wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	2LZU
Title	:	Solution structure of LIMD2
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Deposited on	:	2012-10-10

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
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

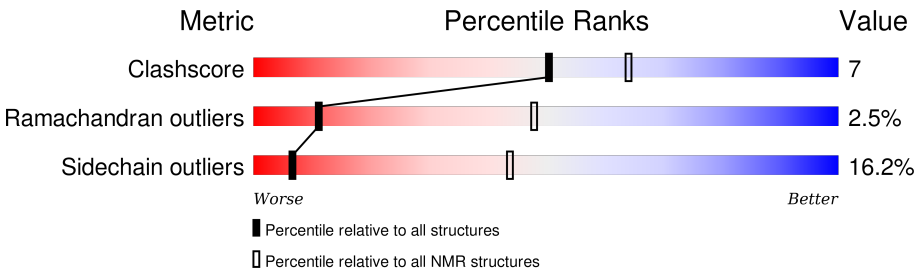
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 71%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	72	54% 25% • 18%

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 10 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:41-A:99 (59)	0.25	10

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	1, 7, 8, 10
2	2, 5, 9
3	3, 4, 6

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1144 atoms, of which 562 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LIM domain-containing protein 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	72	1142	368	562	102	102	8	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

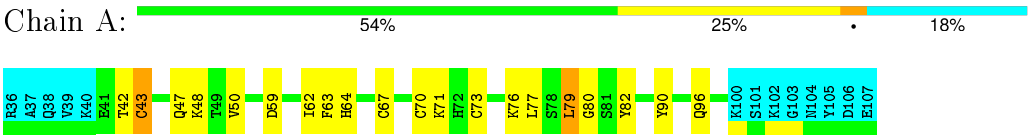
4 Residue-property plots (i)

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: LIM domain-containing protein 2

Chain A:

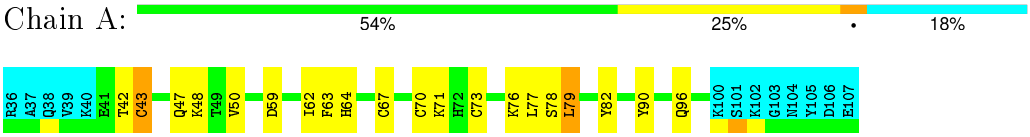


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

- Molecule 1: LIM domain-containing protein 2

Chain A:



5 Refinement protocol and experimental data overview (i)

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

Of the 450 calculated structures, 10 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
ARIA	structure solution	2.3
CNS	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)	2lzu_cs.str
Number of chemical shift lists	3
Total number of shifts	1396
Number of shifts mapped to atoms	1396
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	71%

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)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	A	473	453	451	7±1
All	All	4750	4530	4510	67

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 7.

5 of 16 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:CYS:O	1:A:47:GLN:HA	0.67	1.89	2	10
1:A:64:HIS:HB2	1:A:67:CYS:SG	0.66	2.30	1	10
1:A:70:CYS:HB3	1:A:73:CYS:O	0.55	2.02	8	9
1:A:43:CYS:HA	1:A:62:ILE:O	0.55	2.01	5	9
1:A:43:CYS:HB3	1:A:48:LYS:O	0.53	2.03	5	10

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	59/72 (82%)	54±1 (91±2%)	4±1 (7±2%)	2±1 (3±2%)	11 48
All	All	590/720 (82%)	535 (91%)	40 (7%)	15 (3%)	11 48

All 4 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	79	LEU	6
1	A	80	GLY	5
1	A	59	ASP	3
1	A	60	LYS	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	52/63 (83%)	44±2 (84±3%)	8±2 (16±3%)	7 44
All	All	520/630 (83%)	436 (84%)	84 (16%)	7 44

5 of 12 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	43	CYS	10
1	A	90	TYR	10
1	A	42	THR	10
1	A	79	LEU	10
1	A	63	PHE	10

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)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 71% for the well-defined parts and 61% for the entire structure.

7.1 Chemical shift list 1

File name: 2lzu_cs.str

Chemical shift list name: *assigned_chem_shift_list_1*

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	305
Number of shifts mapped to atoms	305
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

7.1.2 Chemical shift referencing (i)

No chemical shift referencing corrections were calculated (not enough data).

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 34%, i.e. 249 atoms were assigned a chemical shift out of a possible 734. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	54/291 (19%)	54/116 (47%)	0/118 (0%)	0/57 (0%)
Sidechain	150/337 (45%)	150/202 (74%)	0/123 (0%)	0/12 (0%)
Aromatic	45/106 (42%)	45/57 (79%)	0/42 (0%)	0/7 (0%)
Overall	249/734 (34%)	249/375 (66%)	0/283 (0%)	0/76 (0%)

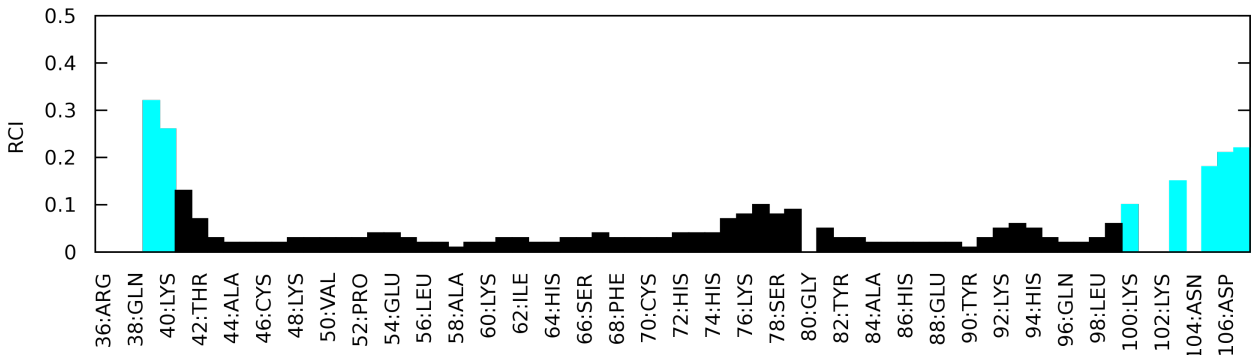
7.1.4 Statistically unusual chemical shifts (i)

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.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: 2lzu_cs.str

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	617
Number of shifts mapped to atoms	617
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	75

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	51	1.64 ± 0.36	Should be applied
$^{13}C_{\beta}$	47	1.37 ± 0.51	Should be applied
$^{13}C'$	0	—	—
^{15}N	60	0.15 ± 0.79	None needed (< 0.5 ppm)

7.2.3 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 71%, i.e. 523 atoms were assigned a chemical shift out of a possible 734. 8 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	217/291 (75%)	112/116 (97%)	51/118 (43%)	54/57 (95%)
Sidechain	261/337 (77%)	178/202 (88%)	83/123 (67%)	0/12 (0%)
Aromatic	45/106 (42%)	45/57 (79%)	0/42 (0%)	0/7 (0%)
Overall	523/734 (71%)	335/375 (89%)	134/283 (47%)	54/76 (71%)

7.2.4 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.

Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	93	PRO	CG	52.90	32.66 – 21.76	23.6
1	A	52	PRO	CG	52.28	32.66 – 21.76	23.0
1	A	49	THR	CG2	46.81	27.15 – 15.95	22.6
1	A	48	LYS	CG	49.84	30.67 – 19.17	21.7
1	A	42	THR	CG2	45.75	27.15 – 15.95	21.6
1	A	56	LEU	CG	51.61	32.55 – 21.05	21.6
1	A	61	LEU	CG	51.58	32.55 – 21.05	21.5
1	A	98	LEU	CG	51.31	32.55 – 21.05	21.3
1	A	85	LEU	CG	50.71	32.55 – 21.05	20.8
1	A	48	LYS	CD	53.09	34.86 – 23.06	20.5
1	A	77	LEU	CG	49.00	32.55 – 21.05	19.3
1	A	62	ILE	CG2	42.83	24.63 – 10.43	17.8
1	A	50	VAL	CG1	45.31	28.40 – 14.60	17.3
1	A	57	VAL	CG1	45.21	28.40 – 14.60	17.2
1	A	78	SER	CB	38.82	71.24 – 56.34	-16.8

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Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	49	THR	CB	41.94	78.10 – 61.30	-16.5
1	A	75	THR	CB	42.23	78.10 – 61.30	-16.3
1	A	56	LEU	CD1	50.80	32.77 – 16.57	16.1
1	A	61	LEU	CD1	50.77	32.77 – 16.57	16.1
1	A	84	ALA	CB	47.32	28.03 – 9.93	15.7
1	A	93	PRO	CA	39.06	71.13 – 55.53	-15.6
1	A	42	THR	CB	43.78	78.10 – 61.30	-15.4
1	A	52	PRO	CA	39.32	71.13 – 55.53	-15.4
1	A	79	LEU	CD1	49.44	32.77 – 16.57	15.3
1	A	77	LEU	CD1	49.40	32.77 – 16.57	15.3
1	A	85	LEU	CD2	49.90	32.60 – 15.60	15.2
1	A	57	VAL	CG2	45.21	29.20 – 13.40	15.1
1	A	56	LEU	CD2	49.62	32.60 – 15.60	15.0
1	A	98	LEU	CD1	48.88	32.77 – 16.57	14.9
1	A	50	VAL	CG2	44.90	29.20 – 13.40	14.9
1	A	45	ALA	CB	45.11	28.03 – 9.93	14.4
1	A	85	LEU	CD1	47.87	32.77 – 16.57	14.3
1	A	62	ILE	CG1	52.76	36.54 – 18.94	14.2
1	A	79	LEU	CD2	47.81	32.60 – 15.60	13.9
1	A	62	ILE	CD1	37.00	21.91 – 5.01	13.9
1	A	61	LEU	CD2	47.53	32.60 – 15.60	13.8
1	A	98	LEU	CD2	46.84	32.60 – 15.60	13.4
1	A	97	GLN	CB	53.75	38.36 – 19.96	13.4
1	A	77	LEU	CD2	46.79	32.60 – 15.60	13.3
1	A	44	ALA	CB	43.08	28.03 – 9.93	13.3
1	A	60	LYS	CB	55.94	41.68 – 23.88	13.0
1	A	96	GLN	CB	52.53	38.36 – 19.96	12.7
1	A	66	SER	CA	32.63	69.25 – 48.25	-12.4
1	A	76	LYS	CA	30.35	67.97 – 45.97	-12.1
1	A	65	ASN	CA	30.60	63.05 – 44.05	-12.1
1	A	97	GLN	CA	30.87	67.31 – 45.91	-12.0
1	A	47	GLN	CA	31.16	67.31 – 45.91	-11.9
1	A	96	GLN	CA	31.20	67.31 – 45.91	-11.9
1	A	92	LYS	CB	53.91	41.68 – 23.88	11.9
1	A	71	LYS	CA	31.16	67.97 – 45.97	-11.7
1	A	60	LYS	CA	31.16	67.97 – 45.97	-11.7
1	A	53	MET	CA	30.35	67.38 – 44.88	-11.5
1	A	55	ARG	CA	30.35	68.35 – 45.25	-11.5
1	A	47	GLN	CB	50.14	38.36 – 19.96	11.4
1	A	94	HIS	CB	53.88	40.69 – 19.69	11.3
1	A	42	THR	CA	32.75	75.37 – 49.07	-11.2
1	A	62	ILE	CA	31.97	75.08 – 48.18	-11.0

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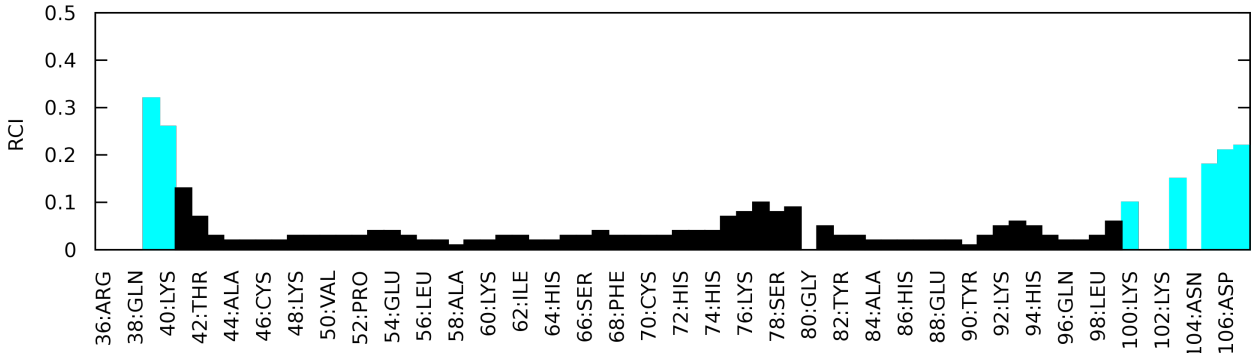
Mol	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	86	HIS	CB	52.74	40.69 – 19.69	10.7
1	A	72	HIS	CA	31.41	68.24 – 44.74	-10.7
1	A	99	PHE	CA	30.75	70.99 – 45.29	-10.7
1	A	89	PHE	CA	30.90	70.99 – 45.29	-10.6
1	A	74	HIS	CB	51.88	40.69 – 19.69	10.3
1	A	53	MET	CB	55.94	44.20 – 21.80	10.2
1	A	50	VAL	CA	33.13	76.93 – 48.03	-10.2
1	A	92	LYS	CA	34.89	67.97 – 45.97	-10.0
1	A	75	THR	CA	35.89	75.37 – 49.07	-10.0
1	A	94	HIS	CA	33.30	68.24 – 44.74	-9.9
1	A	49	THR	CA	36.94	75.37 – 49.07	-9.6
1	A	95	PHE	CA	34.12	70.99 – 45.29	-9.3
1	A	43	CYS	CA	30.35	75.07 – 41.27	-8.2
1	A	91	CYS	CA	30.35	75.07 – 41.27	-8.2
1	A	73	CYS	CA	30.75	75.07 – 41.27	-8.1
1	A	70	CYS	CA	31.16	75.07 – 41.27	-8.0
1	A	46	CYS	CA	31.38	75.07 – 41.27	-7.9
1	A	67	CYS	CA	33.44	75.07 – 41.27	-7.3

7.2.5 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.

Random coil index (RCI) for chain A:



7.3 Chemical shift list 3

File name: 2lzu_cs.str

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	474
Number of shifts mapped to atoms	474
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

7.3.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	—
$^{13}C_{\beta}$	0	—	—
$^{13}C'$	0	—	—
^{15}N	60	0.14 ± 1.22	None needed (< 0.5 ppm)

7.3.3 Completeness of resonance assignments (i)

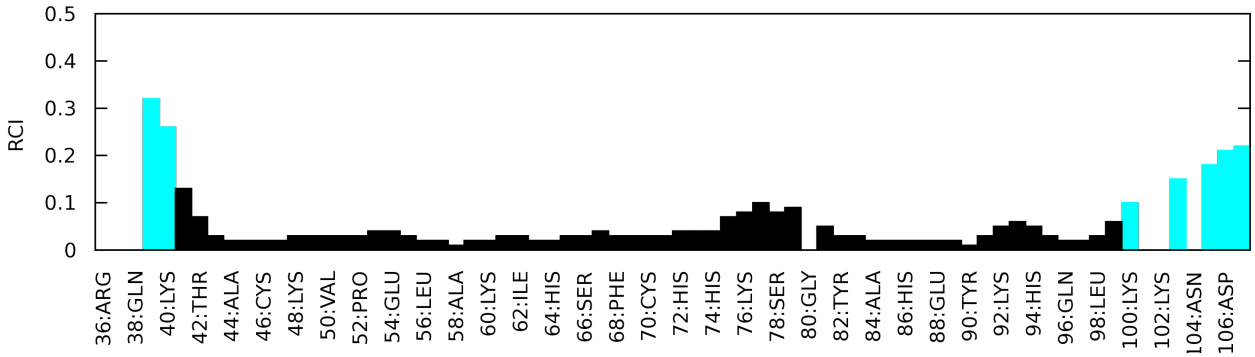
The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 52%, i.e. 382 atoms were assigned a chemical shift out of a possible 734. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	165/291 (57%)	111/116 (96%)	0/118 (0%)	54/57 (95%)
Sidechain	172/337 (51%)	172/202 (85%)	0/123 (0%)	0/12 (0%)
Aromatic	45/106 (42%)	45/57 (79%)	0/42 (0%)	0/7 (0%)
Overall	382/734 (52%)	328/375 (87%)	0/283 (0%)	54/76 (71%)

7.3.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.3.5 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.

Random coil index (RCI) for chain A: