



Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 05:46 AM BST

PDB ID : 2RP4
Title : Solution Structure of the oligomerization domain in Dmp53
Authors : Ou, H.D.; Doetsch, V.
Deposited on : 2008-04-30

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

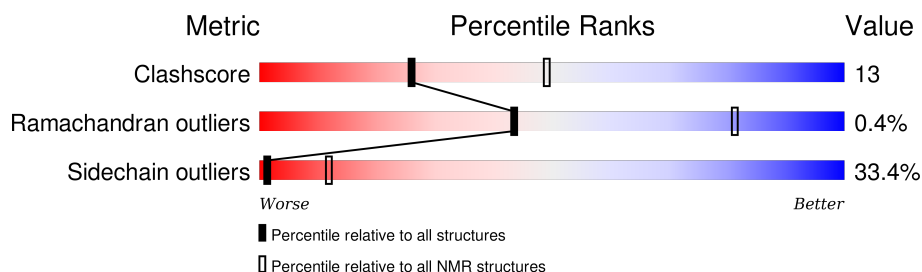
1 Overall quality at a glance

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	76	
1	B	76	
1	C	76	
1	D	76	

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:320-A:326, A:330-A:384, B:320-B:326, B:330-B:384, C:320-C:326, C:330-C:384, D:320-D:325, D:330-D:384 (247)	0.55	18

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4576 atoms, of which 2284 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription factor p53.

Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			1144	355	571	106	110	2	
1	B	71	Total	C	H	N	O	S	0
			1144	355	571	106	110	2	
1	C	71	Total	C	H	N	O	S	0
			1144	355	571	106	110	2	
1	D	71	Total	C	H	N	O	S	0
			1144	355	571	106	110	2	

There are 20 discrepancies between the modelled and reference sequences:

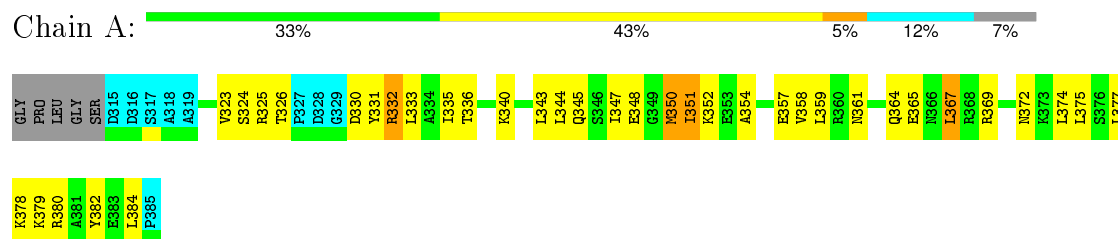
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLY	-	EXPRESSION TAG	UNP Q9N6D8
A	311	PRO	-	EXPRESSION TAG	UNP Q9N6D8
A	312	LEU	-	EXPRESSION TAG	UNP Q9N6D8
A	313	GLY	-	EXPRESSION TAG	UNP Q9N6D8
A	314	SER	-	EXPRESSION TAG	UNP Q9N6D8
B	310	GLY	-	EXPRESSION TAG	UNP Q9N6D8
B	311	PRO	-	EXPRESSION TAG	UNP Q9N6D8
B	312	LEU	-	EXPRESSION TAG	UNP Q9N6D8
B	313	GLY	-	EXPRESSION TAG	UNP Q9N6D8
B	314	SER	-	EXPRESSION TAG	UNP Q9N6D8
C	310	GLY	-	EXPRESSION TAG	UNP Q9N6D8
C	311	PRO	-	EXPRESSION TAG	UNP Q9N6D8
C	312	LEU	-	EXPRESSION TAG	UNP Q9N6D8
C	313	GLY	-	EXPRESSION TAG	UNP Q9N6D8
C	314	SER	-	EXPRESSION TAG	UNP Q9N6D8
D	310	GLY	-	EXPRESSION TAG	UNP Q9N6D8
D	311	PRO	-	EXPRESSION TAG	UNP Q9N6D8
D	312	LEU	-	EXPRESSION TAG	UNP Q9N6D8
D	313	GLY	-	EXPRESSION TAG	UNP Q9N6D8
D	314	SER	-	EXPRESSION TAG	UNP Q9N6D8

4 Residue-property plots

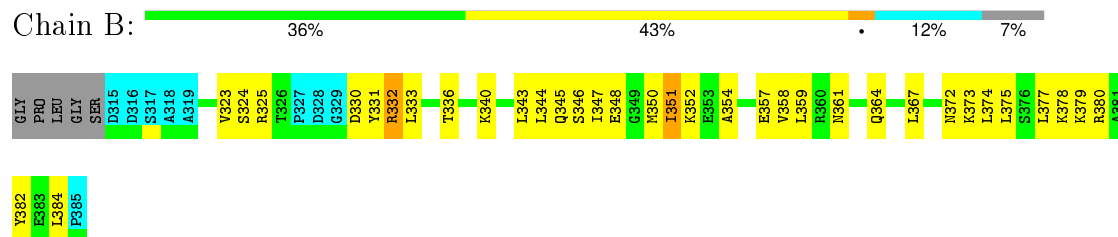
4.1 Average score per residue in the NMR ensemble

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.

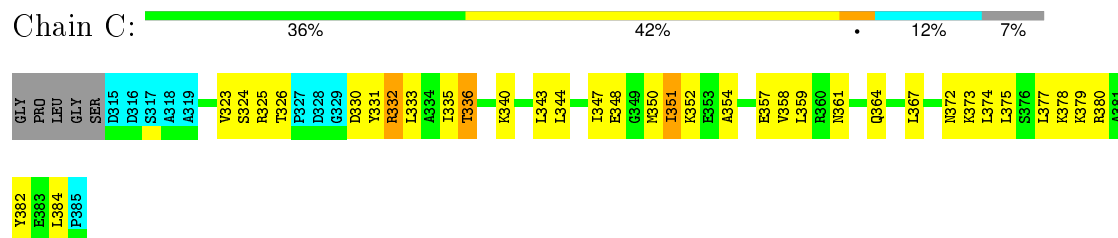
- Molecule 1: Transcription factor p53



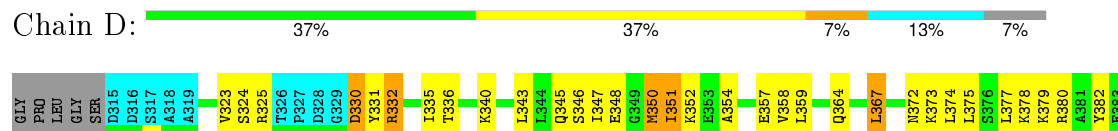
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



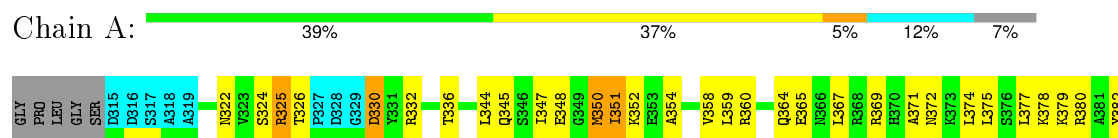


4.2 Scores per residue for each member of the ensemble

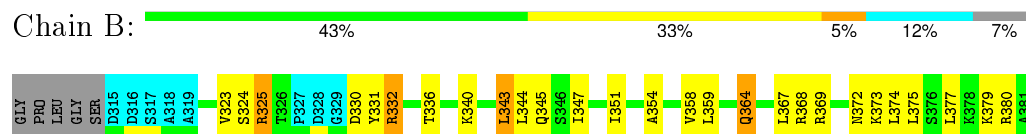
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

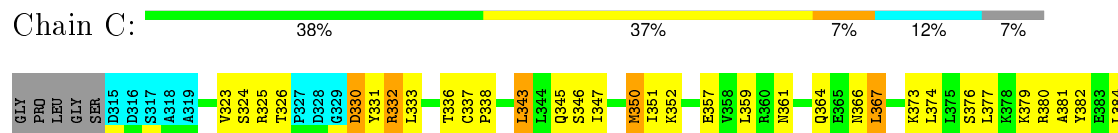
- Molecule 1: Transcription factor p53



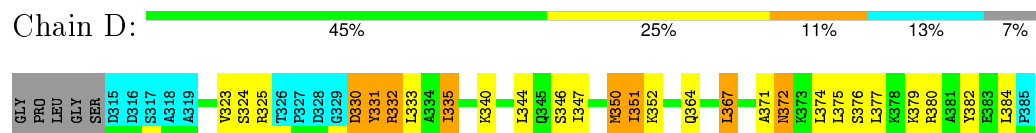
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

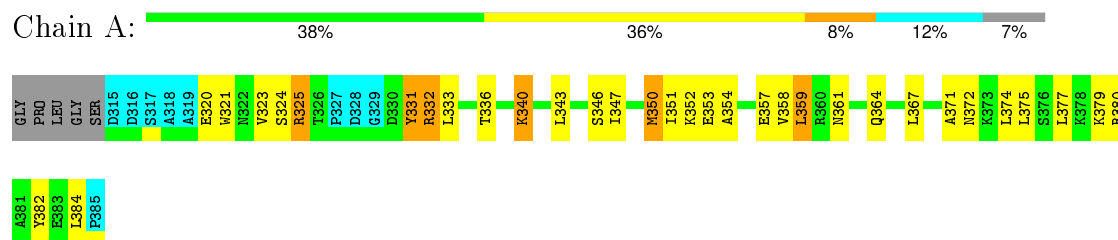


- Molecule 1: Transcription factor p53

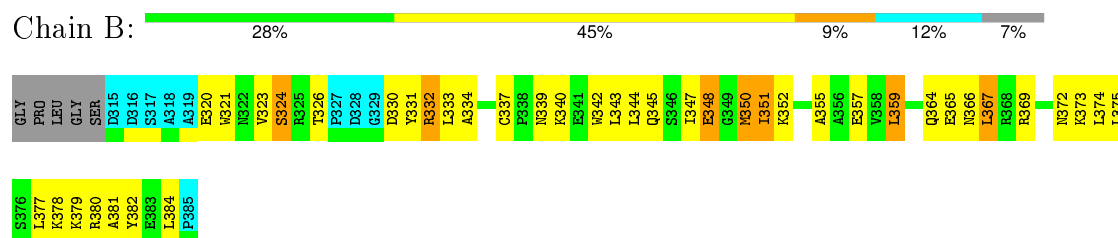


4.2.2 Score per residue for model 2

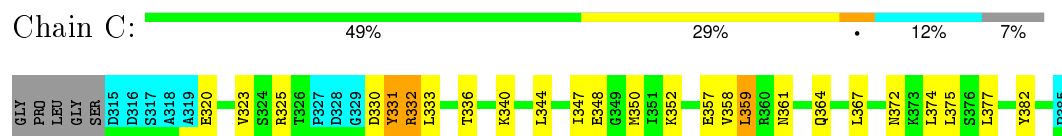
- Molecule 1: Transcription factor p53



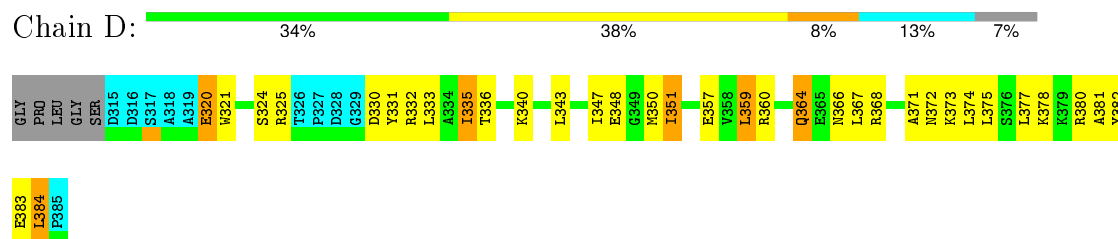
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

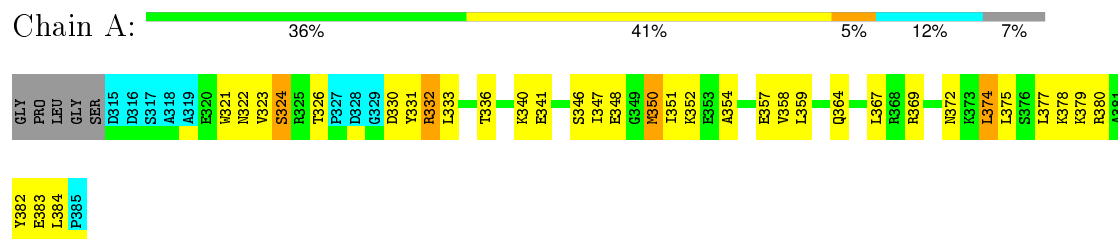


- Molecule 1: Transcription factor p53

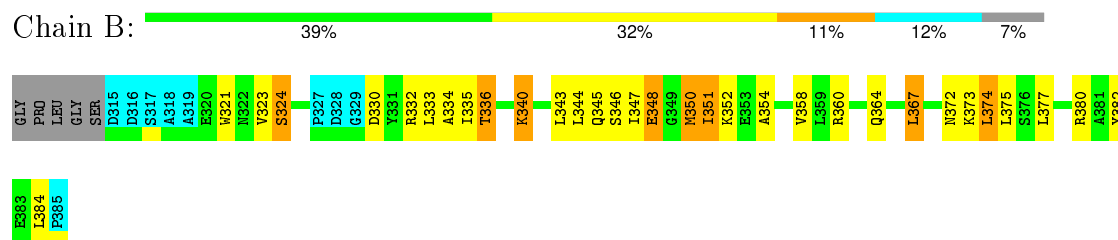


4.2.3 Score per residue for model 3

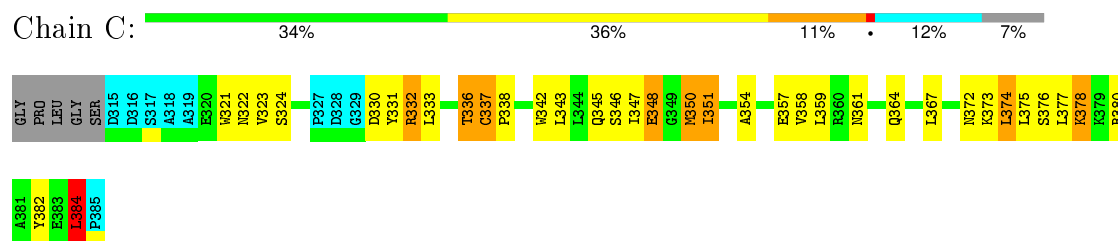
- Molecule 1: Transcription factor p53



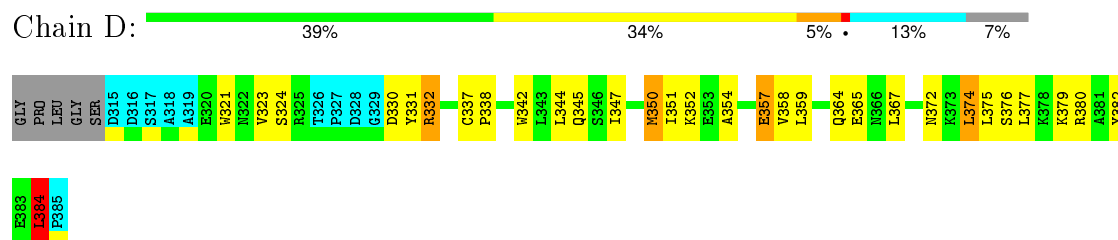
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

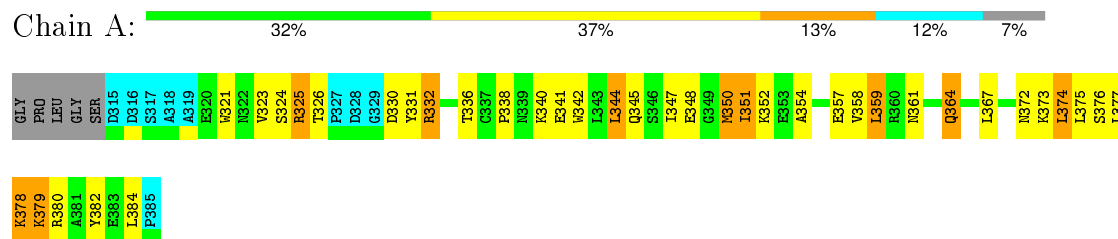


- Molecule 1: Transcription factor p53

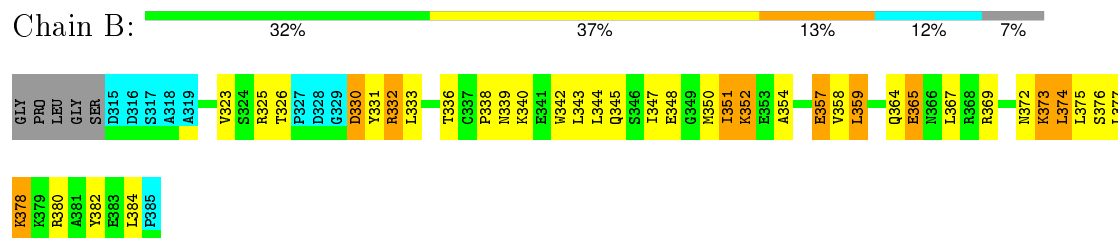


4.2.4 Score per residue for model 4

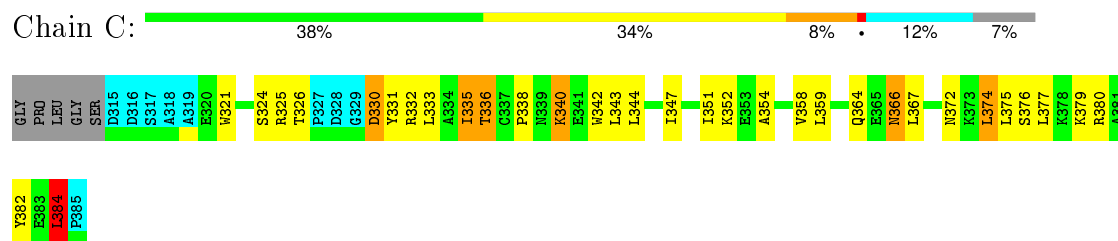
- Molecule 1: Transcription factor p53



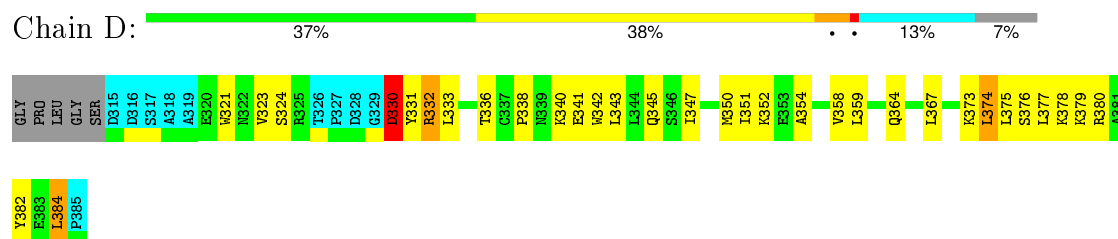
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

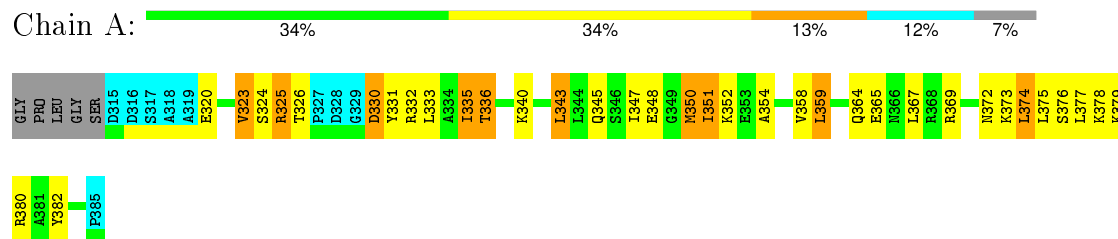


- Molecule 1: Transcription factor p53

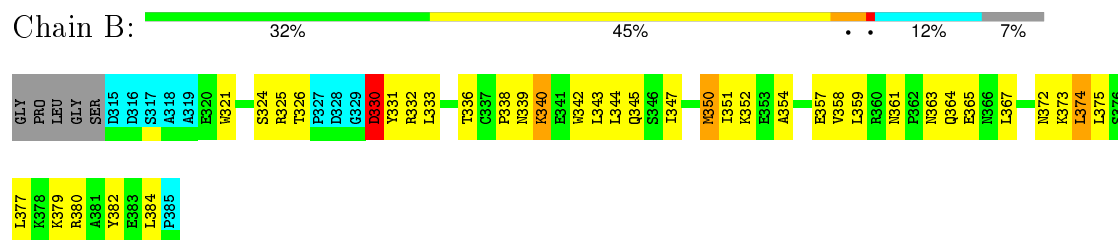


4.2.5 Score per residue for model 5

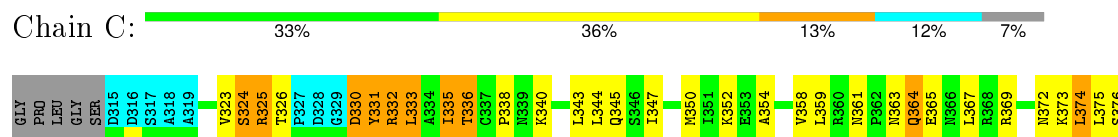
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



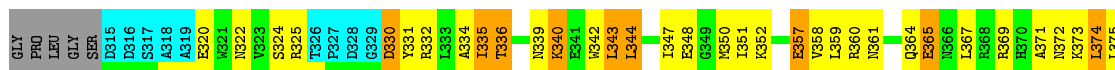
- Molecule 1: Transcription factor p53





• Molecule 1: Transcription factor p53

Chain D: 28% 41% 12% 13% 7%



4.2.6 Score per residue for model 6

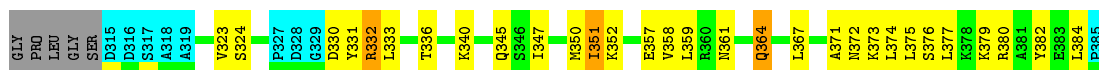
• Molecule 1: Transcription factor p53

Chain A: 43% 28% 11% 12% 7%



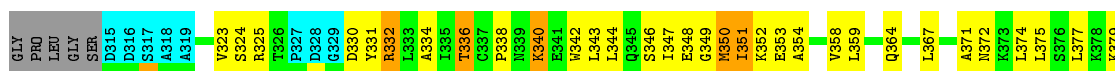
• Molecule 1: Transcription factor p53

Chain B: 42% 36% 12% 7%



• Molecule 1: Transcription factor p53

Chain C: 36% 39% 7% 12% 7%



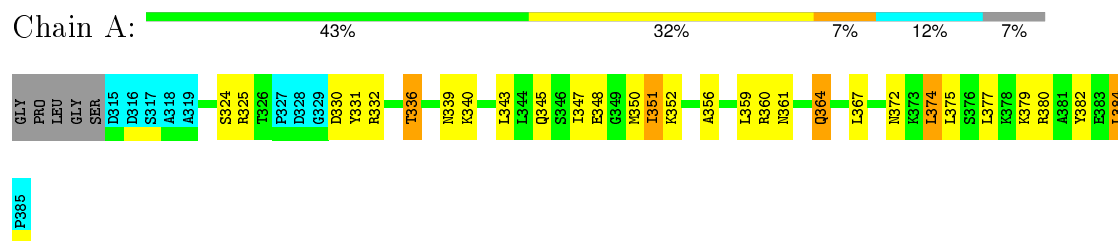
• Molecule 1: Transcription factor p53

Chain D: 36% 38% 7% 13% 7%

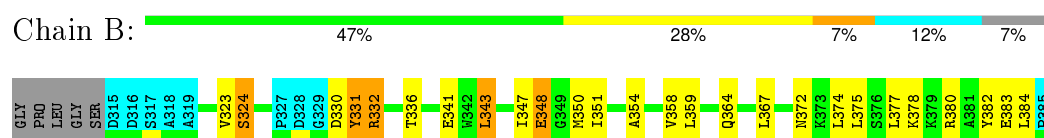


4.2.7 Score per residue for model 7

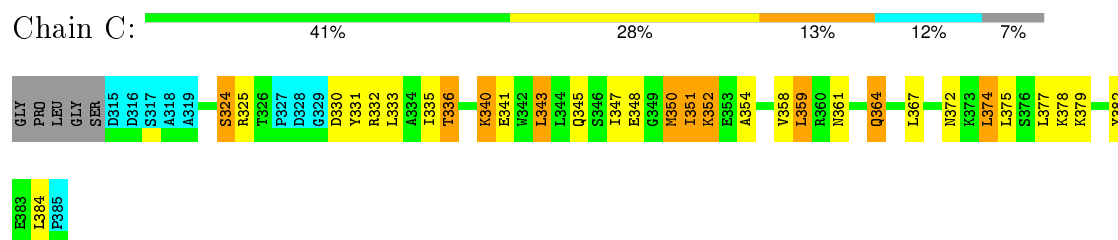
- Molecule 1: Transcription factor p53



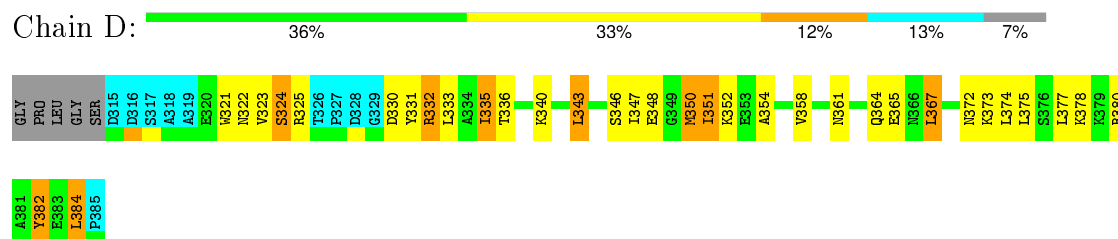
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

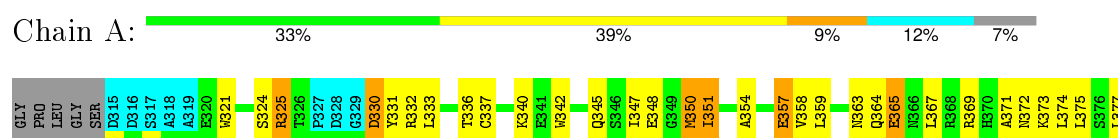


- Molecule 1: Transcription factor p53



4.2.8 Score per residue for model 8

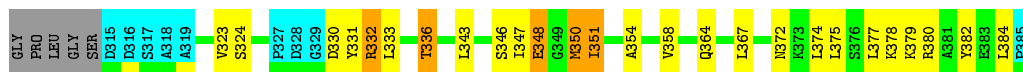
- Molecule 1: Transcription factor p53





- Molecule 1: Transcription factor p53

Chain B:



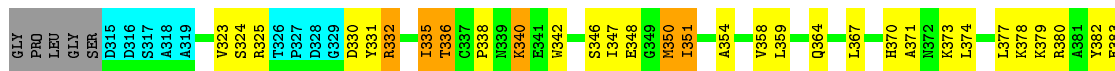
- Molecule 1: Transcription factor p53

Chain C:



- Molecule 1: Transcription factor p53

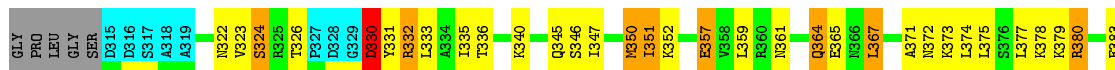
Chain D:



4.2.9 Score per residue for model 9

- Molecule 1: Transcription factor p53

Chain A:



- Molecule 1: Transcription factor p53

Chain B:





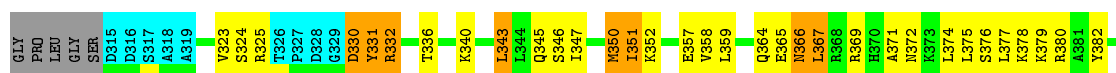
- Molecule 1: Transcription factor p53

Chain C: 33% 43% 5% 12% 7%



- Molecule 1: Transcription factor p53

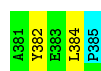
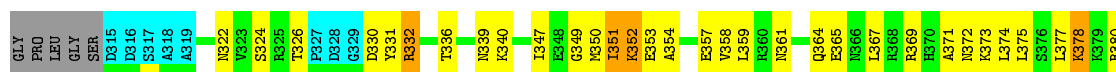
Chain D: 37% 33% 11% 13% 7%



4.2.10 Score per residue for model 10

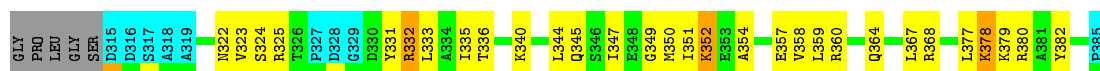
- Molecule 1: Transcription factor p53

Chain A: 37% 39% 5% 12% 7%



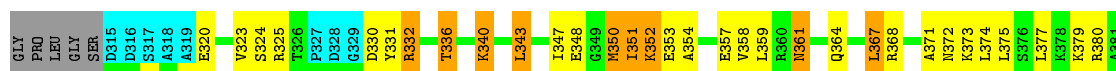
- Molecule 1: Transcription factor p53

Chain B: 42% 36% 12% 7%



- Molecule 1: Transcription factor p53

Chain C: 37% 33% 12% 12% 7%





• Molecule 1: Transcription factor p53

Chain D: 39% 32% 9% 13% 7%



4.2.11 Score per residue for model 11

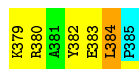
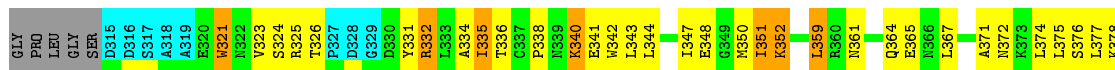
• Molecule 1: Transcription factor p53

Chain A: 34% 33% 14% 12% 7%



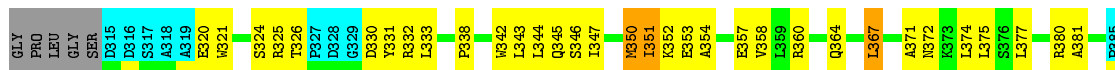
• Molecule 1: Transcription factor p53

Chain B: 32% 39% 11% 12% 7%



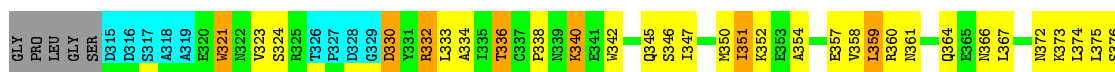
• Molecule 1: Transcription factor p53

Chain C: 38% 39% 12% 7%



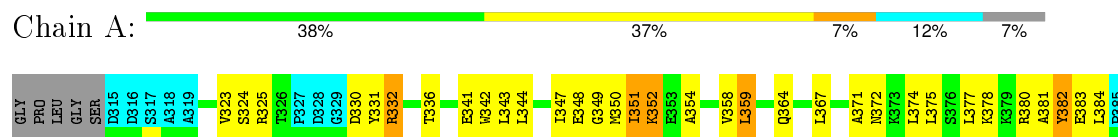
• Molecule 1: Transcription factor p53

Chain D: 33% 38% 9% 13% 7%

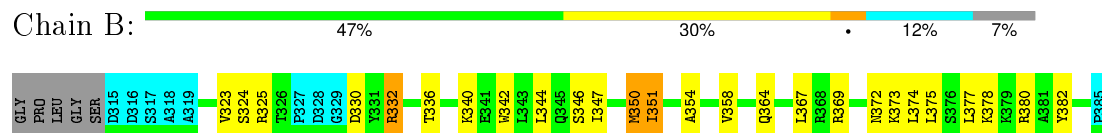


4.2.12 Score per residue for model 12

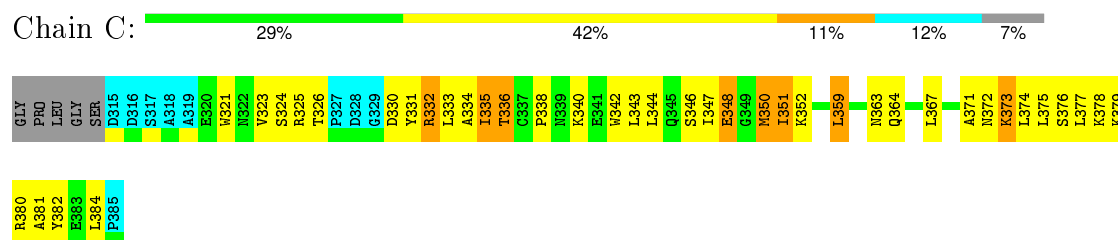
- Molecule 1: Transcription factor p53



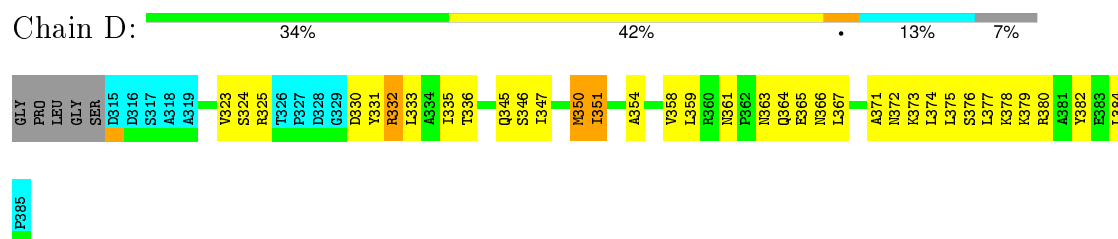
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

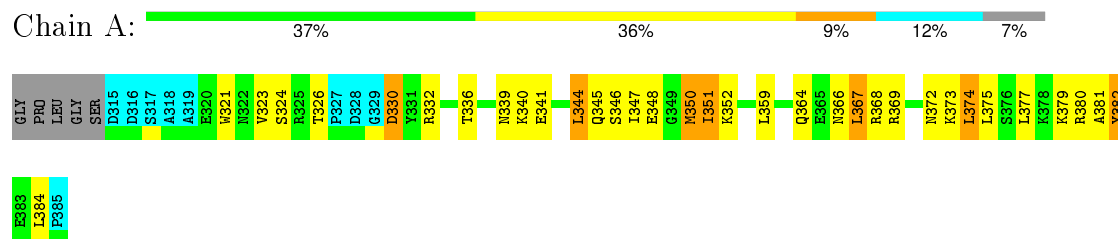


- Molecule 1: Transcription factor p53

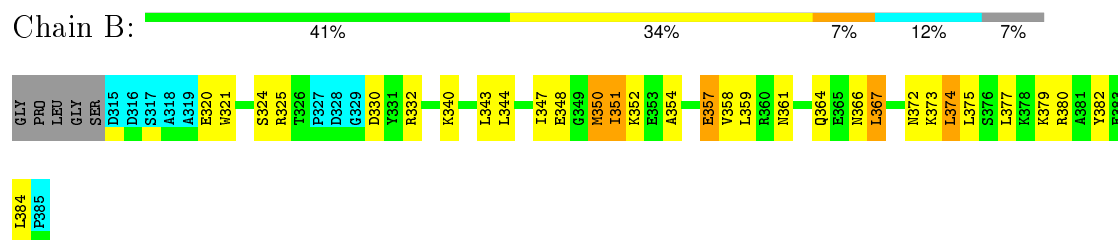


4.2.13 Score per residue for model 13

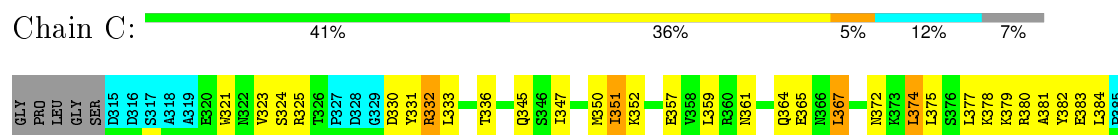
- Molecule 1: Transcription factor p53



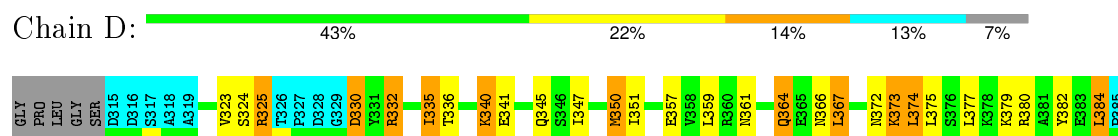
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

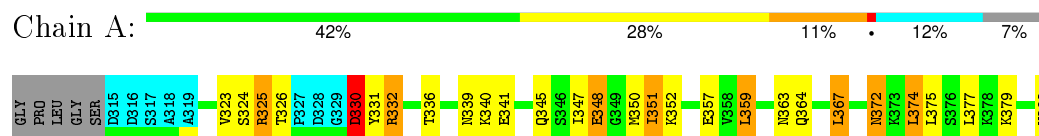


- Molecule 1: Transcription factor p53

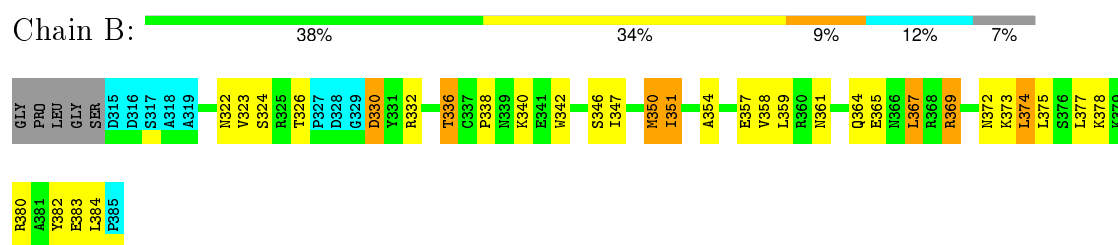


4.2.14 Score per residue for model 14

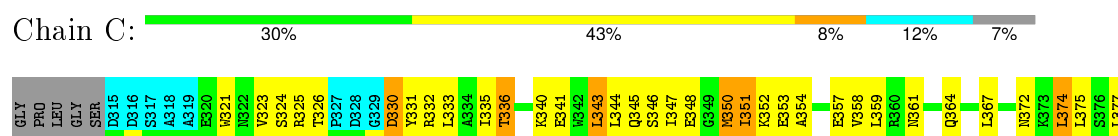
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



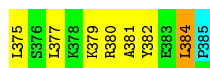
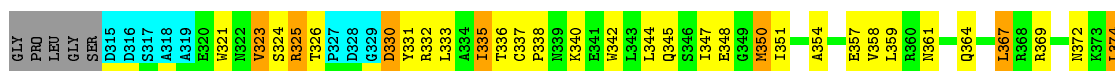


- Molecule 1: Transcription factor p53

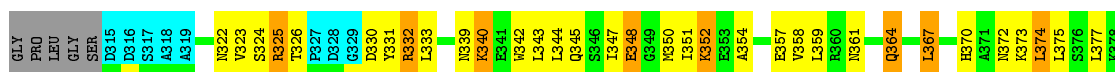
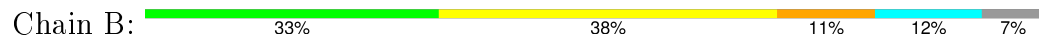


4.2.15 Score per residue for model 15

- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

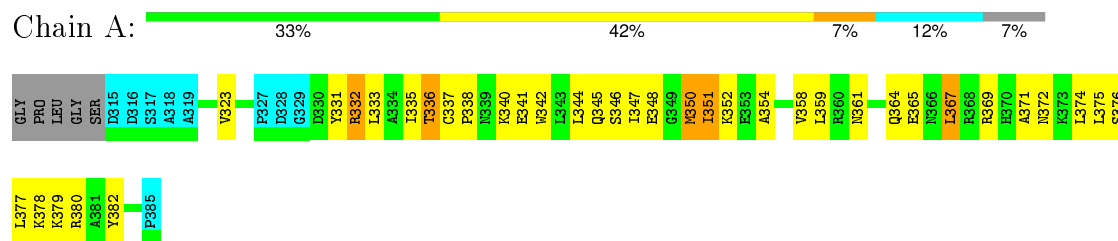


- Molecule 1: Transcription factor p53

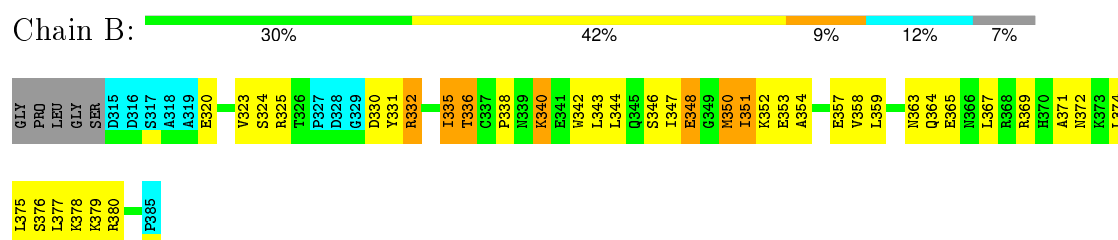


4.2.16 Score per residue for model 16

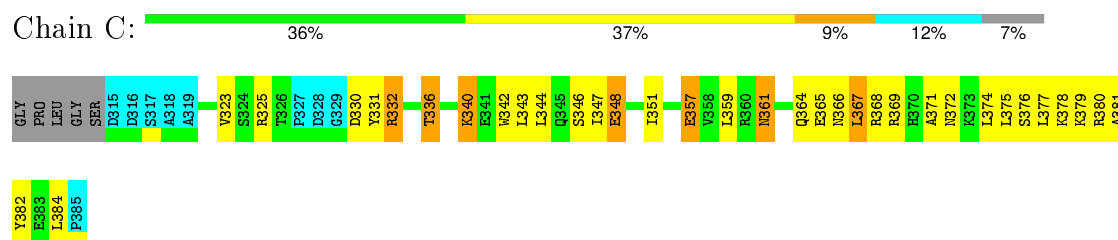
- Molecule 1: Transcription factor p53



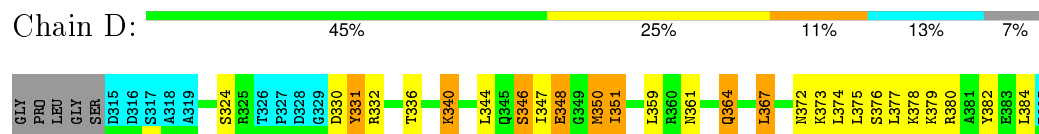
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

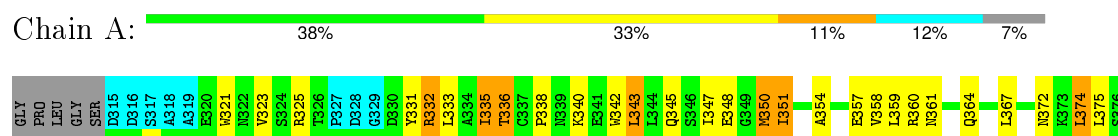


- Molecule 1: Transcription factor p53



4.2.17 Score per residue for model 17

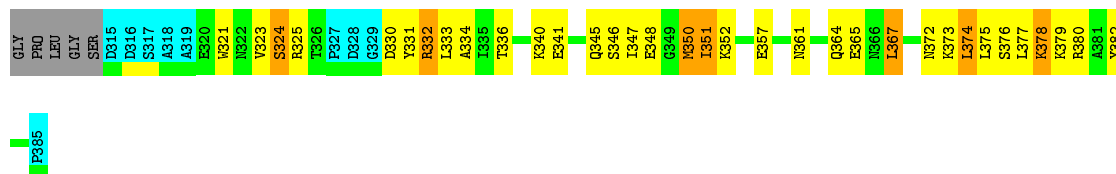
- Molecule 1: Transcription factor p53





• Molecule 1: Transcription factor p53

Chain B: 37% 36% 9% 12% 7%



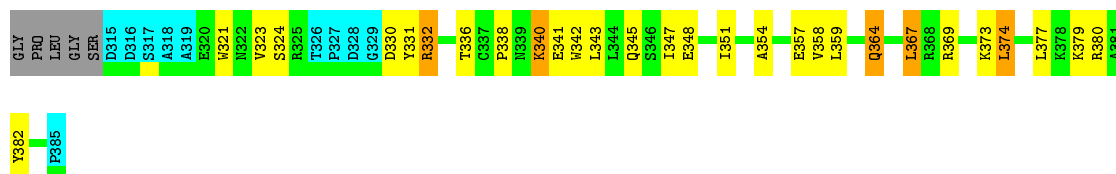
• Molecule 1: Transcription factor p53

Chain C: 43% 33% 5% 12% 7%



• Molecule 1: Transcription factor p53

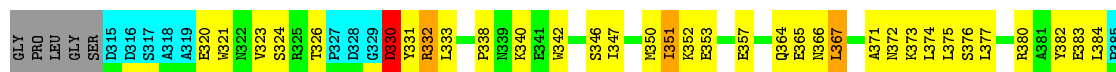
Chain D: 42% 32% 7% 13% 7%



4.2.18 Score per residue for model 18 (medoid)

• Molecule 1: Transcription factor p53

Chain A: 37% 39% 12% 7%

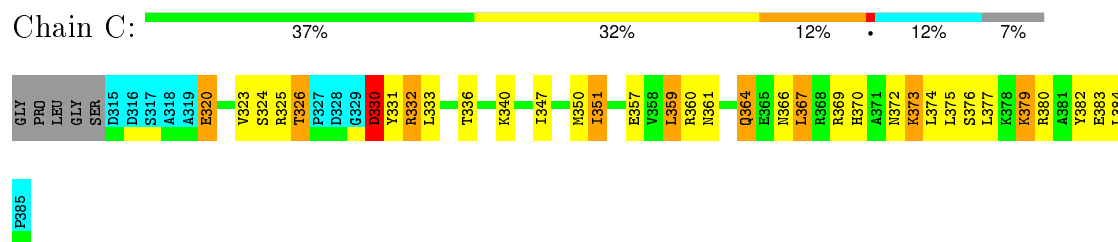


• Molecule 1: Transcription factor p53

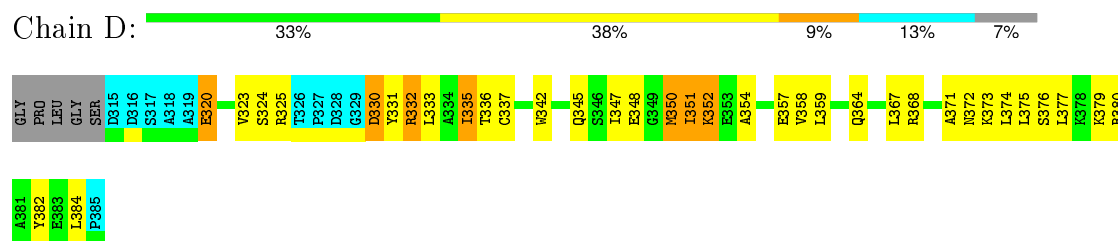
Chain B: 38% 37% 5% 12% 7%



• Molecule 1: Transcription factor p53

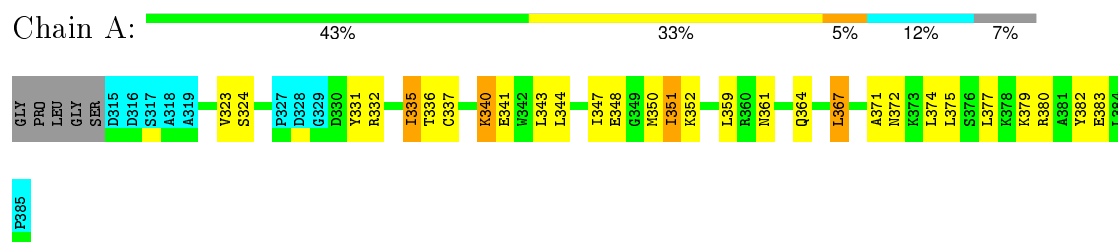


- Molecule 1: Transcription factor p53

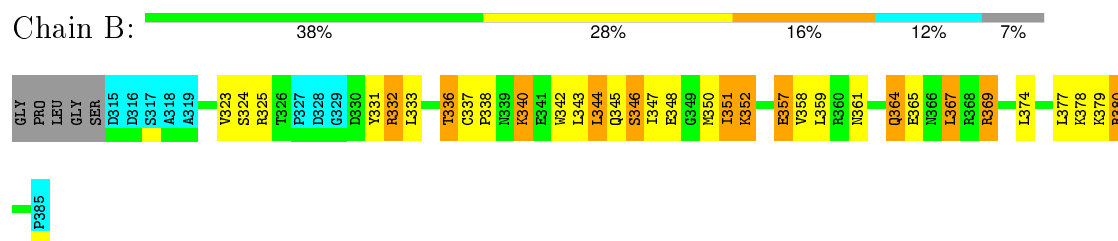


4.2.19 Score per residue for model 19

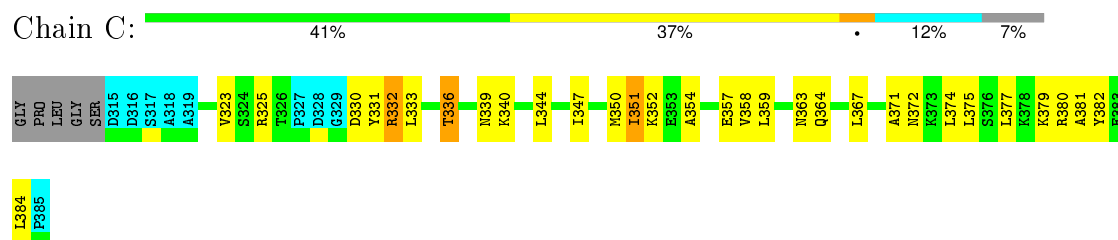
- Molecule 1: Transcription factor p53



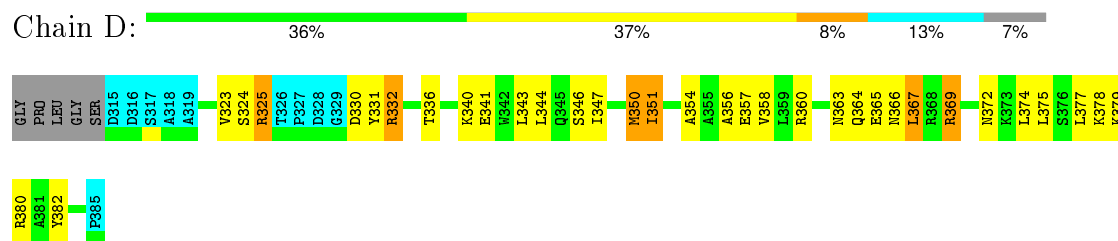
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53

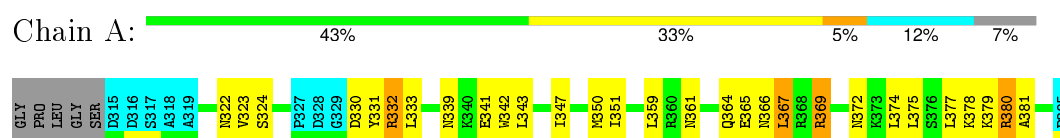


- Molecule 1: Transcription factor p53

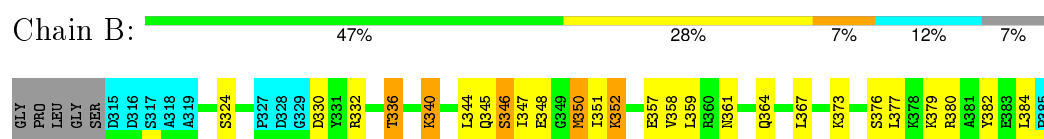


4.2.20 Score per residue for model 20

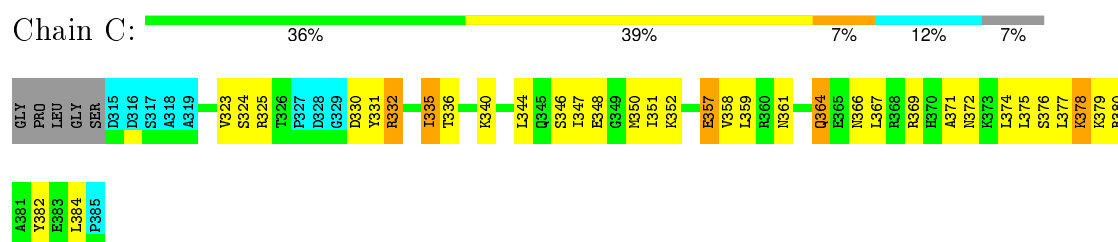
- Molecule 1: Transcription factor p53



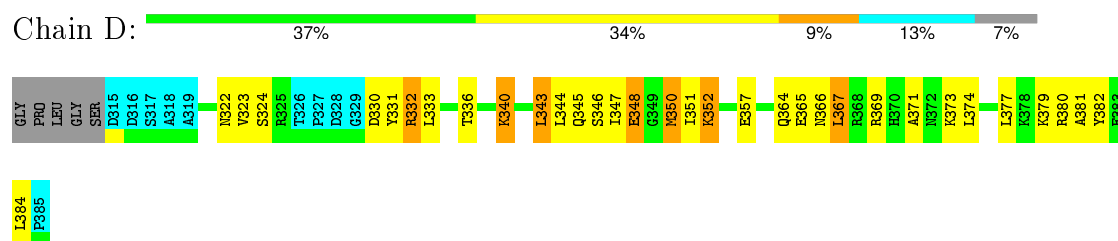
- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



- Molecule 1: Transcription factor p53



5 Refinement protocol and experimental data overview ⓘ

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	refinement	1.2
TALOS	geometry optimization	

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	514	527	526	17±4
1	B	514	527	526	17±4
1	C	514	527	526	17±3
1	D	507	520	519	17±3
All	All	40980	42020	41940	1110

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:347:ILE:HG12	1:C:377:LEU:HD23	0.84	1.48	18	20
1:C:346:SER:HA	1:D:350:MET:HB3	0.80	1.51	12	5
1:A:350:MET:HG3	1:A:374:LEU:HD22	0.80	1.52	12	2
1:B:352:LYS:HB2	1:C:352:LYS:HD3	0.79	1.53	10	1
1:C:350:MET:HG3	1:C:374:LEU:HD22	0.78	1.56	19	3
1:A:350:MET:HB3	1:B:346:SER:HA	0.76	1.54	8	3
1:B:350:MET:HG3	1:B:374:LEU:HD22	0.75	1.59	11	1
1:D:347:ILE:HG12	1:D:377:LEU:HD23	0.75	1.56	11	19
1:B:375:LEU:HD11	1:C:359:LEU:HD11	0.75	1.59	12	3
1:A:347:ILE:HG12	1:A:377:LEU:HD23	0.75	1.58	16	20
1:B:347:ILE:HG12	1:B:377:LEU:HD23	0.74	1.58	2	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:359:LEU:HD11	1:C:375:LEU:HD11	0.74	1.59	4	3
1:B:351:ILE:HG12	1:B:374:LEU:HB2	0.73	1.57	9	9
1:A:352:LYS:HD2	1:D:352:LYS:HA	0.73	1.59	10	1
1:A:359:LEU:HD11	1:D:375:LEU:HD11	0.71	1.62	5	5
1:C:340:LYS:HA	1:C:343:LEU:HD12	0.71	1.63	8	5
1:A:331:TYR:HE2	1:B:340:LYS:HA	0.70	1.47	5	2
1:D:340:LYS:HA	1:D:343:LEU:HD12	0.69	1.63	9	3
1:A:333:LEU:HD11	1:B:377:LEU:HD21	0.68	1.64	15	5
1:D:381:ALA:HA	1:D:384:LEU:HD12	0.67	1.67	2	2
1:A:374:LEU:HD13	1:B:321:TRP:HZ3	0.67	1.49	17	4
1:A:352:LYS:HG3	1:D:352:LYS:HB3	0.67	1.65	11	1
1:B:348:GLU:HG2	1:B:378:LYS:HD2	0.67	1.66	16	6
1:B:340:LYS:HA	1:B:343:LEU:HD12	0.67	1.66	16	4
1:C:351:ILE:HG12	1:C:374:LEU:HB2	0.66	1.68	18	7
1:A:340:LYS:HA	1:A:343:LEU:HD12	0.66	1.68	11	3
1:D:371:ALA:HA	1:D:374:LEU:HD12	0.65	1.68	18	8
1:D:335:ILE:HG12	1:D:336:THR:N	0.65	2.06	5	1
1:D:351:ILE:HG12	1:D:374:LEU:HB2	0.65	1.67	2	11
1:D:321:TRP:HA	1:D:334:ALA:O	0.64	1.91	11	1
1:A:371:ALA:HA	1:A:374:LEU:HD12	0.64	1.69	19	10
1:C:335:ILE:HG12	1:C:336:THR:N	0.64	2.07	5	1
1:A:333:LEU:O	1:B:334:ALA:HA	0.63	1.93	2	5
1:C:377:LEU:HD21	1:D:333:LEU:HD11	0.63	1.70	6	6
1:A:352:LYS:HG3	1:A:353:GLU:N	0.63	2.08	10	1
1:A:343:LEU:HD11	1:B:331:TYR:HB3	0.63	1.71	19	1
1:A:365:GLU:O	1:A:369:ARG:HG2	0.63	1.94	6	5
1:A:326:THR:HG23	1:A:330:ASP:H	0.63	1.54	9	2
1:C:331:TYR:HE2	1:D:340:LYS:HG3	0.62	1.53	11	1
1:C:348:GLU:HG3	1:C:352:LYS:HE3	0.62	1.70	7	2
1:B:321:TRP:HA	1:B:334:ALA:O	0.62	1.94	11	1
1:D:350:MET:HG3	1:D:374:LEU:HD22	0.62	1.71	2	3
1:B:326:THR:HG22	1:B:332:ARG:HB2	0.62	1.70	2	2
1:C:326:THR:HG23	1:C:330:ASP:H	0.61	1.54	18	1
1:A:372:ASN:HA	1:A:375:LEU:HD12	0.61	1.70	7	20
1:C:325:ARG:HA	1:C:330:ASP:O	0.61	1.95	5	3
1:A:352:LYS:HD2	1:D:352:LYS:CA	0.61	2.25	10	1
1:C:324:SER:HA	1:D:384:LEU:HD23	0.61	1.71	7	1
1:A:335:ILE:HG12	1:A:336:THR:N	0.61	2.10	5	1
1:A:352:LYS:HB3	1:D:352:LYS:HD2	0.61	1.71	14	1
1:C:371:ALA:HA	1:C:374:LEU:HD12	0.61	1.72	20	9
1:D:325:ARG:HG3	1:D:331:TYR:CE1	0.61	2.29	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:350:MET:HG2	1:D:374:LEU:HG	0.60	1.71	3	2
1:A:349:GLY:HA3	1:B:349:GLY:HA3	0.60	1.73	10	1
1:A:381:ALA:HA	1:A:384:LEU:HD12	0.60	1.73	12	1
1:B:325:ARG:HG3	1:B:331:TYR:CE1	0.60	2.32	1	3
1:C:358:VAL:HG22	1:C:367:LEU:HB3	0.59	1.73	7	10
1:A:325:ARG:HA	1:A:330:ASP:O	0.59	1.97	5	4
1:B:351:ILE:HG12	1:B:374:LEU:CB	0.59	2.27	12	6
1:C:321:TRP:HZ3	1:D:374:LEU:HD13	0.59	1.56	14	5
1:D:365:GLU:O	1:D:369:ARG:HG2	0.59	1.97	19	5
1:D:349:GLY:HA2	1:D:352:LYS:HE2	0.59	1.73	14	1
1:C:350:MET:HG3	1:C:374:LEU:HG	0.59	1.74	15	3
1:A:323:VAL:HG13	1:A:333:LEU:HD13	0.59	1.74	5	2
1:A:351:ILE:HG12	1:A:374:LEU:HB2	0.58	1.74	8	8
1:A:336:THR:HA	1:B:331:TYR:O	0.58	1.98	7	7
1:D:347:ILE:HA	1:D:350:MET:SD	0.58	2.38	15	2
1:A:351:ILE:HA	1:A:374:LEU:HD13	0.58	1.75	8	9
1:A:321:TRP:HZ3	1:B:374:LEU:HD13	0.58	1.58	3	4
1:C:364:GLN:HG3	1:C:366:ASN:OD1	0.58	1.99	9	3
1:C:351:ILE:HG12	1:C:374:LEU:CB	0.58	2.28	11	1
1:A:352:LYS:HD2	1:D:352:LYS:HB2	0.58	1.75	10	1
1:A:343:LEU:HD11	1:B:333:LEU:HB2	0.58	1.76	5	1
1:D:372:ASN:HA	1:D:375:LEU:HD12	0.58	1.75	14	16
1:D:323:VAL:HA	1:D:332:ARG:O	0.58	1.99	3	15
1:A:347:ILE:HD13	1:A:378:LYS:HA	0.58	1.73	10	2
1:A:377:LEU:HD21	1:B:333:LEU:HD11	0.58	1.75	2	6
1:C:348:GLU:HG2	1:C:378:LYS:HD2	0.57	1.74	3	5
1:A:350:MET:HG2	1:A:374:LEU:HG	0.57	1.76	4	4
1:A:331:TYR:O	1:B:336:THR:HA	0.57	1.99	3	14
1:A:342:TRP:CZ2	1:B:367:LEU:HG	0.57	2.35	8	3
1:B:338:PRO:HD2	1:B:342:TRP:CE3	0.56	2.34	18	5
1:D:348:GLU:HG2	1:D:378:LYS:HD2	0.56	1.77	2	3
1:B:371:ALA:HA	1:B:374:LEU:HD12	0.56	1.78	6	5
1:A:352:LYS:HD2	1:D:352:LYS:CB	0.56	2.30	10	1
1:C:333:LEU:HD11	1:D:377:LEU:HD21	0.56	1.76	11	6
1:C:321:TRP:CZ3	1:D:374:LEU:HD13	0.56	2.36	17	3
1:C:351:ILE:HA	1:C:374:LEU:HD13	0.56	1.78	1	5
1:C:333:LEU:HD23	1:D:335:ILE:HG12	0.55	1.78	2	7
1:B:350:MET:HG2	1:B:374:LEU:HG	0.55	1.77	5	2
1:A:348:GLU:HG2	1:A:378:LYS:HD2	0.55	1.79	1	3
1:C:325:ARG:HG2	1:C:330:ASP:O	0.55	2.02	15	1
1:D:365:GLU:O	1:D:369:ARG:HG3	0.55	2.02	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:338:PRO:HA	1:D:330:ASP:HB2	0.55	1.77	5	2
1:C:331:TYR:CE2	1:D:340:LYS:HG3	0.55	2.36	11	1
1:B:347:ILE:HA	1:B:350:MET:SD	0.54	2.41	11	1
1:D:348:GLU:O	1:D:352:LYS:HE3	0.54	2.02	18	2
1:B:351:ILE:HA	1:B:374:LEU:HD13	0.54	1.79	9	7
1:D:364:GLN:HG3	1:D:366:ASN:OD1	0.54	2.03	20	4
1:C:336:THR:HA	1:D:331:TYR:O	0.54	2.02	17	13
1:B:338:PRO:HD2	1:B:342:TRP:CZ3	0.54	2.38	16	4
1:C:347:ILE:HA	1:C:350:MET:SD	0.54	2.42	5	4
1:C:374:LEU:HD13	1:D:321:TRP:HZ3	0.54	1.60	7	4
1:D:357:GLU:HA	1:D:357:GLU:OE1	0.54	2.02	3	1
1:B:372:ASN:HA	1:B:375:LEU:HD12	0.54	1.79	16	17
1:C:372:ASN:HA	1:C:375:LEU:HD12	0.54	1.80	4	18
1:C:335:ILE:HG12	1:D:333:LEU:HD23	0.54	1.80	4	3
1:C:331:TYR:O	1:D:336:THR:HA	0.54	2.02	13	13
1:C:381:ALA:HA	1:C:384:LEU:HD12	0.54	1.79	19	6
1:B:365:GLU:O	1:B:369:ARG:HG2	0.54	2.03	14	3
1:B:348:GLU:O	1:B:352:LYS:HE3	0.54	2.01	15	4
1:A:333:LEU:HD11	1:B:377:LEU:HD11	0.54	1.80	2	2
1:D:350:MET:HG3	1:D:374:LEU:HG	0.54	1.79	15	2
1:C:333:LEU:O	1:D:334:ALA:HA	0.54	2.03	5	1
1:C:323:VAL:HA	1:C:332:ARG:O	0.53	2.03	14	17
1:A:349:GLY:HA3	1:B:349:GLY:CA	0.53	2.33	10	1
1:D:351:ILE:HG12	1:D:374:LEU:CB	0.53	2.32	2	3
1:B:358:VAL:HG22	1:B:367:LEU:HB3	0.53	1.78	5	7
1:B:352:LYS:CB	1:C:352:LYS:HD3	0.53	2.29	10	1
1:A:384:LEU:HD11	1:B:324:SER:HA	0.53	1.78	2	2
1:D:348:GLU:O	1:D:352:LYS:HG2	0.53	2.04	15	1
1:D:347:ILE:O	1:D:350:MET:HG2	0.53	2.04	15	1
1:A:346:SER:HA	1:B:350:MET:HB3	0.53	1.78	2	4
1:A:331:TYR:CE2	1:B:340:LYS:HA	0.53	2.36	5	1
1:A:349:GLY:HA2	1:A:352:LYS:HE2	0.53	1.80	12	1
1:C:384:LEU:HD21	1:D:324:SER:HA	0.53	1.79	7	1
1:B:364:GLN:HG3	1:B:366:ASN:OD1	0.53	2.04	13	2
1:D:351:ILE:HB	1:D:374:LEU:HB3	0.53	1.79	4	2
1:B:352:LYS:HG3	1:C:352:LYS:HB3	0.52	1.80	19	2
1:A:350:MET:HB2	1:B:346:SER:HA	0.52	1.82	19	1
1:A:365:GLU:O	1:A:369:ARG:HG3	0.52	2.05	16	2
1:D:378:LYS:HE3	1:D:382:TYR:HE2	0.52	1.64	7	1
1:C:365:GLU:O	1:C:369:ARG:HG3	0.52	2.05	16	2
1:B:346:SER:O	1:B:350:MET:HG2	0.52	2.04	8	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:338:PRO:HD2	1:A:342:TRP:CE3	0.52	2.40	18	5
1:C:352:LYS:HG3	1:C:353:GLU:N	0.52	2.19	10	1
1:C:357:GLU:HB3	1:C:367:LEU:HD11	0.52	1.81	10	3
1:B:351:ILE:HB	1:B:374:LEU:HB3	0.52	1.80	4	1
1:B:326:THR:HG21	1:B:332:ARG:HG2	0.52	1.82	18	1
1:C:346:SER:O	1:C:350:MET:HG2	0.52	2.04	12	7
1:A:367:LEU:HG	1:B:342:TRP:CZ2	0.52	2.40	12	2
1:B:358:VAL:HG21	1:C:359:LEU:HD11	0.52	1.81	20	1
1:A:384:LEU:HD21	1:B:324:SER:HA	0.51	1.82	7	2
1:D:325:ARG:HG2	1:D:331:TYR:CE1	0.51	2.40	5	3
1:D:357:GLU:HB3	1:D:367:LEU:HD11	0.51	1.81	13	4
1:D:351:ILE:HA	1:D:374:LEU:HD13	0.51	1.81	8	7
1:D:358:VAL:HG22	1:D:367:LEU:HB3	0.51	1.83	10	8
1:A:340:LYS:HD2	1:A:384:LEU:HD22	0.51	1.82	6	1
1:A:321:TRP:CZ3	1:B:374:LEU:HD13	0.51	2.41	3	4
1:D:325:ARG:HA	1:D:330:ASP:O	0.51	2.06	13	4
1:A:350:MET:HG3	1:A:374:LEU:HG	0.51	1.83	14	2
1:C:348:GLU:O	1:C:352:LYS:HG2	0.51	2.05	6	1
1:A:333:LEU:HD23	1:B:335:ILE:HG12	0.50	1.83	16	2
1:B:357:GLU:HB3	1:B:367:LEU:HD11	0.50	1.84	9	4
1:C:340:LYS:HA	1:D:331:TYR:CE2	0.50	2.42	16	1
1:C:350:MET:HG2	1:C:374:LEU:HG	0.50	1.83	7	1
1:A:326:THR:HG22	1:A:332:ARG:HB2	0.50	1.81	10	2
1:D:338:PRO:HD2	1:D:342:TRP:CE3	0.50	2.41	11	6
1:B:323:VAL:HA	1:B:332:ARG:O	0.50	2.07	7	14
1:A:348:GLU:O	1:A:351:ILE:HG22	0.50	2.07	17	9
1:B:347:ILE:O	1:B:351:ILE:HG22	0.50	2.07	4	2
1:C:347:ILE:O	1:C:351:ILE:HG22	0.49	2.06	16	2
1:D:340:LYS:HE3	1:D:384:LEU:O	0.49	2.07	8	1
1:A:325:ARG:HG2	1:A:330:ASP:O	0.49	2.07	1	2
1:C:331:TYR:CE2	1:D:340:LYS:HA	0.49	2.42	2	1
1:A:374:LEU:HG	1:B:321:TRP:CH2	0.49	2.43	18	2
1:C:367:LEU:HG	1:D:342:TRP:CZ2	0.49	2.43	18	3
1:C:347:ILE:HG23	1:C:374:LEU:HD12	0.49	1.83	7	2
1:C:333:LEU:HB2	1:D:343:LEU:HD11	0.49	1.84	5	2
1:C:351:ILE:HB	1:C:374:LEU:HB3	0.49	1.84	4	1
1:D:338:PRO:HD2	1:D:342:TRP:CZ3	0.49	2.43	4	2
1:D:346:SER:O	1:D:350:MET:HG2	0.49	2.08	16	8
1:D:323:VAL:HB	1:D:333:LEU:HD13	0.49	1.84	18	1
1:D:352:LYS:HG3	1:D:353:GLU:N	0.49	2.23	10	1
1:B:364:GLN:HB3	1:B:367:LEU:HB2	0.49	1.85	2	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:323:VAL:HA	1:A:332:ARG:O	0.49	2.07	13	13
1:A:364:GLN:HB3	1:A:367:LEU:HB2	0.49	1.84	11	20
1:B:365:GLU:O	1:B:369:ARG:HG3	0.49	2.08	4	2
1:C:331:TYR:HB2	1:D:337:CYS:O	0.49	2.07	3	1
1:B:326:THR:HG23	1:B:330:ASP:H	0.49	1.68	18	1
1:A:346:SER:O	1:A:350:MET:HG2	0.48	2.08	2	6
1:A:348:GLU:O	1:A:352:LYS:HE3	0.48	2.07	11	1
1:A:335:ILE:HG12	1:B:333:LEU:HD23	0.48	1.83	17	3
1:A:380:ARG:HD2	1:B:323:VAL:HG13	0.48	1.86	9	1
1:C:353:GLU:HB3	1:D:345:GLN:HG2	0.48	1.84	14	1
1:B:358:VAL:HB	1:C:359:LEU:HD21	0.48	1.84	7	1
1:C:348:GLU:O	1:C:351:ILE:HG22	0.48	2.08	8	7
1:D:364:GLN:HB3	1:D:367:LEU:HB2	0.48	1.86	16	20
1:A:353:GLU:HB3	1:B:345:GLN:NE2	0.48	2.24	2	1
1:D:348:GLU:O	1:D:351:ILE:HG22	0.48	2.08	15	4
1:B:339:ASN:HB2	1:B:342:TRP:CD2	0.48	2.44	5	2
1:A:354:ALA:O	1:A:358:VAL:HG23	0.47	2.09	10	11
1:A:358:VAL:HG22	1:A:367:LEU:HB3	0.47	1.86	17	3
1:B:344:LEU:HD12	1:B:378:LYS:HE2	0.47	1.87	19	1
1:A:321:TRP:CH2	1:B:374:LEU:HG	0.47	2.44	8	1
1:C:354:ALA:O	1:C:358:VAL:HG23	0.47	2.08	5	12
1:C:364:GLN:HB3	1:C:367:LEU:HB2	0.47	1.86	13	19
1:B:348:GLU:HG2	1:B:378:LYS:HG3	0.47	1.86	4	1
1:A:381:ALA:O	1:A:384:LEU:HB2	0.47	2.09	8	3
1:D:347:ILE:HD13	1:D:378:LYS:HA	0.47	1.85	10	1
1:D:371:ALA:HA	1:D:374:LEU:HD22	0.47	1.86	5	1
1:A:321:TRP:HE3	1:B:377:LEU:HD13	0.47	1.70	2	3
1:C:320:GLU:HB2	1:C:336:THR:OG1	0.47	2.09	15	1
1:C:351:ILE:HD13	1:C:374:LEU:HB2	0.47	1.86	20	1
1:A:349:GLY:O	1:A:352:LYS:HG2	0.47	2.10	12	1
1:A:364:GLN:HG3	1:A:366:ASN:OD1	0.47	2.09	20	1
1:C:357:GLU:HG3	1:C:367:LEU:HD11	0.47	1.86	14	1
1:C:342:TRP:CZ2	1:D:367:LEU:HG	0.47	2.45	17	2
1:B:352:LYS:HA	1:C:352:LYS:CD	0.47	2.40	10	1
1:A:339:ASN:HB3	1:A:341:GLU:HG2	0.47	1.86	13	1
1:A:333:LEU:HD11	1:A:335:ILE:HG23	0.47	1.85	16	1
1:A:337:CYS:O	1:B:331:TYR:HB2	0.46	2.09	19	1
1:D:350:MET:SD	1:D:374:LEU:HD11	0.46	2.50	13	1
1:D:335:ILE:HD11	1:D:343:LEU:HD21	0.46	1.87	7	1
1:A:374:LEU:HD13	1:B:321:TRP:CZ3	0.46	2.44	13	3
1:C:325:ARG:HG3	1:C:331:TYR:CE1	0.46	2.45	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:351:ILE:HA	1:C:374:LEU:HD23	0.46	1.86	13	1
1:B:347:ILE:HG23	1:B:374:LEU:HD12	0.46	1.87	15	1
1:A:357:GLU:HB3	1:A:367:LEU:HD11	0.46	1.86	8	2
1:C:379:LYS:O	1:C:383:GLU:HG3	0.46	2.11	18	1
1:C:331:TYR:CB	1:D:343:LEU:HD11	0.46	2.40	9	1
1:B:370:HIS:HA	1:B:373:LYS:HE2	0.46	1.88	15	1
1:A:356:ALA:O	1:A:360:ARG:HG2	0.46	2.10	7	1
1:B:354:ALA:O	1:B:358:VAL:HG23	0.46	2.11	14	12
1:A:350:MET:CG	1:A:374:LEU:HG	0.46	2.41	15	1
1:D:351:ILE:HA	1:D:374:LEU:HD23	0.46	1.88	5	1
1:B:357:GLU:OE1	1:B:357:GLU:HA	0.46	2.10	19	1
1:D:354:ALA:O	1:D:358:VAL:HG23	0.46	2.11	12	11
1:C:336:THR:HG22	1:D:331:TYR:O	0.46	2.11	15	3
1:D:370:HIS:HA	1:D:373:LYS:HE2	0.46	1.87	8	1
1:B:350:MET:SD	1:B:374:LEU:HD22	0.46	2.51	9	2
1:B:347:ILE:HD13	1:B:378:LYS:HA	0.46	1.87	10	1
1:C:338:PRO:HD2	1:C:342:TRP:CE3	0.45	2.46	6	5
1:A:347:ILE:HA	1:A:350:MET:SD	0.45	2.51	12	1
1:A:378:LYS:HG3	1:A:379:LYS:N	0.45	2.25	4	1
1:A:344:LEU:HD11	1:A:382:TYR:HA	0.45	1.87	11	2
1:B:348:GLU:O	1:B:352:LYS:HD3	0.45	2.11	11	1
1:C:325:ARG:HG2	1:C:331:TYR:CE1	0.45	2.46	1	1
1:B:352:LYS:HB3	1:C:352:LYS:HG2	0.45	1.88	2	1
1:A:359:LEU:HD22	1:D:351:ILE:HD12	0.45	1.89	14	1
1:C:347:ILE:HD13	1:C:378:LYS:HA	0.45	1.87	13	1
1:A:347:ILE:HG12	1:A:377:LEU:CD2	0.45	2.40	2	1
1:A:353:GLU:HB3	1:B:345:GLN:HE21	0.45	1.72	10	1
1:C:331:TYR:O	1:D:336:THR:HG22	0.45	2.12	14	2
1:C:340:LYS:HB3	1:C:384:LEU:HD11	0.45	1.88	4	1
1:A:343:LEU:HD11	1:B:331:TYR:CB	0.45	2.40	19	1
1:A:378:LYS:HE2	1:A:382:TYR:HE2	0.45	1.71	12	1
1:A:347:ILE:O	1:A:350:MET:HG2	0.45	2.11	12	1
1:A:325:ARG:HG3	1:A:331:TYR:CE1	0.45	2.46	15	2
1:C:347:ILE:O	1:C:350:MET:HG2	0.45	2.12	5	2
1:A:343:LEU:HD12	1:B:331:TYR:HB3	0.45	1.88	17	1
1:A:330:ASP:CB	1:B:338:PRO:HA	0.45	2.42	5	1
1:A:352:LYS:HB3	1:D:352:LYS:HB3	0.45	1.88	5	1
1:A:330:ASP:OD2	1:B:336:THR:HB	0.45	2.12	8	1
1:A:338:PRO:HA	1:B:330:ASP:CB	0.45	2.42	15	1
1:A:351:ILE:HG12	1:A:374:LEU:CB	0.45	2.42	7	2
1:C:335:ILE:HD11	1:D:333:LEU:HD23	0.44	1.88	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:324:SER:HA	1:B:384:LEU:HD11	0.44	1.89	9	1
1:D:333:LEU:HD11	1:D:335:ILE:HG23	0.44	1.89	12	1
1:C:324:SER:HA	1:D:384:LEU:HD21	0.44	1.89	5	1
1:B:381:ALA:HA	1:B:384:LEU:HD12	0.44	1.87	2	1
1:A:339:ASN:HB2	1:A:342:TRP:CD2	0.44	2.48	20	1
1:A:380:ARG:HA	1:A:380:ARG:HH11	0.44	1.72	20	1
1:C:350:MET:HG3	1:C:374:LEU:CD2	0.44	2.42	20	1
1:A:331:TYR:HE2	1:B:340:LYS:HD3	0.44	1.73	20	1
1:B:348:GLU:HG3	1:B:352:LYS:HE3	0.44	1.89	11	1
1:B:364:GLN:HG3	1:B:367:LEU:HB2	0.44	1.89	1	1
1:B:325:ARG:HH11	1:B:325:ARG:HG3	0.44	1.72	4	1
1:C:340:LYS:HE2	1:C:344:LEU:HD23	0.44	1.89	15	1
1:C:353:GLU:HB3	1:D:345:GLN:HE21	0.44	1.72	10	1
1:B:325:ARG:HA	1:B:330:ASP:O	0.44	2.13	5	3
1:A:352:LYS:HB3	1:D:352:LYS:HG3	0.44	1.88	18	1
1:A:351:ILE:HA	1:A:374:LEU:HD23	0.44	1.90	15	1
1:C:350:MET:HG2	1:C:374:LEU:CG	0.44	2.42	7	1
1:C:361:ASN:HB3	1:C:364:GLN:HB2	0.43	1.90	16	3
1:D:381:ALA:O	1:D:384:LEU:HB2	0.43	2.13	15	2
1:C:377:LEU:HD13	1:D:321:TRP:HE3	0.43	1.72	11	2
1:A:374:LEU:HG	1:B:321:TRP:HH2	0.43	1.73	18	1
1:A:375:LEU:HD11	1:D:359:LEU:HD21	0.43	1.89	11	1
1:C:357:GLU:OE1	1:C:357:GLU:HA	0.43	2.14	16	2
1:B:348:GLU:O	1:B:351:ILE:HG22	0.43	2.14	3	4
1:C:350:MET:HB3	1:D:346:SER:CB	0.43	2.43	12	1
1:B:347:ILE:O	1:B:350:MET:HG2	0.43	2.13	11	1
1:D:347:ILE:HG21	1:D:378:LYS:HB2	0.43	1.90	14	1
1:A:331:TYR:CE1	1:B:384:LEU:HB3	0.43	2.48	5	1
1:C:365:GLU:O	1:C:369:ARG:HG2	0.43	2.13	9	2
1:D:356:ALA:O	1:D:360:ARG:HD3	0.43	2.12	19	1
1:C:343:LEU:HD11	1:D:331:TYR:CB	0.43	2.43	8	3
1:C:347:ILE:HG21	1:C:378:LYS:HB2	0.43	1.90	20	3
1:A:346:SER:HA	1:B:350:MET:HB2	0.43	1.90	9	1
1:C:374:LEU:HD13	1:D:321:TRP:CZ3	0.43	2.49	4	3
1:A:321:TRP:CD2	1:B:373:LYS:HD2	0.43	2.48	4	1
1:B:352:LYS:HG3	1:C:353:GLU:HA	0.43	1.90	11	1
1:B:359:LEU:HD13	1:C:358:VAL:HG11	0.42	1.91	2	1
1:C:370:HIS:HA	1:C:373:LYS:HE2	0.42	1.91	18	1
1:B:340:LYS:HG2	1:B:340:LYS:H	0.42	1.47	5	1
1:C:340:LYS:HE2	1:C:384:LEU:O	0.42	2.14	14	1
1:A:321:TRP:CE3	1:B:377:LEU:HD13	0.42	2.49	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:D:340:LYS:H	1:D:340:LYS:HG3	0.42	1.42	20	2
1:A:345:GLN:NE2	1:B:353:GLU:HB3	0.42	2.29	16	1
1:A:374:LEU:CD1	1:B:321:TRP:HZ3	0.42	2.27	5	1
1:C:350:MET:HB3	1:D:346:SER:HA	0.42	1.90	11	1
1:A:345:GLN:HE22	1:B:357:GLU:HG3	0.42	1.74	13	1
1:D:340:LYS:HE2	1:D:384:LEU:HB3	0.42	1.92	13	1
1:D:320:GLU:HB2	1:D:336:THR:OG1	0.42	2.15	15	1
1:C:321:TRP:HA	1:C:334:ALA:O	0.42	2.15	12	1
1:C:326:THR:HG22	1:C:332:ARG:HB2	0.41	1.92	12	1
1:A:375:LEU:HD11	1:D:359:LEU:HD11	0.41	1.91	2	1
1:C:374:LEU:HG	1:D:321:TRP:CH2	0.41	2.50	2	1
1:A:340:LYS:HG2	1:A:341:GLU:OE1	0.41	2.15	19	1
1:D:350:MET:HG2	1:D:350:MET:H	0.41	1.47	20	2
1:D:344:LEU:HA	1:D:344:LEU:HD13	0.41	1.77	5	1
1:B:333:LEU:HD11	1:B:335:ILE:HG23	0.41	1.92	9	1
1:A:323:VAL:HG12	1:B:380:ARG:HD3	0.41	1.92	19	1
1:C:338:PRO:HA	1:D:330:ASP:CB	0.41	2.45	1	1
1:C:373:LYS:HD2	1:D:321:TRP:CE2	0.41	2.51	17	1
1:C:321:TRP:CE2	1:D:373:LYS:HD2	0.41	2.51	13	1
1:B:351:ILE:HD13	1:B:374:LEU:HB2	0.41	1.92	1	1
1:D:350:MET:H	1:D:350:MET:HG2	0.41	1.48	9	1
1:A:357:GLU:OE1	1:A:357:GLU:HA	0.41	2.16	9	1
1:A:350:MET:SD	1:A:374:LEU:HD22	0.41	2.55	19	1
1:C:353:GLU:HB3	1:D:345:GLN:NE2	0.41	2.30	15	1
1:C:340:LYS:HG2	1:C:340:LYS:H	0.41	1.41	4	1
1:C:350:MET:H	1:C:350:MET:HG2	0.41	1.47	10	1
1:A:331:TYR:HB2	1:B:337:CYS:O	0.41	2.16	19	1
1:A:350:MET:SD	1:A:374:LEU:HD11	0.41	2.55	17	2
1:C:344:LEU:HD13	1:C:344:LEU:HA	0.41	1.74	15	1
1:C:337:CYS:SG	1:C:343:LEU:HG	0.41	2.56	3	1
1:A:325:ARG:HG3	1:A:331:TYR:CE2	0.41	2.51	8	1
1:A:384:LEU:HD21	1:B:331:TYR:CE1	0.41	2.50	6	1
1:B:320:GLU:HG3	1:B:336:THR:HG21	0.41	1.91	16	1
1:B:355:ALA:HB2	1:C:359:LEU:HD22	0.41	1.92	2	1
1:D:320:GLU:HG2	1:D:336:THR:HG21	0.41	1.90	18	1
1:C:337:CYS:HB2	1:C:343:LEU:HD23	0.41	1.91	1	1
1:D:361:ASN:HB3	1:D:364:GLN:HB2	0.41	1.93	10	1
1:C:334:ALA:HA	1:D:333:LEU:O	0.41	2.15	6	1
1:B:325:ARG:HG2	1:B:331:TYR:CE1	0.41	2.50	4	1
1:A:344:LEU:HA	1:A:344:LEU:HD13	0.41	1.75	4	1
1:A:350:MET:H	1:A:350:MET:HG2	0.41	1.53	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:333:LEU:HD11	1:C:335:ILE:HG23	0.41	1.92	7	1
1:B:337:CYS:HB2	1:B:343:LEU:HG	0.41	1.93	2	1
1:B:357:GLU:HA	1:B:357:GLU:OE1	0.41	2.16	4	1
1:C:384:LEU:HD11	1:D:323:VAL:HG22	0.41	1.93	13	1
1:B:361:ASN:HB3	1:B:364:GLN:HB2	0.41	1.93	13	1
1:B:343:LEU:HA	1:B:343:LEU:HD23	0.41	1.74	1	2
1:A:351:ILE:CG1	1:A:374:LEU:HB2	0.40	2.45	19	1
1:A:353:GLU:HA	1:D:352:LYS:HD2	0.40	1.91	18	1
1:D:378:LYS:HE3	1:D:382:TYR:CE2	0.40	2.50	7	1
1:B:343:LEU:HD22	1:B:343:LEU:HA	0.40	1.79	7	1
1:D:340:LYS:H	1:D:340:LYS:HG2	0.40	1.56	5	1
1:B:351:ILE:HB	1:B:374:LEU:CB	0.40	2.47	4	1
1:A:350:MET:CB	1:B:346:SER:HA	0.40	2.46	20	1
1:C:349:GLY:O	1:C:353:GLU:HG2	0.40	2.16	6	1
1:A:348:GLU:HG2	1:A:378:LYS:HG3	0.40	1.93	5	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	62/76 (82%)	59±1 (95±2%)	3±1 (5±2%)	0±0 (0±1%)	43	81
1	B	62/76 (82%)	59±1 (95±1%)	3±1 (5±1%)	0±0 (0±1%)	43	81
1	C	62/76 (82%)	59±1 (95±2%)	3±1 (4±2%)	0±0 (0±1%)	43	81
1	D	61/76 (80%)	58±1 (95±2%)	3±1 (5±1%)	0±1 (0±1%)	38	79
All	All	4940/6080 (81%)	4697 (95%)	222 (4%)	21 (0%)	43	81

All 11 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	330	ASP	3
1	D	330	ASP	3
1	A	330	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	C	330	ASP	2
1	C	384	LEU	2
1	D	384	LEU	2
1	A	384	LEU	2
1	D	321	TRP	1
1	B	384	LEU	1
1	C	321	TRP	1
1	B	321	TRP	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	55/64 (86%)	37±3 (67±6%)	18±3 (33±6%)	1	12
1	B	55/64 (86%)	37±3 (67±5%)	18±3 (33±5%)	1	12
1	C	55/64 (86%)	37±3 (68±5%)	18±3 (32±5%)	1	13
1	D	54/64 (84%)	35±1 (66±3%)	19±1 (34±3%)	1	11
All	All	4380/5120 (86%)	2918 (67%)	1462 (33%)	1	12

All 171 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	324	SER	20
1	D	382	TYR	20
1	D	330	ASP	20
1	B	332	ARG	20
1	D	332	ARG	19
1	D	380	ARG	19
1	C	330	ASP	19
1	B	380	ARG	19
1	C	332	ARG	19
1	A	380	ARG	19
1	A	332	ARG	19
1	A	359	LEU	19
1	B	351	ILE	19

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Mol	Chain	Res	Type	Models (Total)
1	C	359	LEU	18
1	B	382	TYR	18
1	A	382	TYR	18
1	B	324	SER	18
1	A	324	SER	18
1	D	351	ILE	18
1	D	379	LYS	18
1	A	351	ILE	17
1	C	324	SER	17
1	D	359	LEU	16
1	D	350	MET	16
1	C	380	ARG	16
1	A	340	LYS	16
1	B	359	LEU	16
1	B	340	LYS	16
1	B	330	ASP	16
1	A	379	LYS	15
1	A	330	ASP	15
1	C	336	THR	15
1	B	350	MET	15
1	C	382	TYR	15
1	C	379	LYS	15
1	C	325	ARG	15
1	C	351	ILE	14
1	C	340	LYS	14
1	A	350	MET	14
1	B	344	LEU	14
1	A	336	THR	13
1	B	373	LYS	13
1	B	379	LYS	13
1	B	352	LYS	13
1	D	340	LYS	13
1	D	384	LEU	12
1	A	352	LYS	12
1	C	350	MET	12
1	D	357	GLU	12
1	A	325	ARG	12
1	D	373	LYS	12
1	C	352	LYS	11
1	B	336	THR	11
1	C	361	ASN	11
1	A	345	GLN	11

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Mol	Chain	Res	Type	Models (Total)
1	C	343	LEU	11
1	A	361	ASN	11
1	C	344	LEU	11
1	B	384	LEU	11
1	B	357	GLU	10
1	D	367	LEU	10
1	D	336	THR	10
1	D	352	LYS	10
1	A	357	GLU	10
1	C	373	LYS	10
1	B	361	ASN	10
1	D	345	GLN	10
1	A	367	LEU	10
1	C	345	GLN	10
1	B	345	GLN	10
1	A	344	LEU	9
1	D	335	ILE	9
1	C	376	SER	9
1	A	374	LEU	9
1	D	376	SER	8
1	D	344	LEU	8
1	C	374	LEU	8
1	C	384	LEU	8
1	D	374	LEU	8
1	B	374	LEU	8
1	C	357	GLU	8
1	B	325	ARG	8
1	B	367	LEU	8
1	A	373	LYS	8
1	C	326	THR	8
1	D	343	LEU	8
1	A	384	LEU	7
1	A	383	GLU	7
1	A	326	THR	7
1	D	378	LYS	7
1	B	376	SER	7
1	D	325	ARG	7
1	A	341	GLU	7
1	D	366	ASN	6
1	C	348	GLU	6
1	A	343	LEU	6
1	B	343	LEU	6

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Mol	Chain	Res	Type	Models (Total)
1	C	367	LEU	6
1	D	361	ASN	6
1	D	341	GLU	6
1	B	348	GLU	6
1	B	378	LYS	6
1	A	369	ARG	5
1	B	326	THR	5
1	D	348	GLU	5
1	A	335	ILE	5
1	D	364	GLN	5
1	C	341	GLU	5
1	B	364	GLN	5
1	A	322	ASN	5
1	C	364	GLN	4
1	C	378	LYS	4
1	A	365	GLU	4
1	B	365	GLU	4
1	C	335	ILE	4
1	C	366	ASN	4
1	A	364	GLN	4
1	B	369	ARG	4
1	A	376	SER	4
1	C	320	GLU	4
1	C	363	ASN	4
1	C	331	TYR	4
1	D	363	ASN	4
1	B	335	ILE	4
1	A	378	LYS	4
1	B	341	GLU	4
1	D	365	GLU	4
1	D	320	GLU	3
1	D	383	GLU	3
1	A	348	GLU	3
1	B	339	ASN	3
1	C	383	GLU	3
1	A	331	TYR	3
1	D	322	ASN	3
1	B	322	ASN	3
1	C	369	ARG	3
1	D	360	ARG	3
1	D	369	ARG	3
1	B	360	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	B	363	ASN	3
1	B	368	ARG	3
1	B	320	GLU	3
1	B	383	GLU	3
1	C	360	ARG	3
1	D	331	TYR	3
1	A	320	GLU	3
1	A	337	CYS	3
1	A	339	ASN	3
1	A	360	ARG	3
1	A	363	ASN	2
1	C	365	GLU	2
1	D	372	ASN	2
1	A	323	VAL	2
1	B	331	TYR	2
1	B	346	SER	2
1	D	368	ARG	2
1	B	366	ASN	2
1	C	322	ASN	2
1	B	323	VAL	2
1	C	368	ARG	2
1	A	366	ASN	2
1	A	346	SER	1
1	C	337	CYS	1
1	D	337	CYS	1
1	D	346	SER	1
1	A	372	ASN	1
1	D	323	VAL	1
1	D	339	ASN	1
1	C	333	LEU	1
1	A	368	ARG	1
1	C	339	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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