



# Full wwPDB NMR Structure Validation Report ⓘ

Apr 27, 2016 – 04:41 AM BST

PDB ID : 2RML  
Title : Solution structure of the N-terminal soluble domains of Bacillus subtilis CopA  
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Deposited on : 2007-10-30

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](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

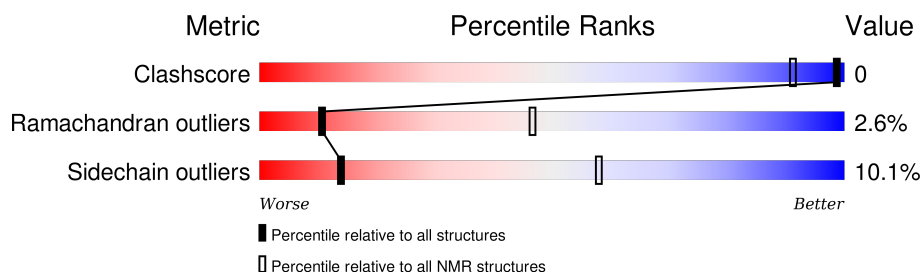
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 77%.

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	147	<div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div>

## 2 Ensemble composition and analysis

This entry contains 25 models. Model 25 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:5-A:147 (143)	0.62	25

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 1 single-model cluster was found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2233 atoms, of which 1124 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Copper-transporting P-type ATPase copA.

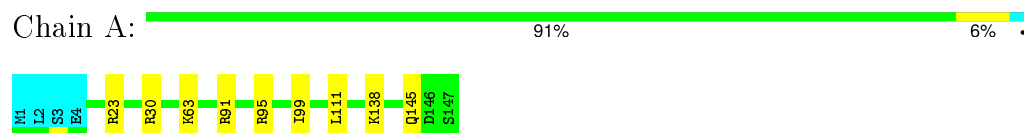
Mol	Chain	Residues	Atoms						Trace
1	A	147	Total	C	H	N	O	S	0
			2233	687	1124	187	226	9	

## 4 Residue-property plots

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

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

- Molecule 1: Copper-transporting P-type ATPase copA

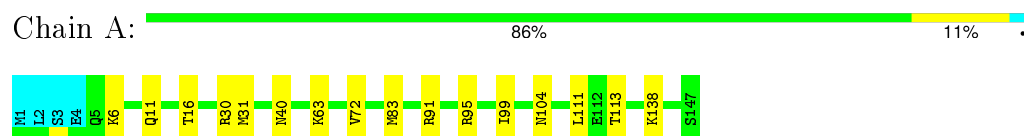


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

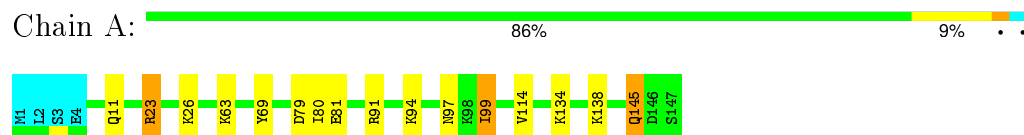
#### 4.2.1 Score per residue for model 1

- Molecule 1: Copper-transporting P-type ATPase copA



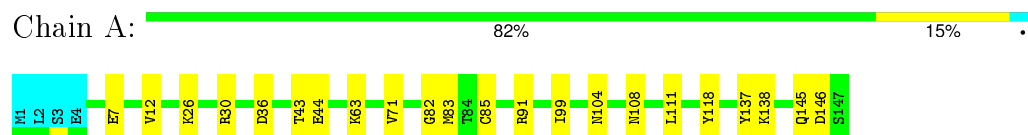
#### 4.2.2 Score per residue for model 2

- Molecule 1: Copper-transporting P-type ATPase copA



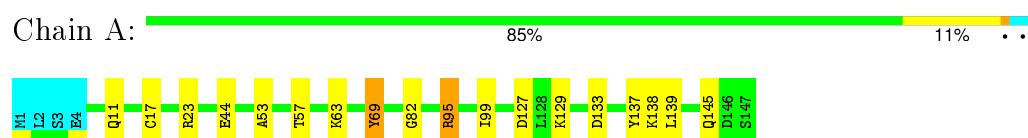
### 4.2.3 Score per residue for model 3

- Molecule 1: Copper-transporting P-type ATPase copA



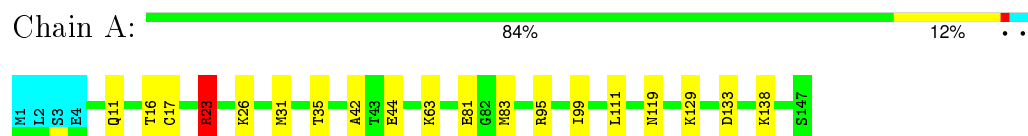
### 4.2.4 Score per residue for model 4

- Molecule 1: Copper-transporting P-type ATPase copA



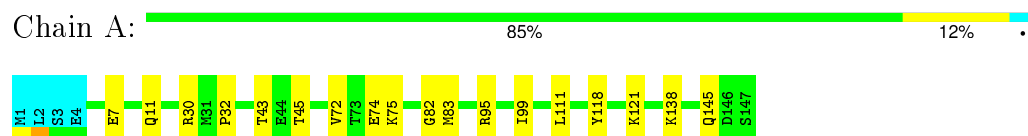
### 4.2.5 Score per residue for model 5

- Molecule 1: Copper-transporting P-type ATPase copA



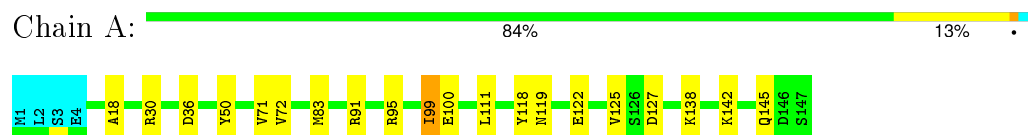
### 4.2.6 Score per residue for model 6

- Molecule 1: Copper-transporting P-type ATPase copA



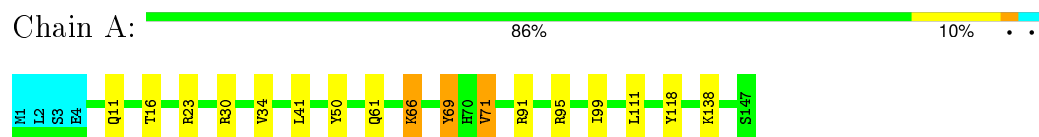
### 4.2.7 Score per residue for model 7

- Molecule 1: Copper-transporting P-type ATPase copA



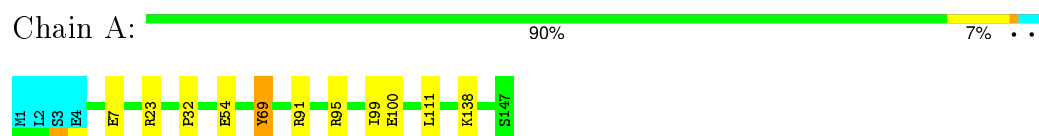
### 4.2.8 Score per residue for model 8

- Molecule 1: Copper-transporting P-type ATPase copA



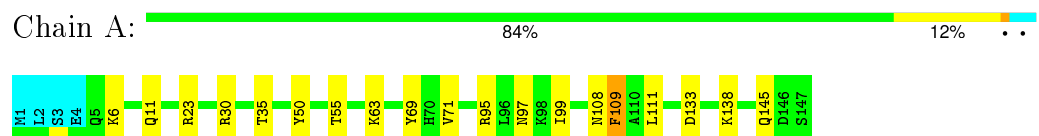
### 4.2.9 Score per residue for model 9

- Molecule 1: Copper-transporting P-type ATPase copA



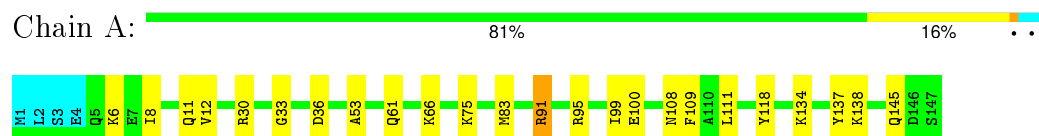
### 4.2.10 Score per residue for model 10

- Molecule 1: Copper-transporting P-type ATPase copA



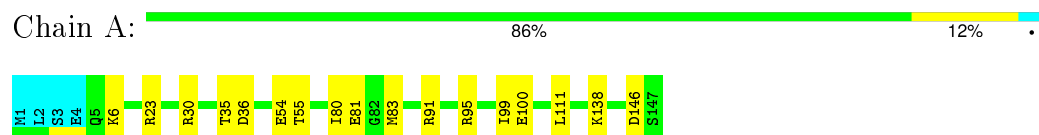
### 4.2.11 Score per residue for model 11

- Molecule 1: Copper-transporting P-type ATPase copA



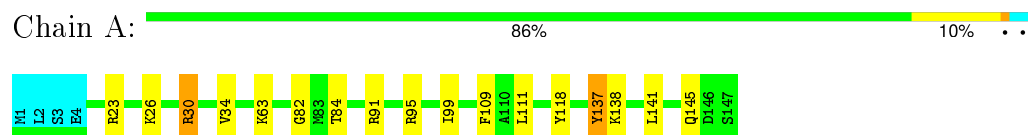
### 4.2.12 Score per residue for model 12

- Molecule 1: Copper-transporting P-type ATPase copA



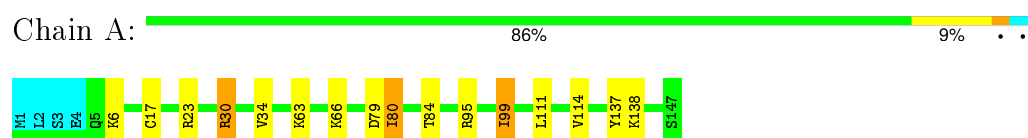
### 4.2.13 Score per residue for model 13

- Molecule 1: Copper-transporting P-type ATPase copA



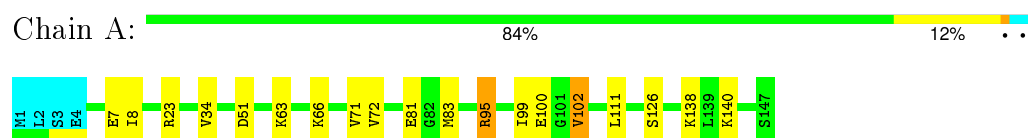
### 4.2.14 Score per residue for model 14

- Molecule 1: Copper-transporting P-type ATPase copA



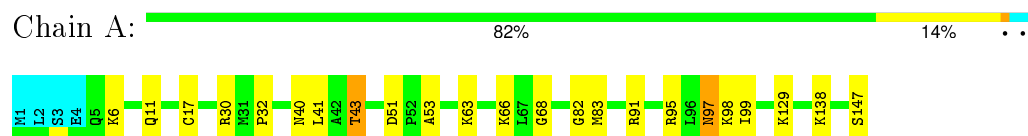
### 4.2.15 Score per residue for model 15

- Molecule 1: Copper-transporting P-type ATPase copA



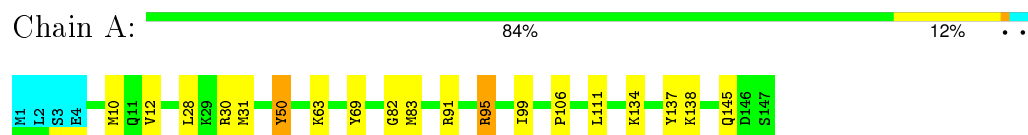
### 4.2.16 Score per residue for model 16

- Molecule 1: Copper-transporting P-type ATPase copA



### 4.2.17 Score per residue for model 17

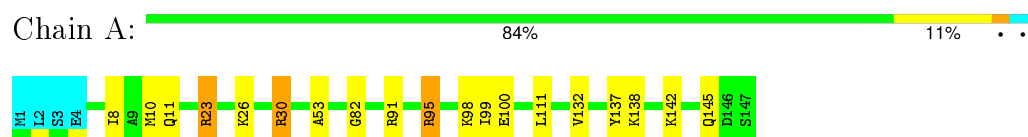
- Molecule 1: Copper-transporting P-type ATPase copA





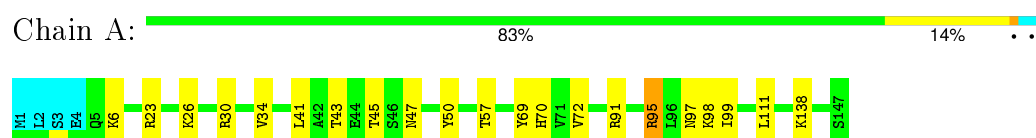
### 4.2.18 Score per residue for model 18

- Molecule 1: Copper-transporting P-type ATPase copA



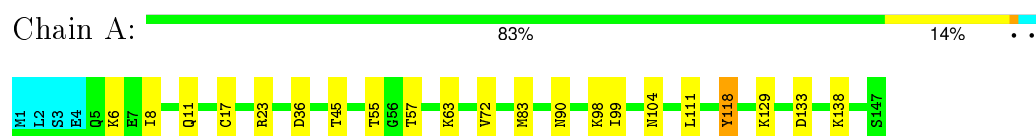
### 4.2.19 Score per residue for model 19

- Molecule 1: Copper-transporting P-type ATPase copA



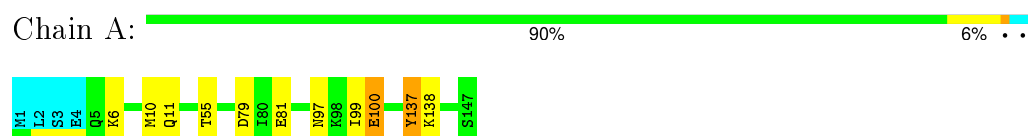
### 4.2.20 Score per residue for model 20

- Molecule 1: Copper-transporting P-type ATPase copA



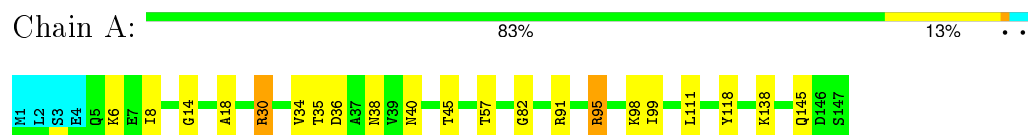
### 4.2.21 Score per residue for model 21

- Molecule 1: Copper-transporting P-type ATPase copA



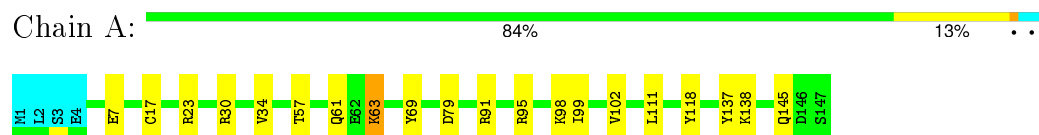
### 4.2.22 Score per residue for model 22

- Molecule 1: Copper-transporting P-type ATPase copA



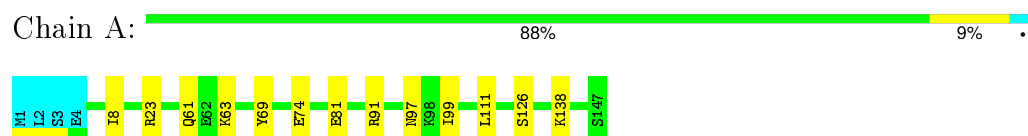
### 4.2.23 Score per residue for model 23

- Molecule 1: Copper-transporting P-type ATPase copA



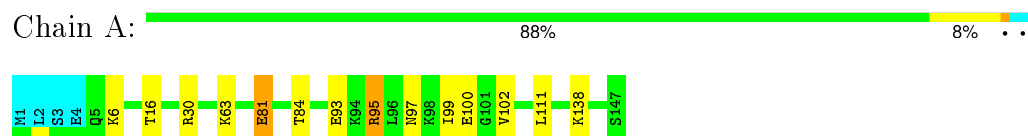
### 4.2.24 Score per residue for model 24

- Molecule 1: Copper-transporting P-type ATPase copA



### 4.2.25 Score per residue for model 25 (medoid)

- Molecule 1: Copper-transporting P-type ATPase copA



## 5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 25 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
DYANA	structure solution	
DYANA	refinement	

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)	BMRB entry 11011
Number of chemical shift lists	1
Total number of shifts	1456
Number of shifts mapped to atoms	1456
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

No validations of the models with respect to experimental NMR restraints is performed at this time.

## 6 Model quality i

### 6.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.63±0.01	0±0/1088 (0.0±0.0%)	1.04±0.02	3±1/1465 (0.2±0.1%)
All	All	0.63	0/27200 (0.0%)	1.04	71/36625 (0.2%)

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	1.0±1.0
All	All	0	26

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	30	ARG	NE-CZ-NH1	11.00	125.80	120.30	6	14
1	A	23	ARG	NE-CZ-NH1	9.59	125.09	120.30	9	14
1	A	95	ARG	NE-CZ-NH1	8.65	124.62	120.30	4	16
1	A	91	ARG	NE-CZ-NH1	8.53	124.56	120.30	9	15
1	A	137	TYR	CB-CG-CD2	-7.56	116.47	121.00	3	5
1	A	30	ARG	NE-CZ-NH2	-6.22	117.19	120.30	14	2
1	A	137	TYR	CB-CG-CD1	5.86	124.51	121.00	3	1
1	A	118	TYR	CB-CG-CD2	-5.42	117.75	121.00	20	1
1	A	95	ARG	NE-CZ-NH2	-5.28	117.66	120.30	1	1
1	A	30	ARG	CD-NE-CZ	5.15	130.81	123.60	6	1
1	A	50	TYR	CB-CG-CD2	-5.10	117.94	121.00	17	1

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	99	ILE	Peptide	6
1	A	69	TYR	Sidechain,Peptide	6
1	A	50	TYR	Sidechain	2
1	A	137	TYR	Sidechain,Peptide	2
1	A	12	VAL	Peptide	1
1	A	108	ASN	Peptide	1
1	A	100	GLU	Peptide	1
1	A	23	ARG	Sidechain	1
1	A	146	ASP	Peptide	1
1	A	68	GLY	Peptide	1
1	A	118	TYR	Sidechain	1
1	A	91	ARG	Sidechain	1
1	A	33	GLY	Peptide	1
1	A	43	THR	Peptide	1

## 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	1078	1091	1091	0±1
All	All	26950	27275	27275	9

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ILE:HD11	1:A:114:VAL:HG12	0.61	1.71	14	2
1:A:99:ILE:HG22	1:A:100:GLU:H	0.54	1.63	18	2
1:A:99:ILE:H	1:A:102:VAL:CG2	0.45	2.24	25	2
1:A:63:LYS:HE3	1:A:63:LYS:HA	0.42	1.92	23	1
1:A:132:VAL:HG13	1:A:137:TYR:CE1	0.41	2.50	18	1
1:A:66:LYS:HA	1:A:66:LYS:HE3	0.40	1.94	8	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	142/147 (97%)	125±3 (88±2%)	14±3 (10±2%)	4±2 (3±1%)	11	47
All	All	3550/3675 (97%)	3116 (88%)	343 (10%)	91 (3%)	11	47

All 25 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	99	ILE	18
1	A	145	GLN	11
1	A	82	GLY	8
1	A	17	CYS	6
1	A	81	GLU	5
1	A	71	VAL	5
1	A	72	VAL	5
1	A	53	ALA	4
1	A	32	PRO	3
1	A	44	GLU	3
1	A	84	THR	3
1	A	100	GLU	3
1	A	18	ALA	2
1	A	109	PHE	2
1	A	108	ASN	2
1	A	98	LYS	2
1	A	41	LEU	1
1	A	42	ALA	1
1	A	12	VAL	1
1	A	43	THR	1
1	A	97	ASN	1
1	A	106	PRO	1
1	A	14	GLY	1
1	A	102	VAL	1
1	A	55	THR	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	115/119 (97%)	103±2 (90±2%)	12±2 (10±2%)	14	58
All	All	2875/2975 (97%)	2586 (90%)	289 (10%)	14	58

All 72 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	138	LYS	25
1	A	111	LEU	21
1	A	63	LYS	15
1	A	11	GLN	12
1	A	6	LYS	11
1	A	95	ARG	11
1	A	83	MET	11
1	A	118	TYR	8
1	A	34	VAL	7
1	A	30	ARG	7
1	A	97	ASN	7
1	A	69	TYR	6
1	A	8	ILE	6
1	A	36	ASP	6
1	A	26	LYS	6
1	A	7	GLU	5
1	A	57	THR	5
1	A	66	LYS	5
1	A	79	ASP	4
1	A	98	LYS	4
1	A	129	LYS	4
1	A	23	ARG	4
1	A	45	THR	4
1	A	133	ASP	4
1	A	16	THR	4
1	A	61	GLN	4
1	A	35	THR	4
1	A	137	TYR	3
1	A	43	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	81	GLU	3
1	A	31	MET	3
1	A	55	THR	3
1	A	40	ASN	3
1	A	50	TYR	3
1	A	100	GLU	3
1	A	104	ASN	3
1	A	10	MET	3
1	A	134	LYS	3
1	A	51	ASP	2
1	A	54	GLU	2
1	A	41	LEU	2
1	A	74	GLU	2
1	A	127	ASP	2
1	A	109	PHE	2
1	A	145	GLN	2
1	A	80	ILE	2
1	A	75	LYS	2
1	A	142	LYS	2
1	A	126	SER	2
1	A	119	ASN	2
1	A	12	VAL	1
1	A	122	GLU	1
1	A	102	VAL	1
1	A	146	ASP	1
1	A	113	THR	1
1	A	28	LEU	1
1	A	71	VAL	1
1	A	47	ASN	1
1	A	85	CYS	1
1	A	91	ARG	1
1	A	141	LEU	1
1	A	70	HIS	1
1	A	147	SER	1
1	A	125	VAL	1
1	A	72	VAL	1
1	A	38	ASN	1
1	A	139	LEU	1
1	A	94	LYS	1
1	A	121	LYS	1
1	A	90	ASN	1
1	A	140	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	93	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 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 77% for the well-defined parts and 75% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 11011

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	1456
Number of shifts mapped to atoms	1456
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	$2.50 \pm 0.20$	Should be applied
$^{13}\text{C}_\beta$	127	$2.71 \pm 0.10$	Should be applied
$^{13}\text{C}'$	1	—	—
$^{15}\text{N}$	137	$0.52 \pm 0.44$	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 77%, i.e. 1279 atoms were assigned a chemical shift out of a possible 1669. 19 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	548/707 (78%)	274/282 (97%)	139/286 (49%)	135/139 (97%)
Sidechain	730/905 (81%)	454/524 (87%)	264/343 (77%)	12/38 (32%)

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	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Aromatic	1/57 (2%)	1/30 (3%)	0/26 (0%)	0/1 (0%)
Overall	1279/1669 (77%)	729/836 (87%)	403/655 (62%)	147/178 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 1295 atoms were assigned a chemical shift out of a possible 1716. 19 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	556/727 (76%)	278/290 (96%)	141/294 (48%)	137/143 (96%)
Sidechain	738/932 (79%)	460/540 (85%)	266/354 (75%)	12/38 (32%)
Aromatic	1/57 (2%)	1/30 (3%)	0/26 (0%)	0/1 (0%)
Overall	1295/1716 (75%)	739/860 (86%)	407/674 (60%)	149/182 (82%)

#### 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	95	ARG	HD2	1.44	4.27 – 1.97	-7.3
1	A	95	ARG	HD3	1.44	4.36 – 1.86	-6.7

#### 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:

