



Full wwPDB NMR Structure Validation Report ⓘ

Aug 8, 2023 – 01:20 pm BST

PDB ID : 8ORY
BMRB ID : 34806
Title : Solution NMR structure of Notch1 L1740-1743 TMD
Authors : Guschtschin-Schmidt, N.; Muhle-Goll, C.
Deposited on : 2023-04-17

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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 : 4.02b-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
BMRB Restraints Analysis : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

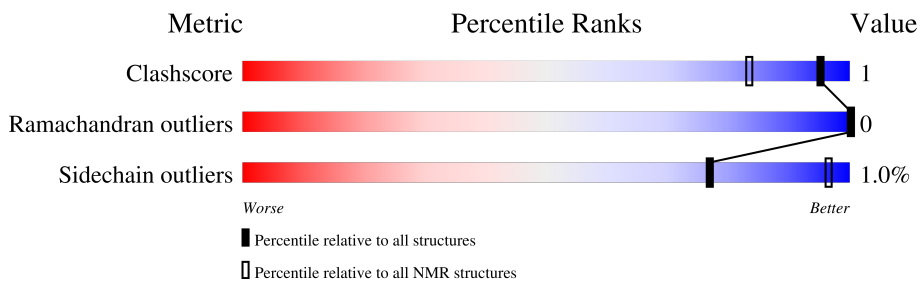
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 76%.

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 ≥ 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	30	 80% 20%

2 Ensemble composition and analysis i

This entry contains 40 models. Model 39 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:1735-A:1749 (15)	0.37	39
2	A:1750-A:1758 (9)	0.52	17

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 8 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 8, 10, 11, 12, 21, 26, 32, 34, 35, 38, 40
2	3, 14, 18, 23, 25, 28, 33
3	7, 15, 17, 19, 30, 37
4	4, 5, 6, 24
5	27, 29, 39
6	2, 20, 22
7	31, 36
8	13, 16
Single-model clusters	9

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 542 atoms, of which 293 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Notch 1 extracellular truncation.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	30	542	176	293	38	33	2	0

There are 10 discrepancies between the modelled and reference sequences:

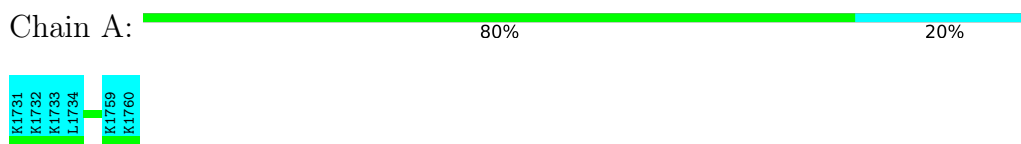
Chain	Residue	Modelled	Actual	Comment	Reference
A	1731	LYS	-	expression tag	UNP P46531
A	1732	LYS	-	expression tag	UNP P46531
A	1733	LYS	-	expression tag	UNP P46531
A	1740	LEU	ALA	engineered mutation	UNP P46531
A	1741	LEU	ALA	engineered mutation	UNP P46531
A	1742	LEU	ALA	engineered mutation	UNP P46531
A	1743	LEU	ALA	engineered mutation	UNP P46531
A	1758	LYS	-	expression tag	UNP P46531
A	1759	LYS	-	expression tag	UNP P46531
A	1760	LYS	-	expression tag	UNP P46531

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: Notch 1 extracellular truncation

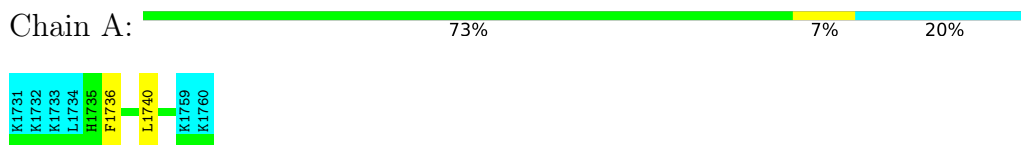


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

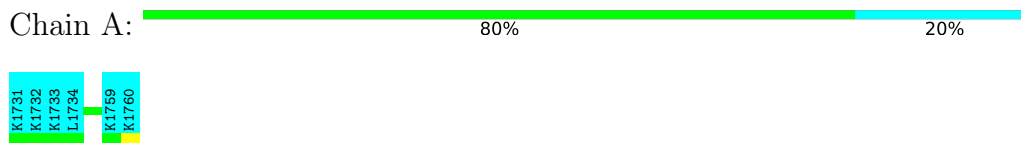
4.2.1 Score per residue for model 1

- Molecule 1: Notch 1 extracellular truncation



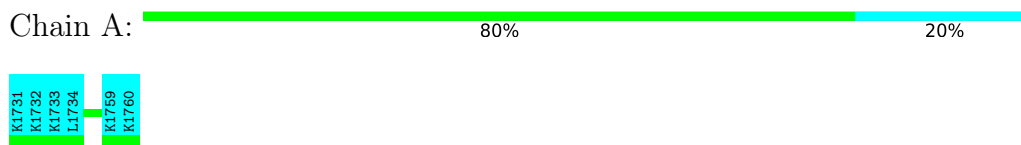
4.2.2 Score per residue for model 2

- Molecule 1: Notch 1 extracellular truncation



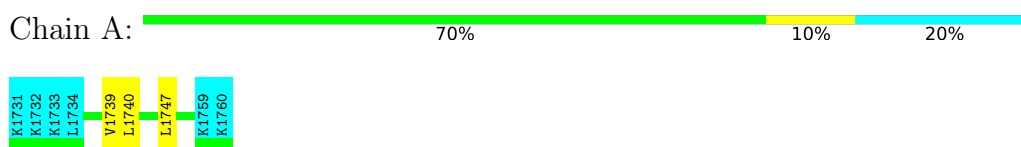
4.2.3 Score per residue for model 3

- Molecule 1: Notch 1 extracellular truncation



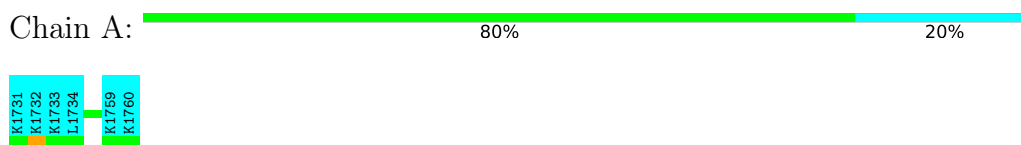
4.2.4 Score per residue for model 4

- Molecule 1: Notch 1 extracellular truncation



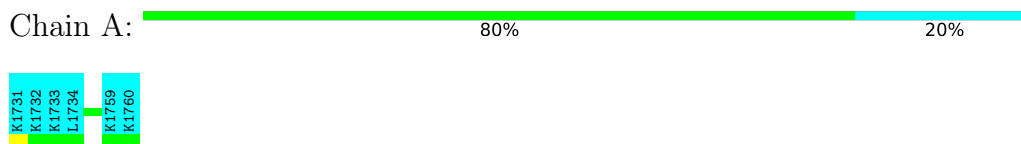
4.2.5 Score per residue for model 5

- Molecule 1: Notch 1 extracellular truncation



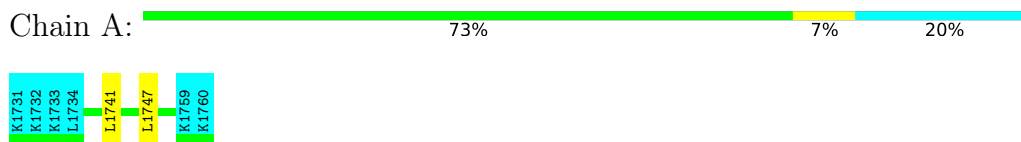
4.2.6 Score per residue for model 6

- Molecule 1: Notch 1 extracellular truncation




4.2.7 Score per residue for model 7

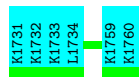
- Molecule 1: Notch 1 extracellular truncation



4.2.8 Score per residue for model 8


- Molecule 1: Notch 1 extracellular truncation

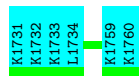
Chain A:  80% 20%



4.2.9 Score per residue for model 9


- Molecule 1: Notch 1 extracellular truncation

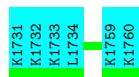
Chain A:  80% 20%



4.2.10 Score per residue for model 10


- Molecule 1: Notch 1 extracellular truncation

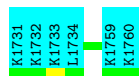
Chain A:  80% 20%



4.2.11 Score per residue for model 11


- Molecule 1: Notch 1 extracellular truncation

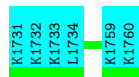
Chain A:  80% 20%



4.2.12 Score per residue for model 12

- Molecule 1: Notch 1 extracellular truncation

Chain A:  80% 20%



4.2.13 Score per residue for model 13


- Molecule 1: Notch 1 extracellular truncation

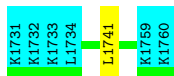
Chain A:  73% 7% 20%



4.2.14 Score per residue for model 14


- Molecule 1: Notch 1 extracellular truncation

Chain A:  77% 1% 20%



4.2.15 Score per residue for model 15

- Molecule 1: Notch 1 extracellular truncation

Chain A:  80% 20%



4.2.16 Score per residue for model 16


- Molecule 1: Notch 1 extracellular truncation

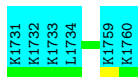
Chain A:  70% 10% 20%



4.2.17 Score per residue for model 17


- Molecule 1: Notch 1 extracellular truncation

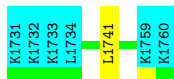
Chain A:  80% 20%



4.2.18 Score per residue for model 18


- Molecule 1: Notch 1 extracellular truncation

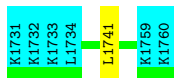
Chain A:  77% 20%



4.2.19 Score per residue for model 19


- Molecule 1: Notch 1 extracellular truncation

Chain A:  77% 20%



4.2.20 Score per residue for model 20

- Molecule 1: Notch 1 extracellular truncation

Chain A:  80% 20%



4.2.21 Score per residue for model 21


- Molecule 1: Notch 1 extracellular truncation

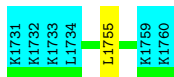
Chain A:  73% 7% 20%



4.2.22 Score per residue for model 22

- Molecule 1: Notch 1 extracellular truncation

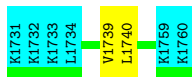
Chain A:  77% 20%



4.2.23 Score per residue for model 23


- Molecule 1: Notch 1 extracellular truncation

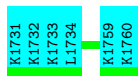
Chain A:  73% 7% 20%



4.2.24 Score per residue for model 24

- Molecule 1: Notch 1 extracellular truncation

Chain A:  80% 20%



4.2.25 Score per residue for model 25


- Molecule 1: Notch 1 extracellular truncation

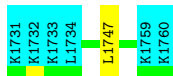
Chain A:  70% 10% 20%



4.2.26 Score per residue for model 26


- Molecule 1: Notch 1 extracellular truncation

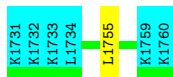
Chain A:  77% 20%



4.2.27 Score per residue for model 27

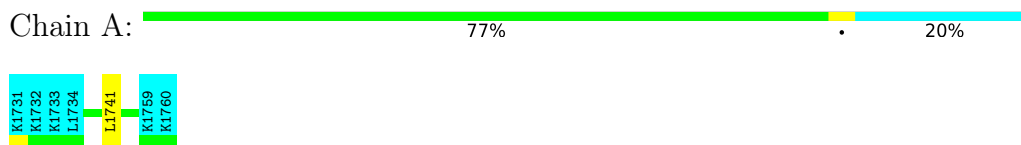
- Molecule 1: Notch 1 extracellular truncation

Chain A:  77% 20%



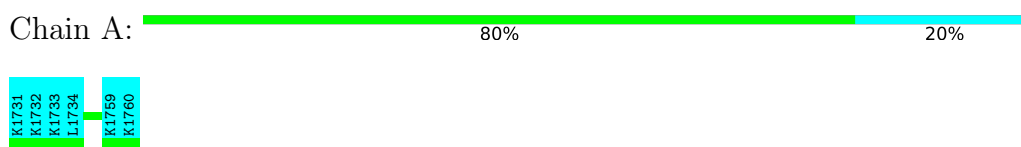
4.2.28 Score per residue for model 28

- Molecule 1: Notch 1 extracellular truncation



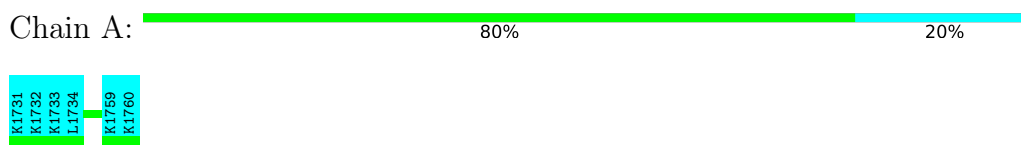
4.2.29 Score per residue for model 29

- Molecule 1: Notch 1 extracellular truncation



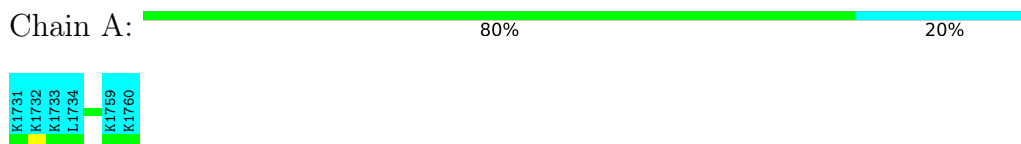
4.2.30 Score per residue for model 30

- Molecule 1: Notch 1 extracellular truncation



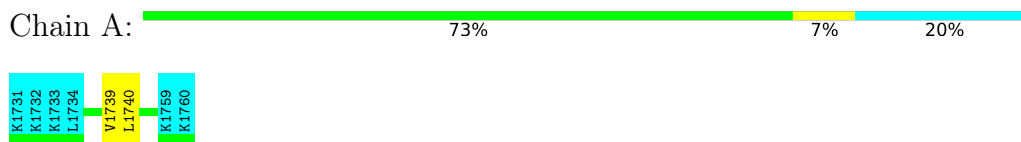
4.2.31 Score per residue for model 31

- Molecule 1: Notch 1 extracellular truncation



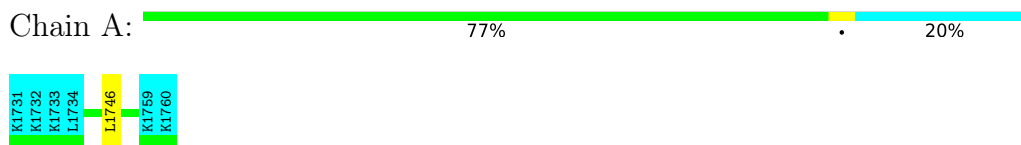
4.2.32 Score per residue for model 32

- Molecule 1: Notch 1 extracellular truncation



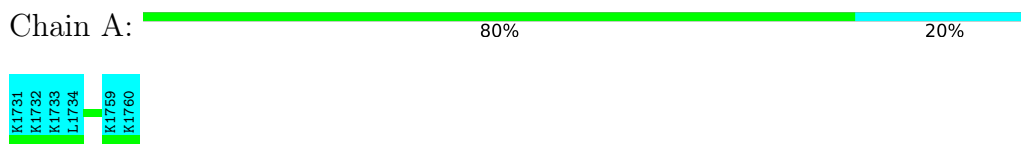
4.2.33 Score per residue for model 33

- Molecule 1: Notch 1 extracellular truncation



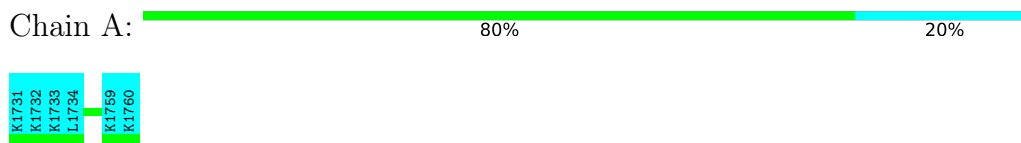
4.2.34 Score per residue for model 34

- Molecule 1: Notch 1 extracellular truncation



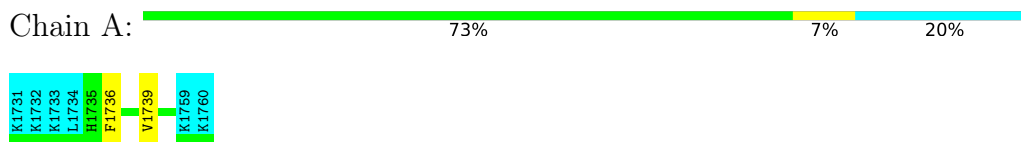
4.2.35 Score per residue for model 35

- Molecule 1: Notch 1 extracellular truncation



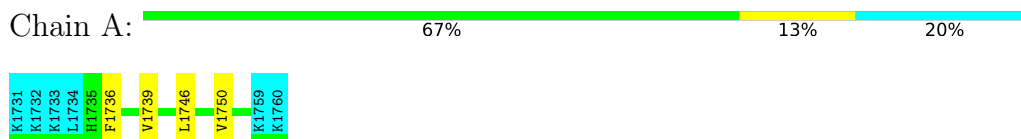
4.2.36 Score per residue for model 36

- Molecule 1: Notch 1 extracellular truncation



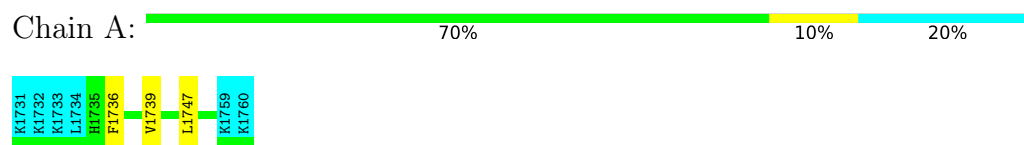
4.2.37 Score per residue for model 37

- Molecule 1: Notch 1 extracellular truncation



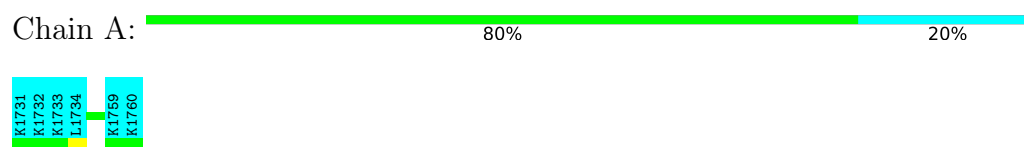
4.2.38 Score per residue for model 38

- Molecule 1: Notch 1 extracellular truncation



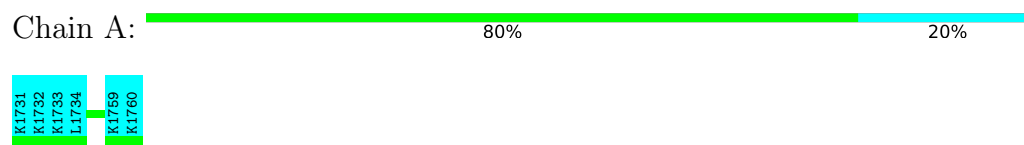
4.2.39 Score per residue for model 39 (medoid)

- Molecule 1: Notch 1 extracellular truncation



4.2.40 Score per residue for model 40

- Molecule 1: Notch 1 extracellular truncation



5 Refinement protocol and experimental data overview

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

Of the 400 calculated structures, 40 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
CNS	refinement	1.2.1
ARIA	structure calculation	2.3.2

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	406
Number of shifts mapped to atoms	406
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	76%

6 Model quality

6.1 Standard geometry

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	195	215	214	0±1
All	All	7800	8600	8560	17

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1736:PHE:O	1:A:1739:VAL:HG22	0.69	1.88	21	4
1:A:1739:VAL:HG23	1:A:1740:LEU:HD12	0.49	1.84	23	5
1:A:1746:LEU:O	1:A:1750:VAL:HG22	0.42	2.14	13	2
1:A:1741:LEU:HD13	1:A:1741:LEU:O	0.42	2.14	19	3
1:A:1741:LEU:O	1:A:1741:LEU:HD13	0.41	2.15	7	2
1:A:1736:PHE:O	1:A:1740:LEU:HD13	0.40	2.17	1	1

6.3 Torsion angles

6.3.1 Protein backbone

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	24/30 (80%)	24±0 (99±2%)	0±0 (1±2%)	0±0 (0±0%)	100	100
All	All	960/1200 (80%)	952 (99%)	8 (1%)	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	22/28 (79%)	22±0 (99±2%)	0±0 (1±2%)	77	96
All	All	880/1120 (79%)	871 (99%)	9 (1%)	77	96

All 4 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	1747	LEU	5
1	A	1755	LEU	2
1	A	1754	VAL	1
1	A	1746	LEU	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 76% for the well-defined parts and 75% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *Notch1L.str*

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	406
Number of shifts mapped to atoms	406
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Chemical shift has been reported more than once. All 46 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1734	LEU	HD12	0.961	.	.
1	A	1734	LEU	HD13	0.961	.	.
1	A	1734	LEU	HD22	0.923	.	.
1	A	1734	LEU	HD23	0.923	.	.
1	A	1739	VAL	HG12	0.994	.	.
1	A	1739	VAL	HG13	0.994	.	.
1	A	1739	VAL	HG22	0.939	.	.
1	A	1739	VAL	HG23	0.939	.	.
1	A	1740	LEU	HD12	0.816	.	.
1	A	1740	LEU	HD13	0.816	.	.
1	A	1741	LEU	HD12	0.919	.	.
1	A	1741	LEU	HD13	0.919	.	.
1	A	1741	LEU	HD22	0.888	.	.
1	A	1741	LEU	HD23	0.888	.	.
1	A	1742	LEU	HD12	0.864	.	.

Continued on next page...

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1742	LEU	HD13	0.864	.	.
1	A	1743	LEU	HD12	0.912	.	.
1	A	1743	LEU	HD13	0.912	.	.
1	A	1743	LEU	HD22	0.866	.	.
1	A	1743	LEU	HD23	0.866	.	.
1	A	1745	VAL	HG12	1.058	.	.
1	A	1745	VAL	HG13	1.058	.	.
1	A	1745	VAL	HG22	1.185	.	.
1	A	1745	VAL	HG23	1.185	.	.
1	A	1746	LEU	HD12	0.925	.	.
1	A	1746	LEU	HD13	0.925	.	.
1	A	1747	LEU	HD12	0.879	.	.
1	A	1747	LEU	HD13	0.879	.	.
1	A	1747	LEU	HD22	0.850	.	.
1	A	1747	LEU	HD23	0.850	.	.
1	A	1750	VAL	HG12	0.952	.	.
1	A	1750	VAL	HG13	0.952	.	.
1	A	1750	VAL	HG22	1.142	.	.
1	A	1750	VAL	HG23	1.142	.	.
1	A	1754	VAL	HG12	1.051	.	.
1	A	1754	VAL	HG13	1.051	.	.
1	A	1754	VAL	HG22	0.923	.	.
1	A	1754	VAL	HG23	0.923	.	.
1	A	1755	LEU	HD12	0.918	.	.
1	A	1755	LEU	HD13	0.918	.	.
1	A	1755	LEU	HD22	0.872	.	.
1	A	1755	LEU	HD23	0.872	.	.
1	A	1756	LEU	HD12	0.890	.	.
1	A	1756	LEU	HD13	0.890	.	.
1	A	1756	LEU	HD22	0.898	.	.
1	A	1756	LEU	HD23	0.898	.	.

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	30	0.15 ± 0.16	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	28	0.86 ± 0.06	Should be checked
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	29	-0.09 ± 0.47	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 76%, i.e. 280 atoms were assigned a chemical shift out of a possible 370. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	97/122 (80%)	50/50 (100%)	24/48 (50%)	23/24 (96%)
Sidechain	153/191 (80%)	104/131 (79%)	49/59 (83%)	0/1 (0%)
Aromatic	30/57 (53%)	20/28 (71%)	10/27 (37%)	0/2 (0%)
Overall	280/370 (76%)	174/209 (83%)	83/134 (62%)	23/27 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 75%, i.e. 359 atoms were assigned a chemical shift out of a possible 478. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	120/152 (79%)	61/62 (98%)	30/60 (50%)	29/30 (97%)
Sidechain	209/269 (78%)	137/180 (76%)	72/83 (87%)	0/6 (0%)
Aromatic	30/57 (53%)	20/28 (71%)	10/27 (37%)	0/2 (0%)
Overall	359/478 (75%)	218/270 (81%)	112/170 (66%)	29/38 (76%)

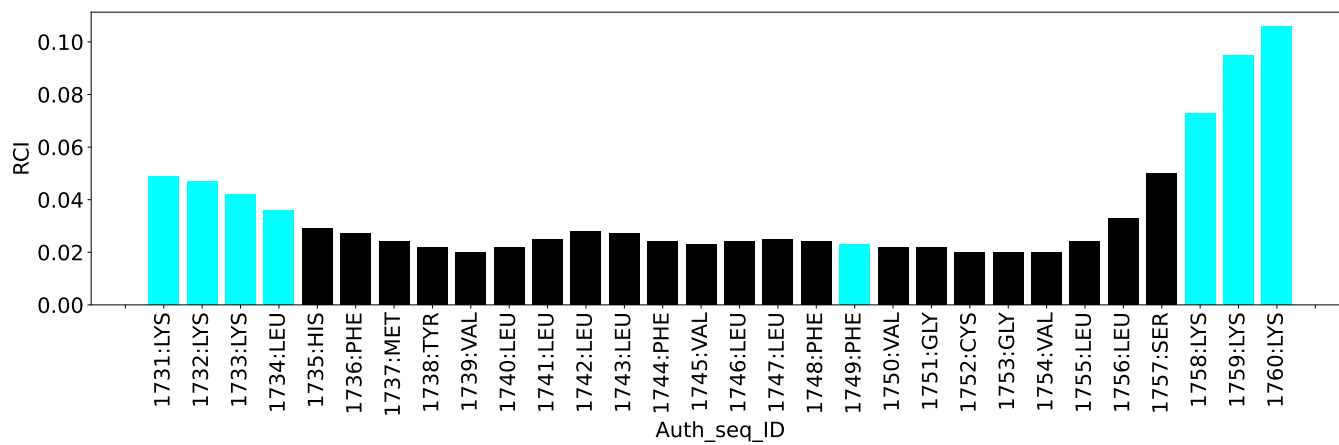
7.1.4 Statistically unusual chemical shifts [i](#)

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:



8 NMR restraints analysis

No restraints data found

9 Distance violation analysis

No distance restraints data found

10 Dihedral-angle violation analysis

No dihedral-angle restraints found