



wwPDB NMR Structure Validation Summary Report ⓘ

May 29, 2020 – 09:42 am BST

PDB ID : 6BA6
Title : Solution structure of Rap1b/talin complex
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Deposited on : 2017-10-12

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:

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

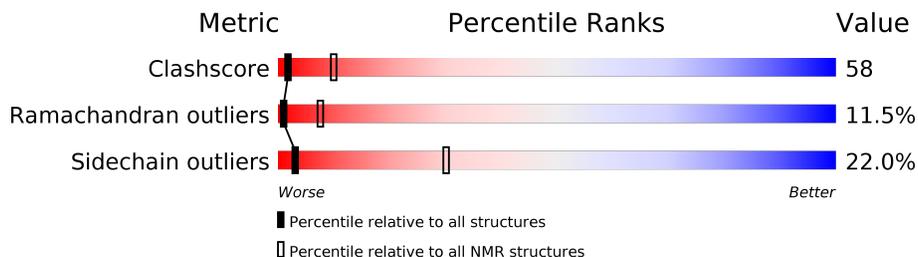
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	93	 16% 59% 14% .. 8%
2	B	168	 15% 68% 15% ..

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 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:2-A:86, B:1-B:167 (252)	0.42	2

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	1, 2, 6, 9, 10, 12, 18
2	3, 4, 5, 11, 15, 16, 20
3	7, 17
Single-model clusters	8; 13; 14; 19

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4045 atoms, of which 2022 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Talin-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	86	1384	437	696	117	127	7	0

There are 7 discrepancies between the modelled and reference sequences:

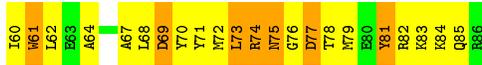
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P26039
A	-5	ALA	-	expression tag	UNP P26039
A	-4	MET	-	expression tag	UNP P26039
A	-3	ASP	-	expression tag	UNP P26039
A	-2	PRO	-	expression tag	UNP P26039
A	-1	GLU	-	expression tag	UNP P26039
A	0	PHE	-	expression tag	UNP P26039

- Molecule 2 is a protein called Ras-related protein Rap-1b.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	167	2661	836	1326	228	263	8	0

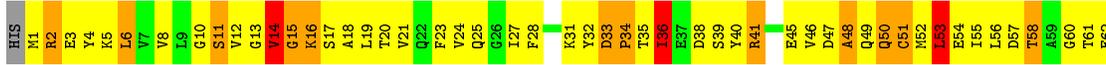
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	HIS	-	expression tag	UNP P61224
B	12	VAL	GLY	engineered mutation	UNP P61224



- Molecule 2: Ras-related protein Rap-1b

Chain B: 23% 58% 16%



5 Refinement protocol and experimental data overview (i)

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *20 structures for lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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	3
Total number of shifts	4180
Number of shifts mapped to atoms	4180
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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
1	A	680	687	687	83±8
2	B	1335	1326	1328	164±13
All	All	40300	40260	40300	4653

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 58.

5 of 1490 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:B:161:LEU:H	2:B:161:LEU:HD23	0.95	1.16	6	7
2:B:161:LEU:HD23	2:B:161:LEU:H	0.92	1.24	13	2
2:B:20:THR:O	2:B:22:GLN:N	0.91	2.04	16	3
1:A:3:ALA:HB1	1:A:19:PHE:O	0.86	1.71	17	15
1:A:35:ARG:NE	1:A:36:ILE:H	0.85	1.70	13	1

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	84/93 (90%)	51±3 (61±3%)	17±3 (20±4%)	16±2 (19±3%)	0	2
2	B	165/168 (98%)	129±3 (78±2%)	24±3 (14±2%)	12±1 (7±1%)	2	15
All	All	4980/5220 (95%)	3602 (72%)	804 (16%)	574 (12%)	1	7

5 of 60 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	14	VAL	20
2	B	124	ARG	20
1	A	56	PRO	20
2	B	48	ALA	20
1	A	53	ASP	20

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	73/79 (92%)	60±3 (82±4%)	13±3 (18±4%)	4	37
2	B	148/149 (99%)	113±4 (76±3%)	35±4 (24±3%)	2	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4420/4560 (97%)	3447 (78%)	973 (22%)	3 30

5 of 146 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)
2	B	83	SER	20
1	A	26	TYR	20
2	B	36	ILE	20
1	A	83	LYS	20
1	A	61	TRP	20

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 74% for the well-defined parts and 74% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

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	1695
Number of shifts mapped to atoms	1695
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	164	-0.10 \pm 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	153	0.55 \pm 0.11	Should be applied
$^{13}\text{C}'$	156	0.32 \pm 0.11	None needed (< 0.5 ppm)
^{15}N	159	0.35 \pm 0.35	None needed (< 0.5 ppm)

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 49%, i.e. 1546 atoms were assigned a chemical shift out of a possible 3164. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	798/1246 (64%)	321/497 (65%)	318/504 (63%)	159/245 (65%)
Sidechain	748/1724 (43%)	443/1006 (44%)	305/628 (49%)	0/90 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/194 (0%)	0/102 (0%)	0/90 (0%)	0/2 (0%)
Overall	1546/3164 (49%)	764/1605 (48%)	623/1222 (51%)	159/337 (47%)

6.1.4 Statistically unusual chemical shifts [i](#)

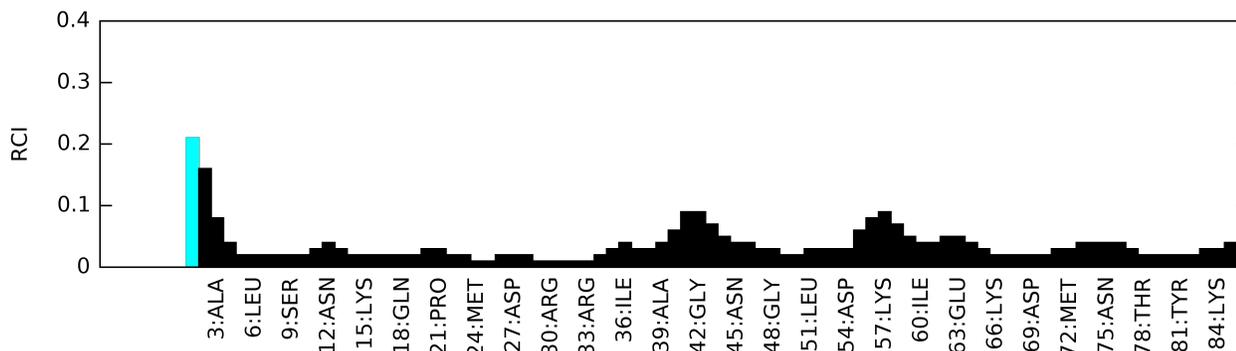
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	134	LEU	HG	-0.28	3.16 – -0.14	-5.4

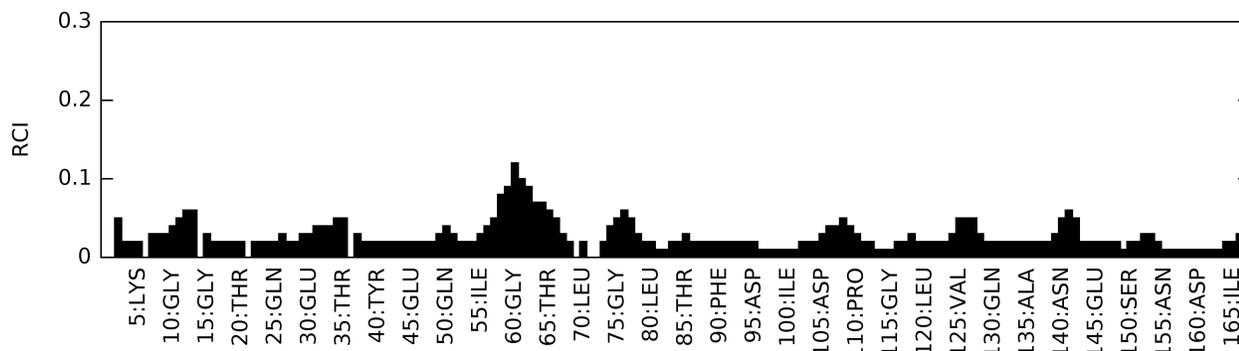
6.1.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:



6.2 Chemical shift list 2

File name: input_cs.cif

Chemical shift list name: rap1b-bound-nc-noesy.str_assigned_chem_shift_list_1

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	1601
Number of shifts mapped to atoms	1601
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

6.2.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	166	0.05 ± 0.13	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	156	0.52 ± 0.19	Should be applied
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	159	0.31 ± 0.27	None needed (< 0.5 ppm)

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 46%, i.e. 1446 atoms were assigned a chemical shift out of a possible 3164. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	648/1246 (52%)	324/497 (65%)	165/504 (33%)	159/245 (65%)
Sidechain	796/1724 (46%)	475/1006 (47%)	320/628 (51%)	1/90 (1%)
Aromatic	2/194 (1%)	1/102 (1%)	0/90 (0%)	1/2 (50%)
Overall	1446/3164 (46%)	800/1605 (50%)	485/1222 (40%)	161/337 (48%)

6.2.4 Statistically unusual chemical shifts [i](#)

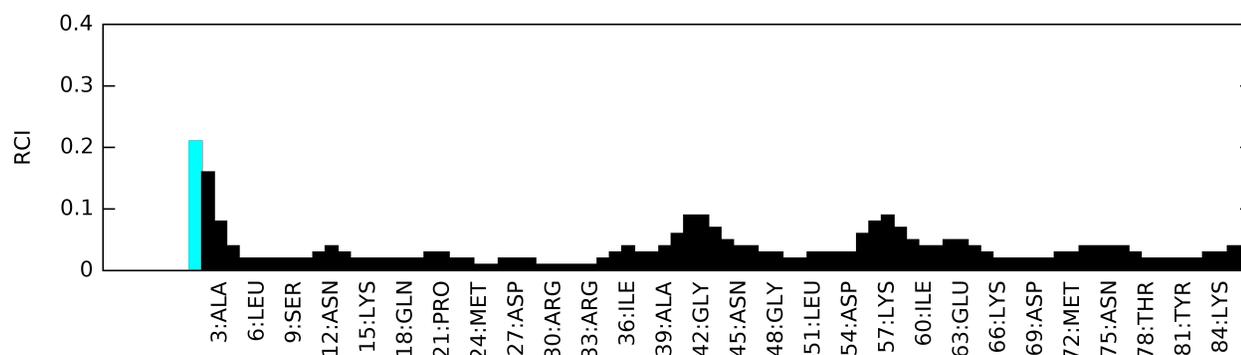
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
2	B	134	LEU	HG	-0.47	3.16 – -0.14	-6.0

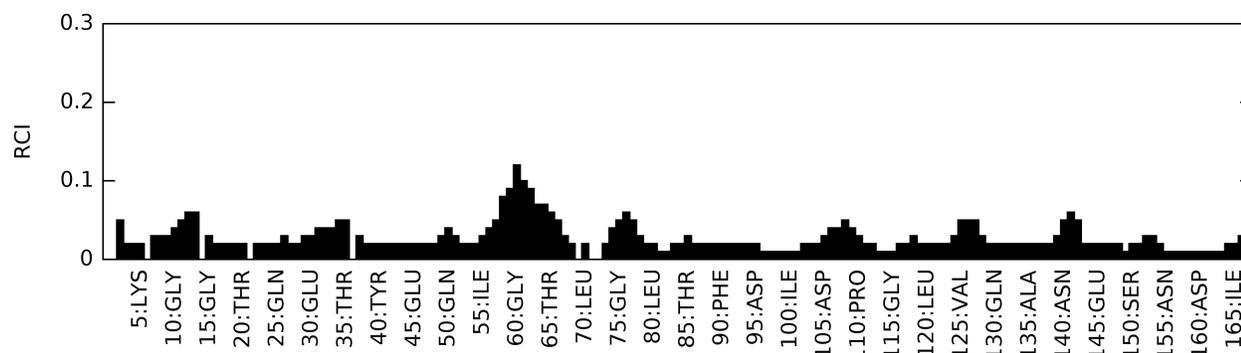
6.2.5 Random Coil Index (RCI) plots [i](#)

The images below report *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:



Random coil index (RCI) for chain B:



6.3 Chemical shift list 3

File name: input_cs.cif

Chemical shift list name: *talin-F0-bound-nc-noesy.str_assigned_chem_shift_list_1*

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	884
Number of shifts mapped to atoms	884
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

6.3.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	84	0.19 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	79	0.43 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	73	-0.15 ± 0.45	None needed (< 0.5 ppm)

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 26%, i.e. 808 atoms were assigned a chemical shift out of a possible 3164. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned

stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	313/1246 (25%)	157/497 (32%)	83/504 (16%)	73/245 (30%)
Sidechain	493/1724 (29%)	307/1006 (31%)	181/628 (29%)	5/90 (6%)
Aromatic	2/194 (1%)	1/102 (1%)	0/90 (0%)	1/2 (50%)
Overall	808/3164 (26%)	465/1605 (29%)	264/1222 (22%)	79/337 (23%)

6.3.4 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	65	GLY	N	130.83	129.07 – 90.27	5.5
1	A	66	LYS	HD3	0.44	2.75 – 0.45	-5.0

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:

