



# Full wwPDB NMR Structure Validation Report ⓘ

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PDB ID : 2LDI  
Title : NMR solution structure of ZiaAN sub mutant  
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Deposited on : 2011-05-26

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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

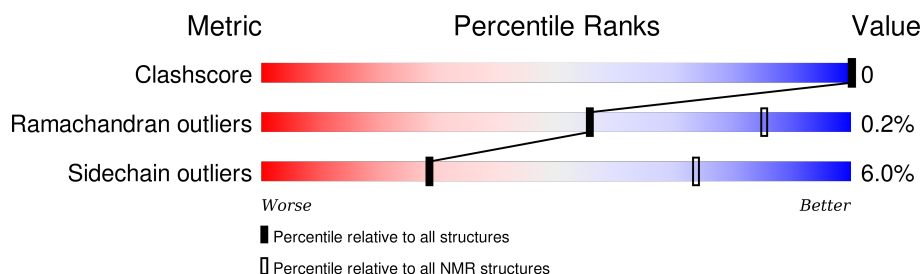
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*


The overall completeness of chemical shifts assignment is 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	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	71	

## 2 Ensemble composition and analysis

This entry contains 30 models. Model 26 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:7-A:17, A:22-A:76 (66)	0.45	26

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 7 clusters and 5 single-model clusters were found.

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

### 3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 997 atoms, of which 469 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc-transporting ATPase.

Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			997	326	469	94	104	4	

There are 8 discrepancies between the modelled and reference sequences:

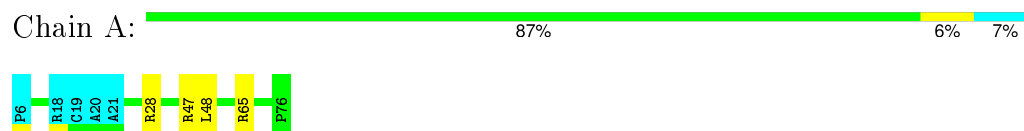
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ARG	ASP	CONFLICT	UNP Q59998
A	20	ALA	THR	CONFLICT	UNP Q59998
A	21	ALA	SER	CONFLICT	UNP Q59998
A	23	ALA	LYS	CONFLICT	UNP Q59998
A	24	SER	LEU	CONFLICT	UNP Q59998
A	25	SER	LYS	CONFLICT	UNP Q59998
A	28	ARG	GLY	CONFLICT	UNP Q59998
A	29	ALA	SER	CONFLICT	UNP Q59998

## 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: Zinc-transporting ATPase

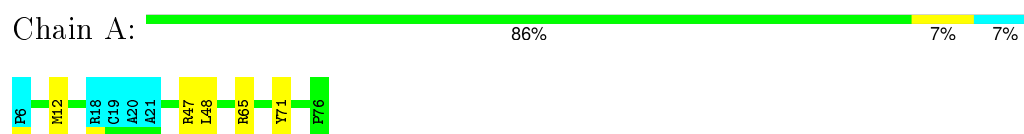


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

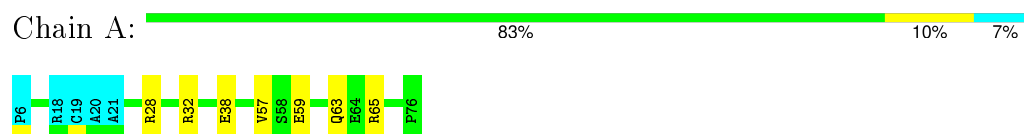
#### 4.2.1 Score per residue for model 1

- Molecule 1: Zinc-transporting ATPase



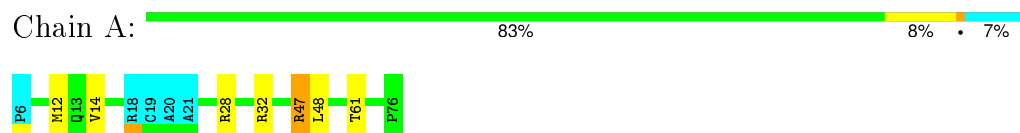
#### 4.2.2 Score per residue for model 2

- Molecule 1: Zinc-transporting ATPase



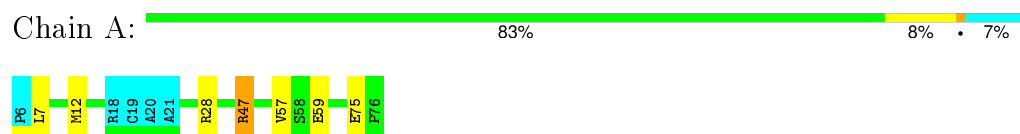
### 4.2.3 Score per residue for model 3

- Molecule 1: Zinc-transporting ATPase



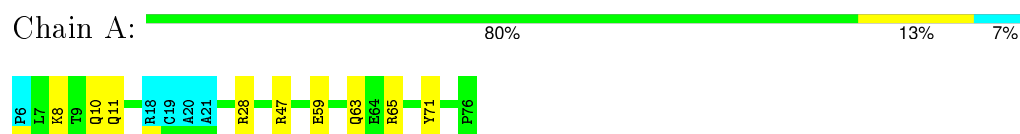
### 4.2.4 Score per residue for model 4

- Molecule 1: Zinc-transporting ATPase



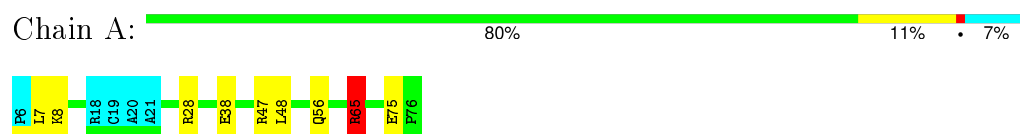
### 4.2.5 Score per residue for model 5

- Molecule 1: Zinc-transporting ATPase



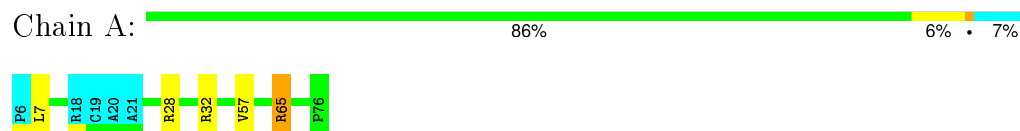
### 4.2.6 Score per residue for model 6

- Molecule 1: Zinc-transporting ATPase



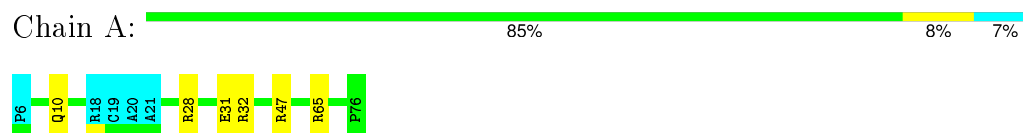
### 4.2.7 Score per residue for model 7

- Molecule 1: Zinc-transporting ATPase



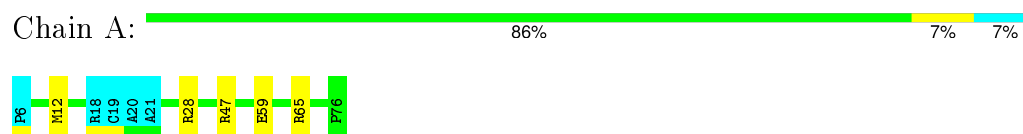
#### 4.2.8 Score per residue for model 8

- Molecule 1: Zinc-transporting ATPase



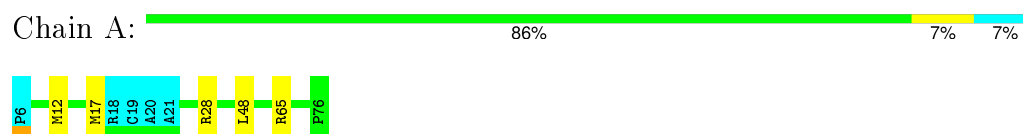
#### 4.2.9 Score per residue for model 9

- Molecule 1: Zinc-transporting ATPase



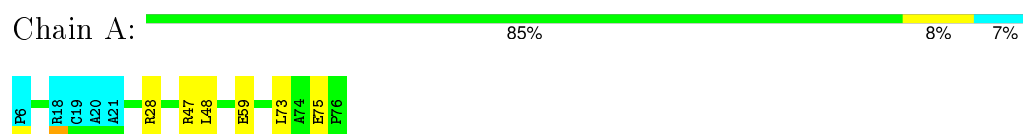
#### 4.2.10 Score per residue for model 10

- Molecule 1: Zinc-transporting ATPase



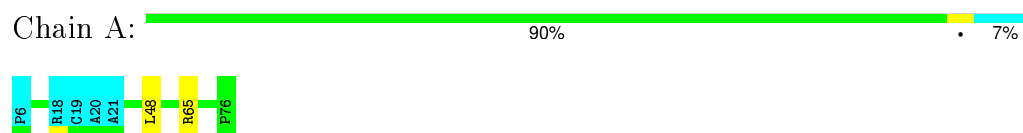
#### 4.2.11 Score per residue for model 11

- Molecule 1: Zinc-transporting ATPase



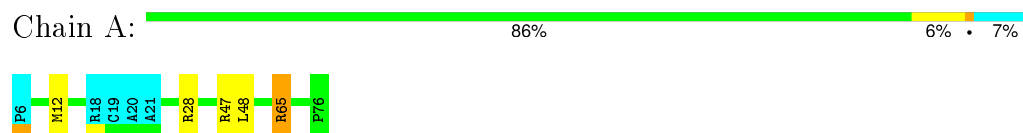
#### 4.2.12 Score per residue for model 12

- Molecule 1: Zinc-transporting ATPase



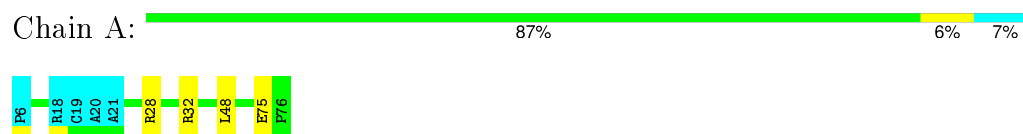
### 4.2.13 Score per residue for model 13

- Molecule 1: Zinc-transporting ATPase



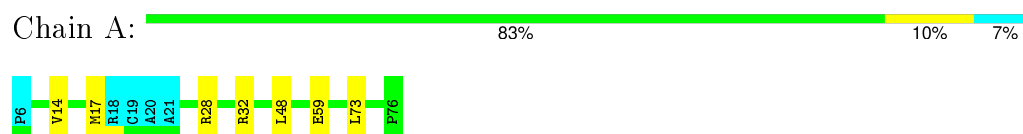
### 4.2.14 Score per residue for model 14

- Molecule 1: Zinc-transporting ATPase



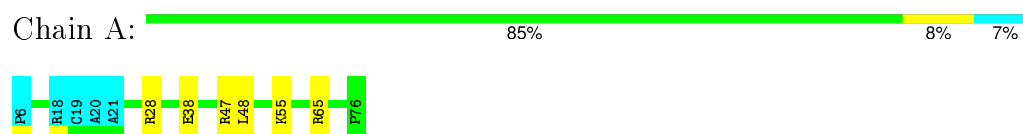
### 4.2.15 Score per residue for model 15

- Molecule 1: Zinc-transporting ATPase



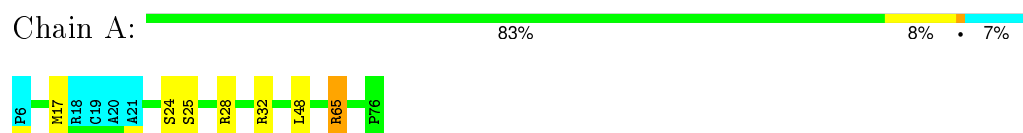
### 4.2.16 Score per residue for model 16

- Molecule 1: Zinc-transporting ATPase



### 4.2.17 Score per residue for model 17

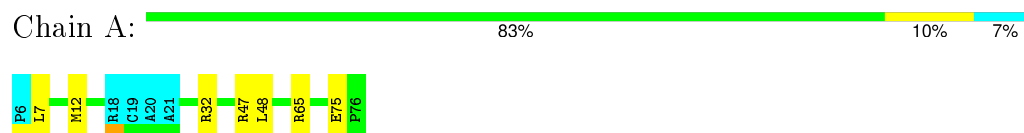
- Molecule 1: Zinc-transporting ATPase





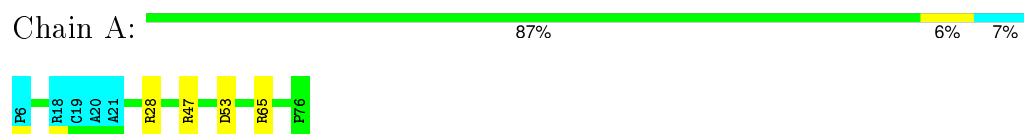
#### 4.2.18 Score per residue for model 18

- Molecule 1: Zinc-transporting ATPase



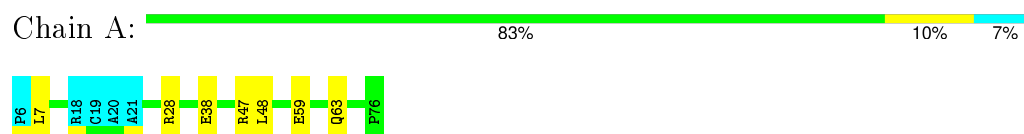
#### 4.2.19 Score per residue for model 19

- Molecule 1: Zinc-transporting ATPase



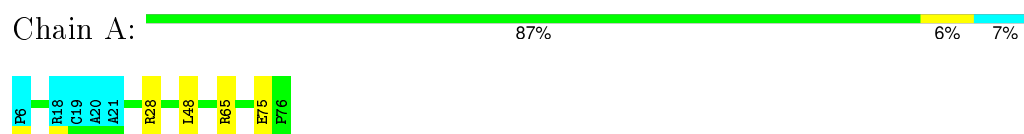
#### 4.2.20 Score per residue for model 20

- Molecule 1: Zinc-transporting ATPase



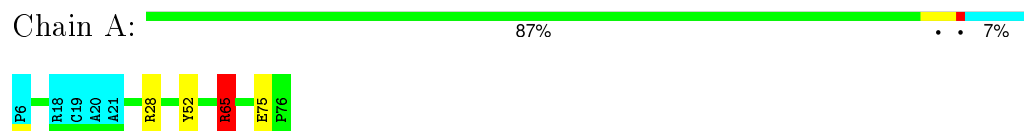
#### 4.2.21 Score per residue for model 21

- Molecule 1: Zinc-transporting ATPase



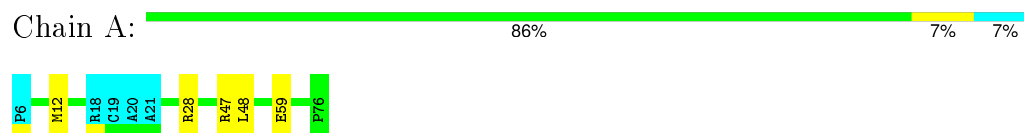
#### 4.2.22 Score per residue for model 22

- Molecule 1: Zinc-transporting ATPase



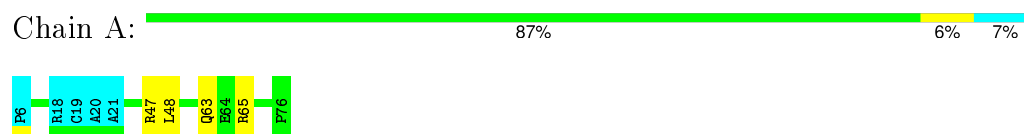
#### 4.2.23 Score per residue for model 23

- Molecule 1: Zinc-transporting ATPase



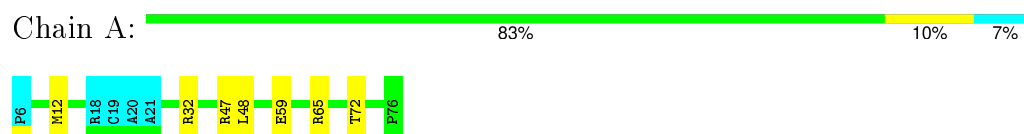
#### 4.2.24 Score per residue for model 24

- Molecule 1: Zinc-transporting ATPase



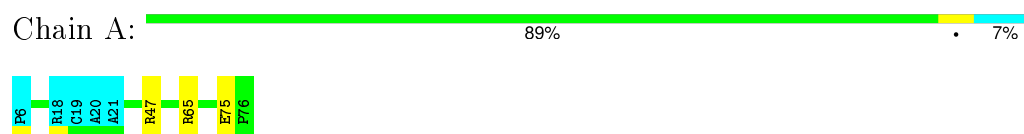
#### 4.2.25 Score per residue for model 25

- Molecule 1: Zinc-transporting ATPase



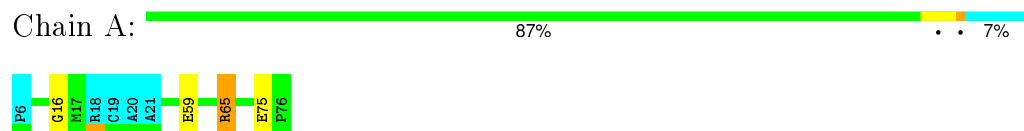
#### 4.2.26 Score per residue for model 26 (medoid)

- Molecule 1: Zinc-transporting ATPase




#### 4.2.27 Score per residue for model 27

- Molecule 1: Zinc-transporting ATPase



#### 4.2.28 Score per residue for model 28


- Molecule 1: Zinc-transporting ATPase

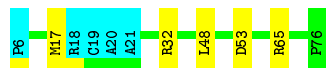
Chain A:  85% 8% 7%



#### 4.2.29 Score per residue for model 29


- Molecule 1: Zinc-transporting ATPase

Chain A:  86% 7% 7%



#### 4.2.30 Score per residue for model 30

- Molecule 1: Zinc-transporting ATPase

Chain A:  85% 7% 7%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *restrained energy minimization*.

Of the 300 calculated structures, 30 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
AMBER	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)	2ldi_cs.str
Number of chemical shift lists	1
Total number of shifts	1014
Number of shifts mapped to atoms	765
Number of unparsed shifts	0
Number of shifts with mapping errors	249
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	80%

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	0.62±0.01	0±0/497 (0.0±0.0%)	1.03±0.03	3±1/670 (0.4±0.1%)
All	All	0.62	0/14910 (0.0%)	1.03	78/20100 (0.4%)

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	0.2±0.5
All	All	0	7

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	47	ARG	NE-CZ-NH1	8.31	124.46	120.30	16	18
1	A	65	ARG	NE-CZ-NH1	7.85	124.23	120.30	27	23
1	A	65	ARG	NE-CZ-NH2	-7.74	116.43	120.30	27	4
1	A	28	ARG	NE-CZ-NH1	7.56	124.08	120.30	4	21
1	A	32	ARG	NE-CZ-NH1	7.29	123.95	120.30	15	11
1	A	47	ARG	NE-CZ-NH2	-5.37	117.62	120.30	20	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	71	TYR	Sidechain	2
1	A	65	ARG	Sidechain	2

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	35	GLY	Peptide	1
1	A	47	ARG	Sidechain	1
1	A	75	GLU	Peptide	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
All	All	14820	13200	15420	-

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 -.

There are no clashes.

## 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	65/71 (92%)	59±2 (90±3%)	6±2 (10±3%)	0±0 (0±1%)	56	85
All	All	1950/2130 (92%)	1759 (90%)	187 (10%)	4 (0%)	56	85

All 2 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	57	VAL	3
1	A	16	GLY	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	53/56 (95%)	50±1 (94±3%)	3±1 (6±3%)	28	74
All	All	1590/1680 (95%)	1495 (94%)	95 (6%)	28	74

All 25 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	48	LEU	19
1	A	59	GLU	10
1	A	75	GLU	10
1	A	12	MET	9
1	A	65	ARG	7
1	A	7	LEU	5
1	A	38	GLU	4
1	A	17	MET	4
1	A	63	GLN	4
1	A	10	GLN	3
1	A	8	LYS	2
1	A	53	ASP	2
1	A	25	SER	2
1	A	73	LEU	2
1	A	14	VAL	2
1	A	72	THR	1
1	A	31	GLU	1
1	A	61	THR	1
1	A	24	SER	1
1	A	11	GLN	1
1	A	9	THR	1
1	A	55	LYS	1
1	A	47	ARG	1
1	A	52	TYR	1
1	A	56	GLN	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 80% for the well-defined parts and 79% for the entire structure.

### 7.1 Chemical shift list 1

File name: 2ldi\_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	1014
Number of shifts mapped to atoms	765
Number of unparsed shifts	0
Number of shifts with mapping errors	249
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. All 249 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	87	HIS	H	8.201	0.02	1
A	106	ASN	H	8.172	0.02	1
A	95	GLY	H	8.341	0.02	1
A	90	SER	HB2	3.957	0.02	1
A	84	GLY	H	8.257	0.02	1
A	111	LEU	CD1	25.136	0.3	1
A	92	ARG	CA	56.257	0.3	1
A	110	GLU	HB3	1.695	0.02	2
A	86	LYS	CG	24.72	0.3	1
A	81	THR	C	176.589	0.3	1
A	111	LEU	CD2	23.668	0.3	1
A	83	ASN	C	176.583	0.3	1
A	107	LEU	N	121.914	0.3	1
A	107	LEU	CB	42.261	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	111	LEU	HD21	0.715	0.02	1
A	101	GLY	CA	45.266	0.3	1
A	88	PRO	CG	27.169	0.3	1
A	83	ASN	N	124.102	0.3	1
A	110	GLU	N	123.008	0.3	1
A	89	HIS	CA	56.236	0.3	1
A	88	PRO	C	177.79	0.3	1
A	80	VAL	CB	32.753	0.3	1
A	82	LEU	HD13	0.795	0.02	1
A	80	VAL	CA	62.251	0.3	1
A	79	SER	N	118.086	0.3	1
A	111	LEU	CA	56.821	0.3	1
A	88	PRO	CB	31.719	0.3	1
A	109	GLN	H	8.256	0.02	1
A	80	VAL	CG1	21.031	0.3	1
A	109	GLN	HB2	1.995	0.02	1
A	82	LEU	CG	26.948	0.3	1
A	106	ASN	N	119.727	0.3	1
A	82	LEU	C	176.241	0.3	1
A	81	THR	HG23	1.042	0.02	1
A	96	HIS	H	8.06	0.02	1
A	95	GLY	N	109.336	0.3	1
A	79	SER	C	174.515	0.3	1
A	85	HIS	CB	30.241	0.3	1
A	86	LYS	N	121.914	0.3	1
A	102	ALA	HB2	1.259	0.02	1
A	83	ASN	HB2	2.649	0.02	2
A	77	LYS	CB	30.616	0.3	1
A	86	LYS	HG2	1.232	0.02	1
A	107	LEU	H	8.06	0.02	1
A	108	LYS	HA	4.229	0.02	1
A	80	VAL	HG21	0.796	0.02	1
A	111	LEU	HG	1.45	0.02	1
A	111	LEU	HA	4.065	0.02	1
A	102	ALA	N	123.555	0.3	1
A	107	LEU	HD11	0.747	0.02	1
A	81	THR	CG2	21.903	0.3	1
A	82	LEU	CD1	24.823	0.3	1
A	88	PRO	HD2	3.33	0.02	1
A	109	GLN	CB	29.732	0.3	1
A	108	LYS	CB	32.733	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	110	GLU	CA	56.246	0.3	1
A	109	GLN	N	121.914	0.3	1
A	97	SER	CA	58.258	0.3	1
A	82	LEU	HG	1.475	0.02	1
A	90	SER	CB	63.886	0.3	1
A	111	LEU	N	129.023	0.3	1
A	107	LEU	HD13	0.747	0.02	1
A	108	LYS	CA	56.24	0.3	1
A	93	GLU	H	8.088	0.02	1
A	94	GLU	CG	36.274	0.3	1
A	97	SER	H	8.116	0.02	1
A	83	ASN	H	7.92	0.02	1
A	77	LYS	HA	4.158	0.02	1
A	77	LYS	HG2	1.314	0.02	1
A	108	LYS	C	176.413	0.3	1
A	100	HIS	CA	56.254	0.3	1
A	88	PRO	HG2	1.832	0.02	1
A	108	LYS	H	8.145	0.02	1
A	79	SER	CB	63.76	0.3	1
A	94	GLU	HB3	1.777	0.02	2
A	104	GLU	CA	56.759	0.3	1
A	92	ARG	N	122.461	0.3	1
A	106	ASN	HA	4.528	0.02	1
A	100	HIS	H	8.312	0.02	1
A	109	GLN	C	175.716	0.3	1
A	109	GLN	CG	36.499	0.3	1
A	107	LEU	CG	26.901	0.3	1
A	110	GLU	C	175.545	0.3	1
A	100	HIS	N	120.82	0.3	1
A	104	GLU	C	176.413	0.3	1
A	77	LYS	HD2	1.532	0.02	1
A	89	HIS	CB	30.257	0.3	1
A	89	HIS	N	119.18	0.3	1
A	86	LYS	CA	56.242	0.3	1
A	88	PRO	CD	50.653	0.3	1
A	109	GLN	HG2	2.077	0.02	1
A	111	LEU	HD23	0.715	0.02	1
A	105	PHE	H	8.117	0.02	1
A	82	LEU	HD22	0.742	0.02	1
A	104	GLU	H	8.06	0.02	1
A	97	SER	N	115.812	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	83	ASN	CB	41.23	0.3	1
A	109	GLN	CA	55.756	0.3	1
A	93	GLU	CB	30.723	0.3	1
A	82	LEU	H	8.257	0.02	1
A	103	GLY	H	8.285	0.02	1
A	89	HIS	C	175.554	0.3	1
A	108	LYS	HG3	1.123	0.02	2
A	82	LEU	HD11	0.795	0.02	1
A	110	GLU	HB2	1.913	0.02	2
A	93	GLU	HA	4.202	0.02	1
A	77	LYS	HB2	1.695	0.02	2
A	102	ALA	HA	4.214	0.02	1
A	101	GLY	H	8.313	0.02	1
A	111	LEU	HB2	1.45	0.02	1
A	111	LEU	HD22	0.715	0.02	1
A	111	LEU	HD11	0.769	0.02	1
A	91	HIS	CA	56.242	0.3	1
A	92	ARG	H	8.144	0.02	1
A	108	LYS	HB2	1.559	0.02	2
A	81	THR	H	8.172	0.02	1
A	89	HIS	H	8.538	0.02	1
A	104	GLU	N	119.727	0.3	1
A	94	GLU	HB2	1.912	0.02	2
A	103	GLY	N	107.696	0.3	1
A	104	GLU	CB	30.236	0.3	1
A	84	GLY	N	113.711	0.3	1
A	96	HIS	N	118.633	0.3	1
A	79	SER	HB2	3.712	0.02	1
A	108	LYS	HG2	1.181	0.02	2
A	99	SER	CB	63.755	0.3	1
A	80	VAL	HG23	0.796	0.02	1
A	111	LEU	H	7.835	0.02	1
A	110	GLU	CB	30.241	0.3	1
A	86	LYS	CB	32.71	0.3	1
A	92	ARG	C	177.447	0.3	1
A	93	GLU	N	121.367	0.3	1
A	79	SER	H	8.313	0.02	1
A	105	PHE	N	120.273	0.3	1
A	91	HIS	C	175.204	0.3	1
A	107	LEU	C	177.446	0.3	1
A	83	ASN	CA	54.753	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	90	SER	N	116.445	0.3	1
A	98	HIS	N	118.633	0.3	1
A	78	SER	CA	58.258	0.3	1
A	111	LEU	CB	43.447	0.3	1
A	80	VAL	HB	1.941	0.02	1
A	78	SER	CB	63.76	0.3	1
A	80	VAL	C	176.241	0.3	1
A	85	HIS	H	8.229	0.02	1
A	108	LYS	CG	24.836	0.3	1
A	78	SER	N	116.445	0.3	1
A	77	LYS	HB3	1.614	0.02	2
A	108	LYS	N	121.914	0.3	1
A	84	GLY	HA2	3.739	0.02	1
A	80	VAL	CG2	20.438	0.3	1
A	82	LEU	HD23	0.742	0.02	1
A	106	ASN	CB	38.753	0.3	1
A	95	GLY	C	174.213	0.3	1
A	82	LEU	HB2	1.463	0.02	1
A	82	LEU	HD21	0.742	0.02	1
A	108	LYS	HB3	1.505	0.02	2
A	102	ALA	C	178.484	0.3	1
A	105	PHE	CA	57.743	0.3	1
A	85	HIS	CA	56.246	0.3	1
A	95	GLY	CA	45.276	0.3	1
A	105	PHE	HB2	3.003	0.02	2
A	105	PHE	C	175.547	0.3	1
A	92	ARG	CG	27.772	0.3	1
A	94	GLU	N	122.461	0.3	1
A	77	LYS	HE2	2.867	0.02	1
A	81	THR	HG22	1.042	0.02	1
A	81	THR	N	118.633	0.3	1
A	80	VAL	HG22	0.796	0.02	1
A	86	LYS	CE	42.145	0.3	1
A	82	LEU	CB	42.701	0.3	1
A	99	SER	C	179.517	0.3	1
A	100	HIS	C	175.896	0.3	1
A	103	GLY	CA	45.241	0.3	1
A	102	ALA	HB3	1.259	0.02	1
A	102	ALA	CA	52.736	0.3	1
A	110	GLU	CG	36.279	0.3	1
A	86	LYS	C	176.07	0.3	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	111	LEU	HD12	0.769	0.02	1
A	82	LEU	CD2	23.592	0.3	1
A	111	LEU	HD13	0.769	0.02	1
A	80	VAL	H	8.032	0.02	1
A	107	LEU	HD22	0.688	0.02	1
A	94	GLU	HG3	1.914	0.02	2
A	91	HIS	CB	30.235	0.3	1
A	81	THR	HG21	1.042	0.02	1
A	78	SER	C	174.857	0.3	1
A	110	GLU	HG2	2.13	0.02	1
A	84	GLY	C	174.343	0.3	1
A	87	HIS	N	116.992	0.3	1
A	81	THR	CA	61.725	0.3	1
A	92	ARG	HB2	1.913	0.02	1
A	108	LYS	CD	28.888	0.3	1
A	81	THR	CB	69.776	0.3	1
A	94	GLU	CB	30.252	0.3	1
A	77	LYS	N	121.367	0.3	1
A	107	LEU	CD1	24.834	0.3	1
A	90	SER	H	8.144	0.02	1
A	82	LEU	CA	55.247	0.3	1
A	107	LEU	HD12	0.747	0.02	1
A	100	HIS	CB	30.254	0.3	1
A	78	SER	HB2	3.656	0.02	1
A	103	GLY	C	174.342	0.3	1
A	82	LEU	N	125.195	0.3	1
A	107	LEU	HD21	0.688	0.02	1
A	105	PHE	HB3	2.84	0.02	2
A	111	LEU	CG	27.188	0.3	1
A	94	GLU	C	177.274	0.3	1
A	97	SER	CB	63.754	0.3	1
A	108	LYS	HD2	1.482	0.02	1
A	107	LEU	HD23	0.688	0.02	1
A	94	GLU	HG2	1.967	0.02	2
A	107	LEU	CA	55.249	0.3	1
A	102	ALA	HB1	1.259	0.02	1
A	88	PRO	CA	66.239	0.3	1
A	102	ALA	CB	19.237	0.3	1
A	96	HIS	C	178.658	0.3	1
A	78	SER	H	8.285	0.02	1
A	80	VAL	HA	4.093	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	81	THR	HB	4.038	0.02	1
A	88	PRO	HB2	1.668	0.02	1
A	101	GLY	N	109.883	0.3	1
A	90	SER	CA	58.565	0.3	1
A	82	LEU	HD12	0.795	0.02	1
A	109	GLN	HA	4.201	0.02	1
A	99	SER	CA	58.256	0.3	1
A	94	GLU	HA	4.147	0.02	1
A	79	SER	CA	58.257	0.3	1
A	108	LYS	CE	42.144	0.3	1
A	106	ASN	C	175.547	0.3	1
A	105	PHE	CB	39.499	0.3	1
A	82	LEU	HA	4.256	0.02	1
A	94	GLU	CA	56.702	0.3	1
A	107	LEU	CD2	23.512	0.3	1
A	77	LYS	CD	29.331	0.3	1
A	77	LYS	CE	42.144	0.3	1
A	77	LYS	C	176.93	0.3	1
A	80	VAL	N	121.367	0.3	1
A	106	ASN	CA	53.225	0.3	1
A	92	ARG	CB	30.241	0.3	1
A	105	PHE	HA	4.474	0.02	1
A	81	THR	HA	4.229	0.02	1
A	84	GLY	CA	45.625	0.3	1
A	93	GLU	CA	56.224	0.3	1
A	85	HIS	N	118.633	0.3	1
A	110	GLU	HA	4.147	0.02	1
A	83	ASN	HB3	2.54	0.02	2
A	77	LYS	CA	56.246	0.3	1
A	77	LYS	CG	24.837	0.3	1

### 7.1.2 Chemical shift referencing [①](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	103	$-0.05 \pm 0.14$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	94	$-0.01 \pm 0.17$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	93	$-0.19 \pm 0.22$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	99	$0.30 \pm 0.36$	None needed ( $< 0.5$ ppm)

### 7.1.3 Completeness of resonance assignments [i](#)

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. 617 atoms were assigned a chemical shift out of a possible 774. 12 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	311/326 (95%)	118/130 (91%)	129/132 (98%)	64/64 (100%)
Sidechain	306/432 (71%)	169/250 (68%)	137/162 (85%)	0/20 (0%)
Aromatic	0/16 (0%)	0/8 (0%)	0/8 (0%)	0/0 (—%)
Overall	617/774 (80%)	287/388 (74%)	266/302 (88%)	64/84 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 653 atoms were assigned a chemical shift out of a possible 831. 12 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	326/349 (93%)	122/139 (88%)	137/142 (96%)	67/68 (99%)
Sidechain	327/466 (70%)	181/271 (67%)	146/172 (85%)	0/23 (0%)
Aromatic	0/16 (0%)	0/8 (0%)	0/8 (0%)	0/0 (—%)
Overall	653/831 (79%)	303/418 (72%)	283/322 (88%)	67/91 (74%)

### 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:



