



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:23 AM BST

PDB ID : 2MW4  
Title : Tetramerization domain of the Ciona intestinalis p53/p73-b transcription factor protein  
Authors : Heering, J.P.; Jonker, H.R.A.; Loehr, F.; Schwalbe, H.; Doetsch, V.  
Deposited on : 2014-10-27

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/NMRValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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

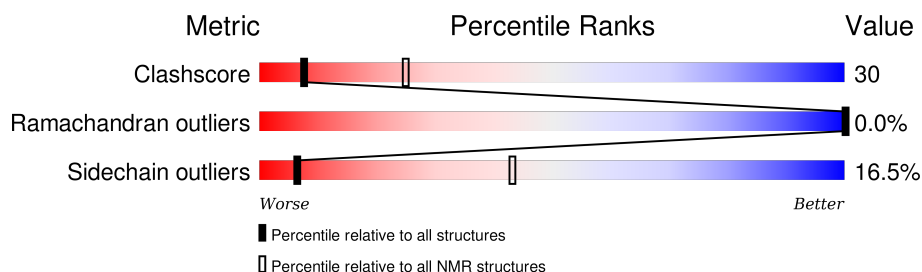
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 22%.

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	47	<div> <div>36%</div> <div>51%</div> <div>9%</div> <div>.</div> </div>
1	B	47	<div> <div>40%</div> <div>49%</div> <div>11%</div> </div>
1	C	47	<div> <div>38%</div> <div>51%</div> <div>11%</div> </div>
1	D	47	<div> <div>38%</div> <div>53%</div> <div>9%</div> </div>

## 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:105-A:149, B:203-B:249, C:303-C:349, D:403-D:449 (186)	0.24	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 4 clusters and 3 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3140 atoms, of which 1592 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription factor protein.

Mol	Chain	Residues	Atoms						Trace
1	A	47	Total	C	H	N	O	S	0
			785	243	398	68	74	2	
1	B	47	Total	C	H	N	O	S	0
			785	243	398	68	74	2	
1	C	47	Total	C	H	N	O	S	0
			785	243	398	68	74	2	
1	D	47	Total	C	H	N	O	S	0
			785	243	398	68	74	2	

There are 4 discrepancies between the modelled and reference sequences:

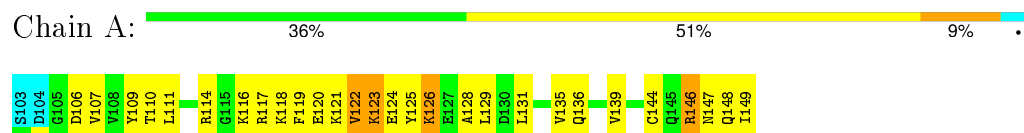
Chain	Residue	Modelled	Actual	Comment	Reference
A	103	SER	-	EXPRESSION TAG	UNP Q4H2Z8
B	203	SER	-	EXPRESSION TAG	UNP Q4H2Z8
C	303	SER	-	EXPRESSION TAG	UNP Q4H2Z8
D	403	SER	-	EXPRESSION TAG	UNP Q4H2Z8

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

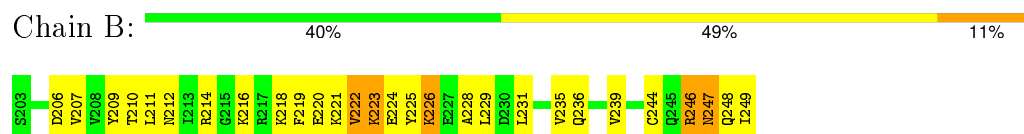
### 4.1 Average score per residue in the NMR ensemble

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

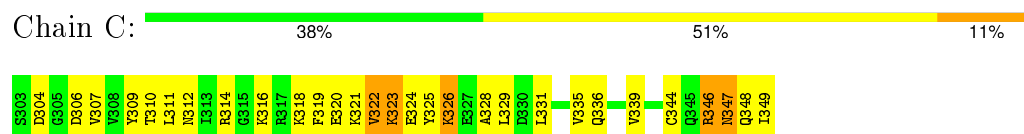
- Molecule 1: Transcription factor protein



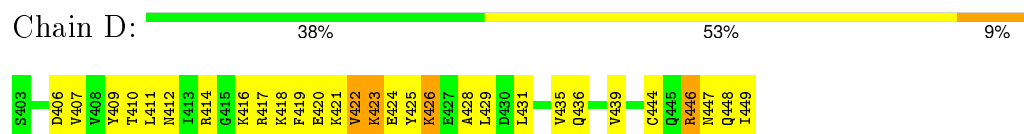
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

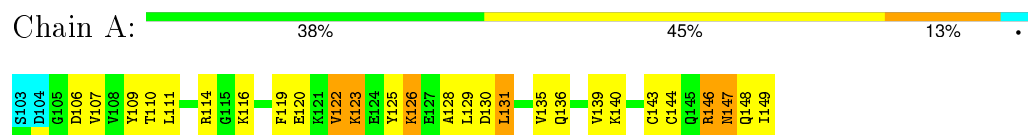


### 4.2 Scores per residue for each member of the ensemble

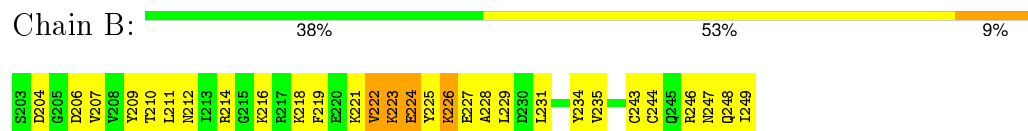
Colouring as in section 4.1 above.

### 4.2.1 Score per residue for model 1

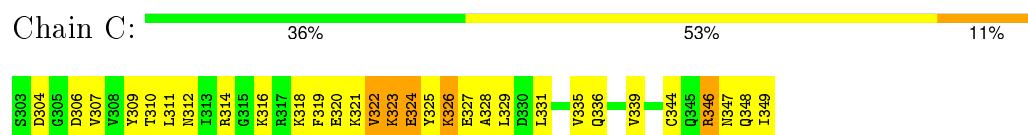
- Molecule 1: Transcription factor protein



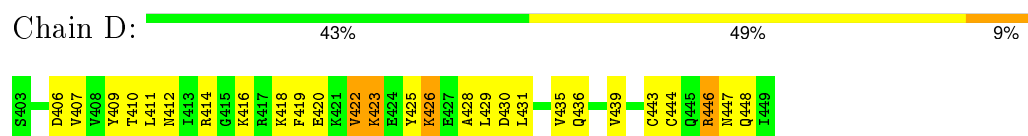
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

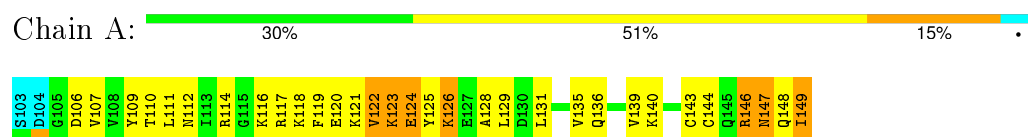


- Molecule 1: Transcription factor protein

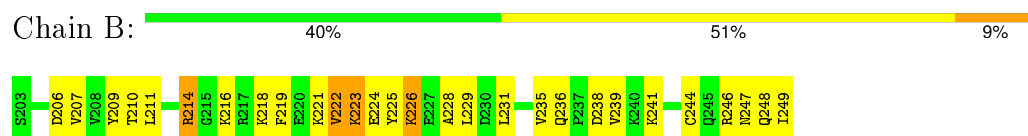


### 4.2.2 Score per residue for model 2

- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein





- Molecule 1: Transcription factor protein



#### 4.2.3 Score per residue for model 3

- Molecule 1: Transcription factor protein



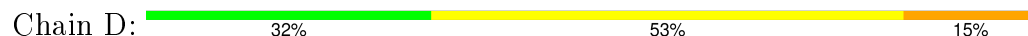
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

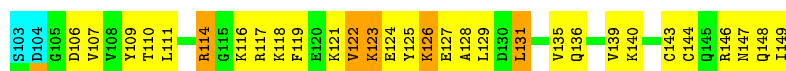


- Molecule 1: Transcription factor protein

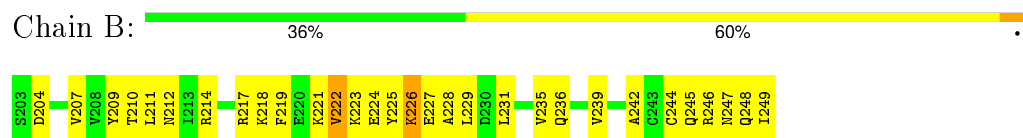


#### 4.2.4 Score per residue for model 4

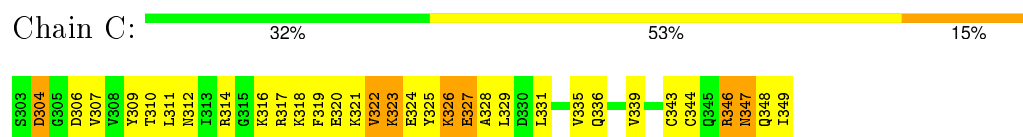
- Molecule 1: Transcription factor protein



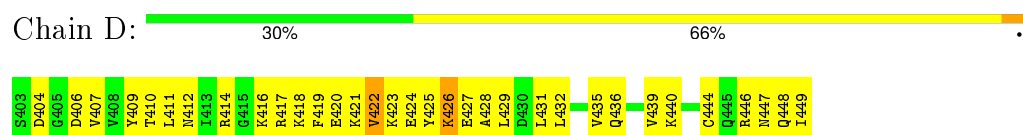
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

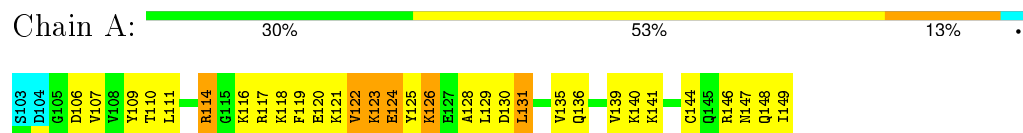


- Molecule 1: Transcription factor protein

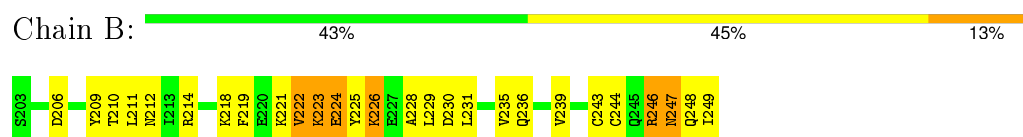


#### 4.2.5 Score per residue for model 5

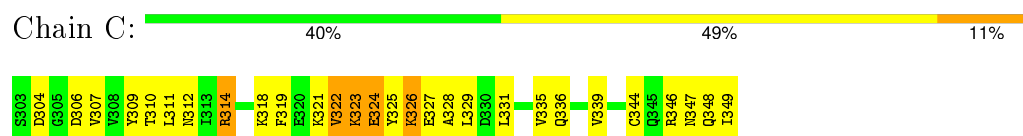
- Molecule 1: Transcription factor protein



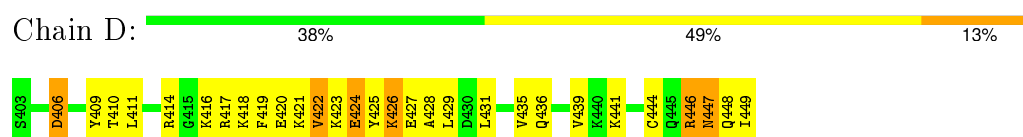
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



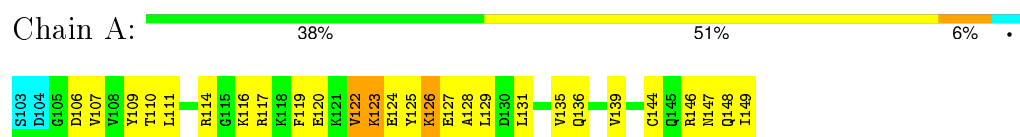
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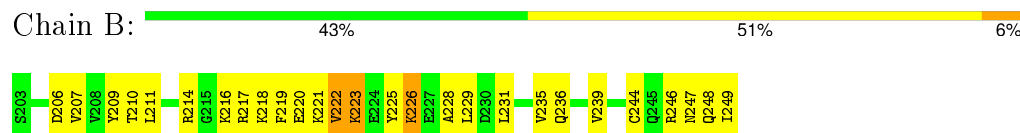


### 4.2.6 Score per residue for model 6

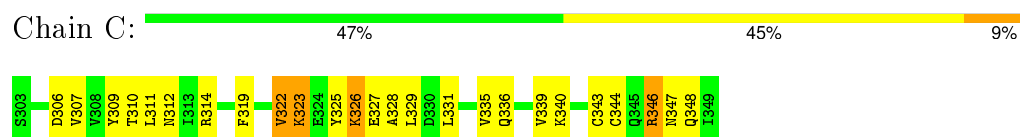
- Molecule 1: Transcription factor protein



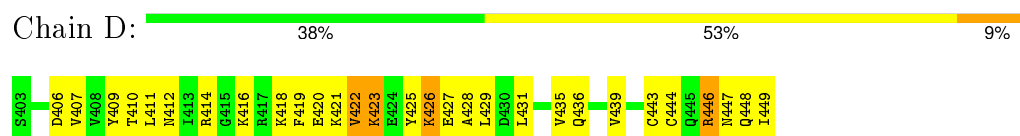
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

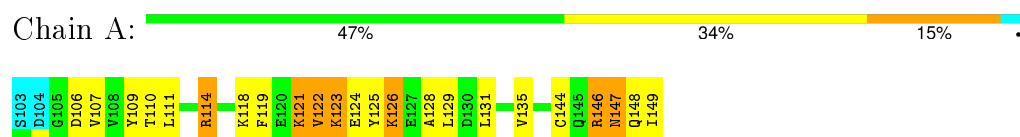


- Molecule 1: Transcription factor protein

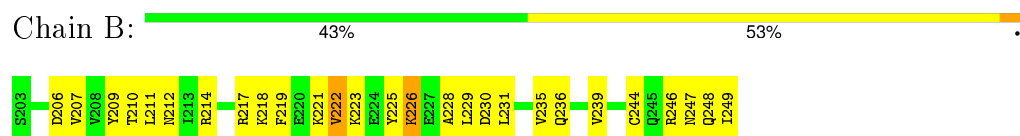


### 4.2.7 Score per residue for model 7

- Molecule 1: Transcription factor protein

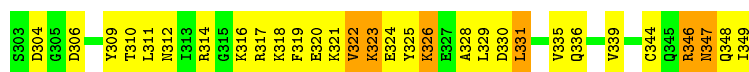


- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



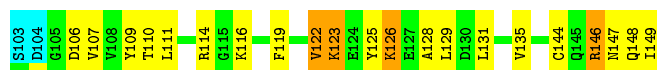


- Molecule 1: Transcription factor protein



#### 4.2.8 Score per residue for model 8

- Molecule 1: Transcription factor protein



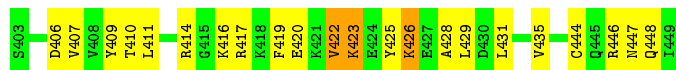
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

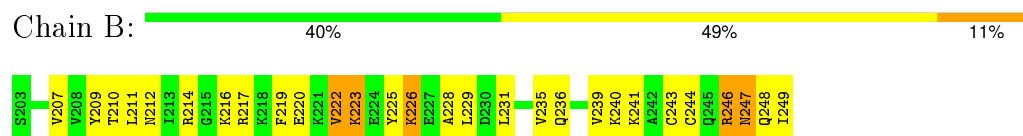


#### 4.2.9 Score per residue for model 9

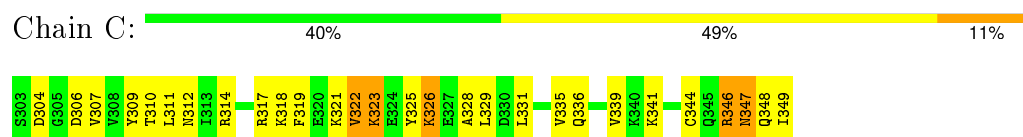
- Molecule 1: Transcription factor protein



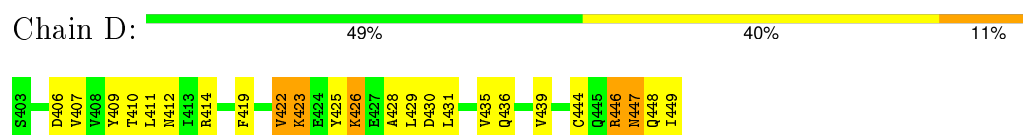
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

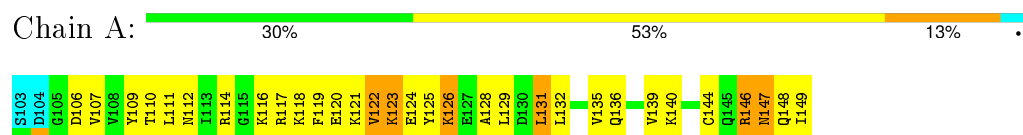


- Molecule 1: Transcription factor protein

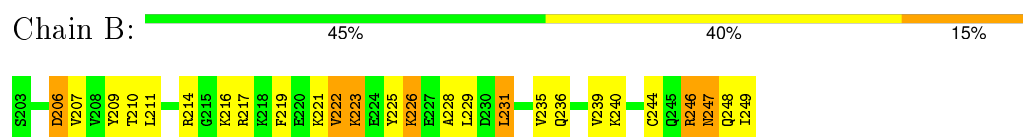


#### 4.2.10 Score per residue for model 10

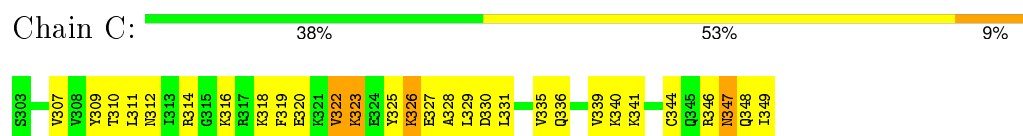
- Molecule 1: Transcription factor protein



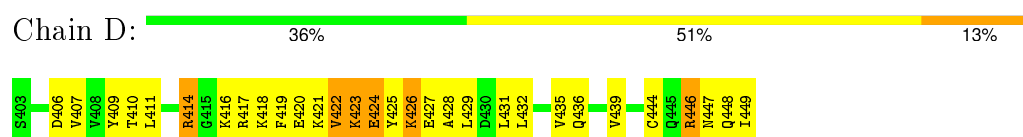
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

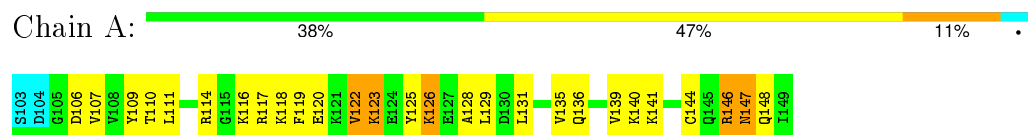


- Molecule 1: Transcription factor protein

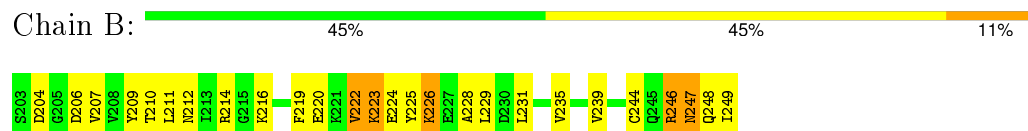


### 4.2.11 Score per residue for model 11

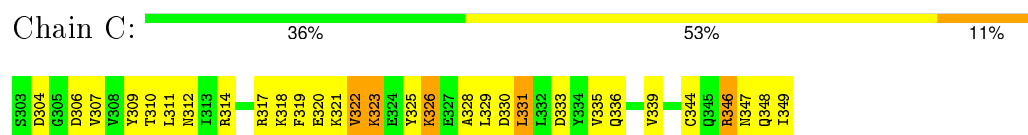
- Molecule 1: Transcription factor protein



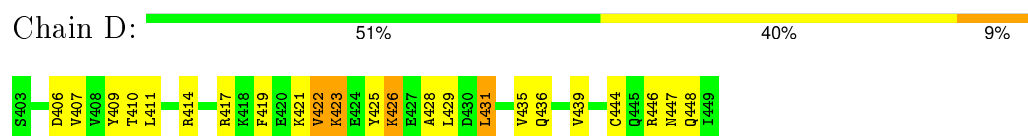
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

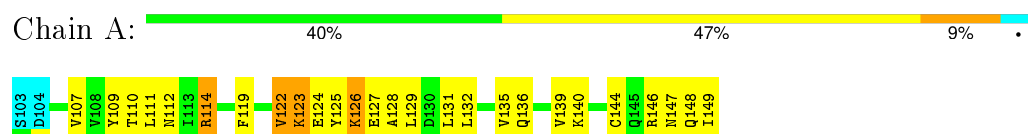


- Molecule 1: Transcription factor protein

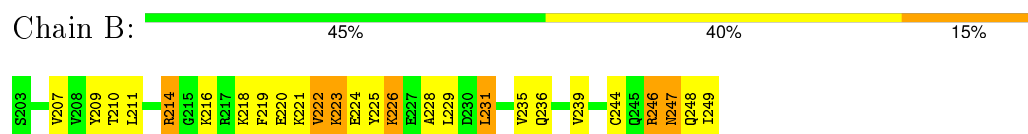


### 4.2.12 Score per residue for model 12

- Molecule 1: Transcription factor protein

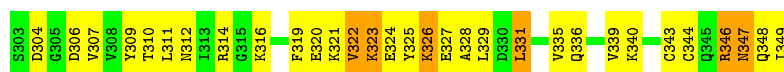


- Molecule 1: Transcription factor protein

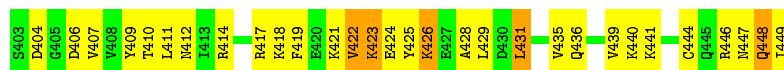


- Molecule 1: Transcription factor protein



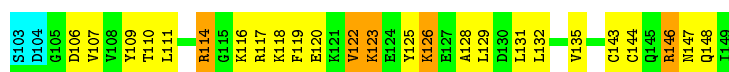


- Molecule 1: Transcription factor protein



#### 4.2.13 Score per residue for model 13

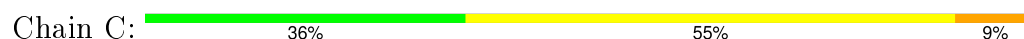
- Molecule 1: Transcription factor protein



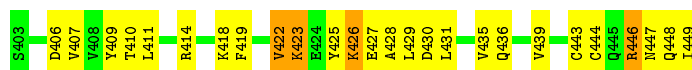
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

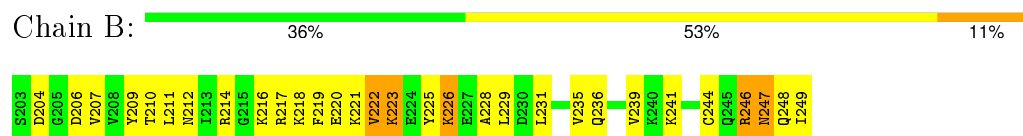


#### 4.2.14 Score per residue for model 14

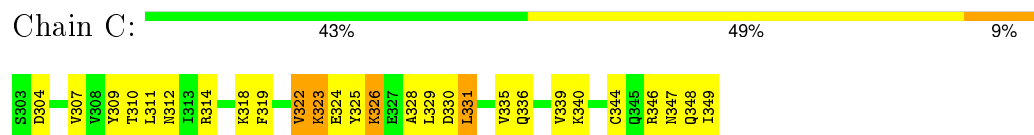
- Molecule 1: Transcription factor protein



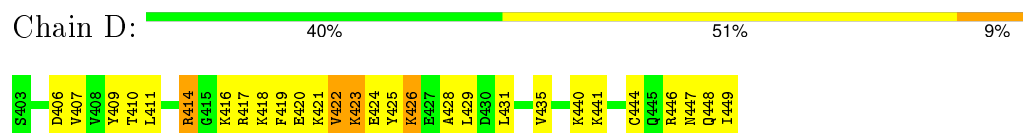
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

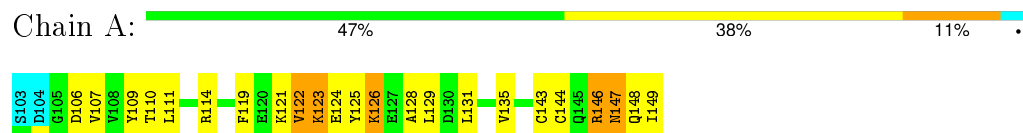


- Molecule 1: Transcription factor protein

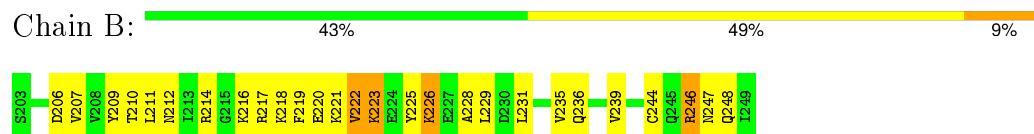


#### 4.2.15 Score per residue for model 15

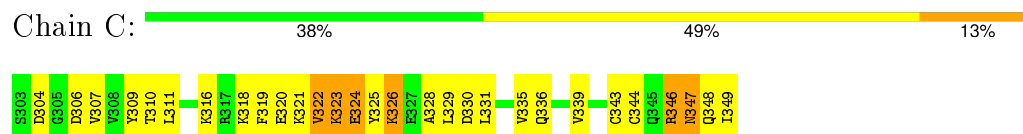
- Molecule 1: Transcription factor protein



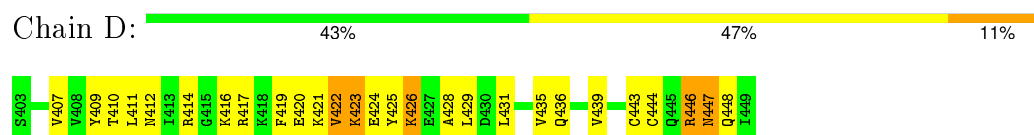
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



### 4.2.16 Score per residue for model 16

- Molecule 1: Transcription factor protein

Chain A: 

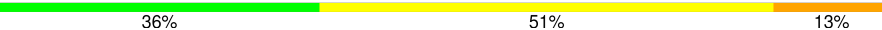


- Molecule 1: Transcription factor protein

Chain B: 



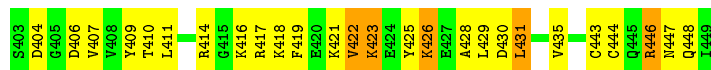
- Molecule 1: Transcription factor protein

Chain C: 



- Molecule 1: Transcription factor protein

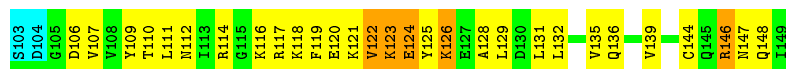
Chain D: 



### 4.2.17 Score per residue for model 17

- Molecule 1: Transcription factor protein

Chain A: 



- Molecule 1: Transcription factor protein

Chain B: 



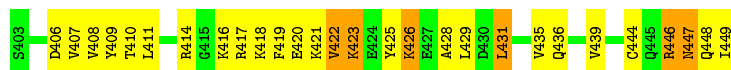
- Molecule 1: Transcription factor protein

Chain C: 



- Molecule 1: Transcription factor protein

Chain D: 40% 47% 13%



#### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Transcription factor protein

Chain A: 38% 47% 11%



- Molecule 1: Transcription factor protein

Chain B: 45% 47% 9%



- Molecule 1: Transcription factor protein

Chain C: 60% 28% 13%



- Molecule 1: Transcription factor protein

Chain D: 53% 40% 6%



#### 4.2.19 Score per residue for model 19

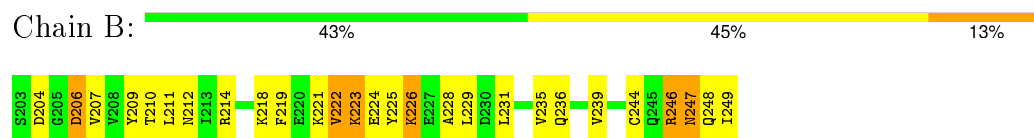
- Molecule 1: Transcription factor protein

Chain A: 43% 40% 13%

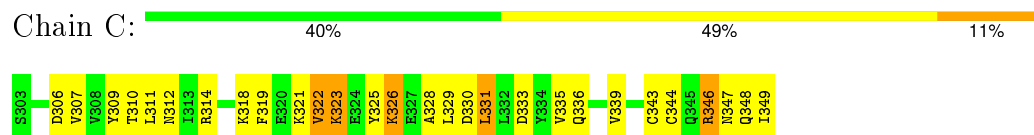




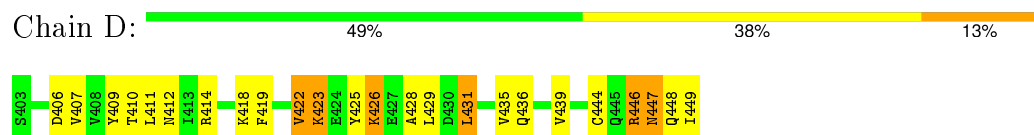
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein

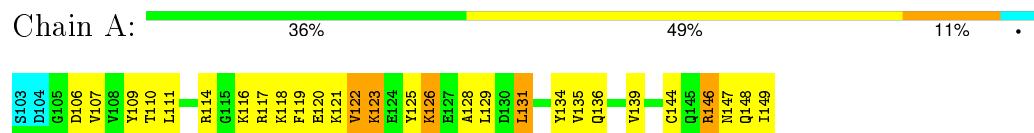


- Molecule 1: Transcription factor protein

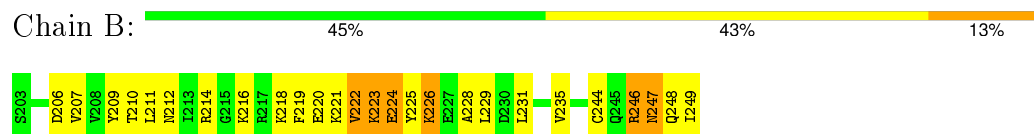


#### 4.2.20 Score per residue for model 20

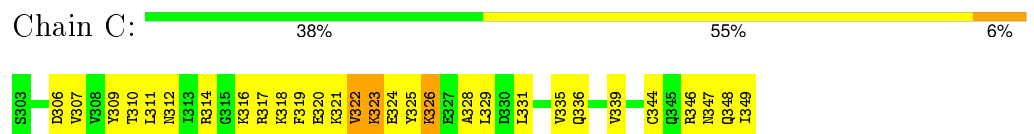
- Molecule 1: Transcription factor protein



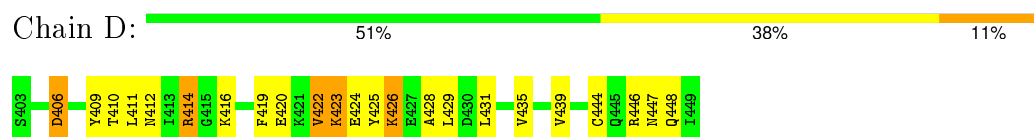
- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



- Molecule 1: Transcription factor protein



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	3.9
CNS	structure solution	1.1
ARIA	structure solution	1.2
ARIA	refinement	1.2

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	2mw4_cs.str
Number of chemical shift lists	1
Total number of shifts	611
Number of shifts mapped to atoms	611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	22%

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	373	387	387	40±4
1	B	387	398	395	38±3
1	C	387	398	395	41±4
1	D	387	398	395	39±5
All	All	30680	31620	31440	1844

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 30.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:235:VAL:HG11	1:D:435:VAL:HG11	0.78	1.55	1	20
1:B:228:ALA:HB1	1:D:428:ALA:HB1	0.76	1.58	12	20
1:A:135:VAL:HG11	1:C:335:VAL:HG11	0.75	1.59	5	20
1:A:128:ALA:HB1	1:C:328:ALA:HB1	0.74	1.59	9	20
1:C:322:VAL:HG12	1:D:422:VAL:HG12	0.73	1.58	9	20
1:A:124:GLU:HG2	1:D:421:LYS:HD3	0.71	1.60	10	10
1:C:329:LEU:HD12	1:D:422:VAL:HG22	0.68	1.64	5	19
1:A:121:LYS:HD3	1:D:424:GLU:HG2	0.68	1.64	10	7
1:A:146:ARG:CZ	1:A:147:ASN:HB3	0.68	2.19	13	13
1:A:122:VAL:HG12	1:B:222:VAL:HG12	0.67	1.67	3	20
1:A:129:LEU:HD12	1:B:222:VAL:HG22	0.66	1.66	1	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:228:ALA:HB1	1:D:428:ALA:CB	0.66	2.21	12	20
1:C:346:ARG:CZ	1:C:347:ASN:HB3	0.66	2.20	13	11
1:A:128:ALA:HB1	1:C:328:ALA:CB	0.65	2.21	10	20
1:C:322:VAL:HG22	1:D:429:LEU:HD12	0.65	1.68	12	19
1:C:310:THR:HG23	1:D:410:THR:HG23	0.65	1.68	18	20
1:A:128:ALA:CB	1:C:328:ALA:HB1	0.64	2.23	8	20
1:B:228:ALA:CB	1:D:428:ALA:HB1	0.64	2.22	6	20
1:A:122:VAL:HG22	1:B:229:LEU:HD12	0.64	1.69	11	20
1:D:446:ARG:CZ	1:D:447:ASN:HB3	0.63	2.23	13	9
1:D:444:CYS:HA	1:D:448:GLN:HB3	0.62	1.71	2	20
1:D:444:CYS:HA	1:D:448:GLN:CB	0.62	2.24	2	9
1:A:110:THR:HG23	1:B:210:THR:HG23	0.62	1.72	13	20
1:A:119:PHE:CD2	1:B:209:TYR:HB3	0.62	2.30	18	13
1:D:423:LYS:O	1:D:426:LYS:HG3	0.62	1.94	9	19
1:B:246:ARG:CZ	1:B:247:ASN:HB3	0.62	2.25	12	12
1:C:344:CYS:HA	1:C:348:GLN:HB3	0.61	1.72	4	20
1:B:223:LYS:O	1:B:226:LYS:HG3	0.61	1.95	7	20
1:B:224:GLU:HG2	1:C:321:LYS:HD3	0.60	1.71	1	6
1:C:323:LYS:O	1:C:326:LYS:HG3	0.60	1.96	9	18
1:B:244:CYS:HA	1:B:248:GLN:HB3	0.60	1.73	12	20
1:C:319:PHE:CD2	1:D:409:TYR:HB3	0.60	2.31	15	8
1:B:221:LYS:HD3	1:C:324:GLU:HG2	0.60	1.71	1	7
1:A:144:CYS:HA	1:A:148:GLN:HB3	0.59	1.74	17	20
1:A:109:TYR:HB3	1:B:219:PHE:CD2	0.59	2.33	9	8
1:C:319:PHE:CD1	1:D:409:TYR:HB3	0.59	2.33	14	12
1:C:309:TYR:HB3	1:D:419:PHE:CD2	0.58	2.33	20	11
1:A:119:PHE:CD1	1:B:209:TYR:HB3	0.58	2.33	15	7
1:A:123:LYS:O	1:A:126:LYS:HG3	0.57	2.00	10	20
1:D:446:ARG:HD3	1:D:447:ASN:OD1	0.57	1.99	3	4
1:A:146:ARG:HD3	1:A:147:ASN:OD1	0.57	1.99	9	6
1:A:109:TYR:HB3	1:B:219:PHE:CD1	0.57	2.35	17	12
1:A:134:TYR:CD1	1:C:346:ARG:HD2	0.57	2.35	20	1
1:A:114:ARG:HG3	1:D:449:ILE:HD11	0.56	1.77	4	6
1:B:246:ARG:HD3	1:B:247:ASN:OD1	0.56	2.00	15	1
1:C:344:CYS:HA	1:C:348:GLN:CB	0.56	2.30	6	6
1:C:340:LYS:HZ3	1:C:340:LYS:HB3	0.56	1.61	10	1
1:B:234:TYR:CD1	1:D:446:ARG:HD2	0.56	2.36	1	1
1:B:244:CYS:HA	1:B:248:GLN:CB	0.56	2.31	15	7
1:A:116:LYS:HB3	1:B:204:ASP:HB3	0.55	1.78	8	9
1:A:135:VAL:CG1	1:C:335:VAL:HG11	0.55	2.30	5	20
1:C:346:ARG:HD3	1:C:347:ASN:OD1	0.55	2.02	1	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:309:TYR:HB3	1:D:419:PHE:CD1	0.54	2.37	5	9
1:C:340:LYS:HZ2	1:C:340:LYS:HB3	0.54	1.62	12	1
1:A:126:LYS:HG2	1:B:211:LEU:HD11	0.54	1.80	8	20
1:B:235:VAL:HG11	1:D:435:VAL:CG1	0.54	2.33	20	20
1:A:125:TYR:CD1	1:C:325:TYR:CD1	0.54	2.96	19	20
1:C:317:ARG:HH11	1:C:317:ARG:HG3	0.54	1.62	20	1
1:B:225:TYR:CD1	1:D:425:TYR:CD1	0.54	2.96	7	20
1:C:314:ARG:HG2	1:D:406:ASP:C	0.53	2.23	4	15
1:B:214:ARG:HG3	1:C:349:ILE:HD11	0.53	1.80	10	6
1:A:121:LYS:HB3	1:B:225:TYR:OH	0.53	2.03	7	9
1:A:135:VAL:HG11	1:C:335:VAL:CG1	0.53	2.33	9	20
1:A:111:LEU:HD11	1:B:226:LYS:HG2	0.53	1.81	5	20
1:B:243:CYS:SG	1:D:431:LEU:HD22	0.53	2.44	5	5
1:D:417:ARG:HD3	1:D:420:GLU:OE2	0.52	2.03	8	1
1:C:326:LYS:HG2	1:D:411:LEU:HD11	0.52	1.81	16	19
1:C:321:LYS:HD2	1:D:429:LEU:HD22	0.52	1.80	7	1
1:B:235:VAL:CG1	1:D:435:VAL:HG11	0.52	2.31	8	20
1:B:231:LEU:HD22	1:D:443:CYS:SG	0.52	2.44	13	6
1:C:317:ARG:HD3	1:C:320:GLU:OE1	0.52	2.04	2	4
1:A:149:ILE:HD11	1:D:414:ARG:HG3	0.52	1.80	7	7
1:A:149:ILE:HB	1:D:412:ASN:HB2	0.52	1.82	2	2
1:B:236:GLN:O	1:B:239:VAL:HG22	0.52	2.05	10	13
1:A:114:ARG:HG2	1:B:206:ASP:HA	0.51	1.82	17	12
1:A:144:CYS:HA	1:A:148:GLN:CB	0.51	2.34	2	9
1:C:306:ASP:C	1:D:414:ARG:HG2	0.51	2.25	2	15
1:A:119:PHE:CE1	1:B:211:LEU:HD13	0.51	2.40	15	4
1:A:106:ASP:C	1:B:214:ARG:HG2	0.51	2.25	5	18
1:A:143:CYS:SG	1:C:331:LEU:HD22	0.51	2.46	13	9
1:B:216:LYS:O	1:B:220:GLU:HG3	0.51	2.06	12	11
1:C:321:LYS:HB3	1:D:425:TYR:OH	0.50	2.06	3	10
1:A:129:LEU:HB3	1:B:218:LYS:HG3	0.50	1.83	14	11
1:A:136:GLN:O	1:A:139:VAL:HG22	0.50	2.05	1	13
1:C:311:LEU:HD11	1:D:426:LYS:HG2	0.50	1.82	14	20
1:B:249:ILE:HB	1:C:312:ASN:O	0.50	2.06	17	17
1:A:148:GLN:HG3	1:C:330:ASP:OD2	0.50	2.07	15	7
1:A:118:LYS:O	1:A:122:VAL:HG23	0.50	2.07	2	6
1:C:316:LYS:O	1:C:320:GLU:HG3	0.50	2.06	3	10
1:A:131:LEU:HD22	1:C:343:CYS:SG	0.50	2.47	18	8
1:A:129:LEU:CD1	1:B:222:VAL:HG22	0.50	2.37	15	13
1:A:114:ARG:HG2	1:B:206:ASP:C	0.50	2.27	2	9
1:B:235:VAL:HG21	1:D:431:LEU:HD12	0.50	1.83	19	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:VAL:HG22	1:B:229:LEU:CD1	0.50	2.37	7	9
1:C:314:ARG:HG2	1:D:406:ASP:HA	0.50	1.84	16	11
1:A:146:ARG:NE	1:A:147:ASN:HB3	0.50	2.22	16	4
1:C:306:ASP:HA	1:D:414:ARG:HG2	0.49	1.84	19	13
1:A:148:GLN:HG2	1:A:149:ILE:N	0.49	2.23	5	2
1:B:217:ARG:O	1:B:221:LYS:HG3	0.49	2.08	4	8
1:A:131:LEU:HD12	1:C:335:VAL:HG21	0.49	1.84	19	16
1:D:416:LYS:O	1:D:420:GLU:HG3	0.49	2.08	14	11
1:A:148:GLN:OE1	1:C:327:GLU:HA	0.49	2.08	12	1
1:B:248:GLN:HG3	1:D:430:ASP:OD2	0.49	2.08	9	5
1:C:318:LYS:HG3	1:D:429:LEU:HB3	0.49	1.85	1	13
1:A:149:ILE:HB	1:D:412:ASN:O	0.49	2.07	2	11
1:B:246:ARG:NE	1:B:247:ASN:HB3	0.49	2.23	5	6
1:A:116:LYS:O	1:A:120:GLU:HG3	0.49	2.07	1	12
1:A:121:LYS:HD3	1:B:229:LEU:HD22	0.49	1.84	7	1
1:C:318:LYS:O	1:C:322:VAL:HG23	0.49	2.07	9	7
1:A:135:VAL:HG21	1:C:331:LEU:HD12	0.48	1.85	19	19
1:C:304:ASP:HB2	1:D:417:ARG:HG2	0.48	1.85	14	6
1:A:125:TYR:OH	1:B:221:LYS:HB3	0.48	2.08	12	12
1:C:326:LYS:HG2	1:D:411:LEU:HD21	0.48	1.86	5	17
1:C:318:LYS:CG	1:D:429:LEU:HB3	0.48	2.38	5	1
1:B:231:LEU:HD12	1:D:435:VAL:HG21	0.48	1.85	3	17
1:D:436:GLN:O	1:D:439:VAL:HG22	0.48	2.08	3	14
1:C:311:LEU:HD13	1:D:419:PHE:CE2	0.48	2.43	2	9
1:C:336:GLN:O	1:C:339:VAL:HG22	0.48	2.08	6	15
1:B:230:ASP:OD2	1:D:448:GLN:HG3	0.48	2.09	18	3
1:B:217:ARG:HD3	1:B:220:GLU:OE1	0.48	2.08	6	1
1:C:346:ARG:NE	1:C:347:ASN:HB3	0.48	2.24	12	5
1:A:119:PHE:O	1:A:123:LYS:HB3	0.48	2.09	3	6
1:D:418:LYS:O	1:D:422:VAL:HG23	0.48	2.09	10	8
1:A:106:ASP:HA	1:B:214:ARG:HG2	0.47	1.85	20	9
1:A:117:ARG:O	1:A:121:LYS:HG3	0.47	2.09	10	2
1:B:249:ILE:HD11	1:C:314:ARG:HG3	0.47	1.87	3	5
1:C:325:TYR:OH	1:D:421:LYS:HB3	0.47	2.10	3	11
1:A:126:LYS:HG2	1:B:211:LEU:HD21	0.47	1.86	14	18
1:C:341:LYS:O	1:C:344:CYS:HB3	0.47	2.10	2	4
1:A:116:LYS:HB3	1:B:204:ASP:CB	0.47	2.40	19	3
1:B:212:ASN:O	1:C:349:ILE:HB	0.47	2.09	20	12
1:D:417:ARG:O	1:D:421:LYS:HG3	0.46	2.11	12	12
1:C:322:VAL:HG11	1:D:426:LYS:HB3	0.46	1.86	5	2
1:C:311:LEU:HD13	1:D:419:PHE:CE1	0.46	2.45	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:LEU:HD13	1:B:219:PHE:CE2	0.46	2.45	3	7
1:C:317:ARG:O	1:C:321:LYS:HG3	0.46	2.10	7	5
1:C:329:LEU:CD1	1:D:422:VAL:HG22	0.46	2.39	20	13
1:A:110:THR:HG23	1:B:210:THR:CG2	0.46	2.41	11	10
1:A:112:ASN:HB2	1:D:449:ILE:HB	0.46	1.88	2	1
1:C:304:ASP:HB2	1:D:416:LYS:HB3	0.46	1.88	16	1
1:C:304:ASP:HB3	1:D:416:LYS:HB3	0.46	1.87	2	7
1:A:117:ARG:HD3	1:A:120:GLU:OE1	0.46	2.11	10	7
1:A:118:LYS:HG3	1:B:229:LEU:HB3	0.46	1.86	3	9
1:C:319:PHE:CE2	1:D:411:LEU:HD13	0.46	2.46	7	8
1:C:329:LEU:HB3	1:D:418:LYS:HG3	0.46	1.87	3	13
1:A:117:ARG:HA	1:A:120:GLU:OE1	0.46	2.10	17	1
1:A:119:PHE:CE2	1:B:211:LEU:HD13	0.46	2.46	7	13
1:A:110:THR:CG2	1:B:210:THR:HG23	0.46	2.40	8	16
1:D:441:LYS:O	1:D:444:CYS:HB3	0.46	2.11	14	2
1:C:319:PHE:O	1:C:323:LYS:HB3	0.46	2.11	3	9
1:C:304:ASP:CB	1:D:416:LYS:HB3	0.46	2.41	2	1
1:A:112:ASN:O	1:D:449:ILE:HB	0.45	2.12	17	6
1:C:316:LYS:HB3	1:D:404:ASP:HB3	0.45	1.89	2	4
1:A:140:LYS:NZ	1:A:140:LYS:HB3	0.45	2.27	2	2
1:C:310:THR:HG23	1:D:410:THR:CG2	0.45	2.40	18	14
1:A:111:LEU:HD21	1:B:226:LYS:HG2	0.45	1.89	5	14
1:B:218:LYS:O	1:B:222:VAL:HG23	0.45	2.12	12	9
1:B:240:LYS:HB3	1:B:240:LYS:NZ	0.45	2.27	10	2
1:B:231:LEU:O	1:B:235:VAL:HG22	0.45	2.12	3	2
1:C:311:LEU:HD21	1:D:426:LYS:HG2	0.45	1.89	5	19
1:C:340:LYS:HB3	1:C:340:LYS:NZ	0.45	2.25	10	2
1:A:111:LEU:HD13	1:B:219:PHE:CE1	0.44	2.48	19	3
1:C:346:ARG:NH1	1:C:347:ASN:HB3	0.44	2.26	11	1
1:A:130:ASP:OD2	1:C:348:GLN:HG3	0.44	2.13	18	3
1:B:249:ILE:HB	1:C:312:ASN:HB2	0.44	1.88	5	3
1:A:140:LYS:HB3	1:A:140:LYS:NZ	0.44	2.27	10	2
1:D:436:GLN:HB2	1:D:439:VAL:HG13	0.44	1.89	4	2
1:C:304:ASP:CB	1:D:417:ARG:HG2	0.44	2.42	12	2
1:A:129:LEU:HD22	1:B:221:LYS:HD2	0.44	1.90	19	1
1:D:441:LYS:O	1:D:444:CYS:HB2	0.44	2.13	3	2
1:D:446:ARG:NE	1:D:447:ASN:HB3	0.44	2.28	5	1
1:C:322:VAL:HG22	1:D:429:LEU:CD1	0.44	2.43	7	10
1:A:123:LYS:HD3	1:A:124:GLU:N	0.44	2.27	12	2
1:C:319:PHE:CE1	1:D:411:LEU:HD13	0.43	2.48	8	8
1:C:340:LYS:NZ	1:C:340:LYS:HB3	0.43	2.28	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:C:310:THR:CG2	1:D:410:THR:HG23	0.43	2.43	5	5
1:A:149:ILE:HD11	1:D:414:ARG:HB2	0.43	1.90	4	1
1:A:148:GLN:HG3	1:C:330:ASP:CG	0.43	2.34	11	1
1:C:335:VAL:HB	1:C:339:VAL:HG21	0.43	1.90	12	1
1:B:239:VAL:HG23	1:D:431:LEU:HD11	0.43	1.90	7	5
1:A:141:LYS:O	1:A:144:CYS:HB2	0.43	2.12	5	1
1:C:331:LEU:O	1:C:335:VAL:HG22	0.43	2.13	20	1
1:B:247:ASN:C	1:B:247:ASN:HD22	0.43	2.16	18	1
1:C:336:GLN:HB2	1:C:339:VAL:HG13	0.43	1.90	16	4
1:A:132:LEU:HD22	1:A:140:LYS:HE2	0.43	1.90	12	1
1:B:241:LYS:O	1:B:244:CYS:HB3	0.43	2.13	8	5
1:D:419:PHE:O	1:D:423:LYS:HB3	0.43	2.14	5	3
1:A:122:VAL:HG11	1:B:226:LYS:HB3	0.43	1.90	4	2
1:B:212:ASN:HB2	1:C:349:ILE:HB	0.42	1.90	14	1
1:C:314:ARG:HG2	1:D:406:ASP:CA	0.42	2.44	4	6
1:C:326:LYS:HB3	1:D:422:VAL:HG11	0.42	1.90	9	1
1:A:126:LYS:HB3	1:B:222:VAL:HG11	0.42	1.91	2	1
1:B:231:LEU:HD11	1:D:439:VAL:HG23	0.42	1.91	19	3
1:D:432:LEU:HD22	1:D:440:LYS:HE2	0.42	1.91	4	1
1:A:131:LEU:HD11	1:C:339:VAL:HG23	0.42	1.90	7	2
1:A:136:GLN:HB2	1:A:139:VAL:HG13	0.42	1.92	16	4
1:A:114:ARG:HG2	1:B:206:ASP:CA	0.42	2.44	17	3
1:B:231:LEU:HD21	1:D:440:LYS:HA	0.42	1.91	12	1
1:B:242:ALA:HA	1:B:245:GLN:HG2	0.42	1.90	4	1
1:A:139:VAL:HG23	1:C:331:LEU:HD11	0.42	1.91	11	1
1:A:117:ARG:HG2	1:B:204:ASP:HB2	0.42	1.90	4	2
1:C:348:GLN:HG2	1:C:349:ILE:N	0.42	2.29	10	1
1:A:132:LEU:HG	1:C:328:ALA:HA	0.42	1.92	10	3
1:C:347:ASN:C	1:C:347:ASN:HD22	0.42	2.18	8	1
1:D:448:GLN:HG2	1:D:449:ILE:N	0.41	2.30	19	1
1:D:426:LYS:HB2	1:D:426:LYS:HE2	0.41	1.77	8	1
1:A:141:LYS:O	1:A:144:CYS:HB3	0.41	2.14	11	2
1:B:228:ALA:HA	1:D:432:LEU:HG	0.41	1.91	10	4
1:A:140:LYS:HG2	1:C:331:LEU:HD21	0.41	1.91	11	1
1:D:431:LEU:O	1:D:435:VAL:HG22	0.41	2.15	7	1
1:B:240:LYS:HB3	1:B:240:LYS:HZ3	0.41	1.75	9	1
1:B:240:LYS:NZ	1:B:240:LYS:HB3	0.41	2.31	13	1
1:C:306:ASP:CA	1:D:414:ARG:HG2	0.41	2.46	19	1
1:A:139:VAL:CG2	1:C:331:LEU:HD11	0.41	2.45	11	1
1:A:128:ALA:HB1	1:C:328:ALA:C	0.41	2.35	15	2
1:A:147:ASN:N	1:A:147:ASN:HD22	0.41	2.14	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:LEU:HD23	1:C:331:LEU:HG	0.41	1.93	13	1
1:A:118:LYS:HA	1:A:121:LYS:HD2	0.41	1.92	7	1
1:A:106:ASP:CA	1:B:214:ARG:HG2	0.41	2.45	1	2
1:A:128:ALA:C	1:C:328:ALA:HB1	0.41	2.36	11	2
1:A:135:VAL:CG2	1:C:331:LEU:HD12	0.41	2.46	5	1
1:C:329:LEU:HD22	1:D:421:LYS:HD2	0.41	1.92	14	1
1:A:149:ILE:HD11	1:C:308:VAL:HG22	0.41	1.92	16	1
1:B:236:GLN:HB2	1:B:239:VAL:HG13	0.41	1.93	12	2
1:A:117:ARG:HD3	1:A:120:GLU:OE2	0.41	2.15	11	1
1:D:426:LYS:HE2	1:D:426:LYS:HB2	0.41	1.77	3	1
1:B:228:ALA:HB1	1:D:428:ALA:C	0.41	2.36	15	1
1:A:140:LYS:NZ	1:C:327:GLU:OE1	0.40	2.55	4	1
1:C:323:LYS:HD3	1:C:324:GLU:N	0.40	2.31	3	1
1:C:313:ILE:HD13	1:C:322:VAL:CG2	0.40	2.47	13	1
1:B:248:GLN:NE2	1:D:427:GLU:HA	0.40	2.31	6	1
1:C:347:ASN:HD22	1:C:347:ASN:C	0.40	2.18	10	2
1:C:314:ARG:HG3	1:D:408:VAL:HG22	0.40	1.92	17	1
1:A:131:LEU:O	1:A:135:VAL:HG22	0.40	2.15	7	1
1:D:417:ARG:HD3	1:D:420:GLU:OE1	0.40	2.17	18	2
1:B:217:ARG:HD3	1:B:220:GLU:OE2	0.40	2.16	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	44/47 (94%)	41±1 (93±1%)	3±1 (7±1%)	0±0 (0±0%)	100	100
1	B	45/47 (96%)	41±1 (91±2%)	4±1 (9±2%)	0±0 (0±0%)	59	88
1	C	45/47 (96%)	41±0 (91±1%)	4±0 (9±1%)	0±0 (0±0%)	100	100
1	D	45/47 (96%)	41±1 (91±2%)	4±1 (9±2%)	0±0 (0±0%)	100	100
All	All	3580/3760 (95%)	3271 (91%)	308 (9%)	1 (0%)	100	100

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	B	208	VAL	1

### 6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	41/43 (95%)	34±1 (83±3%)	7±1 (17±3%)	6	42
1	B	43/43 (100%)	36±1 (84±3%)	7±1 (16±3%)	7	44
1	C	43/43 (100%)	36±1 (83±3%)	7±1 (17±3%)	6	43
1	D	43/43 (100%)	36±1 (84±3%)	7±1 (16±3%)	6	43
All	All	3400/3440 (99%)	2838 (83%)	562 (17%)	6	43

All 56 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	146	ARG	20
1	B	226	LYS	20
1	B	222	VAL	20
1	D	426	LYS	20
1	C	322	VAL	20
1	B	246	ARG	20
1	A	126	LYS	20
1	C	326	LYS	20
1	A	123	LYS	20
1	D	422	VAL	20
1	A	107	VAL	20
1	A	122	VAL	20
1	D	446	ARG	20
1	C	346	ARG	19
1	B	207	VAL	19
1	C	307	VAL	19
1	C	323	LYS	19
1	B	247	ASN	18
1	D	423	LYS	18
1	D	407	VAL	18
1	B	223	LYS	16

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Mol	Chain	Res	Type	Models (Total)
1	C	347	ASN	14
1	D	447	ASN	14
1	A	147	ASN	13
1	B	224	GLU	9
1	C	324	GLU	8
1	A	131	LEU	8
1	A	114	ARG	7
1	C	331	LEU	7
1	C	327	GLU	6
1	D	424	GLU	6
1	D	431	LEU	6
1	A	124	GLU	5
1	A	127	GLU	5
1	D	414	ARG	5
1	D	427	GLU	5
1	C	304	ASP	5
1	B	206	ASP	4
1	B	238	ASP	3
1	B	231	LEU	3
1	B	227	GLU	3
1	C	314	ARG	2
1	C	333	ASP	2
1	D	406	ASP	2
1	C	306	ASP	2
1	B	214	ARG	2
1	D	439	VAL	1
1	D	438	ASP	1
1	A	149	ILE	1
1	A	121	LYS	1
1	D	440	LYS	1
1	D	448	GLN	1
1	D	404	ASP	1
1	A	106	ASP	1
1	D	449	ILE	1
1	C	348	GLN	1

### 6.3.3 RNA ⓘ

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

The completeness of assignment taking into account all chemical shift lists is 22% for the well-defined parts and 22% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2mw4\_cs.str

Chemical shift list name: *assigned\_chem\_shift\_list\_1*

#### 7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	611
Number of shifts mapped to atoms	611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	47	$-0.62 \pm 0.11$	Should be applied
$^{13}\text{C}_\beta$	45	$0.03 \pm 0.19$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	45	$-0.06 \pm 0.09$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	45	$-0.67 \pm 0.50$	None needed (imprecise)

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 22%, i.e. 542 atoms were assigned a chemical shift out of a possible 2455. 8 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	221/922 (24%)	89/368 (24%)	88/372 (24%)	44/182 (24%)
Sidechain	288/1401 (21%)	181/820 (22%)	106/497 (21%)	1/84 (1%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	33/132 (25%)	17/68 (25%)	16/64 (25%)	0/0 (—%)
Overall	542/2455 (22%)	287/1256 (23%)	210/933 (23%)	45/266 (17%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 22%, i.e. 556 atoms were assigned a chemical shift out of a possible 2472. 8 out of 36 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	229/932 (25%)	92/372 (25%)	92/376 (24%)	45/184 (24%)
Sidechain	294/1408 (21%)	185/824 (22%)	108/500 (22%)	1/84 (1%)
Aromatic	33/132 (25%)	17/68 (25%)	16/64 (25%)	0/0 (—%)
Overall	556/2472 (22%)	294/1264 (23%)	216/940 (23%)	46/268 (17%)

#### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

