



# Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:21 pm BST

PDB ID : 2LWR  
Title : Solution Structure of RING2 Domain from Parkin  
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Deposited on : 2012-08-06

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:

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
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 : 2.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

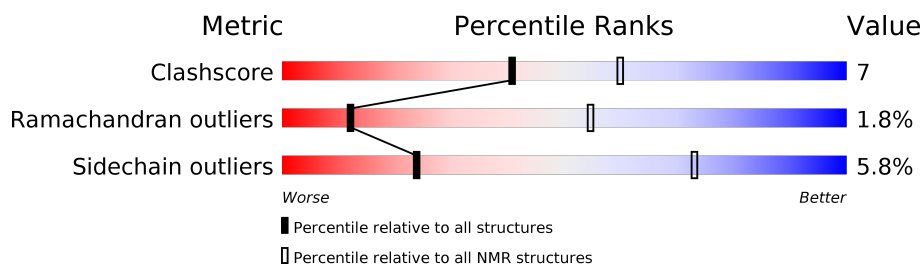
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 85%.

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	68	

## 2 Ensemble composition and analysis

This entry contains 19 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:418-A:427 (10)	1.06	16
2	A:431-A:482 (52)	0.61	18

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 1 single-model cluster was found.

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

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

There are 2 unique types of molecules in this entry. The entry contains 1014 atoms, of which 482 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called SD01679p.

Mol	Chain	Residues	Atoms						Trace
1	A	68	Total	C	H	N	O	S	0
			1012	325	482	97	97	11	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q95TI4
A	0	SER	-	EXPRESSION TAG	UNP Q95TI4

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

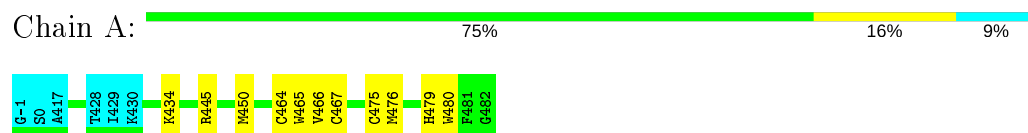
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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

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

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

- Molecule 1: SD01679p

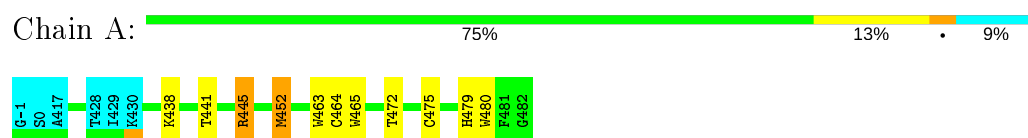


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

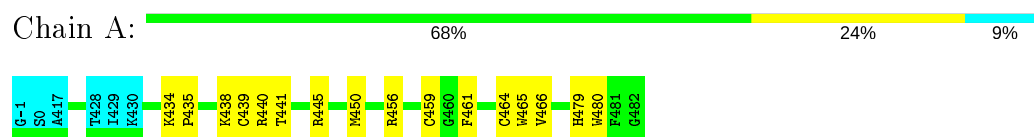
#### 4.2.1 Score per residue for model 1

- Molecule 1: SD01679p



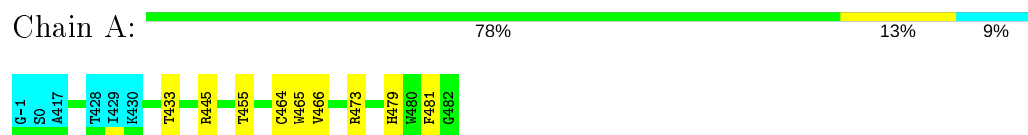
#### 4.2.2 Score per residue for model 2

- Molecule 1: SD01679p



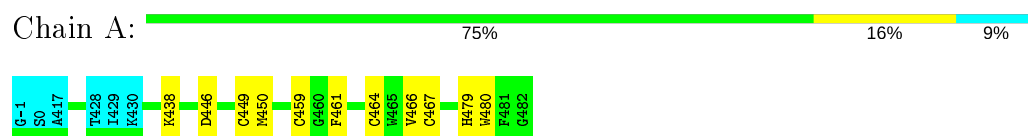
### 4.2.3 Score per residue for model 3

- Molecule 1: SD01679p



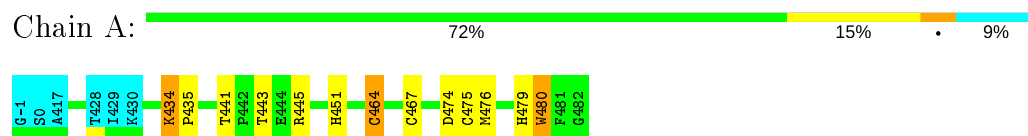
### 4.2.4 Score per residue for model 4

- Molecule 1: SD01679p



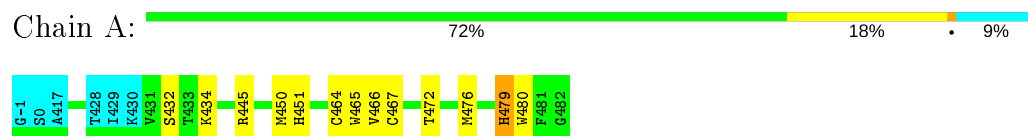
### 4.2.5 Score per residue for model 5

- Molecule 1: SD01679p



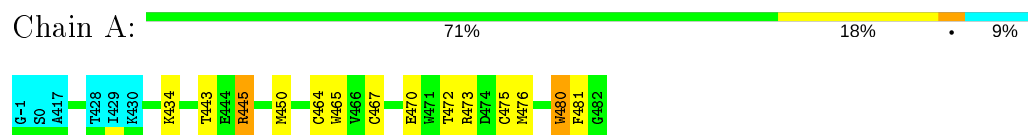
### 4.2.6 Score per residue for model 6

- Molecule 1: SD01679p



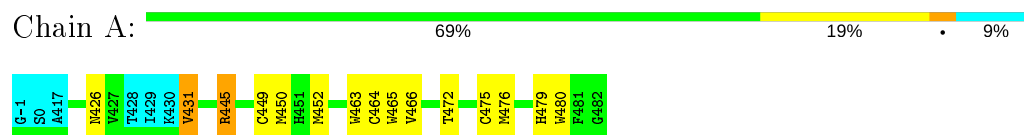
### 4.2.7 Score per residue for model 7

- Molecule 1: SD01679p



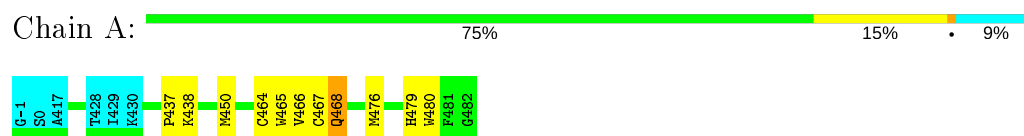
### 4.2.8 Score per residue for model 8

- Molecule 1: SD01679p



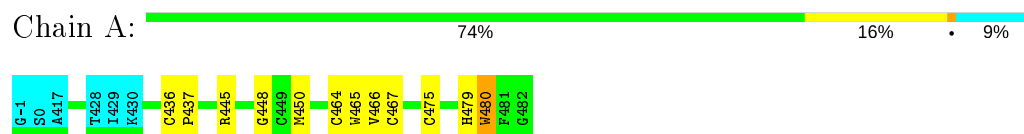
### 4.2.9 Score per residue for model 9

- Molecule 1: SD01679p



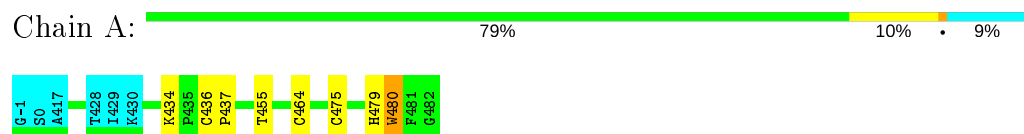
### 4.2.10 Score per residue for model 10

- Molecule 1: SD01679p



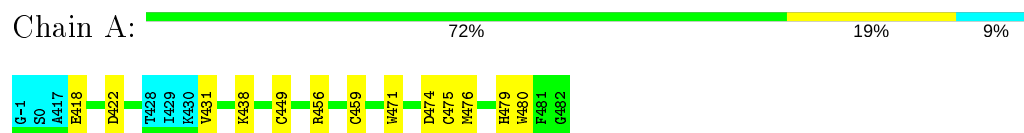
### 4.2.11 Score per residue for model 11

- Molecule 1: SD01679p



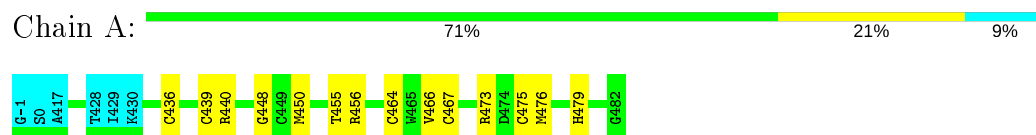
### 4.2.12 Score per residue for model 12

- Molecule 1: SD01679p



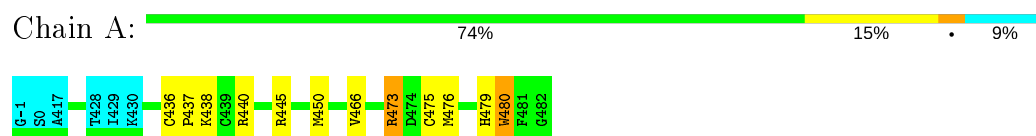
### 4.2.13 Score per residue for model 13

- Molecule 1: SD01679p



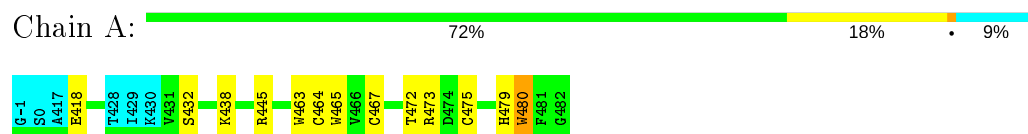
### 4.2.14 Score per residue for model 14

- Molecule 1: SD01679p



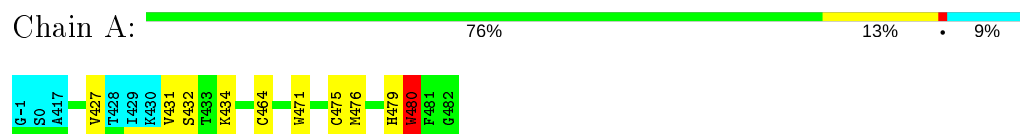
### 4.2.15 Score per residue for model 15

- Molecule 1: SD01679p



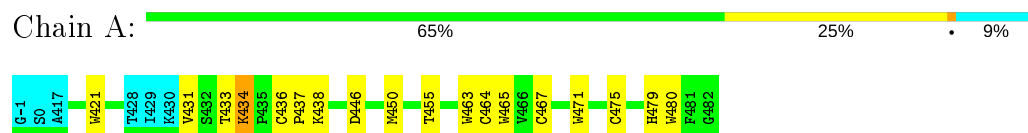
### 4.2.16 Score per residue for model 16

- Molecule 1: SD01679p



### 4.2.17 Score per residue for model 17

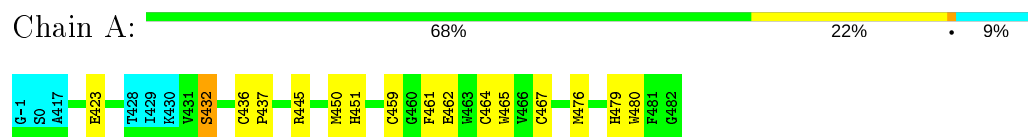
- Molecule 1: SD01679p





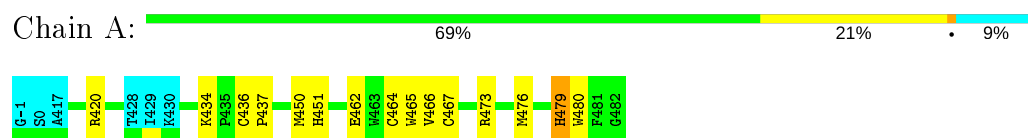
#### 4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: SD01679p



#### 4.2.19 Score per residue for model 19

- Molecule 1: SD01679p



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 20 calculated structures, 19 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	structure solution	2.1
X-PLOR NIH	refinement	2.31
TALOS	geometry optimization	TALOSPlus

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	707
Number of shifts mapped to atoms	707
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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

## 6 Model quality ⓘ

### 6.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	491	436	436	7±2
All	All	9367	8284	8284	132

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 7.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:472:THR:HB	1:A:475:CYS:SG	0.72	2.24	7	4
1:A:466:VAL:HB	1:A:479:HIS:CE1	0.70	2.21	8	9
1:A:450:MET:SD	1:A:465:TRP:HB3	0.69	2.28	6	2
1:A:459:CYS:SG	1:A:461:PHE:HB2	0.65	2.31	2	3
1:A:476:MET:HA	1:A:480:TRP:CZ2	0.63	2.28	5	7
1:A:464:CYS:HB2	1:A:479:HIS:ND1	0.63	2.08	8	7
1:A:464:CYS:HB2	1:A:479:HIS:CE1	0.61	2.31	9	4
1:A:450:MET:SD	1:A:466:VAL:HG23	0.60	2.36	6	2
1:A:466:VAL:HB	1:A:479:HIS:NE2	0.60	2.11	19	2
1:A:464:CYS:SG	1:A:467:CYS:HB2	0.59	2.37	19	11
1:A:464:CYS:HB3	1:A:480:TRP:CZ3	0.59	2.33	15	5
1:A:475:CYS:HB2	1:A:479:HIS:NE2	0.55	2.16	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:445:ARG:HB2	1:A:465:TRP:CH2	0.55	2.37	3	4
1:A:451:HIS:HE2	1:A:462:GLU:HB3	0.54	1.61	18	1
1:A:475:CYS:HB2	1:A:479:HIS:CD2	0.54	2.38	16	8
1:A:450:MET:HB3	1:A:480:TRP:HA	0.53	1.80	6	1
1:A:445:ARG:HD2	1:A:445:ARG:O	0.53	2.04	6	2
1:A:450:MET:O	1:A:465:TRP:HB2	0.53	2.04	17	1
1:A:450:MET:HG3	1:A:465:TRP:CB	0.52	2.35	7	1
1:A:475:CYS:HB3	1:A:479:HIS:CD2	0.52	2.39	10	1
1:A:450:MET:CB	1:A:480:TRP:HA	0.50	2.37	6	1
1:A:434:LYS:O	1:A:443:THR:HB	0.49	2.08	5	2
1:A:471:TRP:HB2	1:A:480:TRP:CH2	0.49	2.43	16	1
1:A:449:CYS:O	1:A:480:TRP:HA	0.49	2.08	8	3
1:A:432:SER:O	1:A:445:ARG:HG3	0.48	2.07	6	1
1:A:439:CYS:SG	1:A:456:ARG:HD3	0.48	2.49	13	2
1:A:473:ARG:HA	1:A:476:MET:SD	0.48	2.49	13	1
1:A:450:MET:HG2	1:A:465:TRP:HB3	0.48	1.85	2	3
1:A:436:CYS:SG	1:A:437:PRO:HD2	0.48	2.47	11	6
1:A:445:ARG:HB3	1:A:452:MET:HE3	0.48	1.85	1	1
1:A:450:MET:SD	1:A:479:HIS:HA	0.47	2.49	18	1
1:A:450:MET:HB3	1:A:479:HIS:O	0.47	2.09	14	1
1:A:451:HIS:NE2	1:A:462:GLU:HB3	0.46	2.26	19	2
1:A:450:MET:HB3	1:A:480:TRP:O	0.46	2.11	2	1
1:A:473:ARG:HG3	1:A:476:MET:SD	0.45	2.51	7	1
1:A:450:MET:O	1:A:450:MET:HG2	0.44	2.11	8	1
1:A:435:PRO:HA	1:A:441:THR:O	0.44	2.12	2	2
1:A:450:MET:CG	1:A:465:TRP:HB3	0.44	2.42	8	2
1:A:456:ARG:HD3	1:A:459:CYS:SG	0.44	2.52	12	1
1:A:436:CYS:O	1:A:440:ARG:HA	0.43	2.13	13	2
1:A:473:ARG:O	1:A:476:MET:HG2	0.43	2.14	14	1
1:A:445:ARG:HB2	1:A:465:TRP:CZ3	0.43	2.49	3	1
1:A:432:SER:O	1:A:445:ARG:HB3	0.43	2.14	18	1
1:A:445:ARG:HB3	1:A:452:MET:CE	0.42	2.44	1	1
1:A:476:MET:HA	1:A:480:TRP:NE1	0.42	2.29	9	1
1:A:449:CYS:HB3	1:A:480:TRP:O	0.42	2.14	12	1
1:A:426:ASN:OD1	1:A:431:VAL:HA	0.42	2.14	8	1
1:A:450:MET:HG3	1:A:465:TRP:HB3	0.42	1.90	7	1
1:A:451:HIS:HB2	1:A:480:TRP:HB3	0.42	1.92	5	1
1:A:450:MET:HG2	1:A:450:MET:O	0.41	2.13	4	1
1:A:437:PRO:HB3	1:A:468:GLN:O	0.41	2.14	9	1
1:A:431:VAL:HG13	1:A:434:LYS:NZ	0.41	2.30	17	1
1:A:452:MET:SD	1:A:465:TRP:CZ3	0.41	3.13	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:464:CYS:HB2	1:A:479:HIS:CB	0.41	2.46	17	1
1:A:464:CYS:HB2	1:A:479:HIS:CG	0.41	2.50	15	1
1:A:432:SER:O	1:A:445:ARG:HG2	0.40	2.17	15	1
1:A:450:MET:CB	1:A:481:PHE:H	0.40	2.29	7	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	61/68 (90%)	50±3 (82±5%)	10±3 (16±5%)	1±1 (2±1%)	12	54
All	All	1159/1292 (90%)	953 (82%)	185 (16%)	21 (2%)	12	54

All 11 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	480	TRP	6
1	A	431	VAL	3
1	A	465	TRP	2
1	A	448	GLY	2
1	A	446	ASP	2
1	A	432	SER	1
1	A	481	PHE	1
1	A	472	THR	1
1	A	468	GLN	1
1	A	422	ASP	1
1	A	479	HIS	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	52/56 (93%)	49±2 (94±3%)	3±2 (6±3%)	24	73
All	All	988/1064 (93%)	931 (94%)	57 (6%)	24	73

All 22 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	438	LYS	8
1	A	445	ARG	6
1	A	434	LYS	6
1	A	480	TRP	5
1	A	455	THR	4
1	A	463	TRP	4
1	A	473	ARG	4
1	A	471	TRP	2
1	A	433	THR	2
1	A	464	CYS	2
1	A	474	ASP	2
1	A	418	GLU	2
1	A	470	GLU	1
1	A	423	GLU	1
1	A	432	SER	1
1	A	440	ARG	1
1	A	451	HIS	1
1	A	421	TRP	1
1	A	441	THR	1
1	A	479	HIS	1
1	A	420	ARG	1
1	A	452	MET	1

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

## 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 85% for the well-defined parts and 83% for the entire structure.

### 7.1 Chemical shift list 1

File name: input\_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	707
Number of shifts mapped to atoms	707
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	7

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	66	$-0.22 \pm 0.24$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	59	$0.16 \pm 0.13$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}'$	45	$0.14 \pm 0.22$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	56	$-1.76 \pm 0.42$	Should be applied

#### 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 85%, i.e. 626 atoms were assigned a chemical shift out of a possible 740. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	275/304 (90%)	116/121 (96%)	106/124 (85%)	53/59 (90%)
Sidechain	271/344 (79%)	172/206 (83%)	97/119 (82%)	2/19 (11%)

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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	80/92 (87%)	43/48 (90%)	32/37 (86%)	5/7 (71%)
Overall	626/740 (85%)	331/375 (88%)	235/280 (84%)	60/85 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 664 atoms were assigned a chemical shift out of a possible 801. 0 out of 4 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	289/334 (87%)	122/133 (92%)	111/136 (82%)	56/65 (86%)
Sidechain	295/375 (79%)	186/224 (83%)	107/131 (82%)	2/20 (10%)
Aromatic	80/92 (87%)	43/48 (90%)	32/37 (86%)	5/7 (71%)
Overall	664/801 (83%)	351/405 (87%)	250/304 (82%)	63/92 (68%)

#### 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	430	LYS	HE3	1.41	3.86 – 1.96	-7.9
1	A	434	LYS	HD3	-0.10	2.75 – 0.45	-7.4
1	A	445	ARG	HD3	1.63	4.36 – 1.86	-5.9
1	A	452	MET	HB3	0.11	3.70 – 0.30	-5.6
1	A	445	ARG	HB3	0.21	3.17 – 0.37	-5.6
1	A	437	PRO	HD3	1.70	5.52 – 1.72	-5.1
1	A	451	HIS	HB3	1.08	5.00 – 1.10	-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:

