1:A:355:ALA:HB2	0.62	1.94	9	1
1:C:332:ILE:HG21	1:C:338:PHE:N	0.62	2.10	18	1
1:B:346:GLU:O	1:B:350:LEU:HD23	0.62	1.95	9	2
1:A:348:LEU:HD13	1:B:337:ARG:CZ	0.62	2.25	25	1
1:B:344:LEU:HD21	1:C:344:LEU:CD2	0.62	2.24	9	4
1:C:330:LEU:HD23	1:C:331:LYS:N	0.61	2.10	22	1
1:B:344:LEU:HD21	1:C:344:LEU:HG	0.61	1.71	3	4
1:C:337:ARG:CZ	1:D:348:LEU:HD13	0.61	2.24	26	1
1:A:348:LEU:HD13	1:A:351:LYS:HD2	0.61	1.71	6	1
1:A:338:PHE:CD1	1:B:330:LEU:HD12	0.61	2.31	10	2
1:C:348:LEU:HD13	1:D:337:ARG:HD2	0.61	1.71	13	1
1:B:344:LEU:CD2	1:C:344:LEU:HD21	0.61	2.25	6	7
1:A:344:LEU:HD21	1:D:344:LEU:CG	0.61	2.24	28	6
1:B:344:LEU:HG	1:C:344:LEU:HD21	0.60	1.71	25	4
1:B:354:GLN:OE1	1:C:350:LEU:HD21	0.60	1.96	7	1
1:A:330:LEU:HD12	1:B:338:PHE:CE2	0.60	2.32	21	1
1:B:344:LEU:CD2	1:C:344:LEU:HD22	0.60	2.25	10	4
1:A:341:PHE:HA	1:A:344:LEU:HD12	0.60	1.73	16	1
1:B:344:LEU:HD21	1:C:344:LEU:HD11	0.60	1.74	18	7
1:A:330:LEU:CD2	1:A:332:ILE:HD11	0.60	2.24	26	3
1:C:332:ILE:HG21	1:C:338:PHE:CA	0.59	2.27	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:330:LEU:HD12	1:A:332:ILE:HD11	0.59	1.73	29	1
1:A:330:LEU:HD13	1:B:338:PHE:CE2	0.59	2.32	8	3
1:B:344:LEU:HD11	1:C:344:LEU:HD11	0.58	1.74	3	1
1:C:330:LEU:HD12	1:D:338:PHE:CE1	0.58	2.33	18	2
1:C:330:LEU:O	1:C:332:ILE:HD12	0.58	1.98	13	2
1:C:337:ARG:CG	1:D:348:LEU:HD22	0.58	2.29	26	1
1:A:348:LEU:HD13	1:B:337:ARG:HG2	0.58	1.75	10	2
1:B:347:ALA:HB1	1:C:347:ALA:HB1	0.58	1.76	28	6
1:D:348:LEU:HD13	1:D:351:LYS:HD3	0.58	1.74	5	1
1:C:332:ILE:HD12	1:C:341:PHE:CE2	0.58	2.33	1	2
1:B:344:LEU:HD11	1:C:344:LEU:CG	0.58	2.29	26	1
1:B:344:LEU:HD21	1:C:344:LEU:CG	0.58	2.28	30	4
1:C:346:GLU:O	1:C:350:LEU:HD12	0.58	1.98	4	2
1:A:346:GLU:O	1:A:350:LEU:HD12	0.57	1.99	15	4
1:C:338:PHE:CE2	1:D:330:LEU:HD13	0.57	2.34	2	3
1:D:330:LEU:HD23	1:D:332:ILE:CD1	0.57	2.27	8	2
1:A:348:LEU:HD22	1:B:337:ARG:HG2	0.57	1.75	8	1
1:A:345:ASN:ND2	1:B:332:ILE:HG23	0.57	2.15	11	2
1:A:330:LEU:HD13	1:B:338:PHE:CZ	0.57	2.34	22	3
1:B:344:LEU:HD22	1:C:344:LEU:CD2	0.57	2.25	10	3
1:C:337:ARG:NE	1:D:348:LEU:HD13	0.57	2.14	2	3
1:B:344:LEU:CG	1:C:344:LEU:HD21	0.57	2.29	1	4
1:A:348:LEU:HD13	1:B:337:ARG:HD2	0.57	1.75	17	1
1:A:330:LEU:O	1:A:332:ILE:HD12	0.56	2.00	11	1
1:B:330:LEU:O	1:B:332:ILE:HD12	0.56	2.00	19	1
1:A:344:LEU:HD11	1:D:344:LEU:HD22	0.56	1.76	18	1
1:A:330:LEU:N	1:A:330:LEU:HD23	0.56	2.16	29	2
1:C:337:ARG:CD	1:D:348:LEU:HD13	0.56	2.31	8	7
1:C:348:LEU:HD13	1:D:337:ARG:NE	0.56	2.15	14	2
1:B:332:ILE:HD13	1:B:341:PHE:CD1	0.56	2.35	6	1
1:B:340:MET:O	1:B:344:LEU:HD12	0.56	2.00	5	3
1:C:348:LEU:HD13	1:D:337:ARG:CD	0.56	2.31	13	1
1:A:344:LEU:HD21	1:D:344:LEU:HG	0.55	1.77	20	5
1:C:332:ILE:HG23	1:D:345:ASN:OD1	0.55	2.02	26	2
1:A:332:ILE:HD13	1:A:341:PHE:CE1	0.55	2.37	30	1
1:A:330:LEU:HD23	1:A:331:LYS:N	0.55	2.17	21	1
1:B:344:LEU:HD21	1:C:344:LEU:CD1	0.55	2.31	14	2
1:C:338:PHE:CD2	1:D:330:LEU:HD22	0.54	2.36	13	2
1:B:344:LEU:HD11	1:C:344:LEU:CD2	0.54	2.32	26	1
1:D:332:ILE:HD12	1:D:332:ILE:N	0.54	2.18	25	2
1:A:338:PHE:CE2	1:B:330:LEU:HD22	0.54	2.37	25	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:344:LEU:HD11	1:D:344:LEU:CG	0.54	2.32	29	1
1:C:330:LEU:HD13	1:D:338:PHE:CE2	0.54	2.37	10	3
1:D:346:GLU:O	1:D:350:LEU:HD12	0.54	2.02	11	2
1:B:344:LEU:HD23	1:C:344:LEU:HD11	0.54	1.78	20	2
1:C:347:ALA:HA	1:C:350:LEU:HD23	0.54	1.79	6	1
1:B:351:LYS:HE3	1:C:347:ALA:HB2	0.54	1.79	11	1
1:C:340:MET:O	1:C:344:LEU:HD12	0.54	2.03	14	5
1:A:344:LEU:HD22	1:D:344:LEU:CD2	0.54	2.33	7	2
1:A:340:MET:CE	1:B:344:LEU:HD22	0.53	2.33	3	1
1:C:338:PHE:CE2	1:D:330:LEU:HD12	0.53	2.38	5	1
1:D:348:LEU:HD23	1:D:351:LYS:CE	0.53	2.34	22	1
1:C:330:LEU:HD22	1:D:338:PHE:CD2	0.53	2.39	7	1
1:C:338:PHE:CZ	1:D:330:LEU:HD13	0.53	2.38	6	5
1:D:341:PHE:HA	1:D:344:LEU:HD12	0.53	1.79	7	1
1:C:337:ARG:HG2	1:D:348:LEU:HD13	0.52	1.81	6	2
1:D:351:LYS:O	1:D:355:ALA:HB3	0.52	2.05	25	2
1:B:344:LEU:HD21	1:C:344:LEU:HD23	0.52	1.81	24	1
1:C:351:LYS:O	1:C:355:ALA:HB3	0.52	2.05	21	1
1:A:344:LEU:HD11	1:D:344:LEU:HG	0.52	1.82	29	1
1:D:348:LEU:HD23	1:D:351:LYS:HD3	0.51	1.81	8	2
1:A:338:PHE:CE1	1:B:330:LEU:HD12	0.51	2.40	10	2
1:A:348:LEU:HD23	1:A:351:LYS:NZ	0.51	2.21	25	2
1:A:330:LEU:HD23	1:A:332:ILE:CD1	0.51	2.32	30	1
1:B:331:LYS:C	1:B:332:ILE:HD12	0.51	2.27	29	1
1:A:350:LEU:C	1:A:350:LEU:HD12	0.50	2.26	27	1
1:A:344:LEU:HD21	1:D:344:LEU:HD23	0.50	1.82	30	2
1:A:337:ARG:HG3	1:B:348:LEU:HD13	0.50	1.83	12	2
1:B:332:ILE:N	1:B:332:ILE:HD12	0.50	2.22	29	1
1:A:337:ARG:HG3	1:B:348:LEU:HD22	0.50	1.82	14	1
1:D:332:ILE:HD12	1:D:341:PHE:CE2	0.50	2.42	6	1
1:C:328:PHE:CE2	1:D:338:PHE:CD2	0.49	2.99	7	1
1:C:348:LEU:HD13	1:D:337:ARG:HB3	0.49	1.83	8	1
1:B:332:ILE:HD13	1:B:341:PHE:CE1	0.49	2.43	6	1
1:A:341:PHE:CD1	1:B:341:PHE:CD1	0.49	3.00	2	2
1:A:348:LEU:HD23	1:B:337:ARG:CG	0.49	2.37	2	1
1:C:348:LEU:HD13	1:D:337:ARG:HG2	0.49	1.84	16	1
1:A:332:ILE:HD13	1:A:341:PHE:CD1	0.49	2.42	30	1
1:B:330:LEU:HG	1:B:332:ILE:HD11	0.49	1.83	18	1
1:C:330:LEU:HD21	1:D:342:ARG:HA	0.49	1.85	19	1
1:A:347:ALA:HB2	1:D:351:LYS:HE3	0.49	1.85	9	2
1:D:330:LEU:HD12	1:D:332:ILE:CD1	0.48	2.31	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:350:LEU:HD12	1:C:351:LYS:N	0.48	2.24	1	1
1:A:337:ARG:CZ	1:B:348:LEU:HD13	0.48	2.39	14	1
1:C:330:LEU:CD2	1:C:332:ILE:HD11	0.48	2.38	27	3
1:D:332:ILE:HG21	1:D:337:ARG:HG3	0.48	1.85	12	1
1:C:341:PHE:CD1	1:D:341:PHE:CD1	0.48	3.02	1	2
1:A:341:PHE:CD2	1:B:341:PHE:CD1	0.48	3.01	25	1
1:B:351:LYS:CE	1:C:347:ALA:HB2	0.48	2.39	11	2
1:C:348:LEU:HD12	1:C:349:GLU:N	0.48	2.24	18	1
1:A:337:ARG:CD	1:B:348:LEU:HD13	0.48	2.38	21	1
1:D:348:LEU:HD13	1:D:351:LYS:NZ	0.47	2.24	7	1
1:B:350:LEU:HD12	1:B:350:LEU:C	0.47	2.30	2	1
1:C:348:LEU:C	1:C:348:LEU:HD12	0.47	2.30	18	1
1:A:344:LEU:HD21	1:D:344:LEU:HD22	0.47	1.87	18	1
1:C:330:LEU:HD12	1:D:338:PHE:CE2	0.47	2.43	28	1
1:A:348:LEU:HD13	1:B:337:ARG:CD	0.47	2.39	17	1
1:B:350:LEU:C	1:B:350:LEU:HD12	0.47	2.30	17	1
1:A:337:ARG:HD2	1:B:348:LEU:HD12	0.47	1.86	19	1
1:C:330:LEU:HD12	1:D:338:PHE:CD1	0.47	2.45	18	1
1:B:332:ILE:HD12	1:B:332:ILE:N	0.47	2.25	25	1
1:A:344:LEU:CD2	1:D:344:LEU:HD22	0.47	2.40	19	1
1:C:332:ILE:N	1:C:332:ILE:HD12	0.47	2.24	18	1
1:A:330:LEU:HD21	1:B:345:ASN:ND2	0.47	2.25	1	1
1:C:348:LEU:HD22	1:D:337:ARG:HD2	0.47	1.85	9	1
1:A:341:PHE:CD2	1:B:341:PHE:CD2	0.47	3.03	21	2
1:D:348:LEU:HD13	1:D:351:LYS:HD2	0.47	1.86	27	1
1:C:350:LEU:HD12	1:C:350:LEU:C	0.46	2.29	1	1
1:C:341:PHE:CD1	1:D:341:PHE:CD2	0.46	3.03	25	3
1:C:337:ARG:HD3	1:D:348:LEU:HD12	0.46	1.88	13	1
1:A:337:ARG:NH2	1:B:348:LEU:HD13	0.46	2.26	14	1
1:C:328:PHE:N	1:C:328:PHE:CD1	0.46	2.83	7	2
1:A:340:MET:HE1	1:B:344:LEU:HD22	0.46	1.88	3	1
1:A:344:LEU:CD1	1:D:344:LEU:HD21	0.46	2.41	20	1
1:C:341:PHE:CD2	1:C:341:PHE:N	0.46	2.83	22	5
1:B:330:LEU:CD2	1:B:332:ILE:HD11	0.46	2.40	18	1
1:B:330:LEU:HD22	1:B:332:ILE:CG1	0.45	2.41	16	1
1:D:337:ARG:HG3	1:D:341:PHE:CE2	0.45	2.46	15	1
1:A:341:PHE:N	1:A:341:PHE:CD2	0.45	2.84	27	3
1:B:344:LEU:HD11	1:C:344:LEU:HG	0.45	1.87	26	1
1:C:341:PHE:CD2	1:D:341:PHE:CD1	0.45	3.04	23	1
1:B:328:PHE:CD1	1:B:328:PHE:N	0.45	2.85	14	4
1:B:337:ARG:HB3	1:B:341:PHE:CE2	0.45	2.46	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:330:LEU:HD22	1:C:332:ILE:HG13	0.45	1.88	14	1
1:A:331:LYS:CG	1:B:329:PHE:CE2	0.45	3.00	3	1
1:B:328:PHE:N	1:B:328:PHE:CD1	0.45	2.85	3	1
1:B:328:PHE:N	1:B:328:PHE:CD2	0.45	2.85	9	2
1:A:328:PHE:N	1:A:328:PHE:CD1	0.44	2.85	23	2
1:C:329:PHE:CE1	1:D:331:LYS:CG	0.44	3.00	20	1
1:A:351:LYS:CE	1:D:347:ALA:HB2	0.44	2.42	3	1
1:D:348:LEU:HD23	1:D:351:LYS:HD2	0.44	1.86	24	1
1:B:351:LYS:NZ	1:C:347:ALA:HB2	0.44	2.27	7	1
1:A:337:ARG:CD	1:A:341:PHE:CZ	0.44	3.00	14	1
1:D:328:PHE:CD2	1:D:328:PHE:N	0.44	2.85	24	1
1:B:328:PHE:CD2	1:B:328:PHE:N	0.44	2.85	20	1
1:D:329:PHE:N	1:D:329:PHE:CD1	0.44	2.86	30	1
1:B:344:LEU:HD23	1:C:344:LEU:HD21	0.44	1.89	23	1
1:B:332:ILE:HG21	1:B:338:PHE:CA	0.44	2.43	5	1
1:C:344:LEU:HD12	1:C:348:LEU:CD1	0.44	2.42	6	1
1:C:328:PHE:CD1	1:C:328:PHE:N	0.44	2.85	10	1
1:C:332:ILE:HD12	1:C:341:PHE:CE1	0.44	2.47	29	1
1:B:346:GLU:O	1:B:350:LEU:HD12	0.44	2.13	20	1
1:A:329:PHE:CE1	1:B:331:LYS:CE	0.44	3.01	13	1
1:C:338:PHE:CE2	1:D:330:LEU:CD1	0.43	3.00	2	1
1:C:328:PHE:N	1:C:328:PHE:CD2	0.43	2.86	19	1
1:D:340:MET:O	1:D:344:LEU:HD12	0.43	2.13	28	1
1:C:332:ILE:HD12	1:C:332:ILE:N	0.43	2.28	3	1
1:A:341:PHE:CD2	1:A:341:PHE:N	0.43	2.82	11	1
1:C:332:ILE:HD13	1:C:338:PHE:HD1	0.43	1.73	18	1
1:B:330:LEU:HD22	1:B:332:ILE:HG13	0.43	1.91	3	1
1:C:330:LEU:HG	1:C:332:ILE:HD11	0.43	1.90	3	1
1:B:337:ARG:CB	1:B:341:PHE:CE2	0.43	3.02	1	1
1:B:344:LEU:HD12	1:B:348:LEU:CD1	0.43	2.44	23	1
1:A:332:ILE:HG23	1:A:337:ARG:HD2	0.43	1.89	7	1
1:D:328:PHE:CD1	1:D:328:PHE:N	0.43	2.86	5	1
1:C:338:PHE:O	1:C:342:ARG:N	0.43	2.51	2	1
1:C:330:LEU:HD13	1:D:338:PHE:HE2	0.43	1.72	2	1
1:A:332:ILE:HD12	1:B:345:ASN:HD21	0.43	1.74	10	1
1:A:331:LYS:CD	1:B:327:TYR:CD2	0.43	3.02	19	1
1:B:326:GLU:CB	1:B:328:PHE:CZ	0.43	3.02	17	1
1:A:347:ALA:HB2	1:D:351:LYS:CE	0.43	2.43	2	2
1:C:328:PHE:CD2	1:C:328:PHE:N	0.43	2.87	21	2
1:A:330:LEU:HD22	1:B:338:PHE:CD1	0.43	2.48	17	1
1:A:337:ARG:HG3	1:A:341:PHE:CE1	0.42	2.48	21	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:328:PHE:CD2	1:A:328:PHE:N	0.42	2.87	19	2
1:C:345:ASN:OD1	1:C:346:GLU:N	0.42	2.52	11	1
1:C:333:ARG:CG	1:D:327:TYR:CZ	0.42	3.02	20	1
1:C:344:LEU:HD22	1:D:340:MET:SD	0.42	2.55	15	1
1:A:332:ILE:HD12	1:A:332:ILE:N	0.42	2.30	23	2
1:B:337:ARG:HG3	1:B:341:PHE:CE1	0.42	2.50	26	2
1:B:345:ASN:OD1	1:B:346:GLU:N	0.42	2.53	29	1
1:A:351:LYS:NZ	1:D:347:ALA:HB2	0.42	2.29	29	1
1:A:348:LEU:HD23	1:B:337:ARG:HG3	0.42	1.90	2	1
1:B:337:ARG:HG3	1:B:341:PHE:CE2	0.42	2.49	27	1
1:A:337:ARG:HG2	1:A:341:PHE:CE1	0.42	2.49	23	1
1:A:328:PHE:CD1	1:A:328:PHE:N	0.42	2.88	3	1
1:A:337:ARG:HG3	1:A:341:PHE:CE2	0.42	2.49	4	1
1:D:341:PHE:N	1:D:341:PHE:CD2	0.42	2.86	26	1
1:C:332:ILE:HG23	1:D:345:ASN:ND2	0.42	2.29	13	1
1:B:348:LEU:HD23	1:B:351:LYS:NZ	0.42	2.30	25	1
1:D:328:PHE:N	1:D:328:PHE:CD2	0.42	2.87	2	3
1:C:337:ARG:HG3	1:C:341:PHE:CE1	0.42	2.50	18	1
1:C:341:PHE:CD2	1:D:341:PHE:CD2	0.41	3.08	29	4
1:B:337:ARG:O	1:B:341:PHE:CD2	0.41	2.73	1	1
1:A:341:PHE:CD1	1:B:341:PHE:CD2	0.41	3.08	10	2
1:C:344:LEU:HD13	1:D:340:MET:SD	0.41	2.55	29	1
1:A:337:ARG:NE	1:B:348:LEU:HD13	0.41	2.30	14	1
1:A:344:LEU:HG	1:D:344:LEU:HD11	0.41	1.91	9	1
1:C:337:ARG:HE	1:D:348:LEU:HD13	0.41	1.71	2	1
1:D:337:ARG:HG2	1:D:341:PHE:CE1	0.41	2.50	10	1
1:A:330:LEU:HG	1:A:332:ILE:HD11	0.41	1.92	5	1
1:A:347:ALA:HB1	1:D:347:ALA:HB1	0.41	1.91	1	1
1:A:344:LEU:HD11	1:D:344:LEU:CD1	0.41	2.46	12	1
1:A:333:ARG:CG	1:B:327:TYR:CD1	0.41	3.04	18	1
1:A:330:LEU:HD21	1:B:332:ILE:CD1	0.41	2.46	29	1
1:A:340:MET:C	1:A:344:LEU:HD12	0.41	2.36	11	1
1:B:344:LEU:CG	1:C:344:LEU:HD11	0.41	2.45	20	1
1:C:337:ARG:CG	1:D:348:LEU:HD12	0.41	2.46	13	1
1:A:351:LYS:HD2	1:D:347:ALA:HB2	0.41	1.91	13	1
1:B:351:LYS:O	1:B:355:ALA:HB2	0.41	2.16	6	1
1:B:344:LEU:HD11	1:D:340:MET:CE	0.41	2.46	29	1
1:B:330:LEU:CG	1:B:332:ILE:HD11	0.40	2.45	18	1
1:D:329:PHE:CD1	1:D:329:PHE:N	0.40	2.88	9	1
1:B:326:GLU:O	1:B:328:PHE:CE2	0.40	2.75	6	1
1:A:330:LEU:CD1	1:B:338:PHE:CE2	0.40	3.05	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:351:LYS:O	1:B:355:ALA:HB3	0.40	2.16	1	1
1:A:344:LEU:CD2	1:D:344:LEU:HD23	0.40	2.46	30	1
1:A:332:ILE:HG21	1:A:337:ARG:HG2	0.40	1.93	30	1
1:A:344:LEU:CD2	1:D:344:LEU:CD2	0.40	3.00	7	1
1:C:337:ARG:HG2	1:C:341:PHE:CE1	0.40	2.52	3	1
1:C:332:ILE:H	1:C:332:ILE:HD12	0.40	1.75	18	1
1:A:347:ALA:HB2	1:D:351:LYS:HE2	0.40	1.93	30	1
1:A:337:ARG:HG2	1:A:341:PHE:CE2	0.40	2.52	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	29/31 (94%)	27±1 (94±4%)	1±1 (5±4%)	0±0 (1±2%)	19	64
1	B	29/31 (94%)	27±1 (94±3%)	1±1 (4±3%)	1±0 (2±2%)	13	53
1	C	29/31 (94%)	27±1 (94±5%)	1±1 (4±4%)	0±0 (2±2%)	17	61
1	D	29/31 (94%)	27±1 (94±4%)	1±1 (5±3%)	0±0 (2±2%)	17	61
All	All	3480/3720 (94%)	3265 (94%)	157 (5%)	58 (2%)	16	59

All 5 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	B	327	TYR	18
1	D	327	TYR	14
1	C	327	TYR	13
1	A	327	TYR	12
1	C	355	ALA	1

6.3.2 Protein sidechains ⓘ

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	25/26 (96%)	21±2 (82±7%)	4±2 (18±7%)	6	41
1	B	26/26 (100%)	22±2 (84±7%)	4±2 (16±7%)	7	44
1	C	26/26 (100%)	21±2 (81±7%)	5±2 (19±7%)	5	38
1	D	26/26 (100%)	21±1 (82±6%)	5±1 (18±6%)	6	41
All	All	3090/3120 (99%)	2547 (82%)	543 (18%)	6	41

All 85 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	D	344	LEU	16
1	B	342	ARG	16
1	A	344	LEU	15
1	A	335	ARG	14
1	A	342	ARG	14
1	B	344	LEU	13
1	C	344	LEU	13
1	C	331	LYS	13
1	C	333	ARG	13
1	C	350	LEU	12
1	B	333	ARG	12
1	C	337	ARG	12
1	D	337	ARG	12
1	D	342	ARG	11
1	B	350	LEU	11
1	D	351	LYS	11
1	C	351	LYS	11
1	A	350	LEU	10
1	B	337	ARG	10
1	C	342	ARG	10
1	D	350	LEU	10
1	A	333	ARG	9
1	A	331	LYS	9
1	D	333	ARG	9
1	A	348	LEU	9
1	D	343	GLU	8
1	D	348	LEU	8
1	D	331	LYS	8
1	D	335	ARG	8

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Mol	Chain	Res	Type	Models (Total)
1	A	337	ARG	8
1	B	335	ARG	8
1	C	329	PHE	7
1	C	349	GLU	7
1	B	351	LYS	7
1	B	336	GLU	7
1	A	351	LYS	7
1	C	346	GLU	7
1	C	348	LEU	6
1	B	331	LYS	6
1	A	354	GLN	6
1	C	354	GLN	6
1	B	340	MET	6
1	D	339	GLU	6
1	A	352	ASP	5
1	D	336	GLU	5
1	C	352	ASP	5
1	A	346	GLU	5
1	C	335	ARG	5
1	C	343	GLU	4
1	D	346	GLU	4
1	C	339	GLU	4
1	C	326	GLU	4
1	B	352	ASP	4
1	A	340	MET	4
1	D	354	GLN	4
1	D	352	ASP	4
1	B	343	GLU	3
1	B	326	GLU	3
1	B	345	ASN	3
1	B	354	GLN	3
1	A	343	GLU	3
1	B	339	GLU	3
1	D	349	GLU	3
1	A	329	PHE	3
1	C	327	TYR	3
1	A	339	GLU	3
1	B	346	GLU	3
1	D	329	PHE	3
1	D	326	GLU	3
1	C	340	MET	3
1	A	336	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	348	LEU	2
1	B	329	PHE	2
1	A	330	LEU	2
1	A	345	ASN	2
1	C	336	GLU	2
1	B	349	GLU	2
1	C	330	LEU	1
1	D	330	LEU	1
1	B	327	TYR	1
1	D	327	TYR	1
1	D	340	MET	1
1	A	349	GLU	1
1	D	345	ASN	1
1	A	327	TYR	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