

Full wwPDB NMR Structure Validation Report (i)

Nov 6, 2023 – 02:26 PM JST

:	8J3Q
:	36559
:	Solution structure of LL-TILmut1
:	Rami, M.J.; Sarma, S.P.
:	2023-04-18
	: : :

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 https://www.wwpdb.org/validation/2017/NMRValidationReportHelp with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

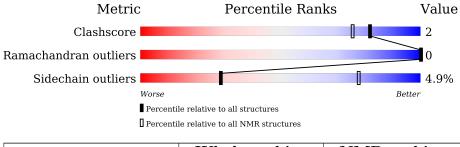
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f NMR} { m archive} \ (\#{ m Entries})$
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 >=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 <=5%

Mol	Chain	Length	Quality of chain	
1	А	58	90%	 9%



2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues								
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model					
1	A:6-A:58 (53)	0.87	15					

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 5 clusters and 2 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 871 atoms, of which 430 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called LL-TIL_mut1.

Mol	Chain	Residues	Atoms						Trace
1	Λ	59	Total	С	Н	Ν	Ο	S	0
	A	99	871	266	430	82	82	11	0



4 Residue-property plots (i)

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: LL-TIL_mut1

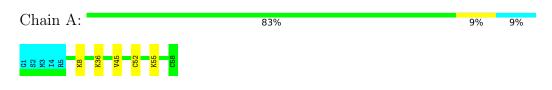
Chain A:	90%	•	9%
8 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2			

4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

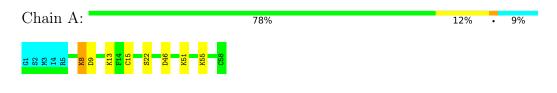
4.2.1 Score per residue for model 1

• Molecule 1: LL-TIL_mut1



4.2.2 Score per residue for model 2

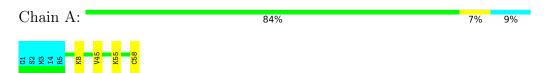
• Molecule 1: LL-TIL_mut1





4.2.3 Score per residue for model 3

• Molecule 1: LL-TIL_mut1



4.2.4 Score per residue for model 4

• Molecule 1: LL-TIL_mut1

Chain A:					83%	7%	•	9%
61 82 85 85 85 85	K36	C52	K55	C58				

4.2.5 Score per residue for model 5

• Molecule 1: LL-TIL_mut1

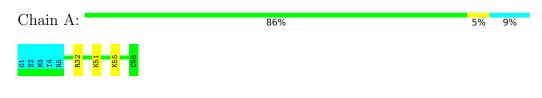
Chain A:	86%	•	·	9%
8 8 1 2 8 1 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 2 8 1 1 1 1				

4.2.6 Score per residue for model 6

• Molecule 1: LL-TIL_mut1

Chain A: 86% • 9%

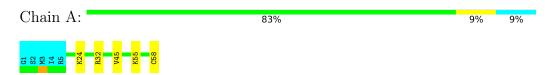
- 4.2.7 Score per residue for model 7
- Molecule 1: LL-TIL_mut1





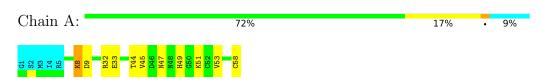
4.2.8 Score per residue for model 8

 \bullet Molecule 1: LL-TIL_mut1



4.2.9 Score per residue for model 9

• Molecule 1: LL-TIL_mut1



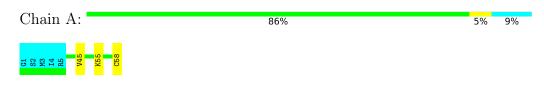
4.2.10 Score per residue for model 10

• Molecule 1: LL-TIL_mut1

Chain A:									79%	10%	·	9%
G1 82 83 85 85 85 85 85 85 85 85 85 85 85 85 85	111	K36	V45	D46 N47	N48	H49	C52	C58				

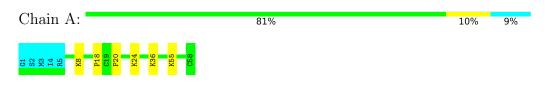
4.2.11 Score per residue for model 11

• Molecule 1: LL-TIL_mut1



4.2.12 Score per residue for model 12

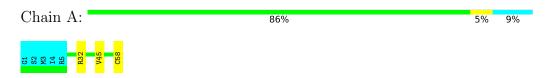
• Molecule 1: LL-TIL_mut1





4.2.13 Score per residue for model 13

• Molecule 1: LL-TIL_mut1



4.2.14 Score per residue for model 14

• Molecule 1: LL-TIL_mut1

Chain A:	79%	12%	9%
<mark>6 11</mark> 8 22 8 23 8 24 7 24 7 23 8 23 8 23 8 23 8 23 8 24 8 25 8 26 8 26 8 26 8 26 8 26 8 26 8 26 8 26			

4.2.15 Score per residue for model 15 (medoid)

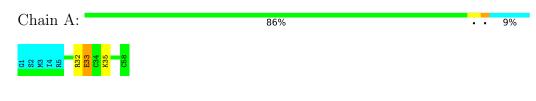
• Molecule 1: LL-TIL_mut1

Chain A:								81%	9%	·	9%
61 82 M3 14 R5 F1 F1	K36	N47 N48	H49	K54	K55 F56	N57	C58				

4.2.16 Score per residue for model 16

• Molecule 1: LL-TIL_mut1

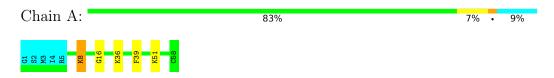
- 4.2.17 Score per residue for model 17
- \bullet Molecule 1: LL-TIL_mut1





4.2.18 Score per residue for model 18

• Molecule 1: LL-TIL_mut1



4.2.19 Score per residue for model 19

• Molecule 1: LL-TIL_mut1

Chain A:	81%	9%	·	9%
G1 82 83 83 83 83 83 83 83 83 83 83 83 85 83 85 83 85 83 85 83 85 83 85 83 85 83 85 83 85 83 85 83 85 83 85 83 85 83 85 85 85 85 85 85 85 85 85 85 85 85 85				

4.2.20 Score per residue for model 20

• Molecule 1: LL-TIL_mut1

Chain 4	4:	-							78%			12%	•	9%
G1 82 85 85	K8	60 0	C19	R32	K36	V45	K51	C58						



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 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
CYANA	structure calculation	
X-PLOR NIH	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	591
Number of shifts mapped to atoms	591
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%



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
1	А	404	387	387	2±1
All	All	8080	7740	7740	39

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 2.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:45:VAL:HG21	1:A:58:CYS:SG	0.68	2.28	9	7	
1:A:54:LYS:HB2	1:A:56:GLU:OE1	0.56	2.01	15	1	
1:A:47:ASN:OD1	1:A:49:HIS:HB2	0.51	2.04	9	3	
1:A:36:LYS:N	1:A:36:LYS:HD2	0.49	2.22	18	5	
1:A:8:LYS:HD2	1:A:9:ASP:N	0.48	2.23	2	3	
1:A:11:ILE:H	1:A:11:ILE:HD13	0.45	1.72	10	1	
1:A:45:VAL:O	1:A:52:CYS:HA	0.45	2.12	10	3	
1:A:8:LYS:HD3	1:A:8:LYS:H	0.44	1.72	18	1	
1:A:51:LYS:HD2	1:A:52:CYS:N	0.44	2.27	19	1	
1:A:33:GLU:OE1	1:A:35:LYS:HE3	0.43	2.13	17	1	
1:A:8:LYS:HD2	1:A:8:LYS:C	0.42	2.35	5	1	
1:A:32:ARG:HD2	1:A:32:ARG:C	0.42	2.34	20	1	
1:A:8:LYS:HD3	1:A:8:LYS:N	0.42	2.30	18	1	
1:A:14:PHE:O	1:A:36:LYS:HG2	0.42	2.15	19	2	

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

Continued on next page...



Atom 1	Atom 2	Clash(Å)	Distance(Å)	Models		
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total	
1:A:44:THR:HB	1:A:53:VAL:O	0.41	2.15	9	1	
1:A:32:ARG:C	1:A:32:ARG:HD2	0.41	2.36	14	1	
1:A:18:PRO:O	1:A:20:PRO:HD3	0.41	2.16	12	1	
1:A:16:GLY:HA3	1:A:39:PHE:CE1	0.41	2.51	18	1	
1:A:22:SER:OG	1:A:24:LYS:HG2	0.41	2.16	14	1	
1:A:22:SER:HB2	1:A:46:ASP:O	0.40	2.16	2	1	
1:A:13:LYS:HE3	1:A:15:CYS:O	0.40	2.17	2	1	
1:A:30:CYS:HB2	1:A:32:ARG:HG3	0.40	1.93	6	1	

Continued from previous page...

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	А	52/58~(90%)	51 ± 1 (97 $\pm2\%$)	$1\pm1 (3\pm2\%)$	0±0 (0±0%)	100 100
All	All	1040/1160~(90%)	1012 (97%)	28 (3%)	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	Analysed Rotameric		Percentiles		
1	А	49/53~(92%)	$47 \pm 1 (95 \pm 2\%)$	$2\pm1 (5\pm2\%)$	29	78	
All	All	980/1060~(92%)	932 (95%)	48 (5%)	29	78	

All 11 unique residues with a non-rotameric side chain are listed below. They are sorted by the frequency of occurrence in the ensemble.



8.]	[3O]
00	JUQ.

Mol	Chain	Res	Type	Models (Total)
1	А	8	LYS	10
1	А	55	LYS	10
1	А	51	LYS	7
1	А	32	ARG	7
1	А	33	GLU	4
1	А	36	LYS	2
1	А	11	ILE	2
1	А	24	LYS	2
1	А	19	CYS	2
1	А	56	GLU	1
1	А	48	ASN	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 monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 80% 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 (i)

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	591
Number of shifts mapped to atoms	591
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	${\rm Correction}\pm{\rm precision},ppm$	Suggested action
$^{13}C_{\alpha}$	54	0.47 ± 0.85	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	50	-0.28 ± 0.25	None needed (< 0.5 ppm)
$^{13}C'$	48	0.09 ± 0.42	None needed (< 0.5 ppm)
^{15}N	49	0.48 ± 0.68	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 84%, i.e. 560 atoms were assigned a chemical shift out of a possible 663. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N
Backbone	247/259~(95%)	103/105~(98%)	97/106~(92%)	$47/48 \ (98\%)$
Sidechain	300/368~(82%)	191/232~(82%)	105/117~(90%)	4/19~(21%)

Continued on next page...



Continuca from pretious page						
	Total	$^{1}\mathbf{H}$	$^{13}\mathrm{C}$	15 N		
Aromatic	13/36~(36%)	9/18~(50%)	4/17~(24%)	0/1~(0%)		
Overall	560/663~(84%)	303/355~(85%)	206/240 (86%)	51/68~(75%)		

Continued from previous page...

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 80%, i.e. 590 atoms were assigned a chemical shift out of a possible 733. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathrm{H}$	$^{13}\mathrm{C}$	15 N
Backbone	259/285~(91%)	108/116~(93%)	102/116~(88%)	49/53~(92%)
Sidechain	318/412~(77%)	202/261~(77%)	112/129~(87%)	4/22 (18%)
Aromatic	13/36~(36%)	9/18~(50%)	4/17~(24%)	0/1~(0%)
Overall	590/733~(80%)	319/395~(81%)	218/262~(83%)	53/76~(70%)

7.1.4 Statistically unusual chemical shifts (i)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	А	44	THR	HG1	5.24	0.08 - 2.19	19.4
1	А	7	PRO	CA	55.54	55.85 - 70.84	-5.2

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:



