



# Full wwPDB NMR Structure Validation Report ⓘ

Sep 30, 2021 – 04:12 PM JST

PDB ID : 6L87  
Title : Solution structure of the tandem PWWP-ARID domains of human RBBP1  
Authors : Gong, W.B.; Perrett, S.; Feng, Y.G.  
Deposited on : 2019-11-05

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.

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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 : 2.23.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

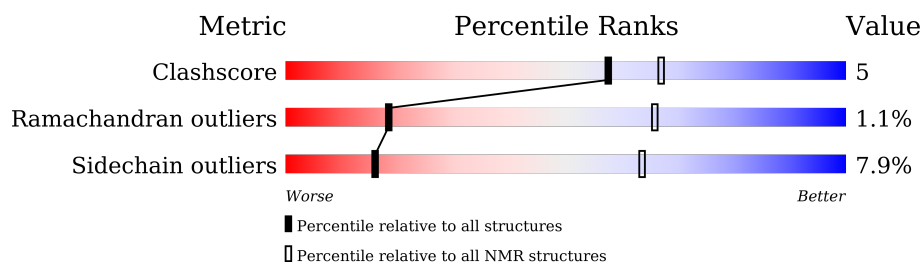
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 88%.

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	229	

## 2 Ensemble composition and analysis

This entry contains 20 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:2-A:103, A:117-A:212 (198)	0.61	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. No single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3730 atoms, of which 1856 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called AT-rich interactive domain-containing protein 4A.

Mol	Chain	Residues	Atoms						Trace
1	A	229	Total	C	H	N	O	S	0
			3730	1193	1856	320	354	7	

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	LYS	ASP	See sequence details	UNP P29374
A	110	LYS	GLU	See sequence details	UNP P29374
A	?	-	ASP	deletion	UNP P29374
A	?	-	GLY	deletion	UNP P29374
A	?	-	PRO	deletion	UNP P29374
A	?	-	ALA	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	ASN	deletion	UNP P29374
A	?	-	ASP	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	ALA	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	LYS	deletion	UNP P29374
A	?	-	THR	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	GLU	deletion	UNP P29374
A	?	-	VAL	deletion	UNP P29374
A	?	-	PRO	deletion	UNP P29374
A	112	LYS	GLU	See sequence details	UNP P29374
A	222	LEU	-	expression tag	UNP P29374
A	223	GLU	-	expression tag	UNP P29374
A	224	HIS	-	expression tag	UNP P29374
A	225	HIS	-	expression tag	UNP P29374
A	226	HIS	-	expression tag	UNP P29374

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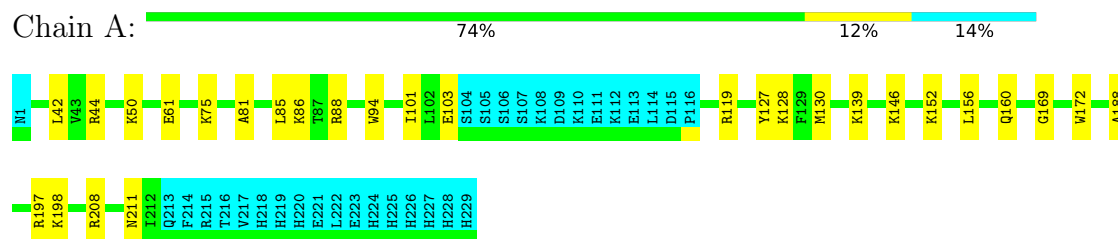
Chain	Residue	Modelled	Actual	Comment	Reference
A	227	HIS	-	expression tag	UNP P29374
A	228	HIS	-	expression tag	UNP P29374
A	229	HIS	-	expression tag	UNP P29374

## 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: AT-rich interactive domain-containing protein 4A

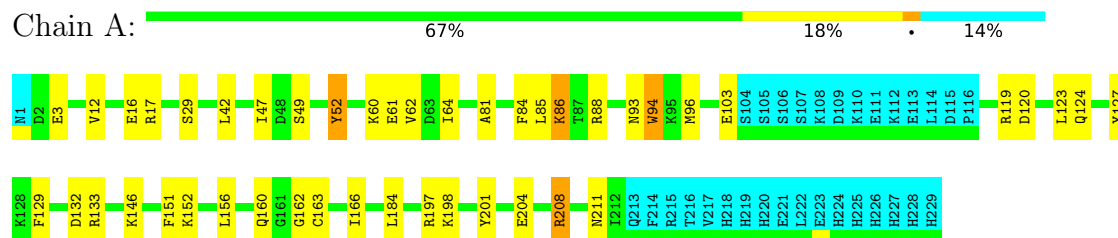


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

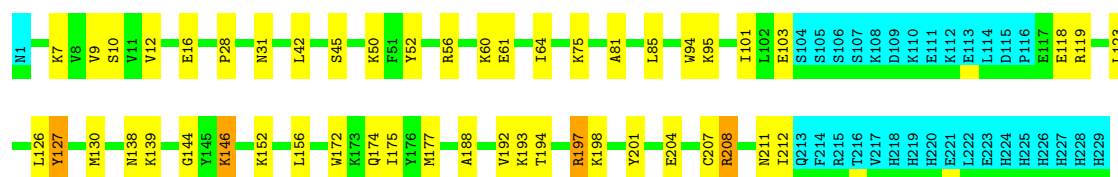
- Molecule 1: AT-rich interactive domain-containing protein 4A



#### 4.2.2 Score per residue for model 2

- Molecule 1: AT-rich interactive domain-containing protein 4A

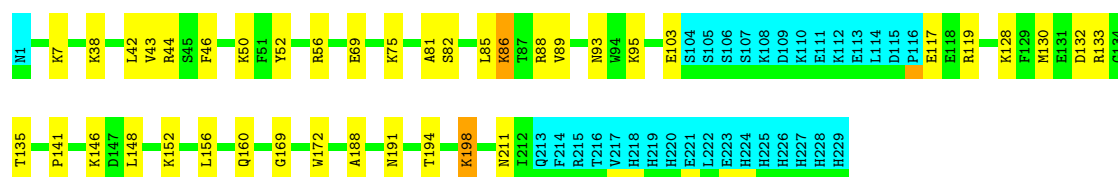




#### 4.2.3 Score per residue for model 3

- Molecule 1: AT-rich interactive domain-containing protein 4A

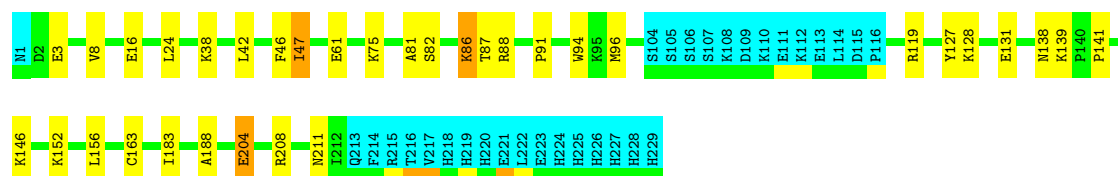
Chain A: 69% 17% 14%



#### 4.2.4 Score per residue for model 4

- Molecule 1: AT-rich interactive domain-containing protein 4A

Chain A: 72% 14% 14%



#### 4.2.5 Score per residue for model 5

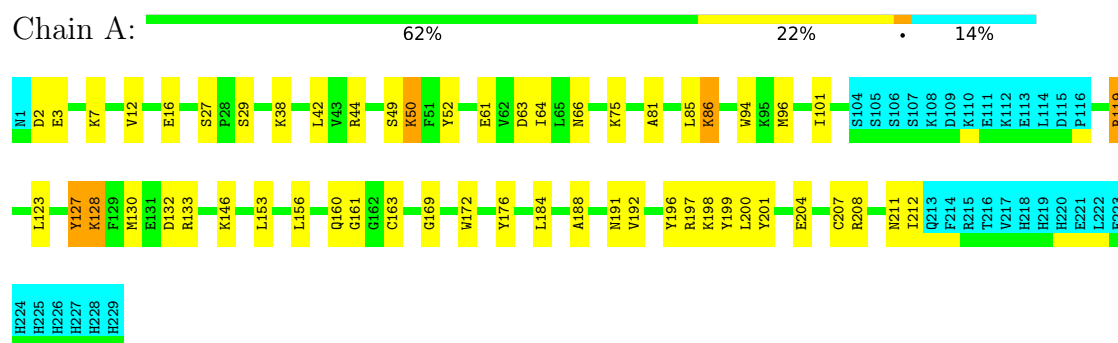
- Molecule 1: AT-rich interactive domain-containing protein 4A

Chain A: 71% 12% 14%



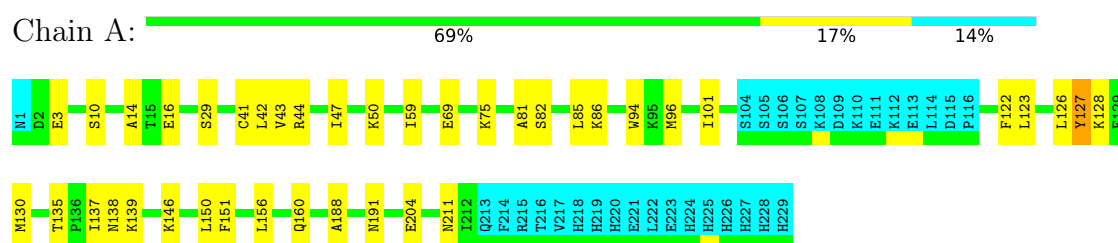
#### 4.2.6 Score per residue for model 6

- Molecule 1: AT-rich interactive domain-containing protein 4A



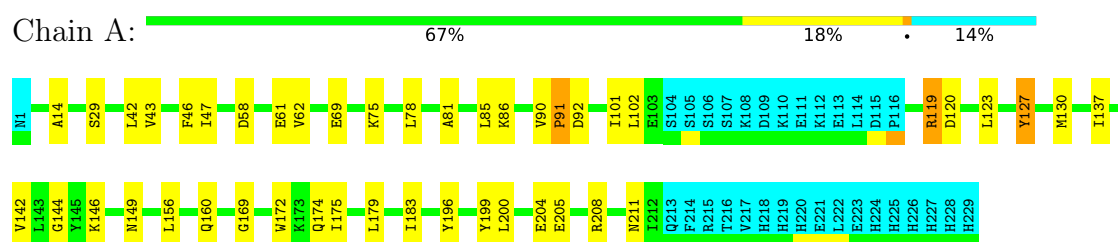
#### 4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: AT-rich interactive domain-containing protein 4A



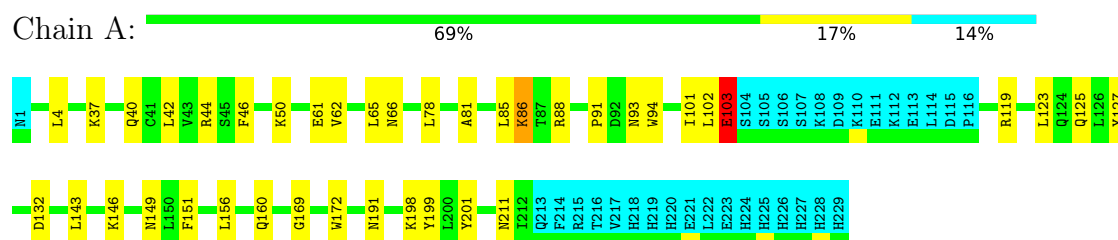
#### 4.2.8 Score per residue for model 8

- Molecule 1: AT-rich interactive domain-containing protein 4A



#### 4.2.9 Score per residue for model 9

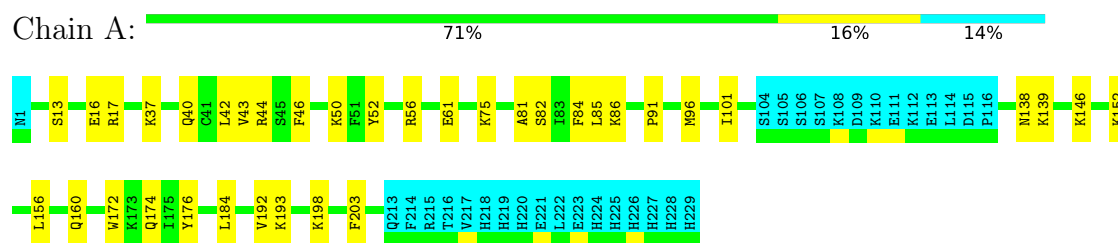
- Molecule 1: AT-rich interactive domain-containing protein 4A





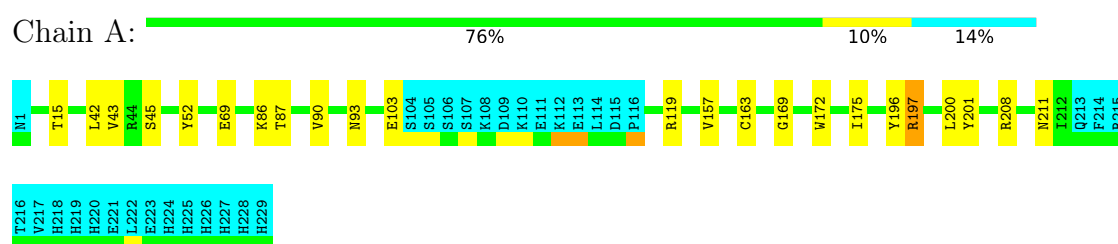
### 4.2.10 Score per residue for model 10

- Molecule 1: AT-rich interactive domain-containing protein 4A



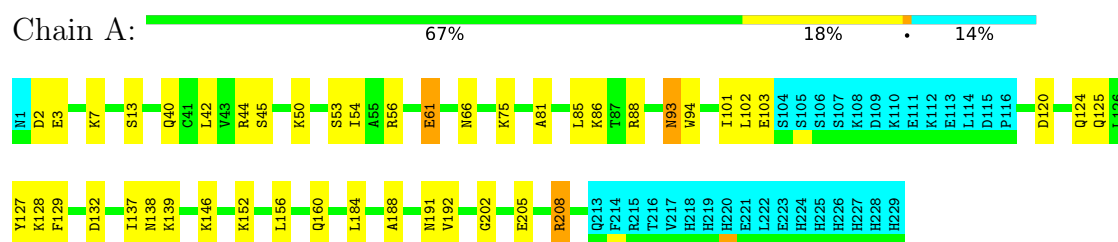
### 4.2.11 Score per residue for model 11

- Molecule 1: AT-rich interactive domain-containing protein 4A



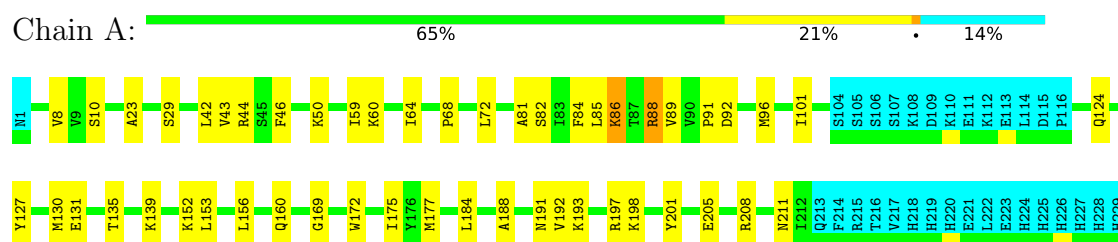
### 4.2.12 Score per residue for model 12

- Molecule 1: AT-rich interactive domain-containing protein 4A



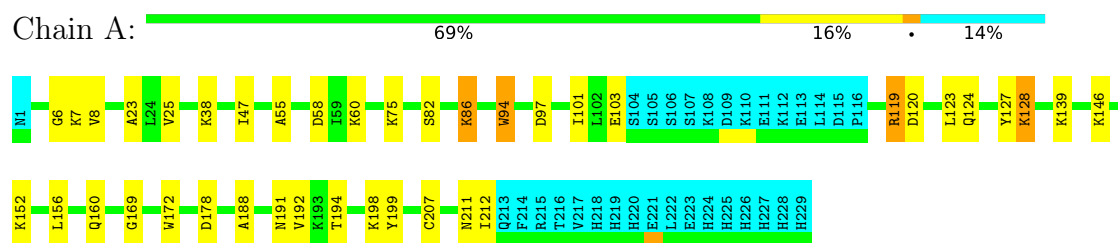
### 4.2.13 Score per residue for model 13

- Molecule 1: AT-rich interactive domain-containing protein 4A



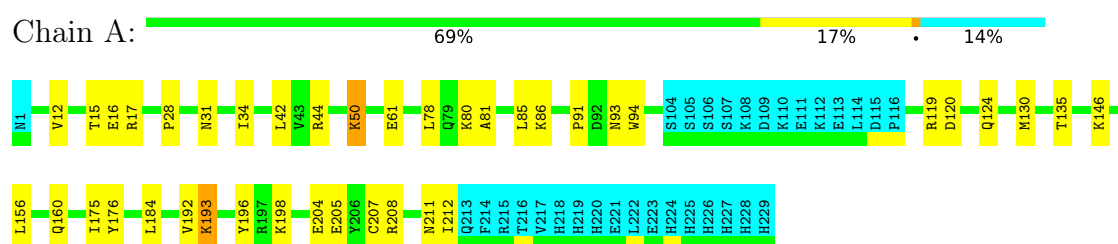
#### 4.2.14 Score per residue for model 14

- Molecule 1: AT-rich interactive domain-containing protein 4A



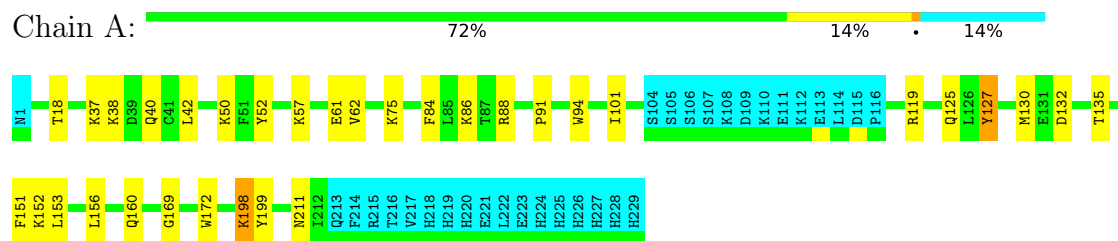
#### 4.2.15 Score per residue for model 15

- Molecule 1: AT-rich interactive domain-containing protein 4A



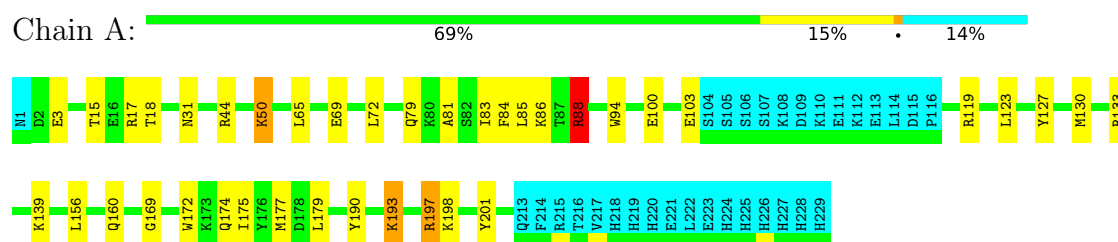
#### 4.2.16 Score per residue for model 16

- Molecule 1: AT-rich interactive domain-containing protein 4A



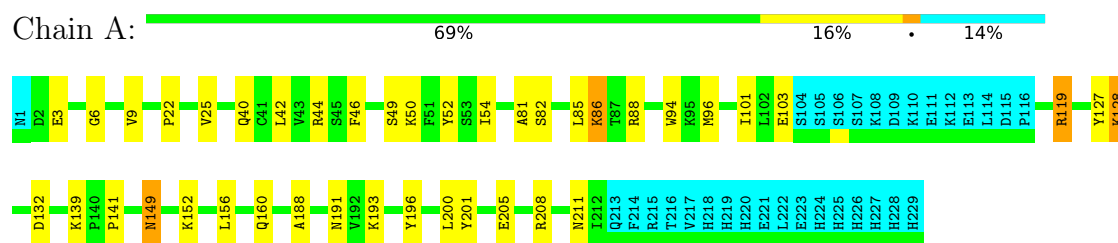
#### 4.2.17 Score per residue for model 17

- Molecule 1: AT-rich interactive domain-containing protein 4A



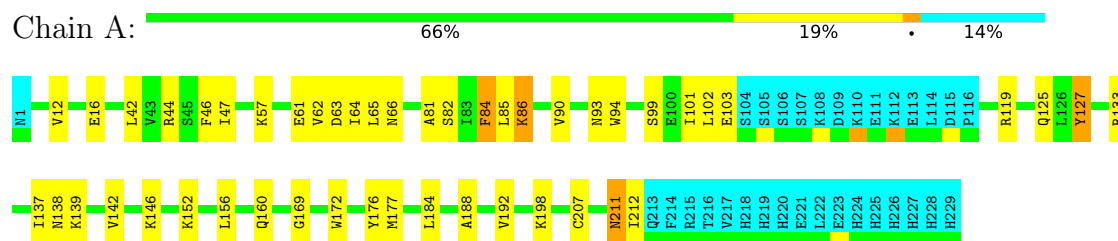
### 4.2.18 Score per residue for model 18

- Molecule 1: AT-rich interactive domain-containing protein 4A



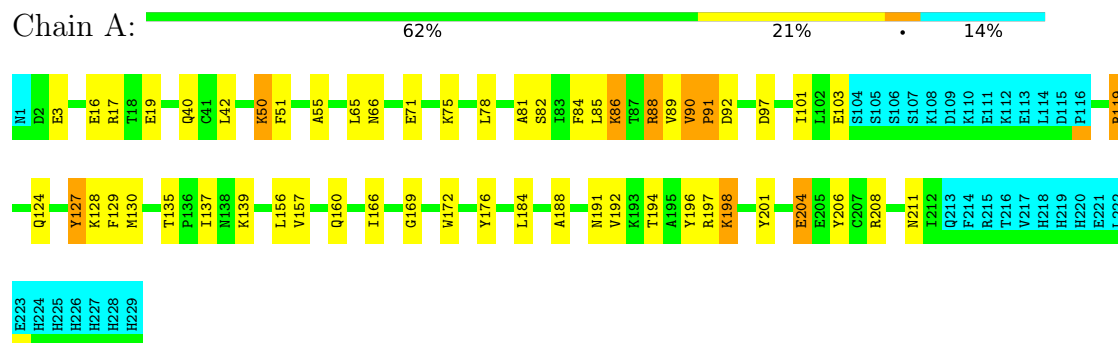
### 4.2.19 Score per residue for model 19

- Molecule 1: AT-rich interactive domain-containing protein 4A



### 4.2.20 Score per residue for model 20

- Molecule 1: AT-rich interactive domain-containing protein 4A



## 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
CNS	refinement	
CYANA	structure calculation	

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	2611
Number of shifts mapped to atoms	2611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

## 6 Model quality [i](#)

### 6.1 Standard geometry [i](#)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.9±0.8
All	All	0	18

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	119	ARG	Sidechain	6
1	A	197	ARG	Sidechain	3
1	A	44	ARG	Sidechain	3
1	A	17	ARG	Sidechain	2
1	A	88	ARG	Sidechain	2
1	A	133	ARG	Sidechain	1
1	A	56	ARG	Sidechain	1

### 6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1604	1610	1609	16±4
All	All	32080	32200	32180	324

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:MET:SD	1:A:133:ARG:HD3	0.64	2.32	5	2
1:A:81:ALA:O	1:A:85:LEU:HG	0.62	1.93	19	15
1:A:169:GLY:HA2	1:A:172:TRP:CE3	0.61	2.30	5	12
1:A:156:LEU:O	1:A:160:GLN:HG2	0.61	1.96	17	15
1:A:204:GLU:O	1:A:208:ARG:HG2	0.60	1.96	6	2
1:A:46:PHE:CE1	1:A:81:ALA:HA	0.59	2.32	13	3
1:A:130:MET:HG3	1:A:135:THR:O	0.59	1.97	7	5
1:A:197:ARG:O	1:A:201:TYR:HB3	0.58	1.98	1	3
1:A:119:ARG:HG3	1:A:120:ASP:N	0.58	2.11	14	2
1:A:84:PHE:O	1:A:88:ARG:HG2	0.57	1.99	16	2
1:A:197:ARG:O	1:A:201:TYR:HB2	0.57	1.99	13	3
1:A:101:ILE:HG21	1:A:123:LEU:HB3	0.56	1.78	9	1
1:A:119:ARG:O	1:A:123:LEU:HG	0.56	2.00	1	4
1:A:152:LYS:O	1:A:156:LEU:HG	0.56	2.00	3	9
1:A:82:SER:O	1:A:86:LYS:HG3	0.56	2.01	10	9
1:A:101:ILE:HG23	1:A:127:TYR:CE2	0.55	2.37	7	4
1:A:188:ALA:O	1:A:192:VAL:HG23	0.55	2.02	14	3
1:A:188:ALA:HA	1:A:191:ASN:ND2	0.55	2.16	12	8
1:A:84:PHE:CE2	1:A:88:ARG:HD2	0.54	2.37	1	1
1:A:163:CYS:SG	1:A:204:GLU:HG3	0.54	2.42	1	1
1:A:193:LYS:O	1:A:197:ARG:HB2	0.54	2.03	2	2
1:A:44:ARG:HG3	1:A:50:LYS:O	0.53	2.02	7	5
1:A:10:SER:O	1:A:59:ILE:HA	0.53	2.03	13	2
1:A:90:VAL:HB	1:A:91:PRO:HD2	0.53	1.80	20	2
1:A:119:ARG:HA	1:A:151:PHE:CD1	0.53	2.38	1	1
1:A:130:MET:SD	1:A:199:TYR:HA	0.53	2.44	8	2
1:A:129:PHE:CE1	1:A:202:GLY:HA3	0.52	2.40	12	1
1:A:86:LYS:O	1:A:93:ASN:HB3	0.52	2.05	1	2
1:A:46:PHE:CE2	1:A:81:ALA:HA	0.52	2.40	18	3
1:A:172:TRP:CZ3	1:A:193:LYS:HA	0.52	2.40	10	1
1:A:198:LYS:HE3	1:A:199:TYR:CZ	0.51	2.40	14	1
1:A:196:TYR:CD1	1:A:200:LEU:HD12	0.51	2.40	8	1
1:A:127:TYR:CE1	1:A:137:ILE:HG13	0.51	2.39	12	1
1:A:101:ILE:HG23	1:A:127:TYR:CE1	0.51	2.41	12	6
1:A:127:TYR:CZ	1:A:137:ILE:HG21	0.51	2.40	7	1
1:A:204:GLU:O	1:A:208:ARG:HG3	0.50	2.06	2	3
1:A:99:SER:O	1:A:103:GLU:HA	0.50	2.06	19	1
1:A:46:PHE:HB2	1:A:84:PHE:CE1	0.50	2.41	19	2
1:A:64:ILE:HD12	1:A:64:ILE:H	0.50	1.66	2	3
1:A:123:LEU:O	1:A:127:TYR:HB2	0.50	2.06	7	1
1:A:96:MET:SD	1:A:101:ILE:HD11	0.50	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:101:ILE:HG23	1:A:127:TYR:CD1	0.49	2.42	16	3
1:A:122:PHE:O	1:A:126:LEU:HG	0.49	2.07	7	1
1:A:37:LYS:HD2	1:A:40:GLN:NE2	0.49	2.22	16	1
1:A:86:LYS:HD2	1:A:87:THR:N	0.48	2.22	4	1
1:A:198:LYS:HE2	1:A:199:TYR:CZ	0.48	2.42	9	1
1:A:6:GLY:HA2	1:A:25:VAL:O	0.48	2.08	18	2
1:A:119:ARG:HH11	1:A:119:ARG:HG3	0.48	1.69	18	1
1:A:176:TYR:CE2	1:A:188:ALA:HB1	0.48	2.44	19	1
1:A:120:ASP:O	1:A:124:GLN:HG2	0.48	2.09	15	1
1:A:193:LYS:HA	1:A:196:TYR:CE1	0.48	2.44	15	1
1:A:196:TYR:CD2	1:A:200:LEU:HD12	0.48	2.43	6	1
1:A:194:THR:O	1:A:198:LYS:HG2	0.48	2.09	20	3
1:A:120:ASP:O	1:A:124:GLN:HG3	0.47	2.09	12	1
1:A:176:TYR:CD2	1:A:192:VAL:HB	0.47	2.44	20	2
1:A:50:LYS:HE3	1:A:50:LYS:N	0.47	2.24	17	1
1:A:163:CYS:SG	1:A:208:ARG:HB3	0.47	2.49	11	1
1:A:196:TYR:HA	1:A:200:LEU:HD23	0.47	1.85	11	2
1:A:40:GLN:HG3	1:A:54:ILE:O	0.47	2.09	5	2
1:A:12:VAL:HB	1:A:16:GLU:O	0.47	2.10	2	3
1:A:205:GLU:OE2	1:A:208:ARG:HD3	0.47	2.09	15	1
1:A:71:GLU:OE2	1:A:75:LYS:HE2	0.47	2.10	20	1
1:A:96:MET:SD	1:A:128:LYS:HG2	0.47	2.49	4	1
1:A:87:THR:HA	1:A:93:ASN:O	0.47	2.10	11	1
1:A:44:ARG:NH2	1:A:132:ASP:HB2	0.47	2.25	18	1
1:A:88:ARG:O	1:A:94:TRP:HB3	0.47	2.09	18	1
1:A:101:ILE:HG23	1:A:127:TYR:CZ	0.47	2.45	18	1
1:A:90:VAL:HG21	1:A:93:ASN:HB2	0.47	1.87	19	1
1:A:84:PHE:HA	1:A:88:ARG:NH2	0.47	2.24	20	1
1:A:102:LEU:O	1:A:103:GLU:HB2	0.47	2.10	9	1
1:A:127:TYR:CE2	1:A:137:ILE:HG13	0.47	2.44	20	1
1:A:207:CYS:HA	1:A:212:ILE:HD12	0.46	1.88	14	4
1:A:88:ARG:HA	1:A:94:TRP:CD1	0.46	2.45	1	1
1:A:172:TRP:CE3	1:A:175:ILE:HD11	0.46	2.44	2	1
1:A:81:ALA:O	1:A:85:LEU:HD13	0.46	2.11	17	1
1:A:46:PHE:CZ	1:A:81:ALA:HA	0.46	2.45	9	2
1:A:156:LEU:HB3	1:A:175:ILE:HG22	0.46	1.86	8	3
1:A:141:PRO:HB2	1:A:148:LEU:O	0.46	2.11	3	1
1:A:31:ASN:ND2	1:A:34:ILE:HB	0.46	2.25	15	1
1:A:130:MET:HG2	1:A:135:THR:O	0.46	2.10	3	1
1:A:28:PRO:HA	1:A:31:ASN:OD1	0.46	2.11	15	2
1:A:12:VAL:HG13	1:A:16:GLU:O	0.46	2.10	6	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LYS:HD3	1:A:40:GLN:NE2	0.46	2.27	9	1
1:A:91:PRO:HA	1:A:94:TRP:O	0.46	2.10	15	1
1:A:43:VAL:HB	1:A:52:TYR:CE1	0.45	2.46	3	1
1:A:41:CYS:SG	1:A:59:ILE:HD12	0.45	2.51	7	1
1:A:205:GLU:OE2	1:A:208:ARG:HD2	0.45	2.11	18	2
1:A:144:GLY:O	1:A:146:LYS:HD3	0.45	2.11	8	1
1:A:50:LYS:HD2	1:A:51:PHE:N	0.45	2.26	20	1
1:A:64:ILE:HG21	1:A:81:ALA:CB	0.45	2.42	1	1
1:A:55:ALA:HB3	1:A:58:ASP:OD2	0.45	2.11	14	1
1:A:10:SER:HB2	1:A:60:LYS:HB2	0.45	1.88	13	1
1:A:156:LEU:O	1:A:160:GLN:HG3	0.44	2.12	19	1
1:A:157:VAL:HG21	1:A:196:TYR:CE1	0.44	2.48	20	1
1:A:144:GLY:O	1:A:146:LYS:HD2	0.44	2.13	5	1
1:A:40:GLN:NE2	1:A:53:SER:HB2	0.44	2.28	12	1
1:A:127:TYR:O	1:A:131:GLU:HG3	0.44	2.13	13	1
1:A:89:VAL:O	1:A:90:VAL:HG22	0.44	2.12	20	1
1:A:176:TYR:CD1	1:A:192:VAL:HB	0.44	2.48	19	3
1:A:17:ARG:HD2	1:A:17:ARG:N	0.44	2.28	10	1
1:A:96:MET:HB3	1:A:124:GLN:OE1	0.44	2.13	1	1
1:A:188:ALA:O	1:A:192:VAL:HG12	0.44	2.13	2	1
1:A:96:MET:CE	1:A:128:LYS:HE2	0.44	2.42	18	1
1:A:45:SER:HB2	1:A:52:TYR:OH	0.43	2.12	2	2
1:A:183:ILE:O	1:A:188:ALA:HB2	0.43	2.13	4	1
1:A:9:VAL:O	1:A:22:PRO:HA	0.43	2.14	18	1
1:A:128:LYS:HD3	1:A:129:PHE:N	0.43	2.28	20	1
1:A:4:LEU:H	1:A:4:LEU:HD23	0.43	1.73	9	1
1:A:152:LYS:O	1:A:156:LEU:HD13	0.43	2.13	16	2
1:A:75:LYS:N	1:A:75:LYS:HD2	0.43	2.28	12	4
1:A:119:ARG:HB3	1:A:151:PHE:CG	0.43	2.48	16	1
1:A:126:LEU:HB3	1:A:130:MET:HE2	0.43	1.89	2	1
1:A:44:ARG:NH1	1:A:132:ASP:HA	0.43	2.28	12	1
1:A:68:PRO:O	1:A:72:LEU:HG	0.43	2.13	13	1
1:A:94:TRP:CZ2	1:A:125:GLN:HA	0.43	2.48	19	1
1:A:157:VAL:HG21	1:A:196:TYR:CE2	0.43	2.49	11	1
1:A:198:LYS:NZ	1:A:198:LYS:HB2	0.43	2.28	16	1
1:A:175:ILE:O	1:A:179:LEU:HD23	0.43	2.14	17	1
1:A:49:SER:HB2	1:A:52:TYR:CE1	0.43	2.49	6	1
1:A:44:ARG:HD2	1:A:132:ASP:OD1	0.43	2.13	9	1
1:A:44:ARG:HG2	1:A:45:SER:N	0.43	2.29	12	1
1:A:40:GLN:HA	1:A:55:ALA:HA	0.43	1.91	20	1
1:A:8:VAL:HA	1:A:23:ALA:O	0.43	2.13	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:125:GLN:HA	1:A:125:GLN:OE1	0.43	2.14	16	1
1:A:8:VAL:HG12	1:A:24:LEU:HD23	0.42	1.92	4	1
1:A:130:MET:CE	1:A:137:ILE:HD11	0.42	2.44	8	1
1:A:207:CYS:HA	1:A:212:ILE:HD13	0.42	1.90	2	1
1:A:130:MET:O	1:A:133:ARG:HG2	0.42	2.14	3	1
1:A:91:PRO:HA	1:A:94:TRP:CZ3	0.42	2.49	4	1
1:A:153:LEU:HD21	1:A:175:ILE:HD12	0.42	1.92	13	1
1:A:64:ILE:HB	1:A:85:LEU:CD1	0.42	2.44	19	1
1:A:29:SER:HB2	1:A:205:GLU:OE1	0.42	2.15	8	1
1:A:90:VAL:HG11	1:A:93:ASN:HD22	0.42	1.74	11	1
1:A:119:ARG:O	1:A:123:LEU:HD13	0.42	2.15	8	2
1:A:128:LYS:HE2	1:A:128:LYS:HA	0.42	1.91	14	1
1:A:137:ILE:HG23	1:A:139:LYS:O	0.42	2.13	19	1
1:A:85:LEU:O	1:A:89:VAL:HB	0.42	2.14	3	1
1:A:119:ARG:HA	1:A:151:PHE:CG	0.42	2.50	5	1
1:A:49:SER:HB2	1:A:52:TYR:CE2	0.42	2.50	18	1
1:A:188:ALA:HA	1:A:191:ASN:CG	0.42	2.35	18	1
1:A:129:PHE:HA	1:A:132:ASP:OD2	0.42	2.14	1	1
1:A:47:ILE:HD13	1:A:47:ILE:O	0.42	2.14	4	1
1:A:160:GLN:HB2	1:A:166:ILE:HD11	0.42	1.92	5	1
1:A:120:ASP:O	1:A:124:GLN:HB2	0.42	2.15	5	1
1:A:86:LYS:HD2	1:A:86:LYS:C	0.42	2.35	6	1
1:A:149:ASN:CB	1:A:179:LEU:HD11	0.42	2.44	8	1
1:A:69:GLU:HA	1:A:72:LEU:HG	0.42	1.91	17	1
1:A:52:TYR:HB3	1:A:54:ILE:HG12	0.42	1.92	18	1
1:A:127:TYR:OH	1:A:141:PRO:HD3	0.42	2.14	18	1
1:A:4:LEU:H	1:A:4:LEU:HD12	0.41	1.75	5	1
1:A:93:ASN:HB3	1:A:94:TRP:CE3	0.41	2.50	12	1
1:A:84:PHE:O	1:A:88:ARG:HG3	0.41	2.15	17	1
1:A:190:TYR:O	1:A:193:LYS:HG3	0.41	2.14	17	1
1:A:29:SER:HB2	1:A:205:GLU:OE2	0.41	2.15	13	1
1:A:172:TRP:HA	1:A:175:ILE:HG12	0.41	1.91	2	1
1:A:44:ARG:HD2	1:A:132:ASP:OD2	0.41	2.15	3	1
1:A:37:LYS:HD3	1:A:40:GLN:OE1	0.41	2.15	10	1
1:A:143:LEU:HD11	1:A:191:ASN:HB3	0.41	1.91	9	1
1:A:49:SER:HB2	1:A:52:TYR:CD1	0.41	2.51	1	1
1:A:144:GLY:O	1:A:146:LYS:HG2	0.41	2.16	2	1
1:A:205:GLU:HA	1:A:208:ARG:HG2	0.41	1.93	13	1
1:A:96:MET:SD	1:A:128:LYS:HB2	0.41	2.56	7	2
1:A:88:ARG:HG3	1:A:89:VAL:N	0.41	2.30	13	1
1:A:64:ILE:HG21	1:A:81:ALA:HB3	0.41	1.91	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:LEU:O	1:A:130:MET:HB2	0.41	2.16	7	1
1:A:9:VAL:HB	1:A:60:LYS:O	0.41	2.15	2	1
1:A:130:MET:HG3	1:A:133:ARG:CZ	0.41	2.45	3	1
1:A:27:SER:C	1:A:29:SER:H	0.41	2.19	6	1
1:A:150:LEU:HD12	1:A:151:PHE:N	0.41	2.30	7	1
1:A:79:GLN:O	1:A:83:ILE:HG13	0.41	2.16	17	1
1:A:101:ILE:HG12	1:A:127:TYR:CD1	0.41	2.51	19	1
1:A:166:ILE:HG21	1:A:172:TRP:NE1	0.41	2.30	20	1
1:A:102:LEU:HD12	1:A:123:LEU:HD21	0.41	1.91	8	1
1:A:119:ARG:HB2	1:A:151:PHE:CG	0.41	2.51	9	1
1:A:96:MET:HE1	1:A:127:TYR:HB3	0.41	1.93	13	1
1:A:162:GLY:O	1:A:166:ILE:HG13	0.40	2.16	1	1
1:A:101:ILE:HG12	1:A:127:TYR:CD2	0.40	2.51	6	1
1:A:130:MET:HE3	1:A:199:TYR:HA	0.40	1.93	16	1
1:A:194:THR:O	1:A:198:LYS:HG3	0.40	2.16	3	1
1:A:14:ALA:HA	1:A:58:ASP:OD2	0.40	2.16	8	1
1:A:172:TRP:O	1:A:175:ILE:HG12	0.40	2.17	11	1
1:A:211:ASN:N	1:A:211:ASN:HD22	0.40	2.14	19	1
1:A:63:ASP:HB2	1:A:66:ASN:OD1	0.40	2.15	6	1
1:A:3:GLU:HB3	1:A:61:GLU:HB3	0.40	1.92	12	1
1:A:149:ASN:N	1:A:149:ASN:HD22	0.40	2.14	18	1
1:A:101:ILE:HA	1:A:127:TYR:CZ	0.40	2.51	2	1
1:A:94:TRP:NE1	1:A:124:GLN:HB3	0.40	2.32	14	1
1:A:204:GLU:OE1	1:A:208:ARG:HD3	0.40	2.17	4	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	198/229 (86%)	182±3 (92±2%)	14±3 (7±1%)	2±1 (1±1%)	18	66
All	All	3960/4580 (86%)	3644 (92%)	272 (7%)	44 (1%)	18	66

All 15 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	103	GLU	10
1	A	184	LEU	8
1	A	91	PRO	6
1	A	92	ASP	3
1	A	15	THR	3
1	A	2	ASP	2
1	A	13	SER	2
1	A	88	ARG	2
1	A	97	ASP	2
1	A	141	PRO	1
1	A	101	ILE	1
1	A	212	ILE	1
1	A	14	ALA	1
1	A	183	ILE	1
1	A	90	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	180/211 (85%)	166±3 (92±2%)	14±3 (8±2%)	16	63
All	All	3600/4220 (85%)	3317 (92%)	283 (8%)	16	63

All 67 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	42	LEU	18
1	A	86	LYS	17
1	A	211	ASN	17
1	A	146	LYS	13
1	A	50	LYS	11
1	A	61	GLU	11
1	A	127	TYR	10
1	A	198	LYS	10
1	A	139	LYS	10
1	A	94	TRP	8
1	A	3	GLU	7

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Mol	Chain	Res	Type	Models (Total)
1	A	47	ILE	6
1	A	138	ASN	6
1	A	75	LYS	6
1	A	62	VAL	5
1	A	7	LYS	5
1	A	177	MET	5
1	A	38	LYS	5
1	A	128	LYS	5
1	A	193	LYS	5
1	A	43	VAL	5
1	A	174	GLN	4
1	A	69	GLU	4
1	A	88	ARG	4
1	A	16	GLU	4
1	A	204	GLU	4
1	A	201	TYR	4
1	A	78	LEU	4
1	A	65	LEU	4
1	A	66	ASN	4
1	A	52	TYR	3
1	A	208	ARG	3
1	A	56	ARG	3
1	A	93	ASN	3
1	A	124	GLN	3
1	A	29	SER	2
1	A	60	LYS	2
1	A	95	LYS	2
1	A	197	ARG	2
1	A	163	CYS	2
1	A	120	ASP	2
1	A	132	ASP	2
1	A	133	ARG	2
1	A	153	LEU	2
1	A	142	VAL	2
1	A	125	GLN	2
1	A	149	ASN	2
1	A	18	THR	2
1	A	57	LYS	2
1	A	17	ARG	2
1	A	10	SER	1
1	A	118	GLU	1
1	A	131	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	156	LEU	1
1	A	119	ARG	1
1	A	103	GLU	1
1	A	203	PHE	1
1	A	178	ASP	1
1	A	80	LYS	1
1	A	160	GLN	1
1	A	31	ASN	1
1	A	100	GLU	1
1	A	40	GLN	1
1	A	63	ASP	1
1	A	84	PHE	1
1	A	19	GLU	1
1	A	206	TYR	1

### 6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 6.5 Carbohydrates [i](#)

There are no 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 88% for the well-defined parts and 82% 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	2611
Number of shifts mapped to atoms	2611
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	216	$-0.62 \pm 0.10$	Should be applied
$^{13}\text{C}_\beta$	206	$0.18 \pm 0.08$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	210	$-0.17 \pm 0.05$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	201	$0.35 \pm 0.21$	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 88%, i.e. 2203 atoms were assigned a chemical shift out of a possible 2516. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	957/972 (98%)	380/387 (98%)	391/396 (99%)	186/189 (98%)
Sidechain	1106/1340 (83%)	681/786 (87%)	405/494 (82%)	20/60 (33%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	140/204 (69%)	83/106 (78%)	55/93 (59%)	2/5 (40%)
Overall	2203/2516 (88%)	1144/1279 (89%)	851/983 (87%)	208/254 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 2404 atoms were assigned a chemical shift out of a possible 2939. 0 out of 37 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	1043/1125 (93%)	416/448 (93%)	426/458 (93%)	201/219 (92%)
Sidechain	1221/1529 (80%)	759/900 (84%)	440/561 (78%)	22/68 (32%)
Aromatic	140/285 (49%)	83/147 (56%)	55/115 (48%)	2/23 (9%)
Overall	2404/2939 (82%)	1258/1495 (84%)	921/1134 (81%)	225/310 (73%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

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	203	PHE	CE1	116.70	137.92 – 123.42	-9.6
1	A	193	LYS	HB2	0.24	3.03 – 0.53	-6.2
1	A	172	TRP	HB2	1.32	4.94 – 1.44	-5.3
1	A	172	TRP	HB3	1.32	4.94 – 1.34	-5.0

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

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:

