



Full wwPDB NMR Structure Validation Report ⓘ

Dec 28, 2016 – 04:59 AM EST

PDB ID : 5JN6
Title : The NMR Solution Structure of RPA3313
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Deposited on : 2016-04-29

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

We welcome your comments at 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.

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-20028442
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

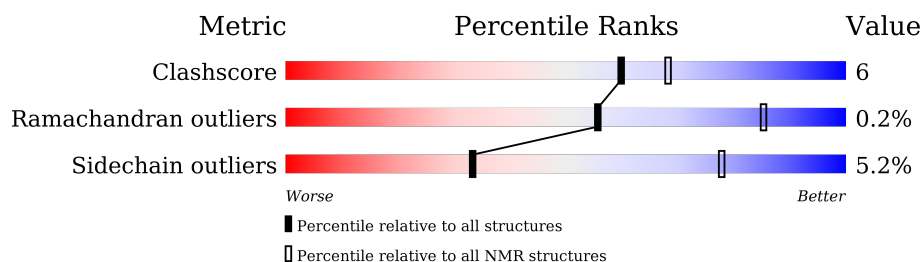
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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 ≥ 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	91	<div> <div style="width: 43%; background-color: green;"></div> <div style="width: 8%; background-color: yellow;"></div> <div style="width: 26%; background-color: cyan;"></div> <div style="width: 23%; background-color: grey;"></div> </div> <div>43% 8% 26% 23%</div>

2 Ensemble composition and analysis

This entry contains 21 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:4-A:20, A:27-A:55 (46)	0.40	1

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 3 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1004 atoms, of which 481 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
1	A	70	Total	C	H	N	O	S	0
			1004	320	481	92	109	2	

There are 21 discrepancies between the modelled and reference sequences:

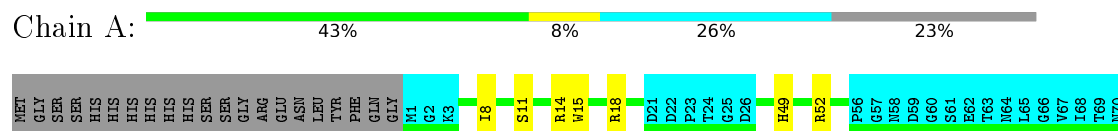
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP Q6N4M4
A	-19	GLY	-	expression tag	UNP Q6N4M4
A	-18	SER	-	expression tag	UNP Q6N4M4
A	-17	SER	-	expression tag	UNP Q6N4M4
A	-16	HIS	-	expression tag	UNP Q6N4M4
A	-15	HIS	-	expression tag	UNP Q6N4M4
A	-14	HIS	-	expression tag	UNP Q6N4M4
A	-13	HIS	-	expression tag	UNP Q6N4M4
A	-12	HIS	-	expression tag	UNP Q6N4M4
A	-11	HIS	-	expression tag	UNP Q6N4M4
A	-10	SER	-	expression tag	UNP Q6N4M4
A	-9	SER	-	expression tag	UNP Q6N4M4
A	-8	GLY	-	expression tag	UNP Q6N4M4
A	-7	ARG	-	expression tag	UNP Q6N4M4
A	-6	GLU	-	expression tag	UNP Q6N4M4
A	-5	ASN	-	expression tag	UNP Q6N4M4
A	-4	LEU	-	expression tag	UNP Q6N4M4
A	-3	TYR	-	expression tag	UNP Q6N4M4
A	-2	PHE	-	expression tag	UNP Q6N4M4
A	-1	GLN	-	expression tag	UNP Q6N4M4
A	0	GLY	-	expression tag	UNP Q6N4M4

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: Uncharacterized protein

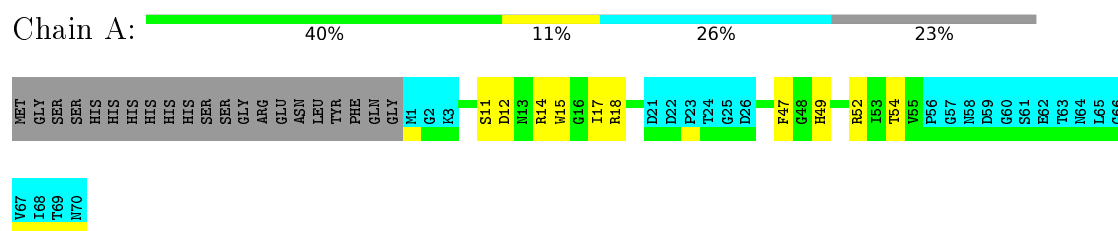


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

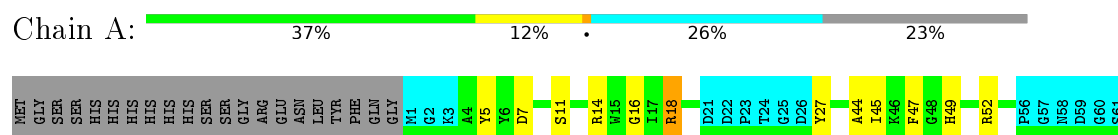
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Uncharacterized protein



4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized protein



E62
T63
N64
L65
G66
V67
I68
T69
N70

4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein

Chain A: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER SER GLY ARG GLU ASN ASN LEU TYR PHE GLN GLY M1 G2 K3 I8 S11 S11 R14 R14 V15 V15 G16 G16 I17 I17 D21 D21 D22 D22 P23 P23 T24 T24 G25 G25 D26 D26 A41 A41 R52 R52 P56 P56 G57 G57 N58 N58 D59 D59 G60 G60 S61 S61 T63 T63 M64 M64 L65 L65 G66 G66 T69 T69 I68 I68 N70 N70

4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein

Chain A: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER SER GLY ARG GLU ASN ASN LEU TYR PHE GLN GLY M1 G2 K3 S11 S11 R14 R14 D21 D21 D22 D22 P23 P23 T24 T24 G25 G25 D26 D26 A44 A44 F47 F47 G48 G48 H49 H49 P56 P56 G57 G57 N58 N58 D59 D59 G60 G60 S61 S61 T63 T63 M64 M64 L65 L65 G66 G66 V67 V67 I68 I68 T69 T69 N70 N70

4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein

Chain A: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER SER GLY ARG GLU ASN ASN LEU TYR PHE GLN GLY M1 G2 K3 A4 A4 Y5 Y5 D7 D7 G10 G10 S11 S11 R14 R14 W15 W15 R18 R18 D21 D21 D22 D22 P23 P23 T24 T24 G25 G25 D26 D26 Y27 Y27 A44 A44 H49 H49 P56 P56 G57 G57 N58 N58 D59 D59 G60 G60 S61 S61 T63 T63 M64 M64 L65 L65 G66 G66

V67
I68
T69
N70

4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein

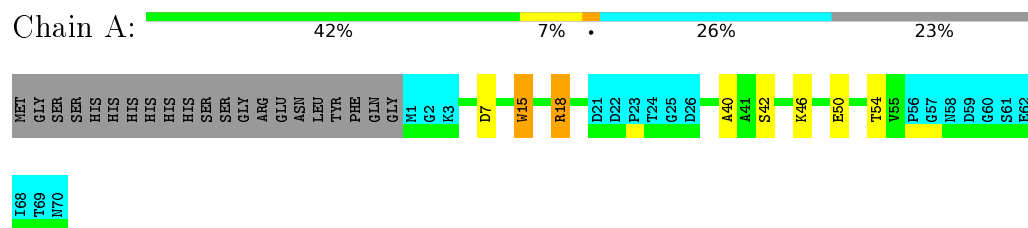
Chain A: 

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER SER GLY ARG GLU ASN ASN LEU TYR PHE GLN GLY M1 G2 K3 Y6 Y6 S11 S11 R14 R14 H19 H19 D20 D20 D21 D21 D22 D22 P23 P23 T24 T24 G25 G25 D26 D26 F34 F34 S42 S42 K46 K46 R52 R52 P56 P56 G57 G57 N58 N58 D59 D59 G60 G60 S61 S61 T63 T63 M64 M64 L65 L65 G66 G66 V67 V67

I68
T69
N70

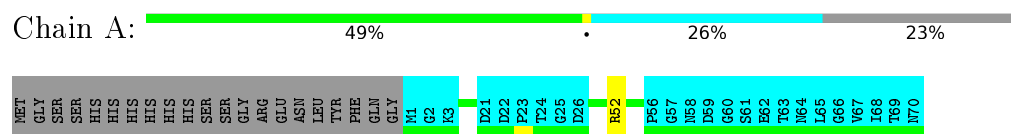
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



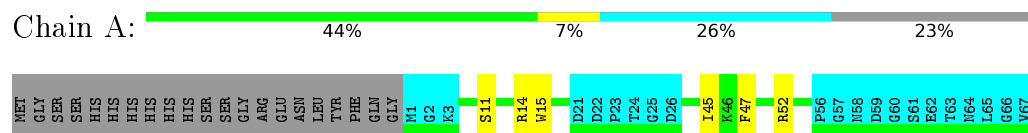
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



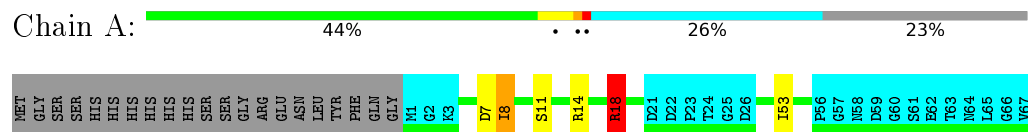
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein

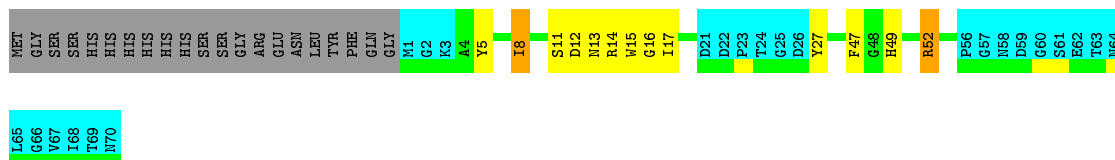




4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein

Chain A: 36% 12% 26% 23%



4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein

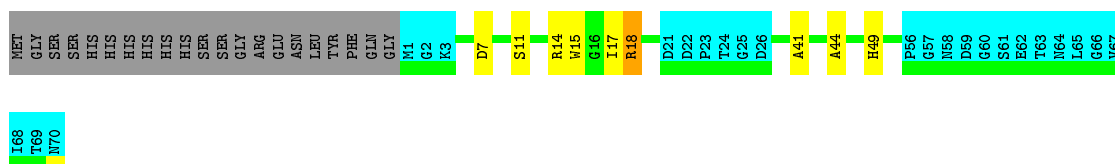
Chain A: 46% 26% 23%



4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein

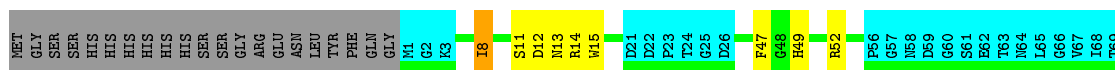
Chain A: 41% 9% 26% 23%



4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein

Chain A: 41% 9% 26% 23%



N70

4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein

Chain A: 

4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein

Chain A: 

4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein

Chain A: G66
V67
I68
T69
N70

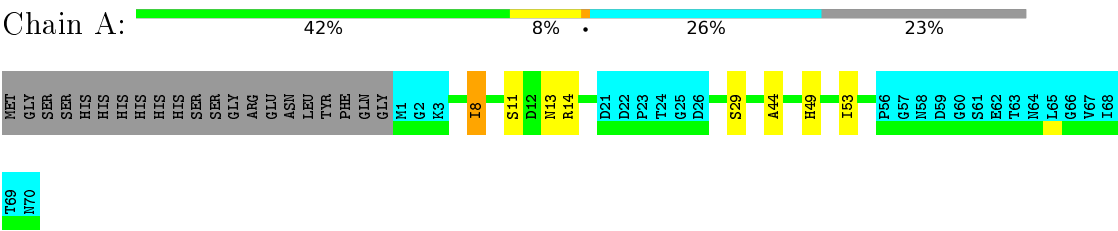
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein

Chain A: 

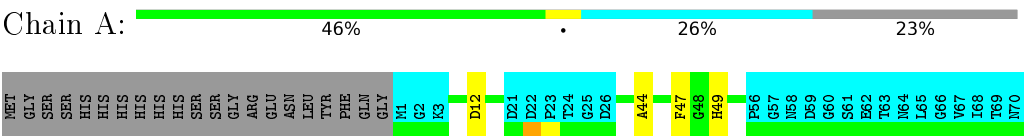
4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



4.2.21 Score per residue for model 21

- Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 1000 calculated structures, 21 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	2.41.1

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)	5jn6_cs.cif
Number of chemical shift lists	1
Total number of shifts	736
Number of shifts mapped to atoms	736
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

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	0.56±0.03	0±0/366 (0.0±0.0%)	0.47±0.04	0±0/497 (0.0±0.0%)
All	All	0.56	0/7686 (0.0%)	0.47	1/10437 (0.0%)

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	0.3±0.5
All	All	0	6

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	18	ARG	NE-CZ-NH1	5.04	122.82	120.30	10	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	18	ARG	Sidechain	6

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	357	333	333	4±2
All	All	7497	6993	6993	84

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 6.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:SER:HB3	1:A:14:ARG:O	0.71	1.86	11	2
1:A:44:ALA:HA	1:A:49:HIS:CG	0.65	2.25	21	3
1:A:7:ASP:HB3	1:A:18:ARG:NH1	0.63	2.09	2	3
1:A:11:SER:HB2	1:A:14:ARG:O	0.62	1.94	16	14
1:A:15:TRP:CH2	1:A:41:ALA:HB2	0.59	2.32	3	3
1:A:7:ASP:HB3	1:A:18:ARG:CZ	0.59	2.28	2	2
1:A:15:TRP:CZ3	1:A:17:ILE:HD11	0.58	2.33	3	2
1:A:12:ASP:HA	1:A:49:HIS:CE1	0.58	2.34	21	3
1:A:47:PHE:HB3	1:A:49:HIS:CD2	0.57	2.34	18	5
1:A:8:ILE:H	1:A:8:ILE:HD13	0.54	1.62	18	5
1:A:42:SER:O	1:A:46:LYS:HG3	0.54	2.03	6	2
1:A:7:ASP:O	1:A:18:ARG:HB3	0.53	2.04	7	4
1:A:10:GLY:HA2	1:A:15:TRP:CZ3	0.51	2.40	5	1
1:A:13:ASN:OD1	1:A:14:ARG:HG2	0.50	2.07	12	1
1:A:8:ILE:HD13	1:A:8:ILE:H	0.50	1.66	12	2
1:A:5:TYR:HB2	1:A:27:TYR:CE2	0.50	2.41	5	1
1:A:12:ASP:HA	1:A:49:HIS:NE2	0.49	2.22	15	1
1:A:44:ALA:HA	1:A:49:HIS:ND1	0.49	2.23	4	6
1:A:47:PHE:HB3	1:A:49:HIS:CE1	0.48	2.44	12	2
1:A:5:TYR:CD1	1:A:27:TYR:HB2	0.47	2.45	12	1
1:A:18:ARG:NH1	1:A:20:ASP:HA	0.46	2.26	11	1
1:A:16:GLY:HA2	1:A:52:ARG:O	0.46	2.11	2	2
1:A:15:TRP:NE1	1:A:40:ALA:HB1	0.46	2.25	7	1
1:A:5:TYR:CE1	1:A:27:TYR:HB3	0.46	2.46	2	1
1:A:18:ARG:HA	1:A:54:THR:O	0.45	2.11	1	1
1:A:6:TYR:CB	1:A:19:HIS:HA	0.44	2.42	6	1
1:A:13:ASN:O	1:A:14:ARG:HD2	0.44	2.12	15	1
1:A:27:TYR:CE2	1:A:30:LYS:HA	0.44	2.48	17	1
1:A:15:TRP:HB3	1:A:49:HIS:CD2	0.44	2.47	19	1
1:A:18:ARG:HG2	1:A:18:ARG:HH11	0.44	1.73	10	2
1:A:15:TRP:CH2	1:A:17:ILE:HD11	0.44	2.48	17	1
1:A:7:ASP:O	1:A:18:ARG:HD3	0.43	2.13	18	2
1:A:18:ARG:HH11	1:A:18:ARG:CG	0.43	2.26	10	1
1:A:10:GLY:HA2	1:A:15:TRP:CE3	0.43	2.48	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:TRP:CZ2	1:A:17:ILE:HD11	0.42	2.48	12	2
1:A:45:ILE:HD13	1:A:45:ILE:O	0.42	2.15	11	1
1:A:6:TYR:OH	1:A:34:PHE:HA	0.41	2.15	6	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	46/91 (51%)	45±1 (98±2%)	1±1 (1±2%)	0±0 (0±1%)	56	85
All	All	966/1911 (51%)	950 (98%)	14 (1%)	2 (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	29	SER	1
1	A	12	ASP	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	34/71 (48%)	32±1 (95±4%)	2±1 (5±4%)	33	78
All	All	714/1491 (48%)	677 (95%)	37 (5%)	33	78

All 11 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	52	ARG	10
1	A	8	ILE	7
1	A	15	TRP	4
1	A	27	TYR	3
1	A	18	ARG	3
1	A	45	ILE	3
1	A	13	ASN	2
1	A	53	ILE	2
1	A	50	GLU	1
1	A	12	ASP	1
1	A	47	PHE	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 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: 5jn6_cs.cif

Chemical shift list name: *assigned_chem_shift_list*

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	736
Number of shifts mapped to atoms	736
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	68	2.52 ± 0.06	Should be applied
$^{13}\text{C}_\beta$	60	2.81 ± 0.07	Should be applied
$^{13}\text{C}'$	67	2.67 ± 0.19	Should be applied
^{15}N	68	-0.59 ± 0.36	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 84%, i.e. 456 atoms were assigned a chemical shift out of a possible 540. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	228/230 (99%)	91/92 (99%)	91/92 (99%)	46/46 (100%)
Sidechain	203/242 (84%)	127/141 (90%)	76/88 (86%)	0/13 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	25/68 (37%)	25/36 (69%)	0/29 (0%)	0/3 (0%)
Overall	456/540 (84%)	243/269 (90%)	167/209 (80%)	46/62 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 83%, i.e. 642 atoms were assigned a chemical shift out of a possible 778. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	336/346 (97%)	133/138 (96%)	135/140 (96%)	68/68 (100%)
Sidechain	281/364 (77%)	174/211 (82%)	107/136 (79%)	0/17 (0%)
Aromatic	25/68 (37%)	25/36 (69%)	0/29 (0%)	0/3 (0%)
Overall	642/778 (83%)	332/385 (86%)	242/305 (79%)	68/88 (77%)

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	22	ASP	CA	43.35	64.88 – 44.48	-5.6

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:

