



# Full wwPDB NMR Structure Validation Report ⓘ

Aug 17, 2022 – 11:32 PM EDT

PDB ID : 2RV8  
Title : Solution Structure of the PhoP DNA-Binding Domain from Mycobacterium tuberculosis  
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Deposited on : 2015-04-17

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.29
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

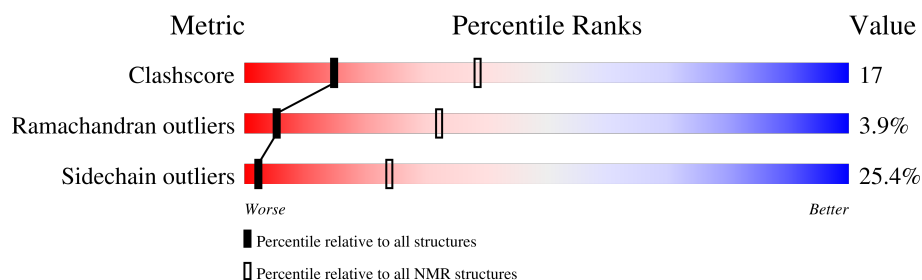
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 80%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	128	<div> <div></div> <div>42%</div> <div>25%</div> <div>5%</div> <div>27%</div> </div>

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 7 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:149-A:205, A:210-A:245 (93)	0.34	7

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 4 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2076 atoms, of which 1036 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called DNA-binding response regulator.

Mol	Chain	Residues	Atoms						Trace
1	A	128	Total	C	H	N	O	S	0
			2076	657	1036	195	186	2	

There are 22 discrepancies between the modelled and reference sequences:

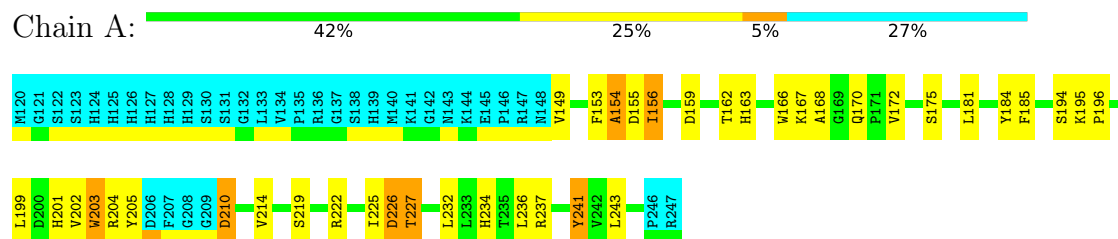
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	MET	-	expression tag	UNP R4MFJ2
A	121	GLY	-	expression tag	UNP R4MFJ2
A	122	SER	-	expression tag	UNP R4MFJ2
A	123	SER	-	expression tag	UNP R4MFJ2
A	124	HIS	-	expression tag	UNP R4MFJ2
A	125	HIS	-	expression tag	UNP R4MFJ2
A	126	HIS	-	expression tag	UNP R4MFJ2
A	127	HIS	-	expression tag	UNP R4MFJ2
A	128	HIS	-	expression tag	UNP R4MFJ2
A	129	HIS	-	expression tag	UNP R4MFJ2
A	130	SER	-	expression tag	UNP R4MFJ2
A	131	SER	-	expression tag	UNP R4MFJ2
A	132	GLY	-	expression tag	UNP R4MFJ2
A	133	LEU	-	expression tag	UNP R4MFJ2
A	134	VAL	-	expression tag	UNP R4MFJ2
A	135	PRO	-	expression tag	UNP R4MFJ2
A	136	ARG	-	expression tag	UNP R4MFJ2
A	137	GLY	-	expression tag	UNP R4MFJ2
A	138	SER	-	expression tag	UNP R4MFJ2
A	139	HIS	-	expression tag	UNP R4MFJ2
A	140	MET	-	expression tag	UNP R4MFJ2
A	141	LYS	-	expression tag	UNP R4MFJ2

## 4 Residue-property plots

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

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: DNA-binding response regulator

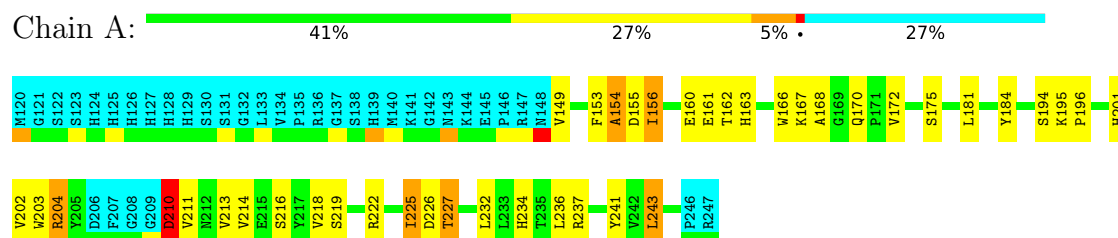


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

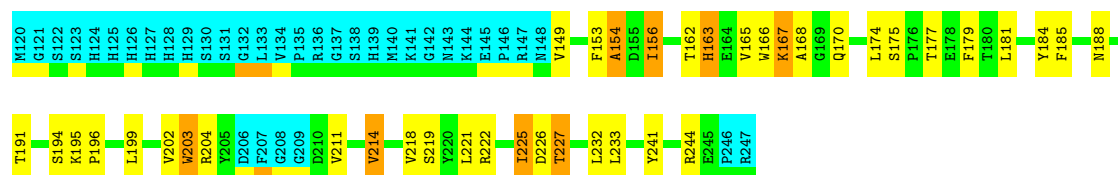
- Molecule 1: DNA-binding response regulator



#### 4.2.2 Score per residue for model 2

- Molecule 1: DNA-binding response regulator

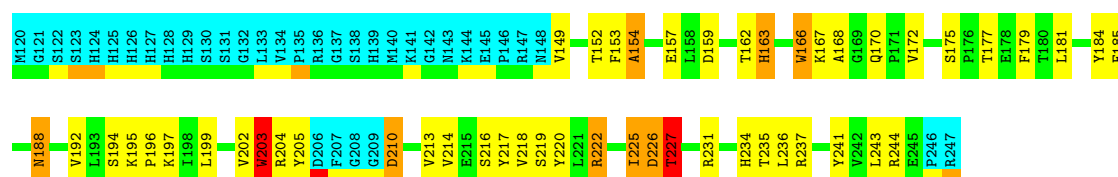




### 4.2.3 Score per residue for model 3

- Molecule 1: DNA-binding response regulator

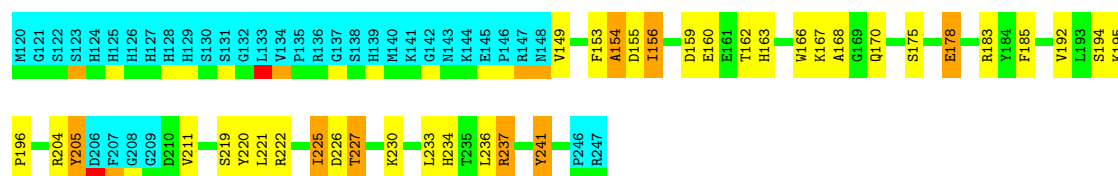
Chain A: 34% 31% 6% 27%



### 4.2.4 Score per residue for model 4

- Molecule 1: DNA-binding response regulator

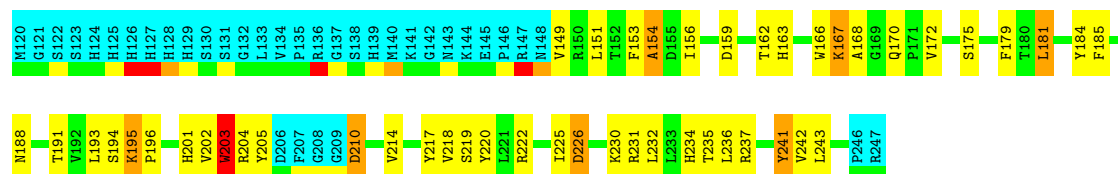
Chain A: 44% 23% 6% 27%



### 4.2.5 Score per residue for model 5

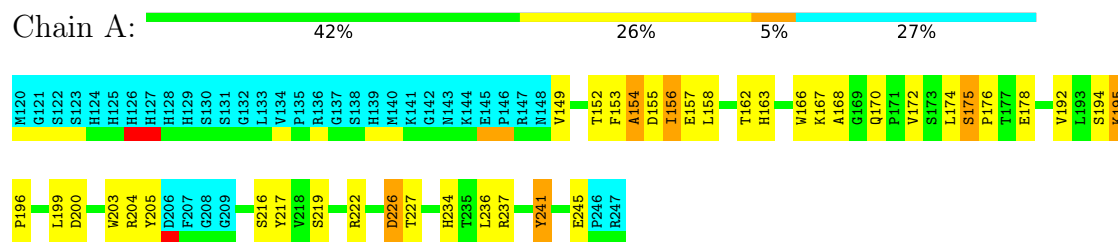
- Molecule 1: DNA-binding response regulator

Chain A: 35% 31% 5% 27%



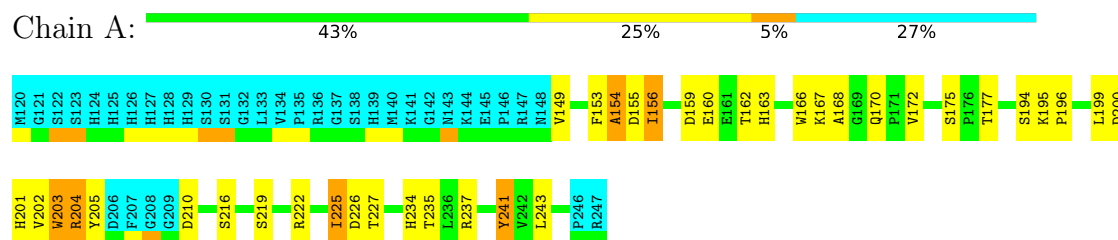
### 4.2.6 Score per residue for model 6

- Molecule 1: DNA-binding response regulator



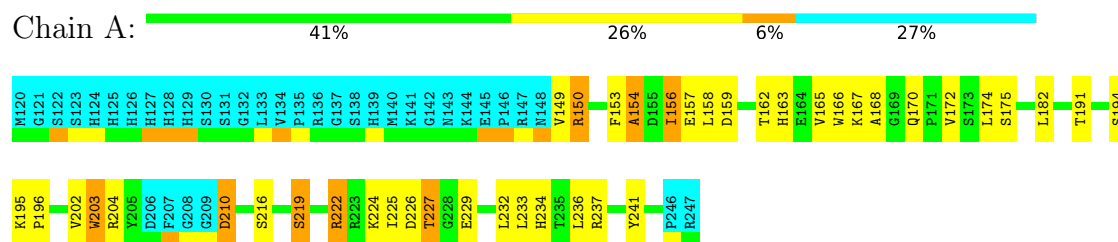
#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: DNA-binding response regulator



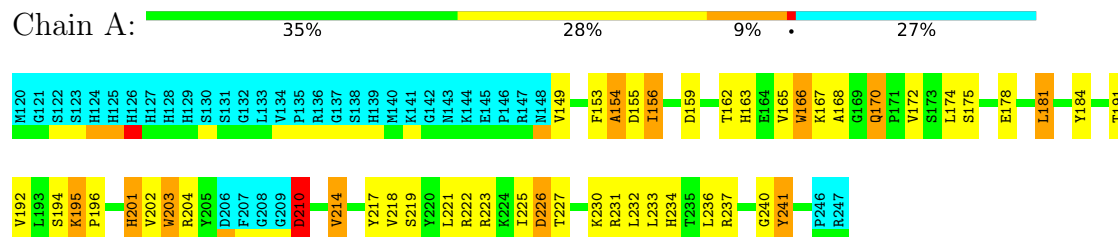
#### 4.2.8 Score per residue for model 8

- Molecule 1: DNA-binding response regulator



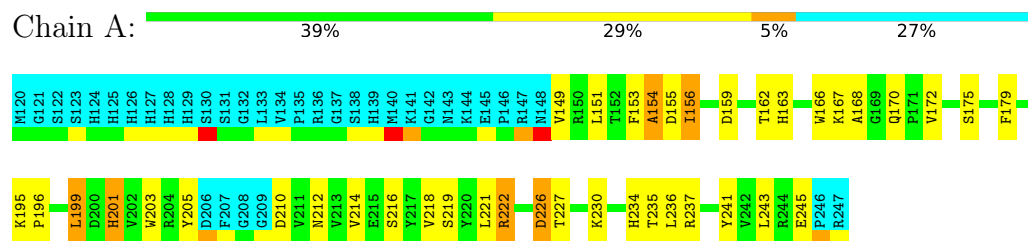
#### 4.2.9 Score per residue for model 9

- Molecule 1: DNA-binding response regulator



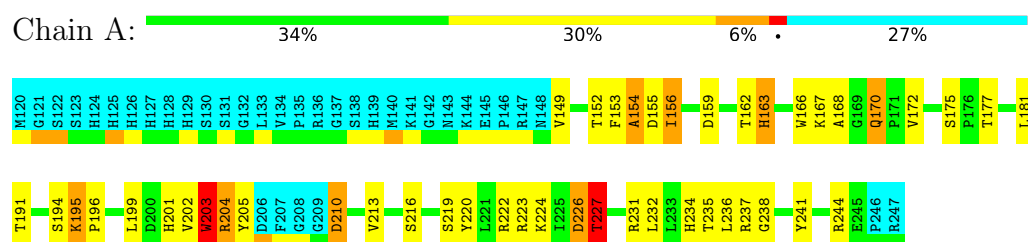
### 4.2.10 Score per residue for model 10

- Molecule 1: DNA-binding response regulator



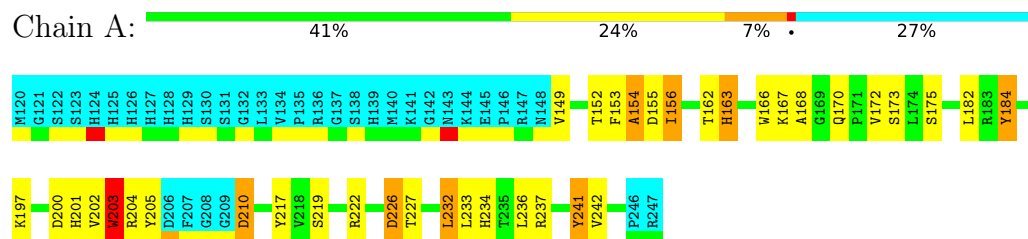
### 4.2.11 Score per residue for model 11

- Molecule 1: DNA-binding response regulator



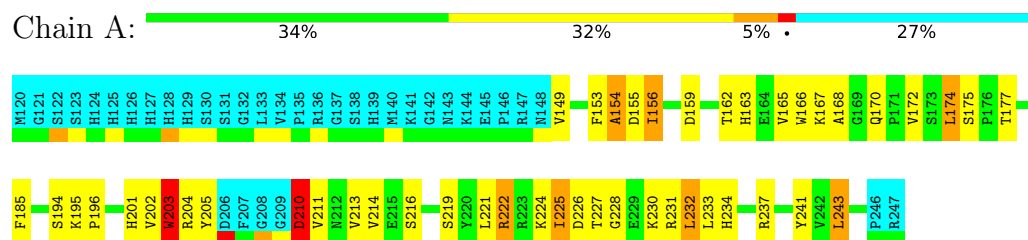
### 4.2.12 Score per residue for model 12

- Molecule 1: DNA-binding response regulator



### 4.2.13 Score per residue for model 13

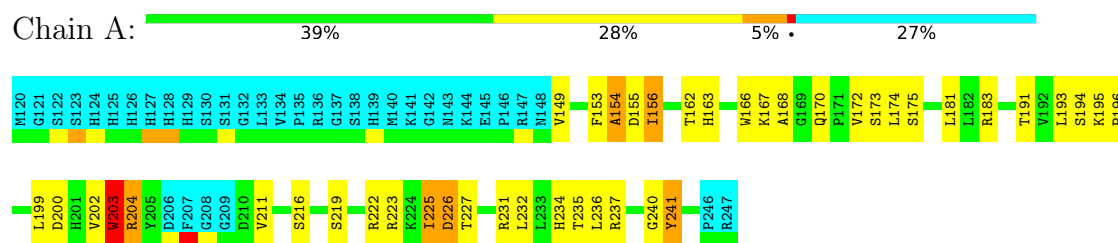
- Molecule 1: DNA-binding response regulator





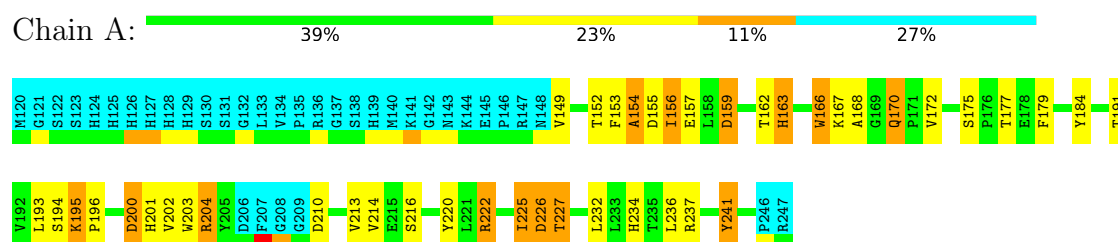
#### 4.2.14 Score per residue for model 14

- Molecule 1: DNA-binding response regulator



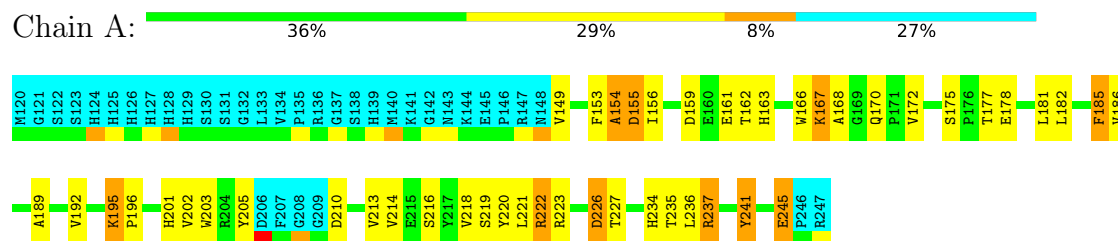
#### 4.2.15 Score per residue for model 15

- Molecule 1: DNA-binding response regulator



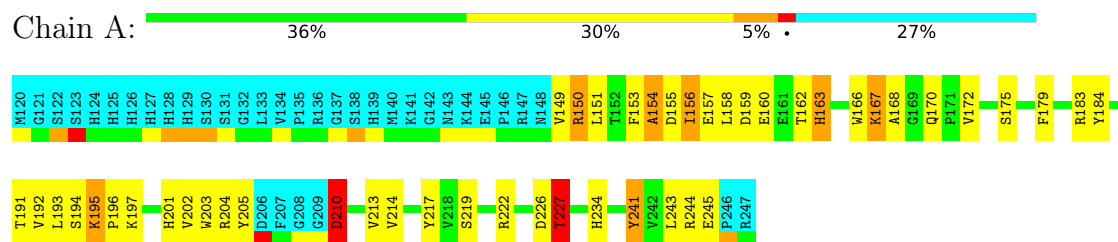
#### 4.2.16 Score per residue for model 16

- Molecule 1: DNA-binding response regulator



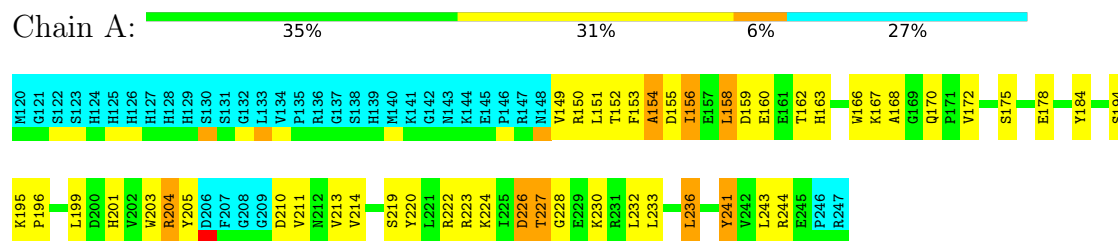
#### 4.2.17 Score per residue for model 17

- Molecule 1: DNA-binding response regulator



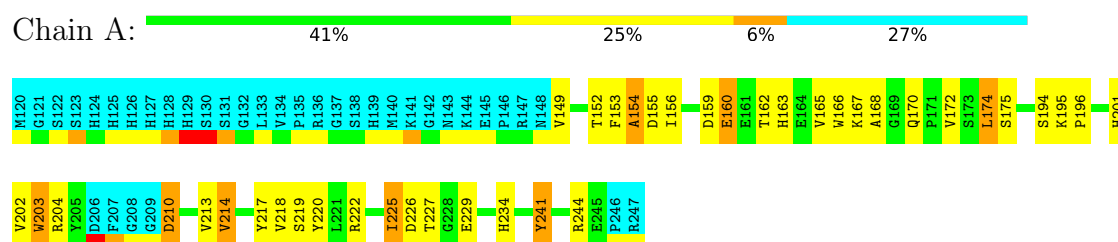
### 4.2.18 Score per residue for model 18

- Molecule 1: DNA-binding response regulator



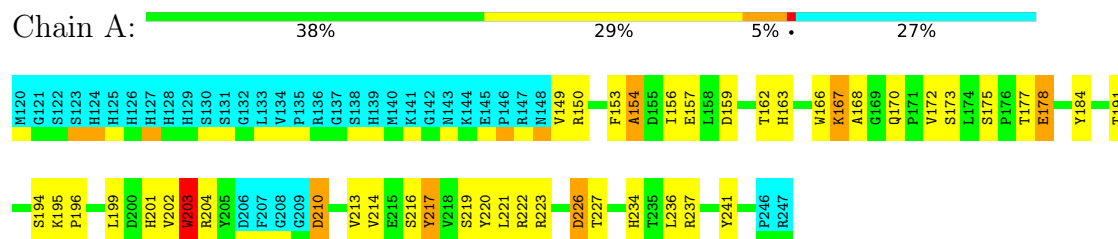
### 4.2.19 Score per residue for model 19

- Molecule 1: DNA-binding response regulator



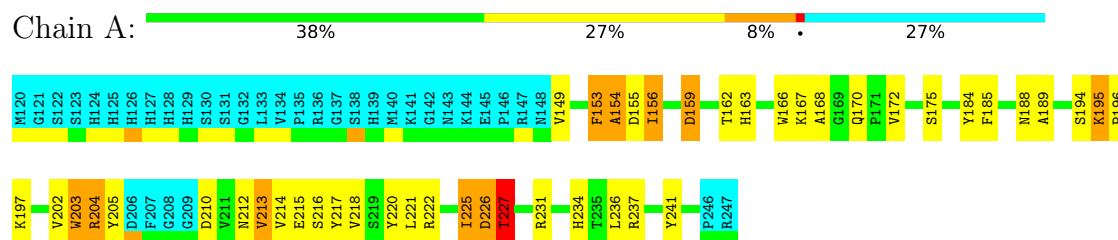
### 4.2.20 Score per residue for model 20

- Molecule 1: DNA-binding response regulator



### 4.2.21 Score per residue for model 21

- Molecule 1: DNA-binding response regulator



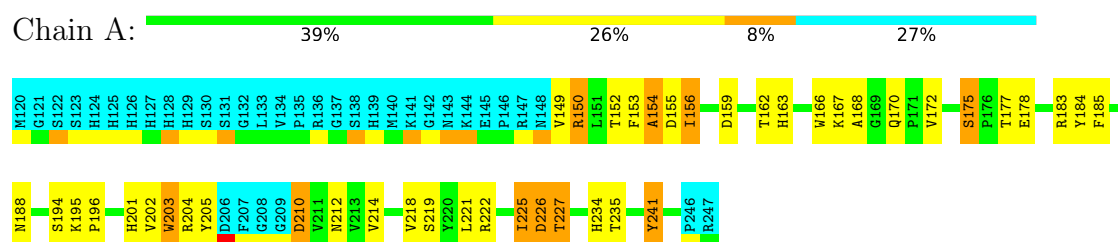
#### 4.2.22 Score per residue for model 22

- Molecule 1: DNA-binding response regulator



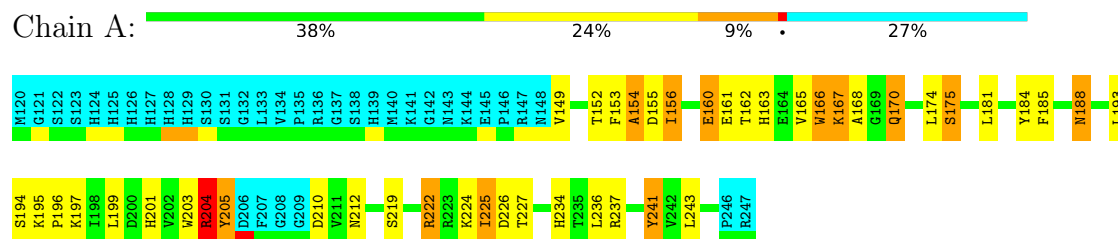
#### 4.2.23 Score per residue for model 23

- Molecule 1: DNA-binding response regulator



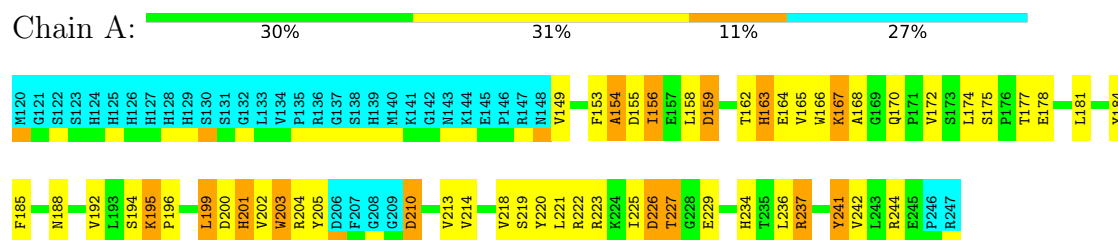
#### 4.2.24 Score per residue for model 24

- Molecule 1: DNA-binding response regulator



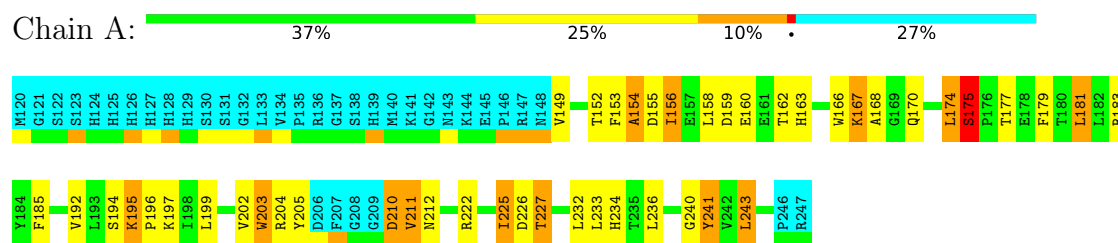
#### 4.2.25 Score per residue for model 25

- Molecule 1: DNA-binding response regulator



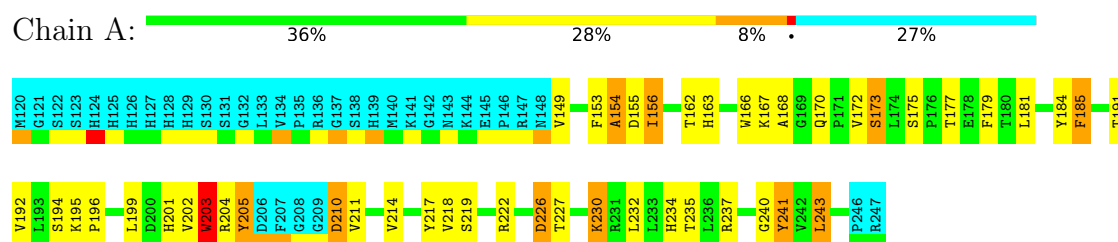
### 4.2.26 Score per residue for model 26

- Molecule 1: DNA-binding response regulator



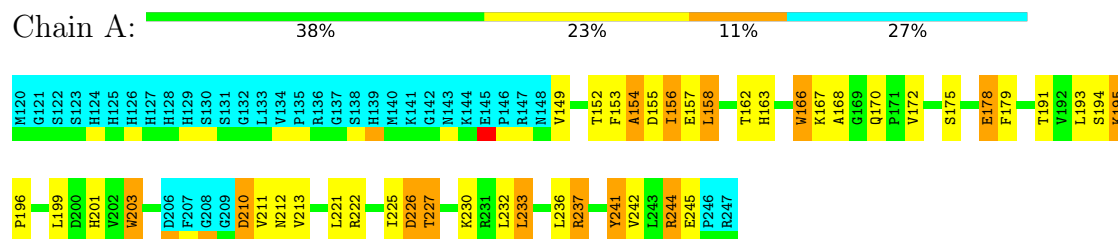
### 4.2.27 Score per residue for model 27

- Molecule 1: DNA-binding response regulator



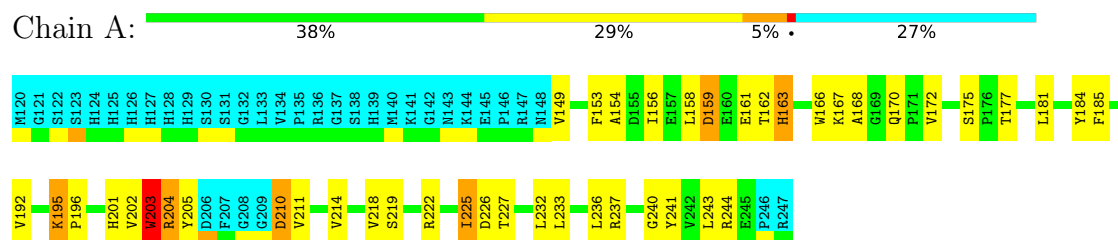
### 4.2.28 Score per residue for model 28

- Molecule 1: DNA-binding response regulator



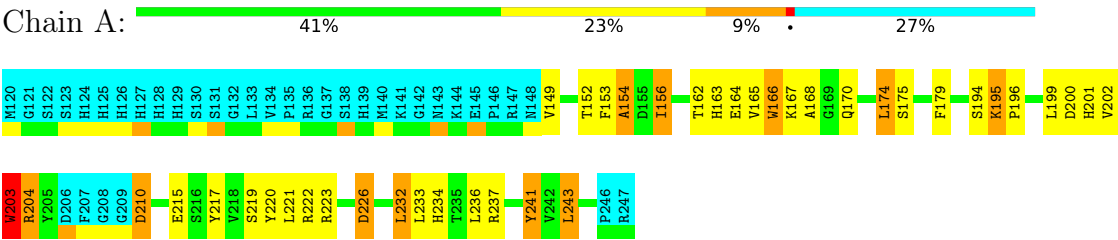
### 4.2.29 Score per residue for model 29

- Molecule 1: DNA-binding response regulator



4.2.30 Score per residue for model 30

- Molecule 1: DNA-binding response regulator



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 30 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
X-PLOR NIH	refinement	2.25
UNIO	structure solution	

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1224
Number of shifts mapped to atoms	1224
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

## 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	768	782	779	26±5
All	All	23040	23460	23370	784

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:174:LEU:HD23	1:A:174:LEU:N	0.85	1.85	13	2
1:A:158:LEU:HD12	1:A:158:LEU:N	0.82	1.90	18	1
1:A:155:ASP:O	1:A:156:ILE:HD13	0.81	1.74	16	1
1:A:225:ILE:O	1:A:225:ILE:HD12	0.79	1.75	7	1
1:A:231:ARG:O	1:A:232:LEU:HD23	0.78	1.78	14	1
1:A:174:LEU:H	1:A:174:LEU:HD12	0.77	1.39	19	1
1:A:165:VAL:HG21	1:A:174:LEU:HD12	0.74	1.57	9	5
1:A:236:LEU:N	1:A:236:LEU:HD22	0.74	1.97	18	1
1:A:214:VAL:O	1:A:218:VAL:HG23	0.73	1.83	25	13
1:A:174:LEU:HD12	1:A:174:LEU:N	0.71	2.00	26	2
1:A:174:LEU:HD12	1:A:174:LEU:H	0.71	1.44	26	1
1:A:151:LEU:HD23	1:A:183:ARG:HH12	0.70	1.46	17	1
1:A:184:TYR:CZ	1:A:201:HIS:NE2	0.69	2.60	10	2
1:A:241:TYR:N	1:A:241:TYR:CD1	0.69	2.61	9	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:TYR:CD1	1:A:201:HIS:NE2	0.69	2.60	22	7
1:A:184:TYR:CE1	1:A:201:HIS:NE2	0.69	2.61	24	10
1:A:232:LEU:O	1:A:243:LEU:HD23	0.65	1.91	27	4
1:A:184:TYR:CZ	1:A:201:HIS:CD2	0.64	2.86	1	3
1:A:153:PHE:CE2	1:A:243:LEU:HD21	0.63	2.28	17	5
1:A:231:ARG:C	1:A:232:LEU:HD12	0.63	2.13	22	3
1:A:232:LEU:N	1:A:232:LEU:HD23	0.63	2.08	30	4
1:A:225:ILE:HD12	1:A:225:ILE:C	0.63	2.14	7	1
1:A:163:HIS:CE1	1:A:179:PHE:CE1	0.62	2.88	28	1
1:A:157:GLU:C	1:A:158:LEU:HD12	0.62	2.14	6	1
1:A:167:LYS:O	1:A:170:GLN:N	0.61	2.33	14	30
1:A:222:ARG:O	1:A:226:ASP:N	0.61	2.33	24	30
1:A:163:HIS:CE1	1:A:179:PHE:CD2	0.61	2.88	2	2
1:A:192:VAL:HG13	1:A:192:VAL:O	0.61	1.96	25	10
1:A:158:LEU:HD12	1:A:158:LEU:H	0.61	1.56	18	1
1:A:163:HIS:N	1:A:163:HIS:ND1	0.60	2.48	12	2
1:A:181:LEU:HD12	1:A:202:VAL:HG21	0.60	1.73	9	3
1:A:174:LEU:H	1:A:174:LEU:CD1	0.60	2.05	19	1
1:A:241:TYR:CD1	1:A:242:VAL:N	0.60	2.69	5	1
1:A:211:VAL:HG12	1:A:211:VAL:O	0.60	1.97	14	2
1:A:195:LYS:NZ	1:A:211:VAL:O	0.59	2.35	18	1
1:A:185:PHE:CZ	1:A:241:TYR:CE2	0.59	2.90	29	1
1:A:163:HIS:NE2	1:A:179:PHE:CE2	0.59	2.70	3	1
1:A:203:TRP:O	1:A:205:TYR:N	0.59	2.36	18	5
1:A:160:GLU:OE2	1:A:161:GLU:N	0.59	2.36	24	1
1:A:160:GLU:OE2	1:A:183:ARG:NH1	0.59	2.36	4	1
1:A:211:VAL:HG22	1:A:211:VAL:O	0.59	1.98	29	4
1:A:233:LEU:H	1:A:233:LEU:HD12	0.59	1.58	28	1
1:A:195:LYS:NZ	1:A:241:TYR:OH	0.58	2.36	3	2
1:A:188:ASN:N	1:A:188:ASN:ND2	0.58	2.51	24	2
1:A:178:GLU:OE2	1:A:221:LEU:HD11	0.58	1.98	16	1
1:A:225:ILE:HD13	1:A:225:ILE:O	0.57	1.99	26	13
1:A:153:PHE:CD1	1:A:154:ALA:N	0.57	2.73	21	4
1:A:174:LEU:N	1:A:174:LEU:CD2	0.56	2.59	13	2
1:A:202:VAL:O	1:A:204:ARG:N	0.56	2.38	22	23
1:A:185:PHE:CG	1:A:241:TYR:OH	0.56	2.57	29	1
1:A:185:PHE:CE2	1:A:241:TYR:CZ	0.56	2.93	29	1
1:A:158:LEU:N	1:A:158:LEU:CD1	0.56	2.60	18	1
1:A:153:PHE:O	1:A:155:ASP:N	0.56	2.39	7	19
1:A:163:HIS:NE2	1:A:179:PHE:CD2	0.56	2.74	3	1
1:A:212:ASN:O	1:A:215:GLU:N	0.56	2.39	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:210:ASP:OD1	1:A:213:VAL:HG23	0.55	2.01	3	1
1:A:184:TYR:CD1	1:A:201:HIS:CE1	0.55	2.95	27	4
1:A:184:TYR:CE1	1:A:201:HIS:CD2	0.55	2.94	1	2
1:A:181:LEU:O	1:A:181:LEU:HD23	0.55	2.02	16	1
1:A:150:ARG:CZ	1:A:159:ASP:OD2	0.55	2.55	23	1
1:A:191:THR:O	1:A:193:LEU:HD12	0.55	2.02	5	4
1:A:153:PHE:CZ	1:A:245:GLU:OE2	0.55	2.59	28	2
1:A:153:PHE:O	1:A:156:ILE:N	0.54	2.40	7	25
1:A:195:LYS:N	1:A:196:PRO:CD	0.54	2.70	2	10
1:A:151:LEU:HD23	1:A:183:ARG:NH1	0.54	2.15	17	1
1:A:236:LEU:HD22	1:A:236:LEU:H	0.54	1.58	18	1
1:A:162:THR:C	1:A:163:HIS:CG	0.54	2.81	27	3
1:A:184:TYR:CE2	1:A:188:ASN:ND2	0.54	2.76	5	4
1:A:199:LEU:HD23	1:A:199:LEU:O	0.54	2.02	24	3
1:A:236:LEU:N	1:A:240:GLY:O	0.54	2.41	29	3
1:A:244:ARG:O	1:A:244:ARG:NE	0.54	2.38	28	1
1:A:199:LEU:O	1:A:203:TRP:N	0.54	2.41	11	4
1:A:235:THR:HG23	1:A:241:TYR:CE2	0.53	2.39	10	1
1:A:200:ASP:O	1:A:204:ARG:CG	0.53	2.56	15	2
1:A:161:GLU:OE1	1:A:161:GLU:N	0.53	2.41	29	1
1:A:162:THR:C	1:A:163:HIS:CD2	0.53	2.81	16	1
1:A:184:TYR:CG	1:A:201:HIS:NE2	0.53	2.77	18	2
1:A:155:ASP:C	1:A:156:ILE:HD13	0.53	2.22	16	1
1:A:178:GLU:CD	1:A:178:GLU:H	0.53	2.06	28	1
1:A:188:ASN:HD22	1:A:188:ASN:N	0.53	2.01	3	1
1:A:162:THR:O	1:A:163:HIS:CB	0.53	2.55	11	5
1:A:199:LEU:CD1	1:A:210:ASP:O	0.53	2.57	7	1
1:A:203:TRP:CZ2	1:A:213:VAL:HG11	0.53	2.39	21	1
1:A:167:LYS:O	1:A:170:GLN:CB	0.52	2.58	18	16
1:A:158:LEU:HD21	1:A:179:PHE:CZ	0.52	2.39	28	1
1:A:232:LEU:N	1:A:232:LEU:CD2	0.52	2.72	30	2
1:A:163:HIS:NE2	1:A:179:PHE:CG	0.52	2.77	2	1
1:A:236:LEU:N	1:A:236:LEU:CD2	0.52	2.69	18	1
1:A:203:TRP:C	1:A:205:TYR:N	0.52	2.63	24	10
1:A:159:ASP:N	1:A:159:ASP:OD1	0.52	2.42	15	3
1:A:163:HIS:CE1	1:A:179:PHE:CD1	0.52	2.98	28	1
1:A:218:VAL:HG21	1:A:241:TYR:CE2	0.51	2.40	23	2
1:A:217:TYR:O	1:A:221:LEU:HD13	0.51	2.05	21	1
1:A:222:ARG:O	1:A:226:ASP:O	0.51	2.29	15	13
1:A:220:TYR:OH	1:A:224:LYS:NZ	0.51	2.44	18	1
1:A:153:PHE:CZ	1:A:243:LEU:HD22	0.51	2.41	26	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ASP:OD1	1:A:155:ASP:N	0.51	2.42	12	2
1:A:182:LEU:O	1:A:186:VAL:HG23	0.51	2.06	16	1
1:A:232:LEU:O	1:A:244:ARG:O	0.51	2.29	18	4
1:A:201:HIS:ND1	1:A:202:VAL:HG23	0.51	2.20	15	1
1:A:233:LEU:H	1:A:233:LEU:CD1	0.51	2.16	28	1
1:A:210:ASP:O	1:A:213:VAL:HG12	0.51	2.06	11	3
1:A:205:TYR:O	1:A:205:TYR:CD2	0.51	2.64	3	2
1:A:184:TYR:CD2	1:A:188:ASN:OD1	0.51	2.64	24	1
1:A:155:ASP:N	1:A:155:ASP:OD1	0.50	2.43	15	3
1:A:165:VAL:HG21	1:A:174:LEU:HD21	0.50	1.84	13	1
1:A:202:VAL:C	1:A:204:ARG:N	0.50	2.65	26	23
1:A:153:PHE:CZ	1:A:243:LEU:HD21	0.50	2.42	10	1
1:A:202:VAL:C	1:A:204:ARG:H	0.50	2.09	22	23
1:A:184:TYR:CE1	1:A:201:HIS:CE1	0.50	3.00	29	4
1:A:185:PHE:CD2	1:A:241:TYR:OH	0.50	2.65	29	2
1:A:213:VAL:CG1	1:A:214:VAL:N	0.49	2.75	25	10
1:A:178:GLU:CD	1:A:178:GLU:N	0.49	2.63	23	3
1:A:241:TYR:CD1	1:A:241:TYR:C	0.49	2.86	29	2
1:A:199:LEU:HG	1:A:214:VAL:HG21	0.49	1.85	25	1
1:A:184:TYR:OH	1:A:201:HIS:NE2	0.49	2.45	10	1
1:A:226:ASP:C	1:A:227:THR:HG22	0.49	2.28	11	1
1:A:160:GLU:N	1:A:160:GLU:CD	0.49	2.66	1	1
1:A:203:TRP:C	1:A:205:TYR:H	0.49	2.11	21	11
1:A:162:THR:O	1:A:163:HIS:CG	0.49	2.65	16	4
1:A:192:VAL:HG22	1:A:242:VAL:HB	0.49	1.85	12	1
1:A:159:ASP:OD2	1:A:162:THR:OG1	0.49	2.30	18	1
1:A:220:TYR:O	1:A:220:TYR:CG	0.49	2.65	18	1
1:A:245:GLU:OE2	1:A:245:GLU:O	0.49	2.31	16	1
1:A:153:PHE:O	1:A:154:ALA:C	0.49	2.52	3	30
1:A:213:VAL:HG13	1:A:214:VAL:N	0.48	2.23	25	2
1:A:225:ILE:C	1:A:225:ILE:CD1	0.48	2.79	7	1
1:A:165:VAL:HG12	1:A:166:TRP:N	0.48	2.24	30	3
1:A:153:PHE:CE1	1:A:154:ALA:HB2	0.48	2.43	21	2
1:A:185:PHE:O	1:A:189:ALA:N	0.48	2.47	16	2
1:A:179:PHE:C	1:A:179:PHE:CD1	0.48	2.86	30	3
1:A:244:ARG:NH2	1:A:245:GLU:O	0.48	2.45	28	1
1:A:167:LYS:O	1:A:168:ALA:C	0.48	2.52	23	30
1:A:199:LEU:C	1:A:199:LEU:HD23	0.48	2.29	28	2
1:A:153:PHE:CD1	1:A:153:PHE:C	0.48	2.86	21	3
1:A:160:GLU:OE1	1:A:183:ARG:NH2	0.48	2.47	26	1
1:A:199:LEU:HD23	1:A:199:LEU:C	0.47	2.29	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:157:GLU:O	1:A:158:LEU:HD12	0.47	2.08	6	1
1:A:222:ARG:O	1:A:226:ASP:OD1	0.47	2.31	21	1
1:A:210:ASP:C	1:A:212:ASN:H	0.47	2.13	26	2
1:A:241:TYR:CD1	1:A:241:TYR:N	0.47	2.82	6	4
1:A:150:ARG:NH1	1:A:159:ASP:OD2	0.47	2.47	18	2
1:A:173:SER:O	1:A:173:SER:OG	0.47	2.33	27	2
1:A:222:ARG:O	1:A:226:ASP:CB	0.47	2.63	1	6
1:A:158:LEU:HD23	1:A:165:VAL:HG22	0.47	1.86	8	2
1:A:242:VAL:HG13	1:A:242:VAL:O	0.47	2.09	28	1
1:A:218:VAL:HG11	1:A:241:TYR:CE2	0.47	2.45	9	1
1:A:150:ARG:NH2	1:A:157:GLU:OE2	0.47	2.48	17	2
1:A:210:ASP:N	1:A:210:ASP:OD1	0.47	2.46	17	1
1:A:160:GLU:CD	1:A:183:ARG:NH1	0.47	2.68	4	1
1:A:167:LYS:NZ	1:A:168:ALA:HB3	0.47	2.25	5	2
1:A:155:ASP:CG	1:A:167:LYS:NZ	0.46	2.68	12	1
1:A:201:HIS:ND1	1:A:204:ARG:NH2	0.46	2.63	19	1
1:A:195:LYS:N	1:A:196:PRO:HD2	0.46	2.24	27	24
1:A:151:LEU:O	1:A:158:LEU:HD12	0.46	2.10	18	1
1:A:178:GLU:OE2	1:A:217:TYR:CE1	0.46	2.68	20	1
1:A:159:ASP:O	1:A:163:HIS:N	0.46	2.48	8	8
1:A:175:SER:CB	1:A:176:PRO:CD	0.46	2.93	6	1
1:A:160:GLU:CD	1:A:161:GLU:N	0.46	2.70	24	1
1:A:192:VAL:O	1:A:192:VAL:CG1	0.46	2.63	25	4
1:A:200:ASP:O	1:A:200:ASP:OD1	0.45	2.34	12	1
1:A:236:LEU:O	1:A:237:ARG:C	0.45	2.55	21	19
1:A:228:GLY:C	1:A:230:LYS:N	0.45	2.69	18	1
1:A:162:THR:O	1:A:163:HIS:C	0.45	2.55	12	25
1:A:210:ASP:C	1:A:212:ASN:N	0.45	2.70	26	2
1:A:211:VAL:O	1:A:211:VAL:CG1	0.45	2.64	14	1
1:A:158:LEU:CD2	1:A:179:PHE:CZ	0.45	3.00	28	1
1:A:162:THR:C	1:A:163:HIS:ND1	0.45	2.70	13	3
1:A:225:ILE:CG2	1:A:226:ASP:N	0.45	2.80	15	7
1:A:228:GLY:C	1:A:230:LYS:H	0.45	2.15	18	1
1:A:219:SER:OG	1:A:222:ARG:NH1	0.44	2.51	8	1
1:A:226:ASP:C	1:A:227:THR:OG1	0.44	2.54	17	2
1:A:226:ASP:O	1:A:227:THR:OG1	0.44	2.33	13	1
1:A:204:ARG:O	1:A:204:ARG:CG	0.44	2.65	18	1
1:A:150:ARG:HH11	1:A:159:ASP:CG	0.44	2.15	22	1
1:A:160:GLU:O	1:A:163:HIS:CD2	0.44	2.70	26	2
1:A:212:ASN:O	1:A:213:VAL:C	0.44	2.55	21	1
1:A:174:LEU:HD23	1:A:174:LEU:H	0.44	1.64	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:PHE:CD1	1:A:179:PHE:C	0.44	2.89	27	1
1:A:185:PHE:CD1	1:A:243:LEU:HD12	0.44	2.48	27	1
1:A:195:LYS:HZ3	1:A:215:GLU:CD	0.44	2.16	21	1
1:A:204:ARG:O	1:A:204:ARG:NE	0.44	2.50	24	1
1:A:184:TYR:CD2	1:A:188:ASN:ND2	0.43	2.87	23	2
1:A:184:TYR:CZ	1:A:188:ASN:ND2	0.43	2.86	5	1
1:A:199:LEU:C	1:A:199:LEU:CD2	0.43	2.87	6	2
1:A:174:LEU:N	1:A:174:LEU:CD1	0.43	2.65	26	1
1:A:174:LEU:O	1:A:175:SER:O	0.43	2.36	26	1
1:A:222:ARG:O	1:A:226:ASP:C	0.43	2.57	13	1
1:A:151:LEU:HD12	1:A:151:LEU:N	0.43	2.28	5	1
1:A:226:ASP:O	1:A:227:THR:CB	0.42	2.67	21	1
1:A:167:LYS:CE	1:A:225:ILE:O	0.42	2.66	5	1
1:A:159:ASP:CB	1:A:162:THR:OG1	0.42	2.67	7	2
1:A:213:VAL:O	1:A:216:SER:OG	0.42	2.33	16	2
1:A:194:SER:OG	1:A:197:LYS:CG	0.42	2.67	17	1
1:A:227:THR:O	1:A:227:THR:OG1	0.42	2.33	3	1
1:A:211:VAL:O	1:A:211:VAL:CG2	0.42	2.65	29	1
1:A:157:GLU:N	1:A:166:TRP:O	0.42	2.52	3	3
1:A:212:ASN:O	1:A:214:VAL:N	0.42	2.52	21	1
1:A:160:GLU:OE2	1:A:160:GLU:N	0.42	2.53	24	1
1:A:210:ASP:O	1:A:212:ASN:N	0.42	2.52	26	1
1:A:204:ARG:O	1:A:204:ARG:CZ	0.42	2.68	30	1
1:A:211:VAL:O	1:A:211:VAL:HG22	0.42	2.15	1	1
1:A:184:TYR:OH	1:A:201:HIS:CE1	0.42	2.73	9	1
1:A:240:GLY:C	1:A:241:TYR:CD1	0.42	2.93	14	2
1:A:167:LYS:NZ	1:A:225:ILE:CG2	0.42	2.83	25	1
1:A:199:LEU:CG	1:A:214:VAL:HG21	0.41	2.45	25	1
1:A:222:ARG:CG	1:A:223:ARG:N	0.41	2.83	25	1
1:A:199:LEU:HD22	1:A:211:VAL:HG22	0.41	1.93	26	1
1:A:150:ARG:HH12	1:A:157:GLU:CG	0.41	2.28	8	1
1:A:222:ARG:O	1:A:226:ASP:CA	0.41	2.68	13	1
1:A:226:ASP:C	1:A:228:GLY:N	0.41	2.73	13	1
1:A:153:PHE:CZ	1:A:243:LEU:HD11	0.41	2.50	18	1
1:A:167:LYS:C	1:A:167:LYS:CD	0.41	2.88	26	1
1:A:230:LYS:CD	1:A:230:LYS:H	0.41	2.27	27	1
1:A:151:LEU:HD22	1:A:186:VAL:HG11	0.41	1.91	10	1
1:A:167:LYS:HZ3	1:A:168:ALA:HB3	0.41	1.75	16	1
1:A:165:VAL:CG2	1:A:174:LEU:HD11	0.41	2.45	19	1
1:A:178:GLU:N	1:A:178:GLU:OE2	0.41	2.54	23	1
1:A:184:TYR:CG	1:A:201:HIS:CE1	0.41	3.09	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:244:ARG:HE	1:A:244:ARG:C	0.41	2.19	28	1
1:A:184:TYR:CE2	1:A:193:LEU:HD21	0.41	2.51	15	1
1:A:184:TYR:O	1:A:188:ASN:ND2	0.41	2.54	3	1
1:A:245:GLU:O	1:A:245:GLU:CD	0.41	2.59	16	1
1:A:159:ASP:OD1	1:A:159:ASP:N	0.41	2.53	25	1
1:A:236:LEU:O	1:A:238:GLY:N	0.40	2.53	11	1
1:A:242:VAL:O	1:A:242:VAL:HG13	0.40	2.16	25	1
1:A:199:LEU:CD2	1:A:203:TRP:CG	0.40	3.04	10	1
1:A:151:LEU:N	1:A:151:LEU:CD1	0.40	2.85	5	1
1:A:178:GLU:CD	1:A:221:LEU:HD11	0.40	2.37	9	1
1:A:199:LEU:O	1:A:203:TRP:CB	0.40	2.70	14	1

## 6.3 Torsion angles [i](#)

### 6.3.1 Protein backbone [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	93/128 (73%)	80±1 (87±2%)	9±2 (10±2%)	4±1 (4±1%)	5	32
All	All	2790/3840 (73%)	2415 (87%)	266 (10%)	109 (4%)	5	32

All 10 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	154	ALA	29
1	A	203	TRP	23
1	A	227	THR	23
1	A	210	ASP	18
1	A	163	HIS	5
1	A	204	ARG	5
1	A	175	SER	3
1	A	237	ARG	1
1	A	213	VAL	1
1	A	211	VAL	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	85/114 (75%)	63±4 (75±4%)	22±4 (25±4%)	2	24
All	All	2550/3420 (75%)	1903 (75%)	647 (25%)	2	24

All 70 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	149	VAL	30
1	A	166	TRP	30
1	A	175	SER	30
1	A	156	ILE	27
1	A	194	SER	27
1	A	234	HIS	26
1	A	241	TYR	26
1	A	172	VAL	25
1	A	219	SER	25
1	A	226	ASP	19
1	A	227	THR	18
1	A	225	ILE	17
1	A	203	TRP	16
1	A	195	LYS	14
1	A	181	LEU	13
1	A	177	THR	13
1	A	233	LEU	12
1	A	152	THR	12
1	A	220	TYR	12
1	A	210	ASP	11
1	A	185	PHE	11
1	A	159	ASP	11
1	A	216	SER	11
1	A	217	TYR	10
1	A	204	ARG	9
1	A	221	LEU	9
1	A	243	LEU	8
1	A	167	LYS	8
1	A	235	THR	8

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Mol	Chain	Res	Type	Models (Total)
1	A	237	ARG	8
1	A	201	HIS	8
1	A	191	THR	7
1	A	222	ARG	7
1	A	244	ARG	7
1	A	230	LYS	7
1	A	223	ARG	7
1	A	178	GLU	6
1	A	205	TYR	6
1	A	174	LEU	6
1	A	200	ASP	6
1	A	158	LEU	6
1	A	197	LYS	5
1	A	232	LEU	5
1	A	160	GLU	5
1	A	173	SER	5
1	A	231	ARG	4
1	A	182	LEU	4
1	A	224	LYS	4
1	A	170	GLN	4
1	A	214	VAL	3
1	A	150	ARG	3
1	A	229	GLU	3
1	A	212	ASN	3
1	A	163	HIS	3
1	A	183	ARG	3
1	A	179	PHE	3
1	A	211	VAL	2
1	A	188	ASN	2
1	A	155	ASP	2
1	A	199	LEU	2
1	A	184	TYR	2
1	A	161	GLU	2
1	A	164	GLU	2
1	A	180	THR	1
1	A	202	VAL	1
1	A	245	GLU	1
1	A	236	LEU	1
1	A	153	PHE	1
1	A	193	LEU	1
1	A	215	GLU	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.5 Carbohydrates [i](#)

There are no monosaccharides 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 80% for the well-defined parts and 65% for the entire structure.

### 7.1 Chemical shift list 1

File name: working\_cs.cif

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	1224
Number of shifts mapped to atoms	1224
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	105	$0.16 \pm 0.11$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	97	$0.47 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	99	$0.19 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	96	$0.22 \pm 0.30$	None needed ( $< 0.5$ ppm)

#### 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 80%, i.e. 968 atoms were assigned a chemical shift out of a possible 1214. 0 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	441/459 (96%)	177/183 (97%)	179/186 (96%)	85/90 (94%)
Sidechain	473/640 (74%)	277/371 (75%)	196/237 (83%)	0/32 (0%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	54/115 (47%)	28/59 (47%)	24/48 (50%)	2/8 (25%)
Overall	968/1214 (80%)	482/613 (79%)	399/471 (85%)	87/130 (67%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 1080 atoms were assigned a chemical shift out of a possible 1650. 0 out of 26 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	501/628 (80%)	201/250 (80%)	204/256 (80%)	96/122 (79%)
Sidechain	525/842 (62%)	307/496 (62%)	218/301 (72%)	0/45 (0%)
Aromatic	54/180 (30%)	28/92 (30%)	24/66 (36%)	2/22 (9%)
Overall	1080/1650 (65%)	536/838 (64%)	446/623 (72%)	98/189 (52%)

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

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

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	164	GLU	HB2	0.92	3.08 – 0.98	-5.3

#### 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:

