



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 02:56 PM BST

PDB ID : 1IBI
Title : QUAIL CYSTEINE AND GLYCINE-RICH PROTEIN, NMR, 15 MINIMIZED MODEL STRUCTURES
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Deposited on : 2001-03-28

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

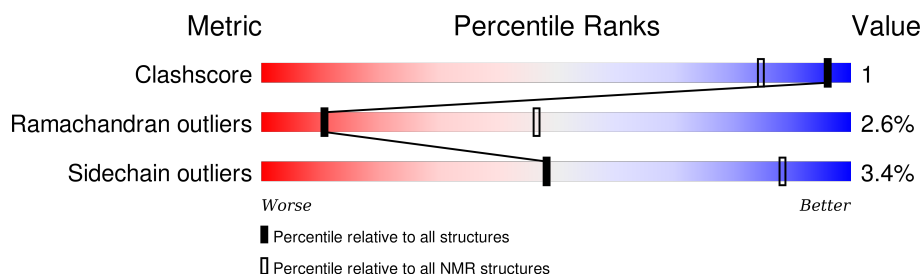
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 83%.

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	113	<div> <div style="width: 50%; background-color: green;"></div> <div style="width: 48%; background-color: grey;"></div> </div>

2 Ensemble composition and analysis

This entry contains 15 models. Model 7 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:118-A:175 (58)	0.59	7

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 4 single-model clusters were found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 882 atoms, of which 434 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called CYSTEINE-RICH PROTEIN 2.

Mol	Chain	Residues	Atoms							Trace
1	A	59	Total	C	H	N	O	S		0
			880	275	434	79	85	7		

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

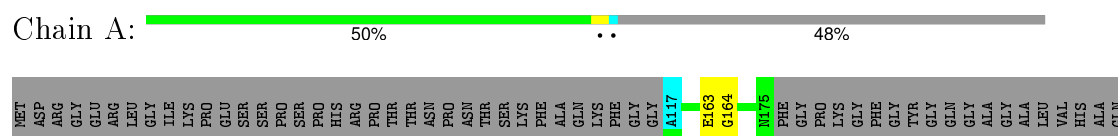
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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: CYSTEINE-RICH PROTEIN 2

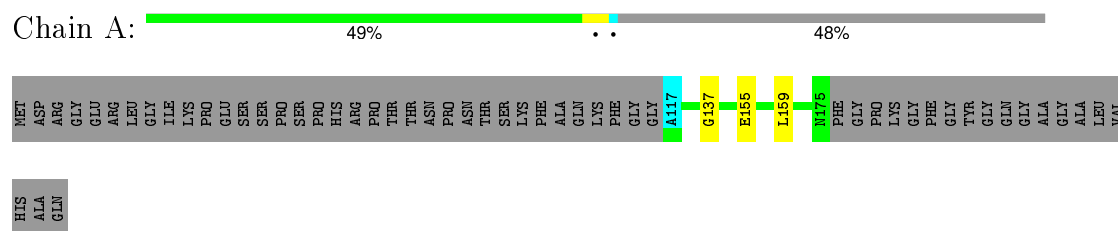


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

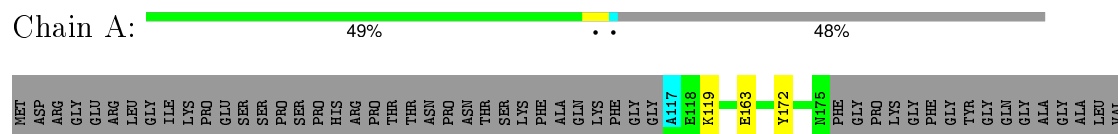
4.2.1 Score per residue for model 1

- Molecule 1: CYSTEINE-RICH PROTEIN 2



4.2.2 Score per residue for model 2

- Molecule 1: CYSTEINE-RICH PROTEIN 2



HIS
ALA
GLN

4.2.3 Score per residue for model 3

- Molecule 1: CYSTEINE-RICH PROTEIN 2

Chain A:  50% 48%

MET ASP ARG GLY GLU ARG LEU LEU GLY ILE LYS LYS PRO GLU SER SER PRO PRO HIS ARG ARG PRO THR THR ASN ASN THR LYS LYS PHE PHE GLY GLY A117 R122 K149 N175 PHE GLY PRO LYS LYS PHE GLY TYR GLY GLN GLY ALA LEU VAL HIS ALA

GLN

4.2.4 Score per residue for model 4

- Molecule 1: CYSTEINE-RICH PROTEIN 2

Chain A:  49% 48%

MET ASP ARG GLY GLU ARG LEU LEU GLY ILE LYS LYS PRO GLU SER SER PRO PRO HIS ARG ARG PRO THR THR ASN ASN THR LYS LYS PHE PHE GLY GLY A117 K132 C171 Y172 N175 PHE GLY PRO LYS LYS PHE GLY TYR GLY GLN GLY ALA LEU VAL HIS

ALA
GLN

4.2.5 Score per residue for model 5

- Molecule 1: CYSTEINE-RICH PROTEIN 2

Chain A:  50% 48%

MET ASP ARG GLY GLU ARG LEU LEU GLY ILE LYS LYS PRO GLU SER SER PRO PRO HIS ARG ARG PRO THR THR ASN ASN THR LYS LYS PHE PHE GLN LYS PHE GLY GLY A117 L159 N175 PHE GLY PRO LYS GLY PHE GLY TYR GLY GLN GLY ALA LEU VAL HIS GLN

4.2.6 Score per residue for model 6

- Molecule 1: CYSTEINE-RICH PROTEIN 2

Chain A:  46% 5% 48%

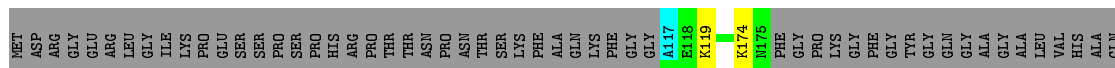
MET ASP ARG GLY GLU ARG LEU LEU GLY ILE LYS LYS PRO GLU SER SER PRO PRO HIS ARG ARG PRO THR THR ASN ASN THR LYS LYS PHE PHE GLN LYS PHE GLY GLY A117 E118 K119 K132 G137 K149 L159 C168 N175 PHE GLY PRO LYS LYS PHE GLY TYR GLY GLN GLY ALA LEU VAL HIS GLN

GLY
ALA
GLY
ALA
LEU
VAL
HIS
ALA
GLN

4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: CYSTEINE-RICH PROTEIN 2

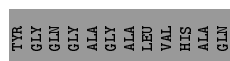
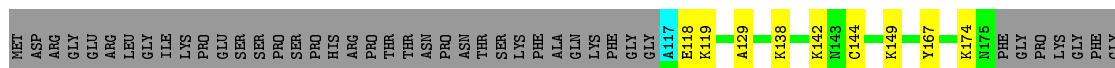
Chain A:  50% 48%



4.2.8 Score per residue for model 8

- Molecule 1: CYSTEINE-RICH PROTEIN 2

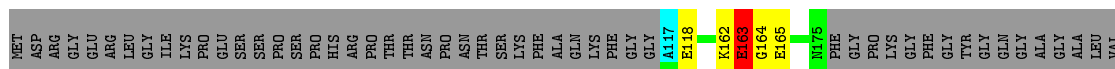
Chain A:  43% 8% 48%



4.2.9 Score per residue for model 9

- Molecule 1: CYSTEINE-RICH PROTEIN 2

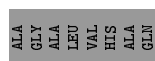
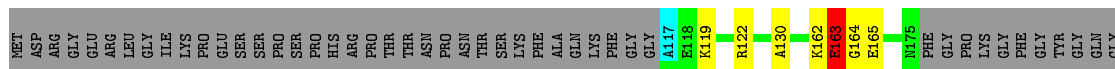
Chain A:  47% 48%



4.2.10 Score per residue for model 10

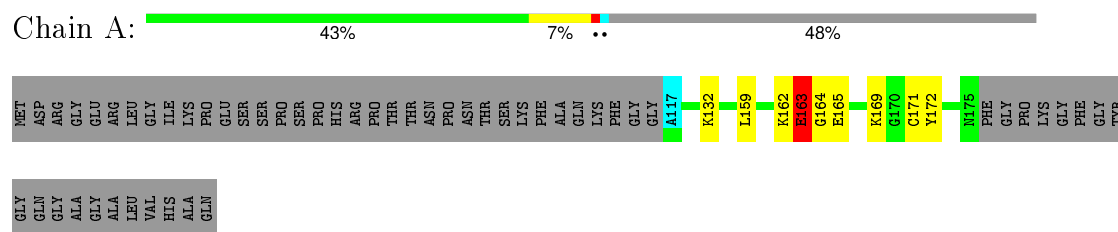
- Molecule 1: CYSTEINE-RICH PROTEIN 2

Chain A:  45% 5% 48%



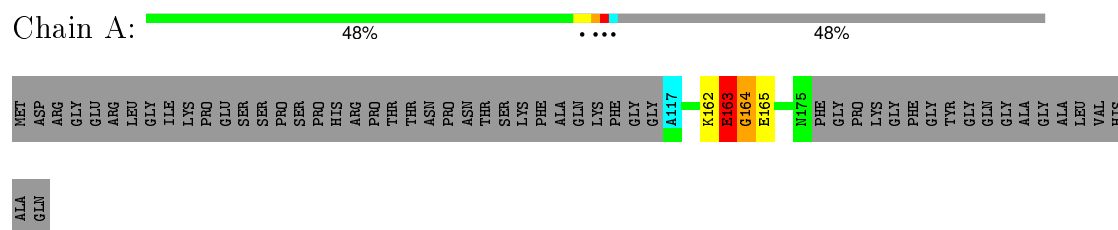
4.2.11 Score per residue for model 11

- Molecule 1: CYSTEINE-RICH PROTEIN 2



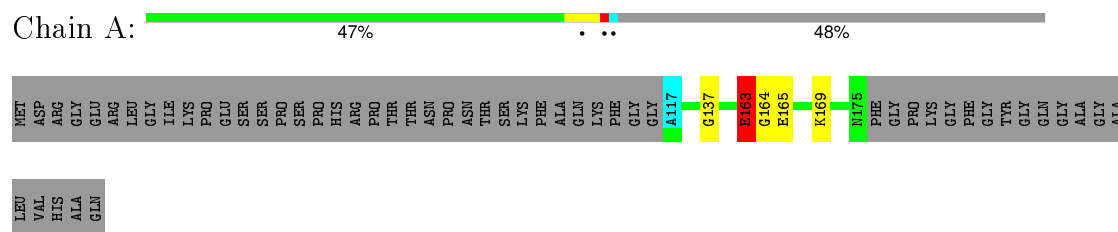
4.2.12 Score per residue for model 12

- Molecule 1: CYSTEINE-RICH PROTEIN 2



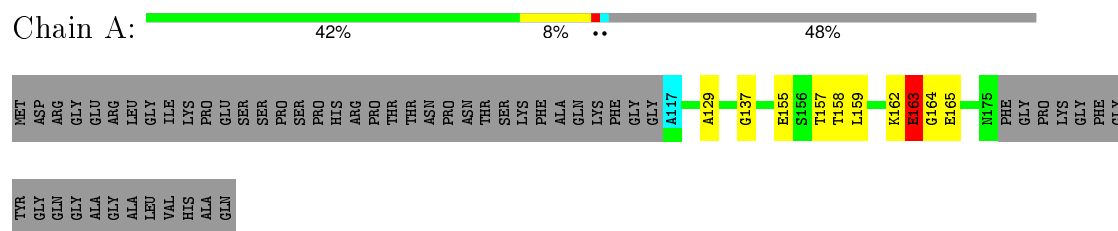
4.2.13 Score per residue for model 13

- Molecule 1: CYSTEINE-RICH PROTEIN 2



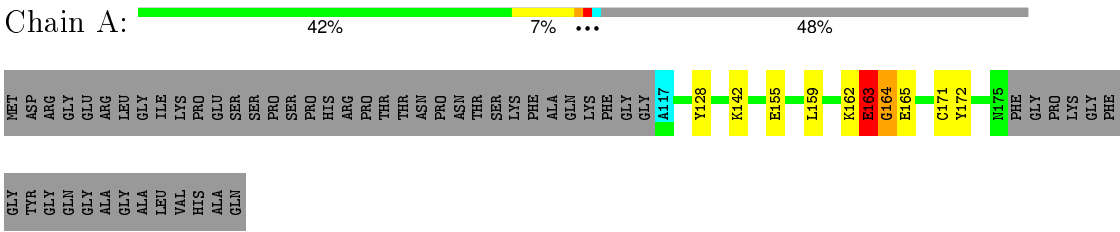
4.2.14 Score per residue for model 14

- Molecule 1: CYSTEINE-RICH PROTEIN 2



4.2.15 Score per residue for model 15

● Molecule 1: CYSTEINE-RICH PROTEIN 2



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 15 were deposited, based on the following criterion: *structures with the least restraint violations, structures with the lowest energy*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	structure solution	1.0
X-PLOR	refinement	3.851

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 5065
Number of chemical shift lists	1
Total number of shifts	623
Number of shifts mapped to atoms	623
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	83%

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	0.93±0.02	0±0/448 (0.0±0.1%)	1.07±0.10	3±2/596 (0.4±0.4%)
All	All	0.93	2/6720 (0.0%)	1.08	39/8940 (0.4%)

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	0.5±0.5
All	All	0	7

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	164	GLY	CA-C	5.08	1.59	1.51	15	2

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	172	TYR	CB-CG-CD2	-7.72	116.37	121.00	11	4
1	A	163	GLU	N-CA-CB	7.72	124.50	110.60	11	7
1	A	172	TYR	CB-CG-CD1	7.08	125.25	121.00	11	4
1	A	163	GLU	O-C-N	-6.53	112.09	123.20	13	7
1	A	163	GLU	C-N-CA	-5.43	110.90	122.30	15	7
1	A	167	TYR	CB-CG-CD2	-5.36	117.78	121.00	8	1
1	A	162	LYS	C-N-CA	-5.25	108.58	121.70	11	6
1	A	163	GLU	CA-C-N	5.09	126.38	116.20	13	3

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	163	GLU	Mainchain	7

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	441	429	430	1±1
2	A	2	0	0	0±0
All	All	6645	6435	6445	16

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:171:CYS:HG	2:A:196:ZN:ZN	0.93	0.63	4	3
1:A:144:CYS:HG	2:A:195:ZN:ZN	0.86	0.68	8	1
1:A:168:CYS:HG	2:A:196:ZN:ZN	0.81	0.54	6	1
1:A:159:LEU:HD23	1:A:159:LEU:H	0.46	1.70	5	2
1:A:163:GLU:O	1:A:165:GLU:N	0.44	2.51	13	7
1:A:159:LEU:H	1:A:159:LEU:HD23	0.43	1.74	11	1
1:A:163:GLU:C	1:A:165:GLU:H	0.40	2.20	12	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	57/113 (50%)	45±2 (79±3%)	11±2 (19±4%)	1±1 (3±3%)	11	47
All	All	855/1695 (50%)	672 (79%)	161 (19%)	22 (3%)	11	47

All 10 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	164	GLY	7
1	A	137	GLY	4
1	A	129	ALA	2
1	A	118	GLU	2
1	A	155	GLU	2
1	A	163	GLU	1
1	A	158	THR	1
1	A	130	ALA	1
1	A	159	LEU	1
1	A	157	THR	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	47/87 (54%)	45±1 (97±3%)	2±1 (3±3%)	48	88
All	All	705/1305 (54%)	681 (97%)	24 (3%)	48	88

All 11 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	119	LYS	5
1	A	132	LYS	3
1	A	149	LYS	3
1	A	174	LYS	2
1	A	122	ARG	2
1	A	159	LEU	2
1	A	169	LYS	2
1	A	142	LYS	2

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Mol	Chain	Res	Type	Models (Total)
1	A	138	LYS	1
1	A	155	GLU	1
1	A	128	TYR	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 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

The completeness of assignment taking into account all chemical shift lists is 83% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5065

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	623
Number of shifts mapped to atoms	623
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	59	-0.32 ± 0.20	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	49	0.13 ± 0.29	None needed (< 0.5 ppm)
$^{13}\text{C}'$	56	0.04 ± 0.24	None needed (< 0.5 ppm)
^{15}N	55	-1.03 ± 0.29	Should be applied

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 83%, i.e. 564 atoms were assigned a chemical shift out of a possible 683. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	271/288 (94%)	107/115 (93%)	111/116 (96%)	53/57 (93%)
Sidechain	252/343 (73%)	156/205 (76%)	96/121 (79%)	0/17 (0%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	41/52 (79%)	24/27 (89%)	16/23 (70%)	1/2 (50%)
Overall	564/683 (83%)	287/347 (83%)	223/260 (86%)	54/76 (71%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 564 atoms were assigned a chemical shift out of a possible 690. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	271/293 (92%)	107/117 (91%)	111/118 (94%)	53/58 (91%)
Sidechain	252/345 (73%)	156/206 (76%)	96/122 (79%)	0/17 (0%)
Aromatic	41/52 (79%)	24/27 (89%)	16/23 (70%)	1/2 (50%)
Overall	564/690 (82%)	287/350 (82%)	223/263 (85%)	54/77 (70%)

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	121	SER	HB3	1.62	5.25 – 2.45	-8.0
1	A	166	ILE	HD11	-0.77	2.13 – -0.77	-5.0
1	A	166	ILE	HD13	-0.77	2.13 – -0.77	-5.0
1	A	166	ILE	HD12	-0.77	2.13 – -0.77	-5.0

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:

