



wwPDB NMR Structure Validation Summary Report ⓘ

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PDB ID : 7SWJ
Title : KirBac1.1 mutant - I131C
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Deposited on : 2021-11-19

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

<https://www.wwpdb.org/validation/2017/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:

MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

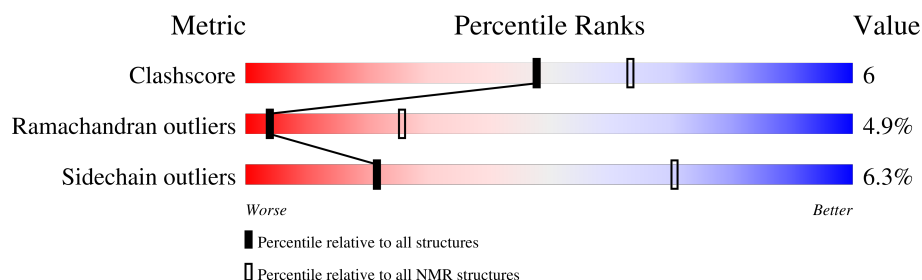
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 10%.

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	333	
1	B	333	
1	C	333	
1	D	333	

2 Ensemble composition and analysis

This entry contains 10 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:3-A:6, A:23-A:31, A:44-A:153, A:161-A:281, B:3-B:6, B:23-B:31, B:44-B:153, B:161-B:281, C:3-C:6, C:23-C:31, C:44-C:153, C:161-C:281, D:3-D:6, D:23-D:31, D:44-D:153, D:161-D:281 (976)	0.30	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 2 clusters and 5 single-model clusters were found.

Cluster number	Models
1	1, 9, 10
2	3, 4
Single-model clusters	2; 5; 6; 7; 8

3 Entry composition

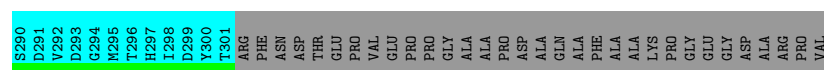
There is only 1 type of molecule in this entry. The entry contains 18860 atoms, of which 9332 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Inward rectifier potassium channel.

Mol	Chain	Residues	Atoms						Trace
1	A	301	Total	C	H	N	O	S	0
			4715	1524	2333	425	415	18	
1	B	301	Total	C	H	N	O	S	0
			4715	1524	2333	425	415	18	
1	C	301	Total	C	H	N	O	S	0
			4715	1524	2333	425	415	18	
1	D	301	Total	C	H	N	O	S	0
			4715	1524	2333	425	415	18	

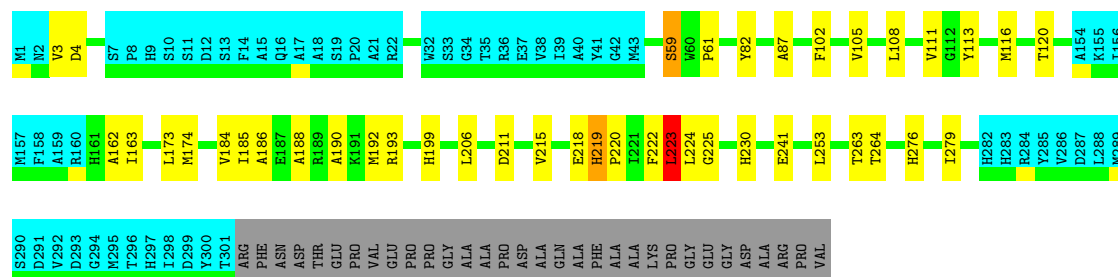
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	CYS	ILE	engineered mutation	UNP P83698
B	131	CYS	ILE	engineered mutation	UNP P83698
C	131	CYS	ILE	engineered mutation	UNP P83698
D	131	CYS	ILE	engineered mutation	UNP P83698



• Molecule 1: Inward rectifier potassium channel

Chain D: 61% 12% 17% 10%

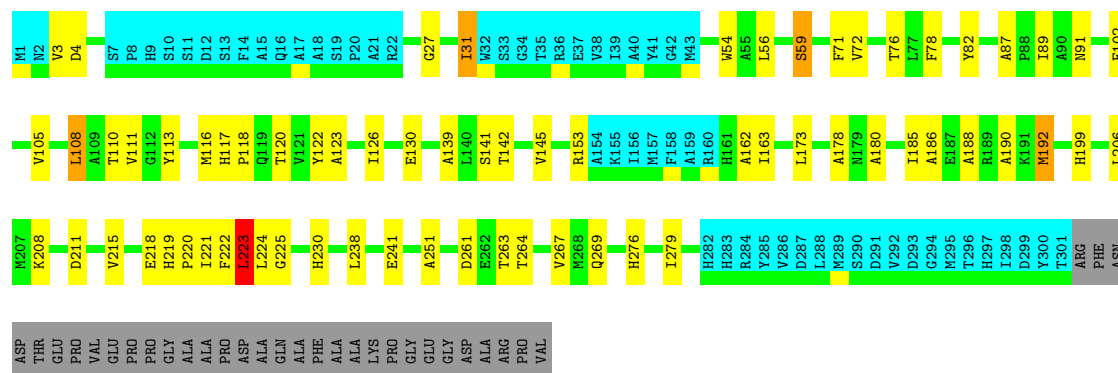


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

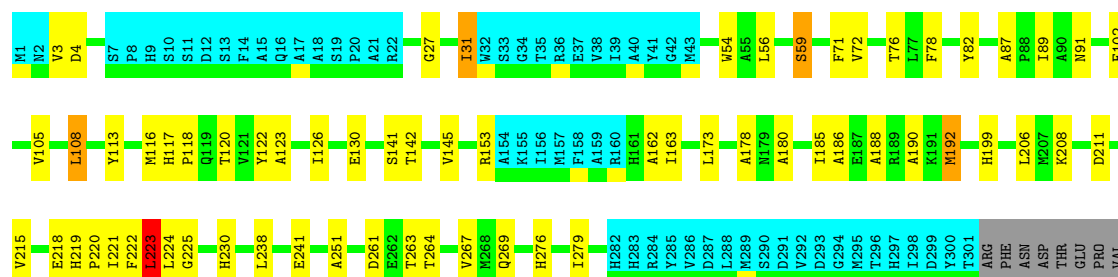
• Molecule 1: Inward rectifier potassium channel

Chain A: 53% 19% 17% 10%



• Molecule 1: Inward rectifier potassium channel

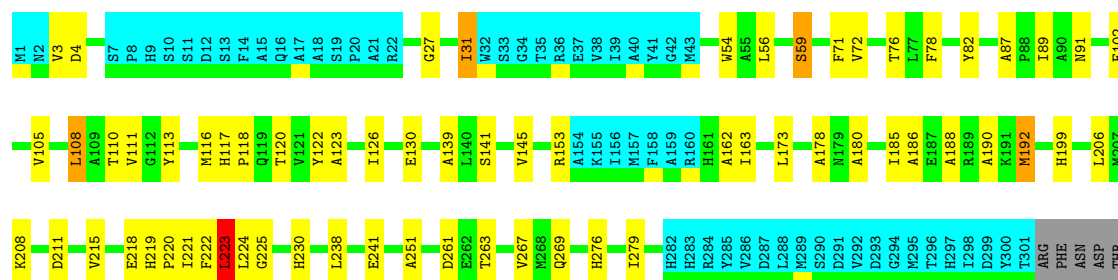
Chain B: 54% 18% 17% 10%



GLU
PRO
PRO
GLY
ALA
ALA
PRO
ASP
ALA
ALA
GLN
ALA
PHE
ALA
ALA
LYS
GLY
GLY
GLY
ASP
ALA
ALA
ARG
PRO
VAL

- Molecule 1: Inward rectifier potassium channel

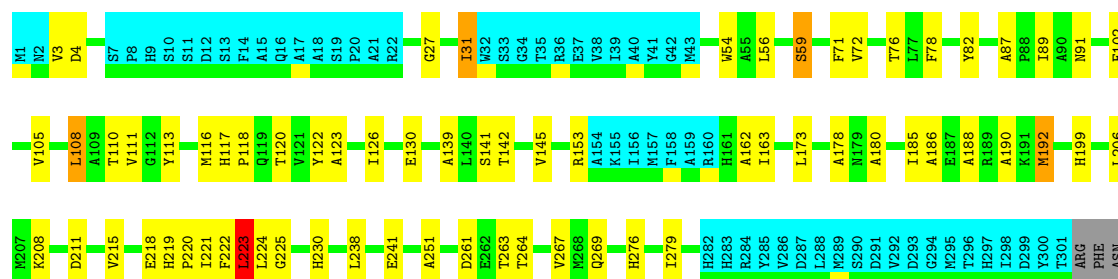
Chain C: 53% 18% 17% 10%



GLU
PRO
VAL
GLU
PRO
PRO
GLY
ALA
ALA
ALA
PRO
ASP
ALA
ALA
GLN
PHE
ALA
LYS
PRO
GLY
GLY
ASP
ALA
ARG
PRO
VAL

- Molecule 1: Inward rectifier potassium channel

Chain D: 53% 19% 17% 10%



ASP
THR
GLU
PRO
PRO
VAL
GLU
PRO
PRO
GLY
ALA
ALA
ALA
PRO
ASP
ALA
ALA
GLN
PHE
ALA
ALA
LYS
PRO
GLY
GLY
GLY
ASP
ALA
ARG
PRO
VAL

5 Refinement protocol and experimental data overview

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

Of the 800 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
X-PLOR NIH	refinement	3.2.9
X-PLOR NIH	structure calculation	3.2.9

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	2
Total number of shifts	1583
Number of shifts mapped to atoms	1583
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	10%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

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	0.98±0.01	0±0/1991 (0.0± 0.0%)	1.03±0.01	0±0/2704 (0.0± 0.0%)
1	B	0.98±0.01	0±0/1991 (0.0± 0.0%)	1.03±0.01	0±0/2704 (0.0± 0.0%)
1	C	0.98±0.01	0±0/1991 (0.0± 0.0%)	1.03±0.01	0±0/2704 (0.0± 0.0%)
1	D	0.98±0.01	0±0/1991 (0.0± 0.0%)	1.03±0.01	0±0/2704 (0.0± 0.0%)
All	All	0.98	0/79640 (0.0%)	1.03	4/108160 (0.0%)

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	220	PRO	N-CA-C	5.05	125.22	112.10	7	1
1	B	220	PRO	N-CA-C	5.05	125.22	112.10	7	1
1	C	220	PRO	N-CA-C	5.05	125.22	112.10	7	1
1	D	220	PRO	N-CA-C	5.05	125.22	112.10	7	1

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	1935	1917	1918	27±6
1	B	1935	1917	1918	27±5
1	C	1935	1917	1918	27±6

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	D	1935	1917	1918	27±5
All	All	77400	76680	76720	974

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 6.

5 of 614 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:219:HIS:CD2	1:A:223:LEU:HD13	0.82	2.10	8	1
1:D:219:HIS:CD2	1:D:223:LEU:HD13	0.81	2.10	8	1
1:C:219:HIS:CD2	1:C:223:LEU:HD13	0.80	2.10	8	1
1:B:219:HIS:CD2	1:B:223:LEU:HD13	0.80	2.10	8	1
1:C:162:ALA:HB1	1:C:173:LEU:HD21	0.80	1.53	9	4

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	244/333 (73%)	210±2 (86±1%)	22±3 (9±1%)	12±2 (5±1%)	4	26
1	B	244/333 (73%)	210±2 (86±1%)	22±3 (9±1%)	12±2 (5±1%)	4	26
1	C	244/333 (73%)	210±2 (86±1%)	22±3 (9±1%)	12±2 (5±1%)	4	26
1	D	244/333 (73%)	210±2 (86±1%)	22±3 (9±1%)	12±2 (5±1%)	4	26
All	All	9760/13320 (73%)	8419 (86%)	861 (9%)	480 (5%)	4	26

5 of 116 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	59	SER	10
1	A	116	MET	10
1	A	223	LEU	10
1	A	225	GLY	10
1	B	59	SER	10

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	200/269 (74%)	188±3 (94±1%)	12±3 (6±1%)	21	70
1	B	200/269 (74%)	187±3 (94±1%)	13±3 (6±1%)	21	70
1	C	200/269 (74%)	188±3 (94±1%)	12±3 (6±1%)	21	70
1	D	200/269 (74%)	188±3 (94±1%)	12±3 (6±1%)	21	70
All	All	8000/10760 (74%)	7499 (94%)	501 (6%)	21	70

5 of 216 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	59	SER	7
1	A	223	LEU	7
1	B	59	SER	7
1	B	223	LEU	7
1	C	59	SER	7

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 10% for the well-defined parts and 10% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1566
Number of shifts mapped to atoms	1566
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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
$^{13}\text{C}_\alpha$	300	-0.39 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	278	0.22 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}'$	294	-0.27 ± 0.12	None needed (< 0.5 ppm)
^{15}N	300	0.09 ± 0.15	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 10%, i.e. 1229 atoms were assigned a chemical shift out of a possible 12200. 38 out of 168 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	714/4768 (15%)	0/1896 (0%)	484/1952 (25%)	230/920 (25%)
Sidechain	507/6164 (8%)	0/3632 (0%)	507/2228 (23%)	0/304 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	8/1268 (1%)	0/684 (0%)	8/528 (2%)	0/56 (0%)
Overall	1229/12200 (10%)	0/6212 (0%)	999/4708 (21%)	230/1280 (18%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

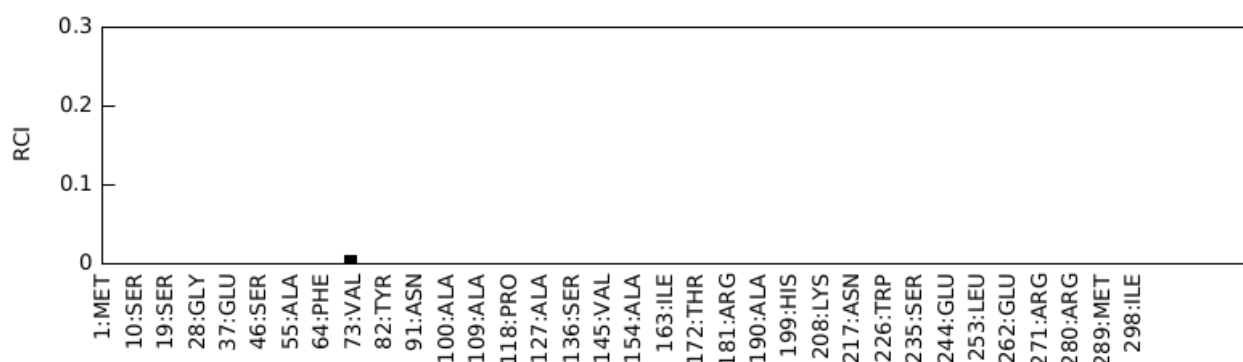
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	14	PHE	CD2	140.31	137.34 – 125.84	7.6
1	A	14	PHE	CD1	140.31	137.63 – 125.43	7.2

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: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	17
Number of shifts mapped to atoms	17
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

7.2.2 Chemical shift referencing [i](#)

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

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 0%, i.e. 17 atoms were assigned a chemical shift out of a possible 12200. 2 out of 168 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	9/4768 (0%)	0/1896 (0%)	6/1952 (0%)	3/920 (0%)
Sidechain	7/6164 (0%)	0/3632 (0%)	7/2228 (0%)	0/304 (0%)
Aromatic	1/1268 (0%)	0/684 (0%)	1/528 (0%)	0/56 (0%)
Overall	17/12200 (0%)	0/6212 (0%)	14/4708 (0%)	3/1280 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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:

