



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 10:49 PM BST

PDB ID : 2KCW
Title : Solution structure of Apo-form YjaB from Escherichia coli
Authors : Lu, J.; Wang, X.; Jin, C.
Deposited on : 2008-12-30

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-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

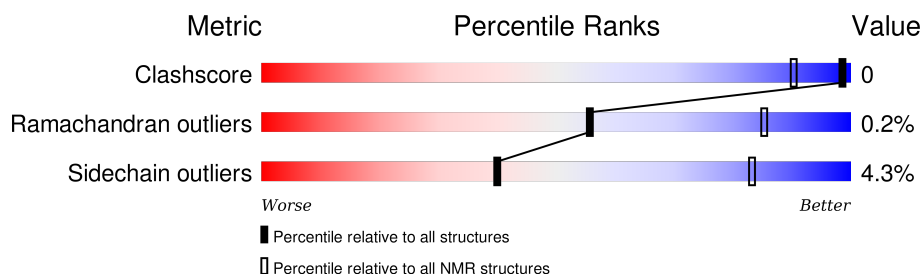
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 89%.

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	147	

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:2-A:128, A:138-A:145 (135)	0.20	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 2 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2292 atoms, of which 1135 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized acetyltransferase yjaB.

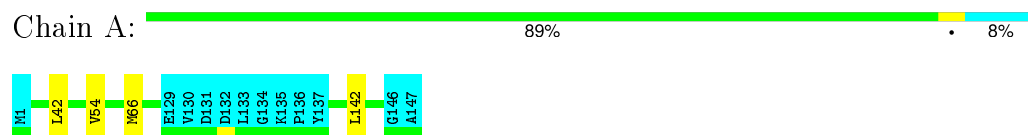
Mol	Chain	Residues	Atoms						Trace
1	A	147	Total	C	H	N	O	S	0
			2292	731	1135	200	220	6	

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 acetyltransferase yjaB

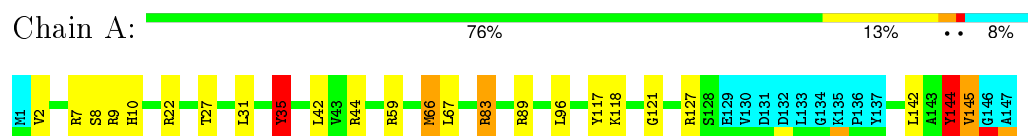


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

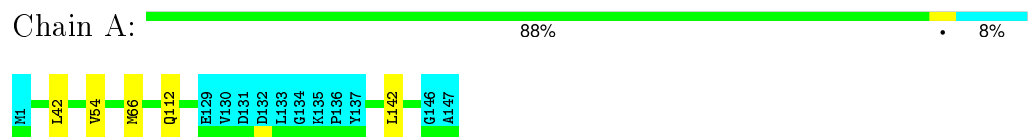
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Uncharacterized acetyltransferase yjaB



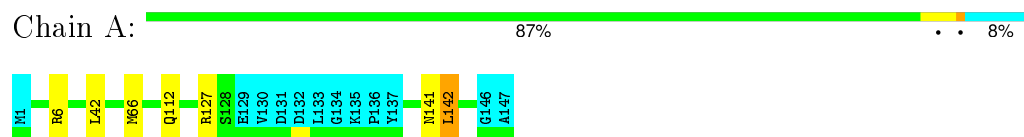
4.2.2 Score per residue for model 2

- Molecule 1: Uncharacterized acetyltransferase yjaB



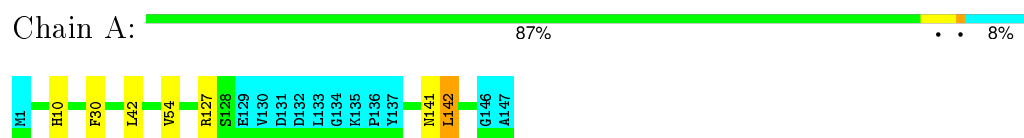
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized acetyltransferase yjaB



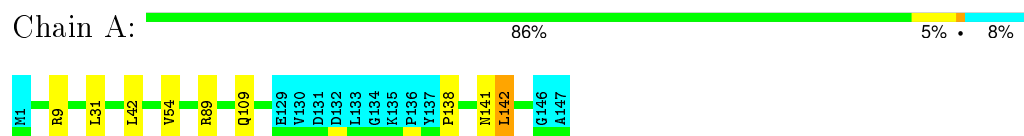
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized acetyltransferase yjaB



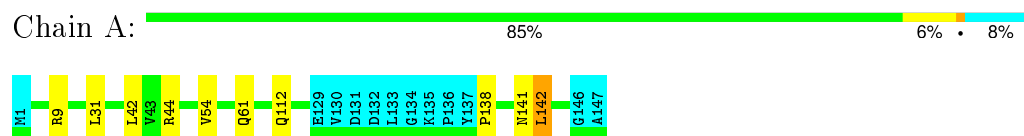
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized acetyltransferase yjaB



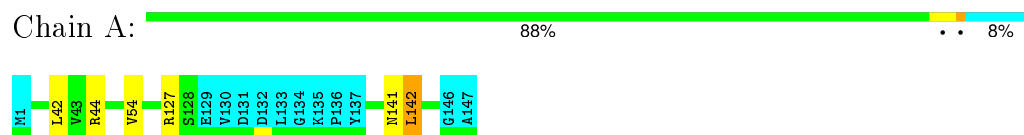
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized acetyltransferase yjaB



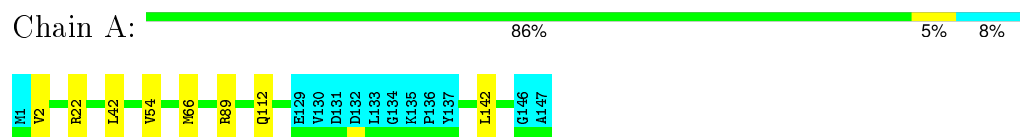
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized acetyltransferase yjaB



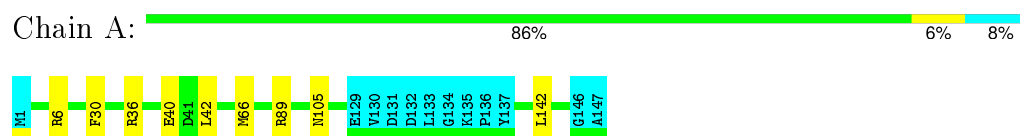
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized acetyltransferase yjaB



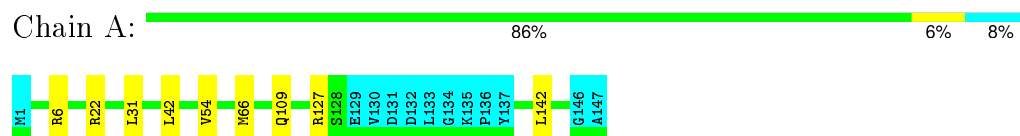
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized acetyltransferase yjaB



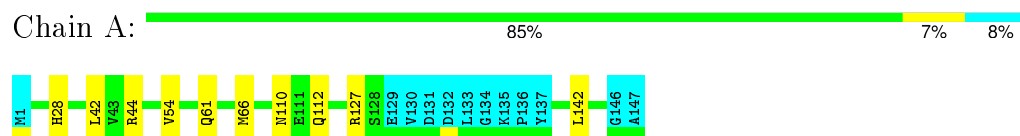
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized acetyltransferase yjaB



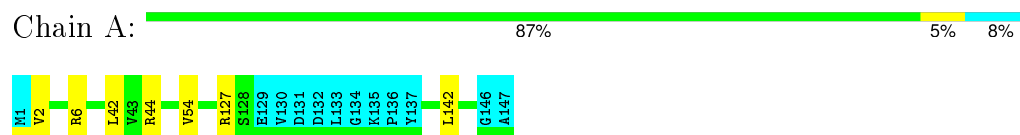
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized acetyltransferase yjaB



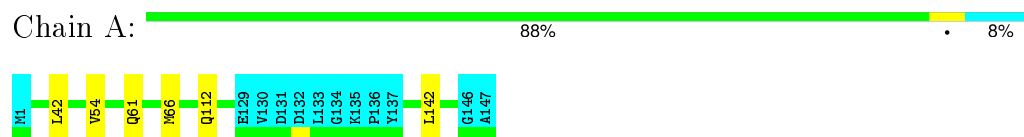
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized acetyltransferase yjaB



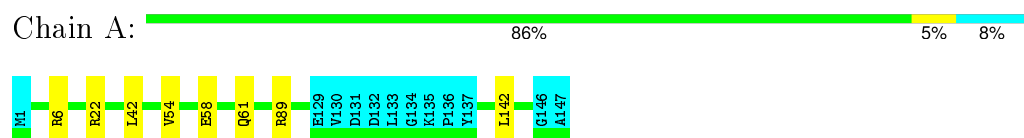
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized acetyltransferase yjaB



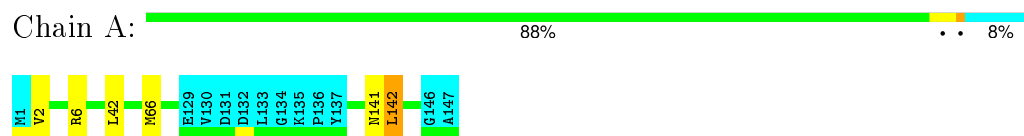
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized acetyltransferase yjaB



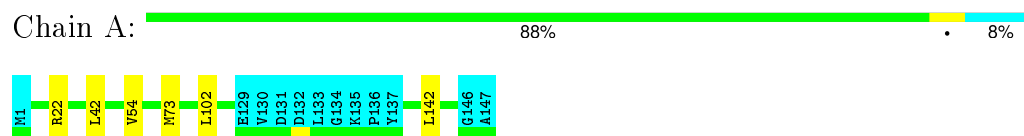
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized acetyltransferase yjaB



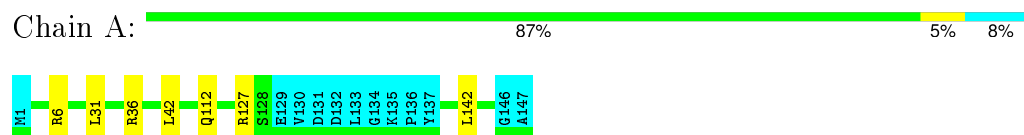
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized acetyltransferase yjaB



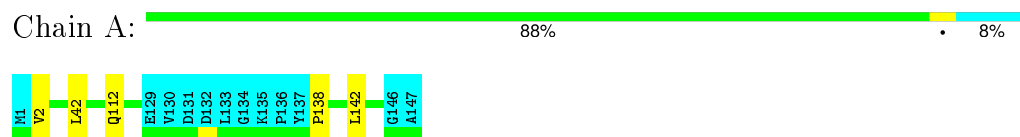
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized acetyltransferase yjaB



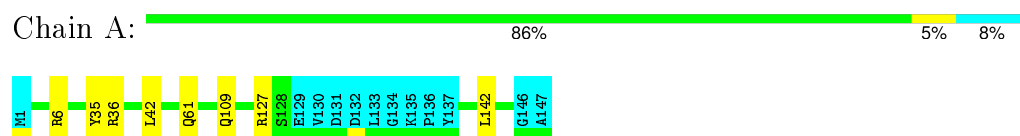
4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized acetyltransferase yjaB



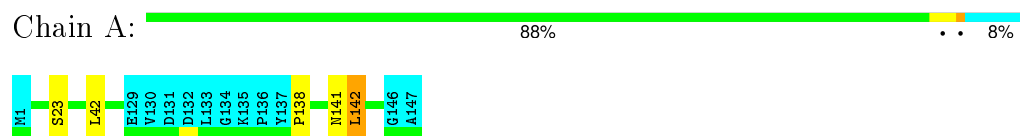
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized acetyltransferase yjaB



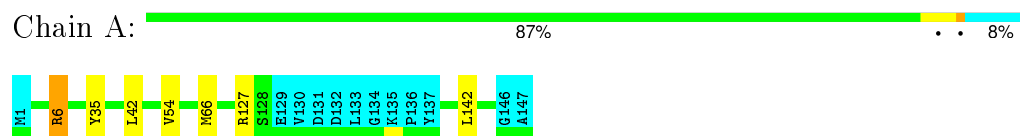
4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized acetyltransferase yjaB



4.2.21 Score per residue for model 21

- Molecule 1: Uncharacterized acetyltransferase yjaB



5 Refinement protocol and experimental data overview

The models were refined using the following method: *MOLECULAR DYNAMICS*.

Of the 100 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
CYANA	structure solution	2.0
AMBER	refinement	7

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)	BMRB entry 16098
Number of chemical shift lists	1
Total number of shifts	1781
Number of shifts mapped to atoms	1781
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	89%

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	0.62±0.01	0±0/1090 (0.0±0.0%)	1.01±0.15	3±5/1480 (0.2±0.3%)
All	All	0.62	0/22890 (0.0%)	1.02	56/31080 (0.2%)

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	0.2±0.7
All	All	0	4

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	59	ARG	NE-CZ-NH2	-18.46	111.07	120.30	1	1
1	A	22	ARG	NE-CZ-NH2	-15.85	112.38	120.30	1	4
1	A	145	VAL	C-N-CA	13.88	151.44	122.30	1	1
1	A	127	ARG	NE-CZ-NH2	-13.13	113.73	120.30	1	10
1	A	9	ARG	NE-CZ-NH2	-11.18	114.71	120.30	1	3
1	A	44	ARG	NE-CZ-NH2	-10.89	114.85	120.30	1	5
1	A	83	ARG	NE-CZ-NH2	-10.46	115.07	120.30	1	1
1	A	66	MET	CA-CB-CG	10.23	130.69	113.30	1	1
1	A	35	TYR	CB-CG-CD2	-10.15	114.91	121.00	1	2
1	A	89	ARG	NE-CZ-NH2	-9.22	115.69	120.30	1	1
1	A	145	VAL	CA-C-O	-9.18	100.81	120.10	1	1
1	A	144	TYR	CB-CG-CD2	-8.47	115.92	121.00	1	1
1	A	145	VAL	O-C-N	7.22	135.48	123.20	1	1
1	A	59	ARG	NH1-CZ-NH2	7.20	127.32	119.40	1	1
1	A	127	ARG	CD-NE-CZ	7.04	133.46	123.60	1	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	22	ARG	NH1-CZ-NH2	6.42	126.46	119.40	1	1
1	A	36	ARG	NE-CZ-NH1	6.25	123.43	120.30	17	1
1	A	59	ARG	CG-CD-NE	-6.05	99.09	111.80	1	1
1	A	6	ARG	NE-CZ-NH1	5.87	123.23	120.30	15	7
1	A	117	TYR	CB-CG-CD2	-5.77	117.54	121.00	1	1
1	A	6	ARG	NE-CZ-NH2	-5.69	117.45	120.30	21	4
1	A	144	TYR	CB-CG-CD1	5.56	124.34	121.00	1	1
1	A	117	TYR	CB-CG-CD1	5.38	124.23	121.00	1	1
1	A	2	VAL	CG1-CB-CG2	-5.36	102.32	110.90	1	1
1	A	7	ARG	NE-CZ-NH2	-5.10	117.75	120.30	1	1
1	A	67	LEU	CB-CG-CD1	5.05	119.59	111.00	1	1
1	A	127	ARG	NE-CZ-NH1	5.05	122.83	120.30	1	1
1	A	2	VAL	CA-CB-CG2	5.01	118.42	110.90	1	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	144	TYR	Sidechain	1
1	A	35	TYR	Sidechain	1
1	A	10	HIS	Sidechain	1
1	A	22	ARG	Sidechain	1

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	1067	1050	1050	1±1
All	All	22407	22050	22050	14

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 0.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:96:LEU:HD21	1:A:144:TYR:HD2	0.63	1.53	1	1
1:A:96:LEU:HD21	1:A:144:TYR:CD2	0.62	2.30	1	1
1:A:96:LEU:HD11	1:A:144:TYR:CE2	0.58	2.33	1	1
1:A:96:LEU:CD1	1:A:144:TYR:CE2	0.49	2.95	1	1
1:A:141:ASN:C	1:A:142:LEU:HD23	0.46	2.31	5	7
1:A:28:HIS:CE1	1:A:110:ASN:HD22	0.46	2.29	11	1
1:A:27:THR:HG21	1:A:83:ARG:HH12	0.45	1.72	1	1
1:A:73:MET:HB2	1:A:102:LEU:HD11	0.40	1.93	16	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	135/147 (92%)	130±1 (96±1%)	4±1 (3±1%)	0±0 (0±0%)	56	85
All	All	2835/3087 (92%)	2735 (96%)	94 (3%)	6 (0%)	56	85

All 3 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	138	PRO	4
1	A	109	GLN	1
1	A	58	GLU	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	116/125 (93%)	111±1 (96±1%)	5±1 (4±1%)	40	83
All	All	2436/2625 (93%)	2331 (96%)	105 (4%)	40	83

All 20 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	42	LEU	21
1	A	142	LEU	21
1	A	54	VAL	13
1	A	66	MET	10
1	A	112	GLN	8
1	A	61	GLN	5
1	A	31	LEU	5
1	A	2	VAL	4
1	A	89	ARG	4
1	A	30	PHE	2
1	A	109	GLN	2
1	A	36	ARG	2
1	A	118	LYS	1
1	A	105	ASN	1
1	A	23	SER	1
1	A	6	ARG	1
1	A	8	SER	1
1	A	10	HIS	1
1	A	40	GLU	1
1	A	144	TYR	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 ⓘ

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 89% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16098

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	1781
Number of shifts mapped to atoms	1781
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	147	-0.56 ± 0.16	Should be applied
$^{13}\text{C}_\beta$	136	-0.06 ± 0.11	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	-0.34 ± 0.14	None needed (< 0.5 ppm)
^{15}N	131	0.35 ± 0.29	None needed (< 0.5 ppm)

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 89%, i.e. 1491 atoms were assigned a chemical shift out of a possible 1666. 31 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	641/663 (97%)	259/264 (98%)	261/270 (97%)	121/129 (94%)
Sidechain	754/873 (86%)	459/508 (90%)	281/323 (87%)	14/42 (33%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	96/130 (74%)	54/70 (77%)	41/54 (76%)	1/6 (17%)
Overall	1491/1666 (89%)	772/842 (92%)	583/647 (90%)	136/177 (77%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 90%, i.e. 1615 atoms were assigned a chemical shift out of a possible 1797. 33 out of 33 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	696/721 (97%)	281/287 (98%)	284/294 (97%)	131/140 (94%)
Sidechain	815/938 (87%)	497/546 (91%)	304/349 (87%)	14/43 (33%)
Aromatic	104/138 (75%)	58/74 (78%)	45/58 (78%)	1/6 (17%)
Overall	1615/1797 (90%)	836/907 (92%)	633/701 (90%)	146/189 (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	6	ARG	NE	117.00	92.63 – 76.73	20.3
1	A	127	ARG	NE	115.91	92.63 – 76.73	19.6
1	A	36	ARG	NE	115.56	92.63 – 76.73	19.4
1	A	44	ARG	NE	114.99	92.63 – 76.73	19.1
1	A	22	ARG	NE	113.22	92.63 – 76.73	17.9
1	A	109	GLN	HB2	0.49	3.30 – 0.80	-6.2
1	A	104	THR	HG22	-0.10	2.29 – -0.01	-5.4
1	A	104	THR	HG21	-0.10	2.29 – -0.01	-5.4
1	A	104	THR	HG23	-0.10	2.29 – -0.01	-5.4

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:

