



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 7NIP / pdb_00007nip
BMRB ID : 50117
Title : titin N2A unique sequence (UN2A) core
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Deposited on : 2021-02-13

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

We welcome your comments at 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 1%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	41	 93% 5% •

2 Ensemble composition and analysis

This entry contains 10 models. Model 8 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:3-A:40 (38)	0.50	8

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. No single-model clusters were found.

Cluster number	Models
1	2, 3, 4, 5
2	1, 7, 8, 10
3	6, 9

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 676 atoms, of which 339 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Isoform 11 of Titin.

Mol	Chain	Residues	Atoms						Trace
1	A	40	Total	C	H	N	O	S	0
			676	217	339	54	64	2	

There is a discrepancy between the modelled and reference sequences:

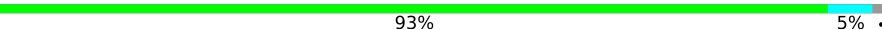
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q8WZ42

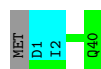
4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Isoform 11 of Titin

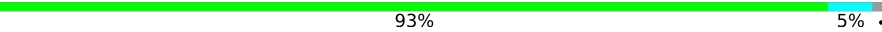
Chain A:  93% 5% •

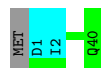


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 8. Colouring as in section 4.1 above.

- Molecule 1: Isoform 11 of Titin

Chain A:  93% 5% •



5 Refinement protocol and experimental data overview

The models were refined using the following method: *na*.

Of the 32500 calculated structures, 10 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CS-ROSETTA	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	403
Number of shifts mapped to atoms	5
Number of unparsed shifts	0
Number of shifts with mapping errors	398
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	1%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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 [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	3210	3240	3240	-

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	37/41 (90%)	37±0 (100±1%)	0±0 (0±1%)	0±0 (0±0%)	100	100
All	All	370/410 (90%)	369 (100%)	1 (0%)	0 (0%)	100	100

There are no Ramachandran outliers.

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	34/37 (92%)	34±0 (100±0%)	0±0 (0±0%)	100	100
All	All	340/370 (92%)	340 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

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 oligosaccharides 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 1% for the well-defined parts and 1% for the entire structure.

7.1 Chemical shift list 1

File name: `working_cs.cif`

Chemical shift list name: *starch_output*

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	403
Number of shifts mapped to atoms	5
Number of unparsed shifts	0
Number of shifts with mapping errors	398
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.

- No matching atom found in the structure. First 5 (of 398) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	MET	CA	56.5	?	1
1	A	1	MET	CB	29.96	?	1
1	A	1	MET	C	176.42	?	1
1	A	2	ASP	H	8.103	?	1
1	A	2	ASP	N	123.071	?	1
1	A	2	ASP	CA	55.44	?	1
1	A	2	ASP	CB	41.58	?	1
1	A	2	ASP	C	176.381	?	1
1	A	3	GLU	H	8.187	?	1
1	A	3	GLU	N	121.433	?	1
1	A	3	GLU	CA	56.473	?	1
1	A	3	GLU	CB	29.459	?	1
1	A	11	GLU	CA	57.885	?	1
1	A	11	GLU	CB	29.525	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	11	GLU	C	177.824	?	1
1	A	12	GLY	H	8.135	?	1
1	A	12	GLY	N	108.676	?	1
1	A	12	GLY	C	176.845	?	1
1	A	12	GLY	CA	45.947	?	1
1	A	13	ASP	H	8.161	?	1
1	A	13	ASP	N	122.991	?	1
1	A	13	ASP	C	177.902	?	1
1	A	13	ASP	CA	56.385	?	1
1	A	13	ASP	CB	40.787	?	1
1	A	14	LEU	H	8.166	?	1
1	A	14	LEU	N	123.311	?	1
1	A	14	LEU	C	178.537	?	1
1	A	14	LEU	CA	57.149	?	1
1	A	14	LEU	CB	40.989	?	1
1	A	15	ARG	H	8.116	?	1
1	A	15	ARG	N	118.6	?	1
1	A	15	ARG	C	178.169	?	1
1	A	15	ARG	CA	62.634	?	1
1	A	15	ARG	CB	29.229	?	1
1	A	16	ALA	H	7.75	?	1
1	A	16	ALA	N	121.471	?	1
1	A	16	ALA	C	179.493	?	1
1	A	16	ALA	CA	53.834	?	1
1	A	16	ALA	CB	17.901	?	1
1	A	17	MET	H	7.768	?	1
1	A	17	MET	N	118.183	?	1
1	A	17	MET	CA	57.094	?	1
1	A	17	MET	CB	32.271	?	1
1	A	18	LEU	CA	54.674	?	1
1	A	18	LEU	CB	41.711	?	1
1	A	18	LEU	C	176.723	?	1
1	A	19	LYS	H	8.136	?	1
1	A	19	LYS	N	122.966	?	1
1	A	19	LYS	C	176.228	?	1
1	A	19	LYS	CA	55.738	?	1
1	A	19	LYS	CB	32.478	?	1
1	A	20	LYS	H	8.302	?	1
1	A	20	LYS	N	123.757	?	1
1	A	20	LYS	C	175.352	?	1
1	A	20	LYS	CA	56.131	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	20	LYS	CB	32.377	?	1
1	A	21	THR	H	7.671	?	1
1	A	21	THR	N	114.811	?	1
1	A	21	THR	CA	58.739	?	1
1	A	21	THR	CB	69.958	?	1
1	A	22	PRO	CA	62.982	?	1
1	A	22	PRO	CB	31.257	?	1
1	A	22	PRO	C	176.592	?	1
1	A	24	LEU	H	8.021	?	1
1	A	24	LEU	N	125.563	?	1
1	A	24	LEU	CA	54.464	?	1
1	A	24	LEU	CB	41.694	?	1
1	A	26	LYS	CA	55.982	?	1
1	A	26	LYS	C	177.08	?	1
1	A	27	GLY	H	8.39	?	1
1	A	27	GLY	N	111.364	?	1
1	A	27	GLY	C	173.796	?	1
1	A	27	GLY	CA	45.079	?	1
1	A	28	ALA	H	8.174	?	1
1	A	28	ALA	N	124.471	?	1
1	A	28	ALA	C	178.315	?	1
1	A	28	ALA	CA	52.309	?	1
1	A	28	ALA	CB	18.356	?	1
1	A	29	GLY	H	8.386	?	1
1	A	29	GLY	N	109.31	?	1
1	A	29	GLY	C	174.362	?	1
1	A	29	GLY	CA	45.148	?	1
1	A	30	GLU	H	8.123	?	1
1	A	30	GLU	N	120.83	?	1
1	A	30	GLU	C	177.44	?	1
1	A	30	GLU	CA	57.069	?	1
1	A	30	GLU	CB	29.437	?	1
1	A	31	GLU	H	8.005	?	1
1	A	31	GLU	N	121.259	?	1
1	A	31	GLU	CA	56.974	?	1
1	A	31	GLU	CB	31.917	?	1
1	A	32	GLU	CA	56.22	?	1
1	A	32	GLU	CB	30.156	?	1
1	A	32	GLU	C	176.105	?	1
1	A	33	GLU	H	8.285	?	1
1	A	33	GLU	N	122.785	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	GLU	C	176.135	?	1
1	A	33	GLU	CA	56.025	?	1
1	A	33	GLU	CB	29.992	?	1
1	A	34	ILE	H	8.111	?	1
1	A	34	ILE	N	122.778	?	1
1	A	34	ILE	C	175.045	?	1
1	A	34	ILE	CA	60.293	?	1
1	A	34	ILE	CB	38.675	?	1
1	A	35	ASP	H	8.288	?	1
1	A	35	ASP	N	126.205	?	1
1	A	35	ASP	C	177.024	?	1
1	A	35	ASP	CA	53.074	?	1
1	A	35	ASP	CB	41.149	?	1
1	A	36	ILE	H	8.3	?	1
1	A	36	ILE	N	125.219	?	1
1	A	36	ILE	C	176.381	?	1
1	A	36	ILE	CA	62.545	?	1
1	A	36	ILE	CB	37.298	?	1
1	A	37	MET	H	8.007	?	1
1	A	37	MET	N	119.227	?	1
1	A	37	MET	C	178.763	?	1
1	A	37	MET	CA	57.236	?	1
1	A	37	MET	CB	30.072	?	1
1	A	38	GLU	H	7.435	?	1
1	A	38	GLU	N	119.404	?	1
1	A	38	GLU	C	178.922	?	1
1	A	38	GLU	CA	58.078	?	1
1	A	38	GLU	CB	28.671	?	1
1	A	39	LEU	H	7.529	?	1
1	A	39	LEU	N	119.918	?	1
1	A	39	LEU	C	179.268	?	1
1	A	39	LEU	CA	57.499	?	1
1	A	39	LEU	CB	41.263	?	1
1	A	40	LEU	H	7.761	?	1
1	A	40	LEU	N	116.939	?	1
1	A	40	LEU	C	178.457	?	1
1	A	40	LEU	CA	56.264	?	1
1	A	40	LEU	CB	40.748	?	1
1	A	41	LYS	H	7.457	?	1
1	A	41	LYS	N	118.411	?	1
1	A	41	LYS	C	177.181	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	41	LYS	CA	58.607	?	1
1	A	41	LYS	CB	31.853	?	1
1	A	42	ASN	H	7.668	?	1
1	A	42	ASN	N	115.507	?	1
1	A	42	ASN	C	174.932	?	1
1	A	42	ASN	CA	53.385	?	1
1	A	42	ASN	CB	39.504	?	1
1	A	43	VAL	H	7.347	?	1
1	A	43	VAL	N	119.994	?	1
1	A	43	VAL	CA	61.621	?	1
1	A	43	VAL	CB	32.446	?	1
1	A	45	PRO	CA	64.385	?	1
1	A	45	PRO	CB	31.797	?	1
1	A	45	PRO	C	178.761	?	1
1	A	46	LYS	H	8.474	?	1
1	A	46	LYS	N	117.949	?	1
1	A	46	LYS	C	179.079	?	1
1	A	46	LYS	CA	58.402	?	1
1	A	46	LYS	CB	31.004	?	1
1	A	47	GLU	H	8.192	?	1
1	A	47	GLU	N	119.047	?	1
1	A	47	GLU	C	177.689	?	1
1	A	47	GLU	CA	56.5	?	1
1	A	47	GLU	CB	29.318	?	1
1	A	48	TYR	H	7.545	?	1
1	A	48	TYR	N	119.101	?	1
1	A	48	TYR	C	177.514	?	1
1	A	48	TYR	CA	59.85	?	1
1	A	48	TYR	CB	36.917	?	1
1	A	49	GLU	H	8.197	?	1
1	A	49	GLU	N	119.158	?	1
1	A	49	GLU	C	178.258	?	1
1	A	49	GLU	CA	59.463	?	1
1	A	49	GLU	CB	28.631	?	1
1	A	50	LYS	H	7.481	?	1
1	A	50	LYS	N	119.686	?	1
1	A	50	LYS	C	178.995	?	1
1	A	50	LYS	CA	59.07	?	1
1	A	50	LYS	CB	31.166	?	1
1	A	51	TYR	H	7.667	?	1
1	A	51	TYR	N	119.195	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	51	TYR	C	177.57	?	1
1	A	51	TYR	CA	61.195	?	1
1	A	51	TYR	CB	37.972	?	1
1	A	52	ALA	H	8.461	?	1
1	A	52	ALA	N	122.435	?	1
1	A	52	ALA	C	180.012	?	1
1	A	52	ALA	CA	55.24	?	1
1	A	52	ALA	CB	17.346	?	1
1	A	53	ARG	H	7.815	?	1
1	A	53	ARG	N	116.862	?	1
1	A	53	ARG	C	179.234	?	1
1	A	53	ARG	CA	58.422	?	1
1	A	53	ARG	CB	29.348	?	1
1	A	54	MET	H	7.717	?	1
1	A	54	MET	N	119.243	?	1
1	A	54	MET	C	177.279	?	1
1	A	54	MET	CA	58.146	?	1
1	A	54	MET	CB	32.427	?	1
1	A	55	TYR	H	7.655	?	1
1	A	55	TYR	N	115.756	?	1
1	A	55	TYR	C	175.841	?	1
1	A	55	TYR	CA	57.972	?	1
1	A	55	TYR	CB	38.464	?	1
1	A	56	GLY	H	7.627	?	1
1	A	56	GLY	N	109.004	?	1
1	A	56	GLY	C	174.489	?	1
1	A	56	GLY	CA	46.17	?	1
1	A	57	ILE	H	7.844	?	1
1	A	57	ILE	N	119.981	?	1
1	A	57	ILE	CA	60.563	?	1
1	A	57	ILE	CB	37.709	?	1
1	A	60	PHE	CA	60.3	?	1
1	A	60	PHE	CB	38.758	?	1
1	A	60	PHE	C	176.854	?	1
1	A	61	ARG	H	8.268	?	1
1	A	61	ARG	N	119.593	?	1
1	A	61	ARG	C	178.991	?	1
1	A	61	ARG	CA	59.216	?	1
1	A	61	ARG	CB	28.603	?	1
1	A	62	GLY	H	8.07	?	1
1	A	62	GLY	N	108.387	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	62	GLY	C	176.424	?	1
1	A	62	GLY	CA	46.489	?	1
1	A	63	LEU	H	7.59	?	1
1	A	63	LEU	N	124.57	?	1
1	A	63	LEU	C	178.016	?	1
1	A	63	LEU	CA	57.493	?	1
1	A	63	LEU	CB	40.849	?	1
1	A	64	LEU	H	7.767	?	1
1	A	64	LEU	N	118.74	?	1
1	A	64	LEU	C	179.665	?	1
1	A	64	LEU	CA	57.588	?	1
1	A	64	LEU	CB	40.422	?	1
1	A	65	GLN	H	7.892	?	1
1	A	65	GLN	N	118.591	?	1
1	A	65	GLN	C	178.339	?	1
1	A	65	GLN	CA	58.235	?	1
1	A	65	GLN	CB	27.787	?	1
1	A	66	ALA	H	7.783	?	1
1	A	66	ALA	N	122.975	?	1
1	A	66	ALA	C	179.749	?	1
1	A	66	ALA	CA	54.597	?	1
1	A	66	ALA	CB	17.45	?	1
1	A	67	PHE	H	8.058	?	1
1	A	67	PHE	N	118.553	?	1
1	A	67	PHE	C	177.404	?	1
1	A	67	PHE	CA	60.036	?	1
1	A	67	PHE	CB	38.144	?	1
1	A	68	GLU	H	8.033	?	1
1	A	68	GLU	N	119.899	?	1
1	A	68	GLU	C	178.849	?	1
1	A	68	GLU	CA	58.898	?	1
1	A	68	GLU	CB	28.698	?	1
1	A	69	LEU	H	7.722	?	1
1	A	69	LEU	N	119.973	?	1
1	A	69	LEU	C	179.517	?	1
1	A	69	LEU	CA	57.068	?	1
1	A	69	LEU	CB	40.956	?	1
1	A	70	LEU	H	7.709	?	1
1	A	70	LEU	N	121.043	?	1
1	A	70	LEU	C	178.913	?	1
1	A	70	LEU	CA	56.887	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	70	LEU	CB	40.974	?	1
1	A	71	LYS	H	7.813	?	1
1	A	71	LYS	N	120.389	?	1
1	A	71	LYS	C	178.216	?	1
1	A	71	LYS	CA	57.844	?	1
1	A	71	LYS	CB	31.482	?	1
1	A	72	GLN	H	7.908	?	1
1	A	72	GLN	N	119.427	?	1
1	A	72	GLN	C	177.436	?	1
1	A	72	GLN	CA	57.156	?	1
1	A	72	GLN	CB	28.16	?	1
1	A	73	SER	H	7.983	?	1
1	A	73	SER	N	116.117	?	1
1	A	73	SER	CA	59.572	?	1
1	A	73	SER	CB	63.527	?	1
1	A	77	GLU	CA	55.999	?	1
1	A	77	GLU	CB	32.223	?	1
1	A	77	GLU	C	176.375	?	1
1	A	78	THR	H	7.847	?	1
1	A	78	THR	N	117.326	?	1
1	A	78	THR	CA	59.736	?	1
1	A	78	THR	CB	69.534	?	1
1	A	80	ARG	CA	56.619	?	1
1	A	80	ARG	CB	30.116	?	1
1	A	80	ARG	C	176.574	?	1
1	A	81	LEU	H	8.239	?	1
1	A	81	LEU	N	122.102	?	1
1	A	81	LEU	CA	54.834	?	1
1	A	81	LEU	CB	40.79	?	1
1	A	82	GLU	CA	56.722	?	1
1	A	82	GLU	CB	29.37	?	1
1	A	82	GLU	C	176.843	?	1
1	A	83	ILE	H	7.876	?	1
1	A	83	ILE	N	121.054	?	1
1	A	83	ILE	C	176.496	?	1
1	A	83	ILE	CA	61.302	?	1
1	A	83	ILE	CB	37.951	?	1
1	A	84	GLU	H	8.223	?	1
1	A	84	GLU	N	123.978	?	1
1	A	84	GLU	C	176.394	?	1
1	A	84	GLU	CA	56.89	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	84	GLU	CB	29.606	?	1
1	A	85	GLU	H	8.143	?	1
1	A	85	GLU	N	122.132	?	1
1	A	85	GLU	C	176.833	?	1
1	A	85	GLU	CA	56.745	?	1
1	A	85	GLU	CB	29.502	?	1
1	A	86	ILE	H	7.892	?	1
1	A	86	ILE	N	122.077	?	1
1	A	86	ILE	C	176.572	?	1
1	A	86	ILE	CA	61.5	?	1
1	A	86	ILE	CB	38.146	?	1
1	A	87	GLU	H	8.26	?	1
1	A	87	GLU	N	124.399	?	1
1	A	87	GLU	C	176.802	?	1
1	A	87	GLU	CA	56.782	?	1
1	A	87	GLU	CB	29.399	?	1
1	A	88	ARG	H	8.184	?	1
1	A	88	ARG	N	121.829	?	1
1	A	88	ARG	C	176.677	?	1
1	A	88	ARG	CA	56.568	?	1
1	A	88	ARG	CB	29.524	?	1
1	A	89	SER	H	8.301	?	1
1	A	89	SER	N	117.605	?	1
1	A	89	SER	CA	58.634	?	1
1	A	89	SER	CB	63.702	?	1
1	A	90	GLU	CA	57.462	?	1
1	A	90	GLU	CB	31.856	?	1
1	A	90	GLU	C	177.944	?	1
1	A	91	ARG	H	8.179	?	1
1	A	91	ARG	N	120.802	?	1
1	A	91	ARG	C	178.224	?	1
1	A	91	ARG	CA	58.009	?	1
1	A	91	ARG	CB	29.095	?	1
1	A	92	ASP	H	7.864	?	1
1	A	92	ASP	N	123.395	?	1
1	A	92	ASP	C	178.094	?	1
1	A	92	ASP	CA	56.887	?	1
1	A	92	ASP	CB	40.826	?	1
1	A	93	GLU	H	7.98	?	1
1	A	93	GLU	N	119.674	?	1
1	A	93	GLU	CA	57.176	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	93	GLU	CB	28.293	?	1
1	A	97	GLU	CA	56.217	?	1
1	A	97	GLU	CB	30.196	?	1
1	A	97	GLU	C	175.045	?	1
1	A	98	GLU	H	8.273	?	1
1	A	98	GLU	N	123.148	?	1
1	A	98	GLU	C	177.734	?	1
1	A	98	GLU	CA	56.271	?	1
1	A	98	GLU	CB	29.778	?	1
1	A	99	LEU	H	8.118	?	1
1	A	99	LEU	N	124.423	?	1
1	A	99	LEU	C	177.278	?	1
1	A	99	LEU	CA	54.915	?	1
1	A	99	LEU	CB	41.436	?	1
1	A	100	VAL	H	7.937	?	1
1	A	100	VAL	N	121.795	?	1
1	A	100	VAL	CA	61.884	?	1
1	A	100	VAL	CB	32.156	?	1
1	A	101	SER	CA	60.636	?	1
1	A	101	SER	CB	62.942	?	1
1	A	101	SER	C	175.915	?	1
1	A	102	PHE	H	7.952	?	1
1	A	102	PHE	N	123.15	?	1
1	A	102	PHE	C	175.836	?	1
1	A	102	PHE	CA	59.931	?	1
1	A	102	PHE	CB	38.853	?	1
1	A	103	ILE	H	8.066	?	1
1	A	103	ILE	N	120.484	?	1
1	A	103	ILE	CA	63.407	?	1
1	A	103	ILE	CB	38.853	?	1
1	A	105	GLN	CA	56.798	?	1
1	A	105	GLN	CB	29.298	?	1
1	A	106	ARG	CA	56.965	?	1
1	A	106	ARG	CB	32.319	?	1
1	A	106	ARG	C	177.615	?	1
1	A	107	LEU	H	7.827	?	1
1	A	107	LEU	N	120.63	?	1
1	A	107	LEU	C	177.828	?	1
1	A	107	LEU	CA	55.678	?	1
1	A	107	LEU	CB	41.073	?	1
1	A	108	SER	H	7.782	?	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	108	SER	N	115.141	?	1
1	A	108	SER	CA	58.648	?	1
1	A	108	SER	CB	63.897	?	1
1	A	109	GLN	CA	57.172	?	1
1	A	109	GLN	CB	29.464	?	1
1	A	109	GLN	C	177.407	?	1
1	A	110	THR	H	7.981	?	1
1	A	110	THR	N	115.568	?	1
1	A	110	THR	C	173.765	?	1
1	A	110	THR	CA	62.962	?	1
1	A	110	THR	CB	69.384	?	1
1	A	111	GLU	H	7.865	?	1
1	A	111	GLU	N	128.524	?	1
1	A	111	GLU	CA	57.93	?	1
1	A	111	GLU	CB	30.52	?	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	92	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	86	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	75	0.00 $\pm$ 0.00	None needed (< 0.5 ppm)
^{15}N	75	0.00 $\pm$ 0.00	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 1%, i.e. 5 atoms were assigned a chemical shift out of a possible 560. 0 out of 7 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	4/190 (2%)	1/77 (1%)	2/76 (3%)	1/37 (3%)
Sidechain	1/323 (0%)	0/208 (0%)	1/101 (1%)	0/14 (0%)
Aromatic	0/47 (0%)	0/22 (0%)	0/25 (0%)	0/0 (—%)
Overall	5/560 (1%)	1/307 (0%)	3/202 (1%)	1/51 (2%)

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

