



Full wwPDB NMR Structure Validation Report ⓘ

Nov 6, 2017 – 06:59 PM EST

PDB ID : 5KQC
Title : Identification and structural characterization of LytU
Authors : Tossavainen, H.; Raulinaitis, V.; Permi, P.
Deposited on : unknown

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20030345
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

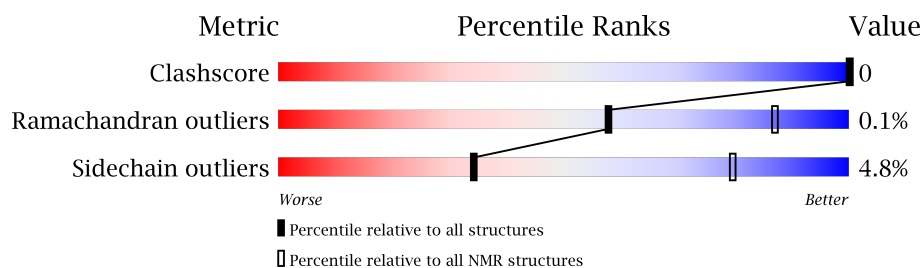
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR


The overall completeness of chemical shifts assignment is 82%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	145	

2 Ensemble composition and analysis ⓘ

This entry contains 15 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:59-A:64, A:77-A:102, A:107-A:114, A:119-A:149, A:157-A:191 (106)	0.19	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 2 clusters and 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2259 atoms, of which 1106 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Peptidase M23.

Mol	Chain	Residues	Atoms						Trace
1	A	145	Total	C	H	N	O	S	0
			2258	734	1106	202	215	1	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP A0A0D6GI13

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

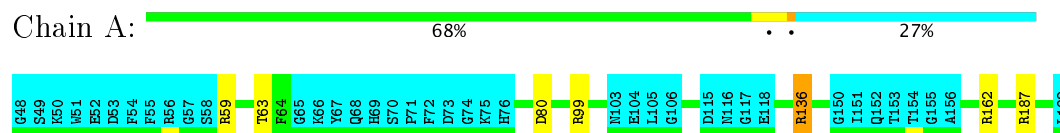
Mol	Chain	Residues	Atoms	
2	A	1	Total	Zn
			1	1

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: Peptidase M23

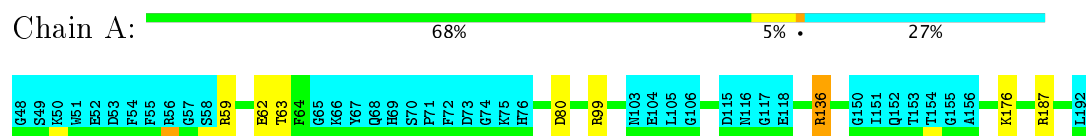


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

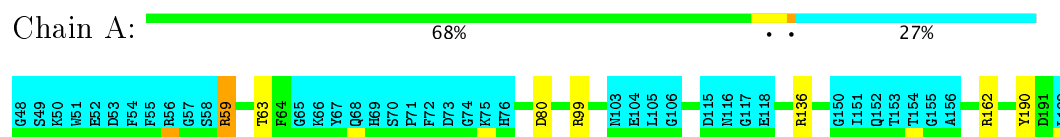
4.2.1 Score per residue for model 1

- Molecule 1: Peptidase M23



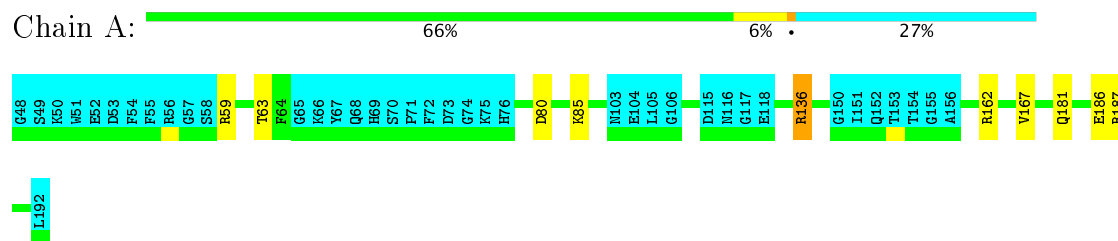
4.2.2 Score per residue for model 2

- Molecule 1: Peptidase M23



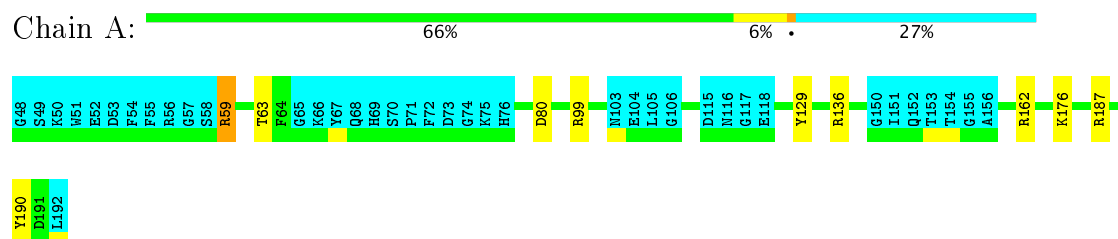
4.2.3 Score per residue for model 3

- Molecule 1: Peptidase M23



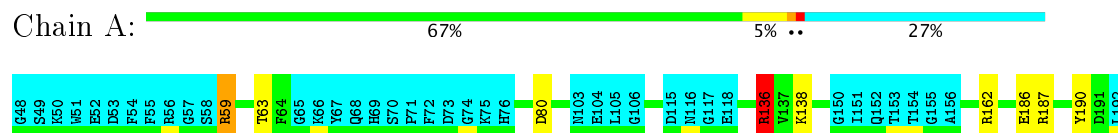
4.2.4 Score per residue for model 4

- Molecule 1: Peptidase M23



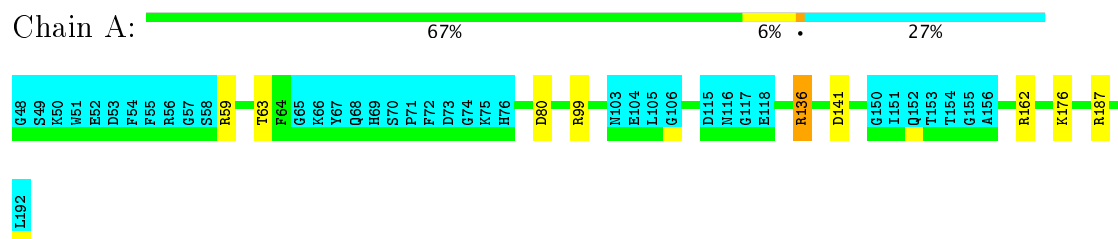
4.2.5 Score per residue for model 5

- Molecule 1: Peptidase M23



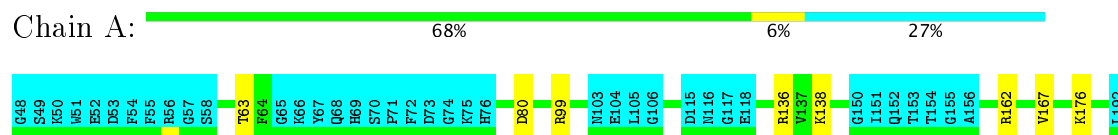
4.2.6 Score per residue for model 6

- Molecule 1: Peptidase M23



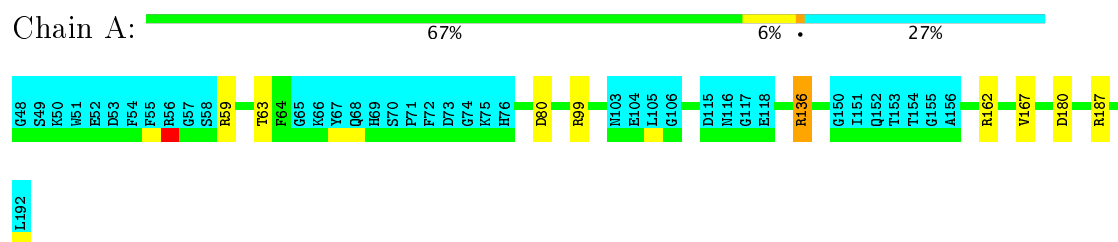
4.2.7 Score per residue for model 7

- Molecule 1: Peptidase M23



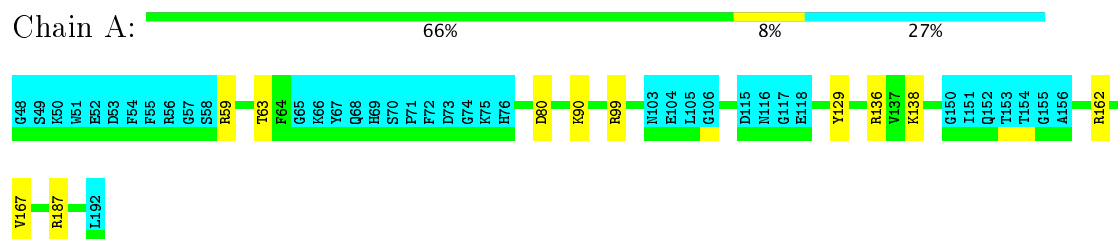
4.2.8 Score per residue for model 8

- Molecule 1: Peptidase M23



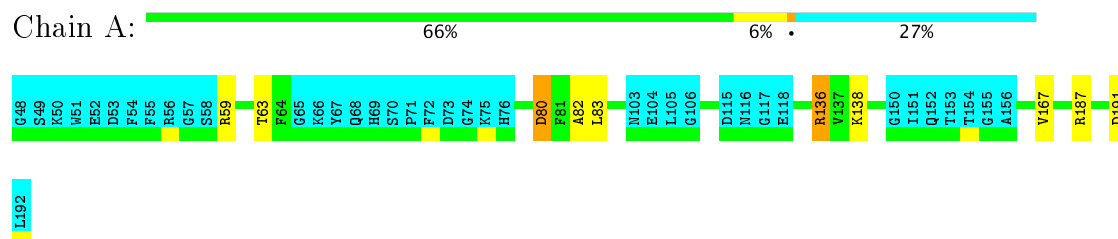
4.2.9 Score per residue for model 9

- Molecule 1: Peptidase M23



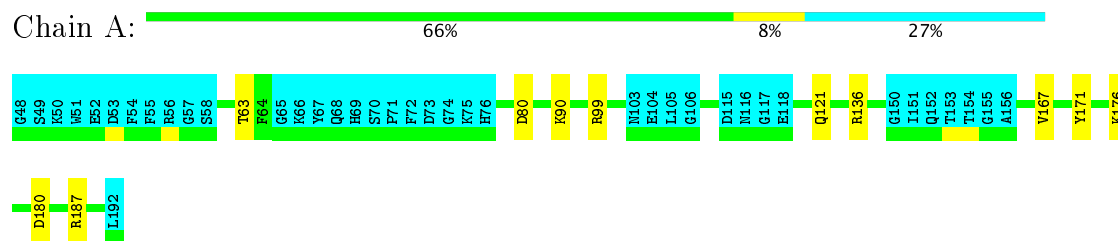
4.2.10 Score per residue for model 10

- Molecule 1: Peptidase M23



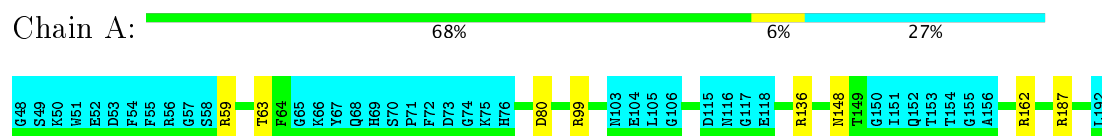
4.2.11 Score per residue for model 11

- Molecule 1: Peptidase M23



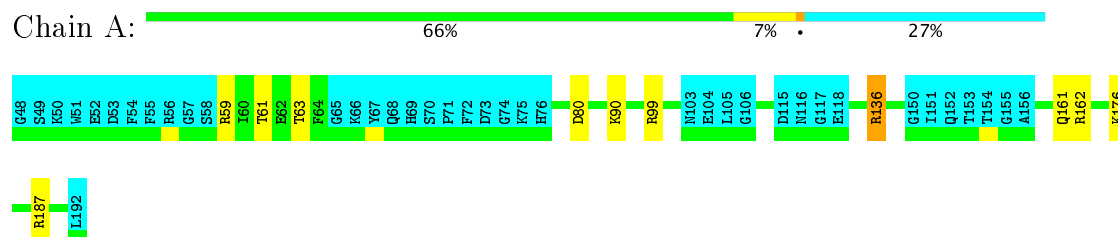
4.2.12 Score per residue for model 12

- Molecule 1: Peptidase M23



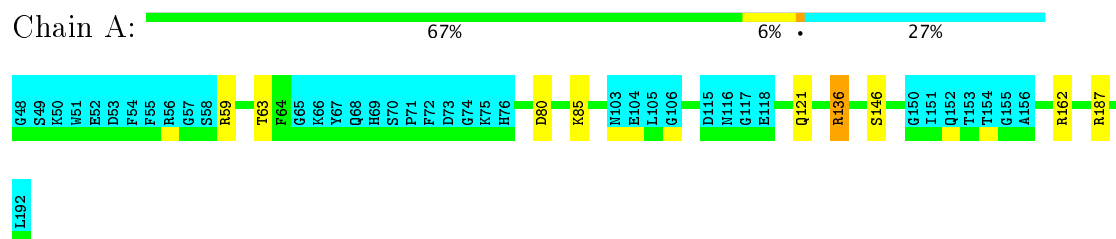
4.2.13 Score per residue for model 13

- Molecule 1: Peptidase M23



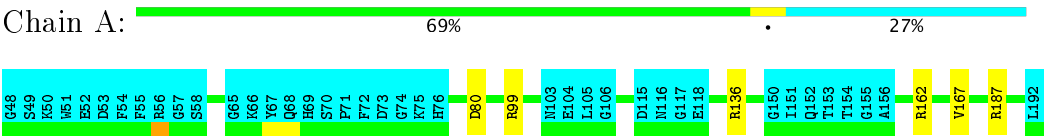
4.2.14 Score per residue for model 14

- Molecule 1: Peptidase M23



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: Peptidase M23



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 15 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	
AMBER	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)	5kqc_cs.cif
Number of chemical shift lists	1
Total number of shifts	1571
Number of shifts mapped to atoms	1571
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

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

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	0.74±0.01	0±0/874 (0.0±0.0%)	1.18±0.03	7±1/1184 (0.6±0.1%)
All	All	0.74	0/13110 (0.0%)	1.18	107/17760 (0.6%)

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	0.7±0.8
All	All	0	10

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	136	ARG	NE-CZ-NH1	11.71	126.16	120.30	6	14
1	A	80	ASP	CB-CG-OD2	11.35	128.51	118.30	15	15
1	A	80	ASP	CB-CG-OD1	9.74	127.07	118.30	5	14
1	A	162	ARG	NE-CZ-NH1	9.59	125.10	120.30	7	11
1	A	80	ASP	OD1-CG-OD2	-9.54	105.18	123.30	10	15
1	A	99	ARG	NE-CZ-NH1	9.29	124.95	120.30	13	11
1	A	59	ARG	NE-CZ-NH1	8.79	124.70	120.30	5	11
1	A	187	ARG	NE-CZ-NH1	8.70	124.65	120.30	12	12
1	A	187	ARG	NE-CZ-NH2	-5.50	117.55	120.30	10	3
1	A	162	ARG	NE-CZ-NH2	-5.31	117.64	120.30	15	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	190	TYR	Sidechain	3
1	A	129	TYR	Sidechain	2
1	A	162	ARG	Sidechain	1
1	A	80	ASP	Sidechain	1
1	A	59	ARG	Sidechain	1
1	A	136	ARG	Sidechain	1
1	A	171	TYR	Sidechain	1

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	850	836	836	0±0
All	All	12765	12540	12540	-

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	106/145 (73%)	102±1 (96±1%)	4±1 (3±1%)	0±0 (0±0%)	58	87
All	All	1590/2175 (73%)	1534 (96%)	55 (3%)	1 (0%)	58	87

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	82	ALA	1

6.3.2 Protein sidechains ⓘ

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	88/118 (75%)	84±1 (95±2%)	4±1 (5±2%)	34	79
All	All	1320/1770 (75%)	1257 (95%)	63 (5%)	34	79

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	63	THR	14
1	A	136	ARG	9
1	A	167	VAL	7
1	A	176	LYS	6
1	A	138	LYS	4
1	A	90	LYS	3
1	A	59	ARG	3
1	A	186	GLU	2
1	A	180	ASP	2
1	A	121	GLN	2
1	A	85	LYS	2
1	A	146	SER	1
1	A	191	ASP	1
1	A	148	ASN	1
1	A	61	THR	1
1	A	141	ASP	1
1	A	62	GLU	1
1	A	181	GLN	1
1	A	161	GLN	1
1	A	83	LEU	1

6.3.3 RNA ⓘ

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 1 ligands modelled in this entry, 1 is 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 82% for the well-defined parts and 79% for the entire structure.

7.1 Chemical shift list 1

File name: 5kqc_cs.cif

Chemical shift list name: 2Zn.bmrB

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	1571
Number of shifts mapped to atoms	1571
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	5

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
$^{13}\text{C}_\alpha$	139	0.28 ± 0.26	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	124	-0.24 ± 0.25	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	119	-0.12 ± 0.40	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 82%, i.e. 1091 atoms were assigned a chemical shift out of a possible 1329. 13 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	399/518 (77%)	199/206 (97%)	106/212 (50%)	94/100 (94%)
Sidechain	584/670 (87%)	364/394 (92%)	208/243 (86%)	12/33 (36%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	108/141 (77%)	70/75 (93%)	37/61 (61%)	1/5 (20%)
Overall	1091/1329 (82%)	633/675 (94%)	351/516 (68%)	107/138 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 79%, i.e. 1401 atoms were assigned a chemical shift out of a possible 1783. 15 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	516/711 (73%)	258/283 (91%)	139/290 (48%)	119/138 (86%)
Sidechain	732/870 (84%)	459/513 (89%)	259/314 (82%)	14/43 (33%)
Aromatic	153/202 (76%)	97/108 (90%)	54/86 (63%)	2/8 (25%)
Overall	1401/1783 (79%)	814/904 (90%)	452/690 (66%)	135/189 (71%)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	109	VAL	HB	-0.04	3.59 – 0.39	-6.3
1	A	162	ARG	HD3	1.56	4.36 – 1.86	-6.2
1	A	169	ASN	HB3	0.75	4.41 – 1.11	-6.1
1	A	80	ASP	HA	6.41	6.15 – 3.05	5.8
1	A	166	GLY	HA3	1.86	5.80 – 2.00	-5.4

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:

