Full wwPDB NMR Structure Validation Report (i)

May 28, 2020 – 11:48 pm BST

PDB ID	:	2MMA
Title	:	NMR-based docking model of GrxS14-BolA2 apo-heterodimer from Arabidopsis thaliana
Authors	:	Roret, T.; Tsan, P.; Couturier, J.; Rouhier, N.; Didierjean, C.
Deposited on	:	2014-03-13

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

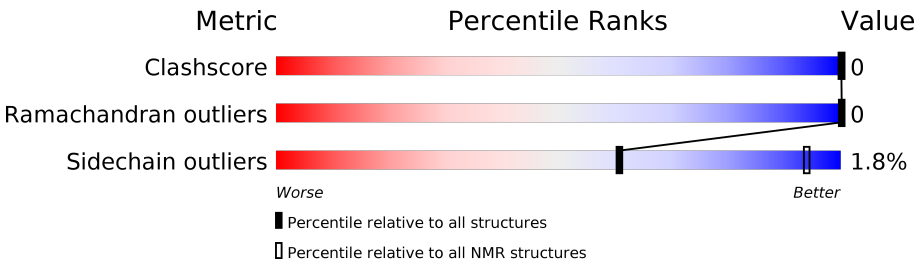
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 15%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	109	96%
2	B	92	80% 7% 13%

2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2978 atoms, of which 1492 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Monothiol glutaredoxin-S14, chloroplastic.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	107	1701	548	847	134	165	7	0

- Molecule 2 is a protein called BolA2.

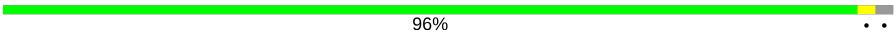
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	80	1277	397	645	110	122	3	0

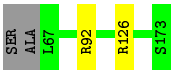
4 Residue-property plots (i)

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: Monothiol glutaredoxin-S14, chloroplastic

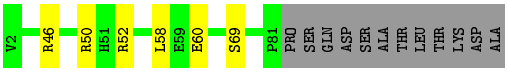
Chain A:





- Molecule 2: BolA2

Chain B:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics, energy minimization.*

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *all calculated structures submitted.*

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

Software name	Classification	Version
GRAMM-X Protein-Protein Docking Web Server	structure solution	1.2.0
YASARA Energy Minimization Server	geometry optimization	
YASARA Energy Minimization Server	refinement	
GRAMM-X Protein-Protein Docking Web Server	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	4
Total number of shifts	756
Number of shifts mapped to atoms	756
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	15%

No validations of the models with respect to experimental NMR restraints is performed at this time.

COVALENT-GEOMETRY INFOmissingINFO

5.1 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
All	All	1486	1492	1492	-

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.

5.2 Torsion angles (i)

5.2.1 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	105/109 (96%)	105 (100%)	0 (0%)	0 (0%)	100	100
2	B	78/92 (85%)	77 (99%)	1 (1%)	0 (0%)	100	100
All	All	183/201 (91%)	182 (99%)	1 (1%)	0 (0%)	100	100

There are no Ramachandran outliers.

5.2.2 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	97/98 (99%)	97 (100%)	0 (0%)	100	100
2	B	71/81 (88%)	68 (96%)	3 (4%)	33	82
All	All	168/179 (94%)	165 (98%)	3 (2%)	61	94

All 3 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
2	B	60	GLU
2	B	58	LEU
2	B	69	SER

5.2.3 RNA (i)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

5.5 Ligand geometry (i)

There are no ligands in this entry.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 15% for the well-defined parts and 15% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *BOLA2-GRXS14*

6.1.1 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	176
Number of shifts mapped to atoms	176
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

6.1.2 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	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	88	0.76 ± 0.39	None needed (imprecise)

6.1.3 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 7%, i.e. 154 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	154/919 (17%)	77/366 (21%)	0/374 (0%)	77/179 (43%)
Sidechain	0/1263 (0%)	0/740 (0%)	0/474 (0%)	0/49 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/151 (0%)	0/82 (0%)	0/64 (0%)	0/5 (0%)
Overall	154/2333 (7%)	77/1188 (6%)	0/912 (0%)	77/233 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 154 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	154/919 (17%)	77/366 (21%)	0/374 (0%)	77/179 (43%)
Sidechain	0/1263 (0%)	0/740 (0%)	0/474 (0%)	0/49 (0%)
Aromatic	0/151 (0%)	0/82 (0%)	0/64 (0%)	0/5 (0%)
Overall	154/2333 (7%)	77/1188 (6%)	0/912 (0%)	77/233 (33%)

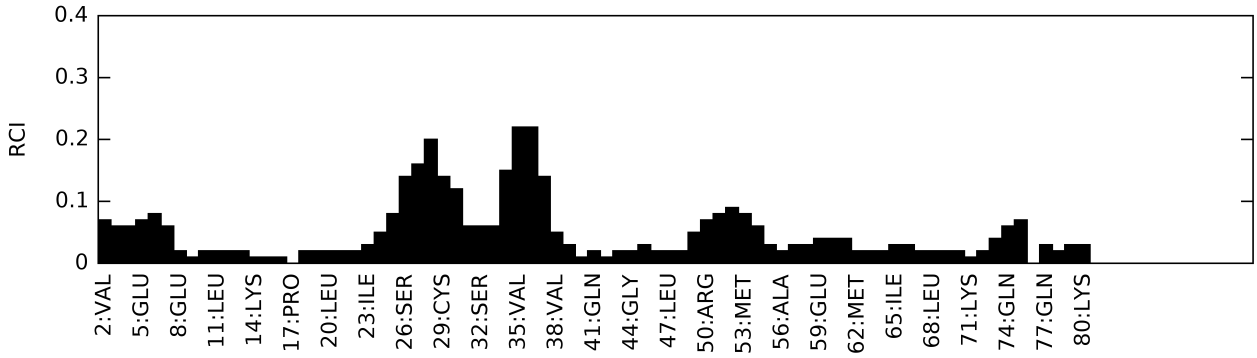
6.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.1.5 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 B:



6.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: *BOLA2_assigned_chem_shifts*

6.2.1 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	176
Number of shifts mapped to atoms	176
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

6.2.2 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	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	88	0.80 ± 0.50	None needed (imprecise)

6.2.3 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 7%, i.e. 154 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	154/919 (17%)	77/366 (21%)	0/374 (0%)	77/179 (43%)
Sidechain	0/1263 (0%)	0/740 (0%)	0/474 (0%)	0/49 (0%)
Aromatic	0/151 (0%)	0/82 (0%)	0/64 (0%)	0/5 (0%)
Overall	154/2333 (7%)	77/1188 (6%)	0/912 (0%)	77/233 (33%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 7%, i.e. 154 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	154/919 (17%)	77/366 (21%)	0/374 (0%)	77/179 (43%)

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	Total	^{1}H	^{13}C	^{15}N
Sidechain	0/1263 (0%)	0/740 (0%)	0/474 (0%)	0/49 (0%)
Aromatic	0/151 (0%)	0/82 (0%)	0/64 (0%)	0/5 (0%)
Overall	154/2333 (7%)	77/1188 (6%)	0/912 (0%)	77/233 (33%)

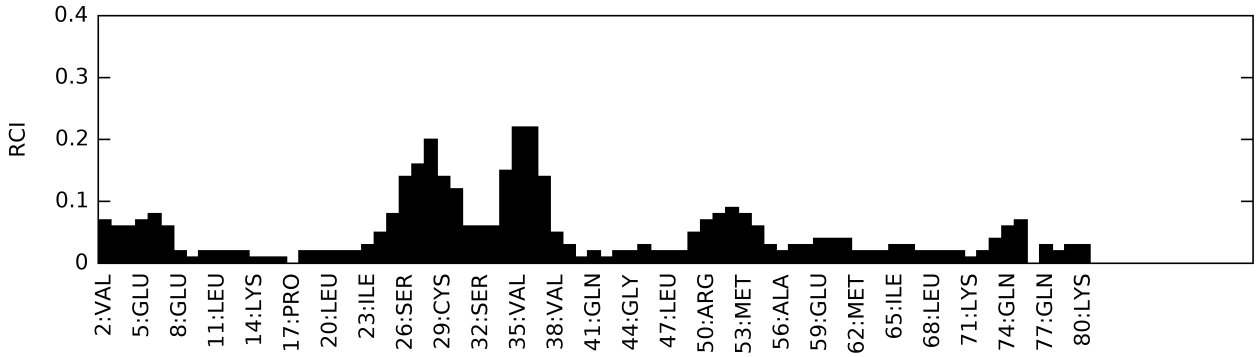
6.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.2.5 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 B:



6.3 Chemical shift list 3

File name: input_cs.cif

Chemical shift list name: *GRXS14-BOLA2*

6.3.1 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	202
Number of shifts mapped to atoms	202

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

6.3.2 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	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	101	0.93 ± 0.47	None needed (imprecise)

6.3.3 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 8%, i.e. 198 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	198/919 (22%)	99/366 (27%)	0/374 (0%)	99/179 (55%)
Sidechain	0/1263 (0%)	0/740 (0%)	0/474 (0%)	0/49 (0%)
Aromatic	0/151 (0%)	0/82 (0%)	0/64 (0%)	0/5 (0%)
Overall	198/2333 (8%)	99/1188 (8%)	0/912 (0%)	99/233 (42%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 198 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
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Aromatic	0/151 (0%)	0/82 (0%)	0/64 (0%)	0/5 (0%)
Overall	198/2333 (8%)	99/1188 (8%)	0/912 (0%)	99/233 (42%)

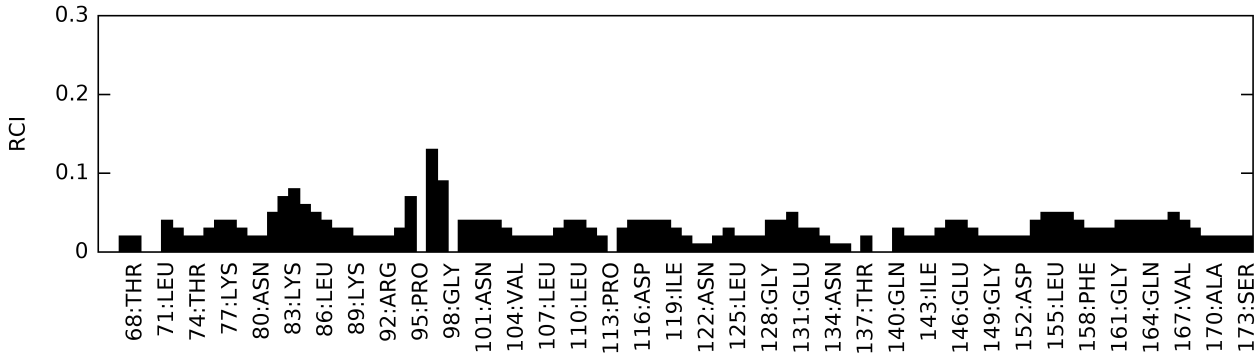
6.3.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.3.5 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:



6.4 Chemical shift list 4

File name: input_cs.cif

Chemical shift list name: *GRXS14_assigned_chem_shifts*

6.4.1 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	202
Number of shifts mapped to atoms	202
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

6.4.2 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
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	101	0.96 ± 0.28	Should be applied

6.4.3 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 8%, i.e. 198 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

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The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 8%, i.e. 198 atoms were assigned a chemical shift out of a possible 2333. 0 out of 35 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

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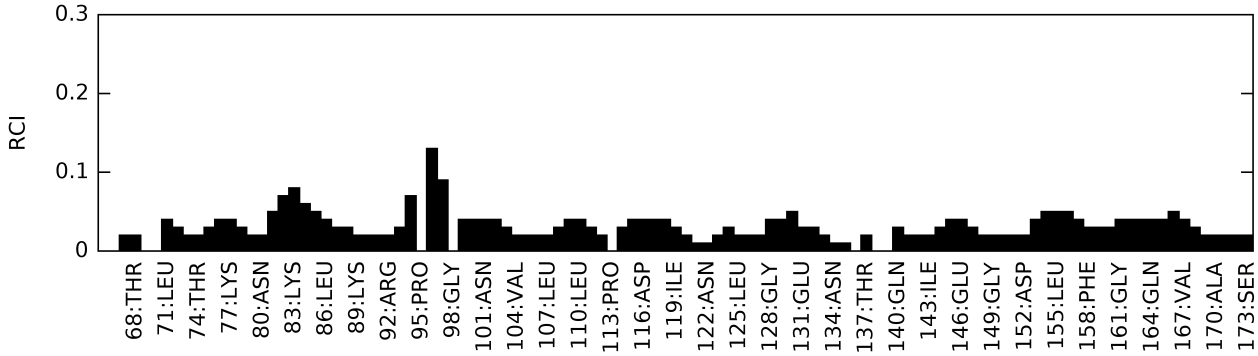
6.4.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

6.4.5 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: