Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 09:33 AM EDT

PDB ID	:	2LV6
BMRB ID	:	18556
Title	:	The complex between Ca-Calmodulin and skeletal muscle myosin light chain kinase from combination of NMR and aqueous and contrast-matched SAXS data
Authors	:	Grishaev, A.V.; Anthis, N.J.; Clore, G.M.
Deposited on	:	2012-06-29

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

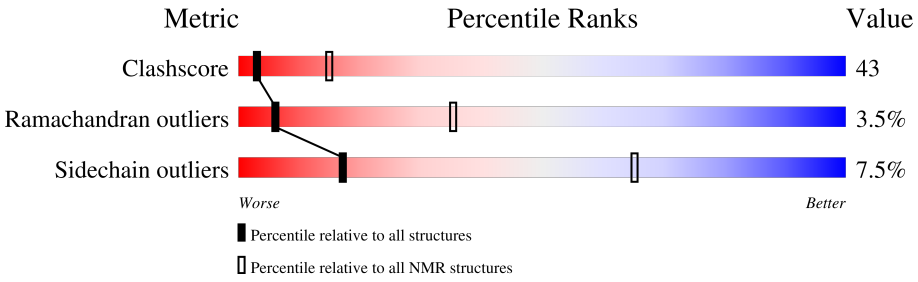
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION SCATTERING, SOLUTION NMR

The overall completeness of chemical shifts assignment is 12%.

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	148	76% 18% 6%
2	B	26	12% 54% 35%

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

There are 3 unique types of molecules in this entry. The entry contains 2700 atoms, of which 1323 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
1	A	148	Total	C	H	N	O	S	0
			2257	713	1094	187	254	9	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	99	PHE	TYR	SEE REMARK 999	UNP P62158
A	143	THR	GLN	SEE REMARK 999	UNP P62158

- Molecule 2 is a protein called Myosin light chain kinase 2, skeletal/cardiac muscle.

Mol	Chain	Residues	Atoms					Trace
2	B	26	Total	C	H	N	O	0
			439	134	229	43	33	

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

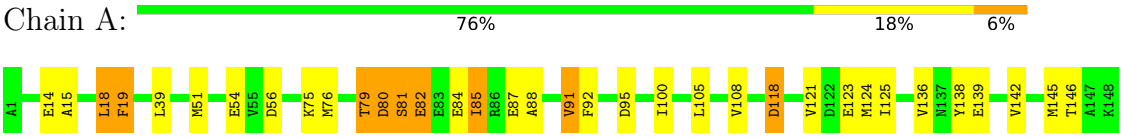
Mol	Chain	Residues	Atoms	
3	A	4	Total	Ca
			4	4

4 Residue-property plots (i)

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

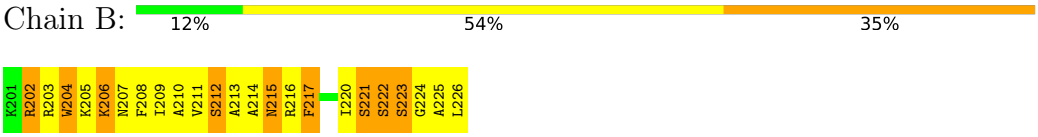
• Molecule 1: Calmodulin

Chain A:



• Molecule 2: Myosin light chain kinase 2, skeletal/cardiac muscle

Chain B:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *rigid-body optimization, simulated annealing.*

Of the 1 calculated structures, 1 were deposited, based on the following criterion: *structures with the least restraint violations.*

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

Software name	Classification	Version
Custom	structure solution	
CNS	refinement	1.0
Custom	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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	288
Number of shifts mapped to atoms	288
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0.55	1/1175 (0.1%)	0.85	3/1576 (0.2%)
2	B	0.94	0/213 (0.0%)	0.92	0/279 (0.0%)
All	All	0.62	1/1388 (0.1%)	0.86	3/1855 (0.2%)

All bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	19	PHE	CB-CG	-5.41	1.42	1.51

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	118	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	56	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	95	ASP	CB-CG-OD1	5.25	123.02	118.30

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts

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	1163	1094	1095	99
2	B	210	229	228	95

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Mol	Chain	Non-H	H(model)	H(added)	Clashes
All	All	1377	1323	1323	117

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 43.

All clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:18:LEU:HB3	2:B:210:ALA:CB	1.13	1.74
1:A:145:MET:SD	2:B:205:LYS:HA	1.04	1.93
1:A:18:LEU:HB3	2:B:210:ALA:HB2	0.94	1.35
1:A:145:MET:CE	2:B:208:PHE:CB	0.88	2.51
1:A:105:LEU:HD22	2:B:204:TRP:CH2	0.86	2.06
1:A:105:LEU:HD22	2:B:204:TRP:CZ2	0.84	2.07
1:A:105:LEU:HD13	2:B:204:TRP:CZ3	0.84	2.07
1:A:145:MET:HE1	2:B:204:TRP:O	0.84	1.71
1:A:85:ILE:HG23	2:B:208:PHE:CZ	0.84	2.08
1:A:105:LEU:HD21	1:A:124:MET:SD	0.80	2.16
2:B:208:PHE:O	2:B:211:VAL:HG22	0.79	1.76
1:A:145:MET:CE	2:B:208:PHE:HB3	0.78	2.08
1:A:18:LEU:CB	2:B:210:ALA:HB2	0.78	2.08
1:A:100:ILE:HD12	1:A:136:VAL:CG2	0.77	2.09
1:A:145:MET:SD	2:B:208:PHE:HB3	0.77	2.18
1:A:79:THR:HG22	1:A:80:ASP:OD1	0.76	1.81
1:A:19:PHE:CE2	2:B:210:ALA:O	0.74	2.39
1:A:138:TYR:O	1:A:142:VAL:HG13	0.74	1.82
1:A:105:LEU:HD13	2:B:204:TRP:CE3	0.74	2.16
1:A:19:PHE:HE2	2:B:213:ALA:HB3	0.72	1.43
1:A:18:LEU:CB	2:B:210:ALA:CB	0.72	2.62
1:A:123:GLU:HG3	2:B:202:ARG:HG2	0.69	1.65
1:A:19:PHE:CE2	2:B:213:ALA:HB3	0.69	2.22
1:A:15:ALA:HB2	2:B:209:ILE:CG2	0.68	2.18
1:A:139:GLU:O	1:A:142:VAL:HG22	0.67	1.90
1:A:87:GLU:OE1	2:B:215:ASN:ND2	0.66	2.28
1:A:145:MET:CE	2:B:208:PHE:HB2	0.66	2.18
1:A:145:MET:HE3	2:B:208:PHE:HB2	0.65	1.69
1:A:145:MET:HE3	2:B:208:PHE:CB	0.65	2.21
1:A:85:ILE:HG23	2:B:208:PHE:CE1	0.64	2.27
1:A:124:MET:HA	2:B:202:ARG:HB2	0.63	1.69
1:A:19:PHE:CZ	2:B:214:ALA:HB2	0.63	2.28
1:A:124:MET:CA	2:B:202:ARG:HB2	0.63	2.23
2:B:217:PHE:HA	2:B:220:ILE:HD12	0.63	1.70
1:A:51:MET:HE2	2:B:217:PHE:HB3	0.62	1.70

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:84:GLU:HG3	2:B:216:ARG:HB2	0.62	1.70
1:A:85:ILE:HA	2:B:208:PHE:CE1	0.62	2.28
1:A:100:ILE:HD12	1:A:136:VAL:HG21	0.61	1.73
1:A:84:GLU:CG	2:B:212:SER:O	0.60	2.49
1:A:39:LEU:HD21	2:B:211:VAL:CG1	0.60	2.26
2:B:208:PHE:CD2	2:B:209:ILE:N	0.60	2.69
1:A:145:MET:SD	2:B:208:PHE:CB	0.60	2.90
1:A:39:LEU:HD22	1:A:91:VAL:HG11	0.59	1.75
1:A:81:SER:O	1:A:82:GLU:CB	0.59	2.51
1:A:18:LEU:HB3	2:B:210:ALA:HB1	0.59	1.70
1:A:123:GLU:HG3	2:B:202:ARG:CG	0.57	2.28
1:A:145:MET:SD	2:B:205:LYS:CA	0.57	2.84
1:A:84:GLU:HG2	2:B:212:SER:CA	0.56	2.30
1:A:87:GLU:HB2	2:B:215:ASN:OD1	0.55	2.00
1:A:145:MET:CG	2:B:208:PHE:CD2	0.55	2.90
1:A:82:GLU:HA	1:A:85:ILE:HD12	0.54	1.77
1:A:18:LEU:HD13	2:B:207:ASN:HA	0.54	1.80
1:A:85:ILE:HA	2:B:208:PHE:HE1	0.54	1.61
1:A:15:ALA:HB2	2:B:209:ILE:HG21	0.52	1.82
1:A:15:ALA:CB	2:B:209:ILE:CG2	0.52	2.88
1:A:124:MET:HG2	2:B:202:ARG:HB2	0.52	1.80
1:A:145:MET:HE1	2:B:208:PHE:CB	0.52	2.34
1:A:118:ASP:O	1:A:121:VAL:CG2	0.52	2.57
1:A:19:PHE:CZ	2:B:210:ALA:O	0.51	2.63
1:A:145:MET:HG3	2:B:208:PHE:CD2	0.51	2.41
1:A:39:LEU:HD21	2:B:211:VAL:HG11	0.51	1.82
1:A:145:MET:HG3	2:B:208:PHE:CG	0.51	2.41
1:A:18:LEU:CD1	2:B:207:ASN:HA	0.50	2.37
1:A:91:VAL:CG2	1:A:92:PHE:N	0.49	2.76
1:A:88:ALA:HB3	2:B:208:PHE:CE1	0.49	2.42
2:B:220:ILE:O	2:B:222:SER:N	0.48	2.46
1:A:145:MET:HE1	2:B:208:PHE:HB3	0.48	1.85
1:A:105:LEU:O	1:A:108:VAL:CG2	0.48	2.62
2:B:207:ASN:O	2:B:211:VAL:HG13	0.48	2.07
2:B:208:PHE:O	2:B:211:VAL:CG2	0.48	2.58
1:A:88:ALA:CB	2:B:208:PHE:CD1	0.47	2.97
1:A:19:PHE:CE1	2:B:214:ALA:HB2	0.47	2.44
1:A:145:MET:SD	2:B:208:PHE:CD2	0.47	3.08
2:B:203:ARG:C	2:B:205:LYS:N	0.47	2.68
1:A:124:MET:HA	2:B:202:ARG:CB	0.46	2.39
1:A:14:GLU:HG2	2:B:206:LYS:HB3	0.46	1.87
1:A:87:GLU:O	1:A:91:VAL:HG13	0.46	2.11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)
2:B:203:ARG:C	2:B:205:LYS:H	0.46	2.13
2:B:205:LYS:O	2:B:209:ILE:HG13	0.46	2.10
1:A:18:LEU:HD22	2:B:210:ALA:HB3	0.46	1.87
1:A:100:ILE:HD12	1:A:136:VAL:HG22	0.45	1.85
1:A:136:VAL:CG2	1:A:136:VAL:O	0.45	2.64
2:B:222:SER:O	2:B:223:SER:O	0.45	2.34
1:A:142:VAL:O	1:A:146:THR:N	0.45	2.41
2:B:222:SER:O	2:B:223:SER:C	0.45	2.55
2:B:225:ALA:C	2:B:226:LEU:HD12	0.45	2.31
1:A:18:LEU:HD13	2:B:207:ASN:CA	0.44	2.43
1:A:88:ALA:O	1:A:91:VAL:HG22	0.44	2.12
2:B:205:LYS:HB3	2:B:209:ILE:HD11	0.44	1.89
1:A:118:ASP:O	1:A:121:VAL:HG23	0.44	2.12
1:A:125:ILE:HD13	2:B:204:TRP:CZ2	0.44	2.48
1:A:84:GLU:O	2:B:215:ASN:OD1	0.44	2.36
1:A:84:GLU:HG2	2:B:212:SER:HA	0.44	1.87
1:A:84:GLU:HA	2:B:215:ASN:OD1	0.44	2.12
1:A:85:ILE:CG2	2:B:208:PHE:CZ	0.44	2.95
1:A:124:MET:CG	2:B:202:ARG:HB2	0.43	2.43
1:A:105:LEU:O	1:A:108:VAL:HG22	0.43	2.13
2:B:221:SER:O	2:B:223:SER:N	0.43	2.51
1:A:145:MET:SD	2:B:208:PHE:CG	0.43	3.12
1:A:145:MET:O	1:A:146:THR:C	0.43	2.56
1:A:84:GLU:CD	2:B:212:SER:CB	0.42	2.87
2:B:205:LYS:O	2:B:206:LYS:C	0.42	2.57
1:A:14:GLU:HG2	2:B:206:LYS:CB	0.42	2.44
2:B:205:LYS:O	2:B:209:ILE:N	0.42	2.50
2:B:223:SER:C	2:B:225:ALA:H	0.42	2.19
1:A:88:ALA:CB	2:B:208:PHE:CE1	0.42	3.03
1:A:75:LYS:HD2	1:A:84:GLU:CD	0.41	2.35
1:A:84:GLU:CG	2:B:212:SER:OG	0.41	2.69
1:A:54:GLU:HB3	2:B:217:PHE:CE1	0.41	2.50
1:A:124:MET:HG2	2:B:202:ARG:CB	0.41	2.46
2:B:224:GLY:O	2:B:225:ALA:C	0.41	2.58
1:A:92:PHE:CD2	1:A:108:VAL:HG21	0.41	2.51
1:A:123:GLU:C	2:B:202:ARG:HG2	0.41	2.37
1:A:124:MET:HB3	2:B:204:TRP:NE1	0.40	2.30
1:A:14:GLU:HG2	2:B:206:LYS:CG	0.40	2.46
1:A:19:PHE:CZ	2:B:214:ALA:CB	0.40	3.01
1:A:145:MET:HE1	2:B:204:TRP:C	0.40	2.34

6.3 Torsion angles

6.3.1 Protein backbone

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	146/148 (99%)	141 (97%)	2 (1%)	3 (2%)	10 50
2	B	24/26 (92%)	17 (71%)	4 (17%)	3 (12%)	1 6
All	All	170/174 (98%)	158 (93%)	6 (4%)	6 (4%)	6 35

All 6 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	79	THR
1	A	80	ASP
1	A	82	GLU
2	B	221	SER
2	B	222	SER
2	B	223	SER

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	126/126 (100%)	121 (96%)	5 (4%)	35 83
2	B	21/21 (100%)	15 (71%)	6 (29%)	2 18
All	All	147/147 (100%)	136 (93%)	11 (7%)	17 65

All 11 residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	18	LEU

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Mol	Chain	Res	Type
1	A	76	MET
1	A	81	SER
1	A	85	ILE
1	A	91	VAL
2	B	202	ARG
2	B	204	TRP
2	B	206	LYS
2	B	212	SER
2	B	215	ASN
2	B	217	PHE

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 12% for the well-defined parts and 12% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

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	288
Number of shifts mapped to atoms	288
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

7.1.2 Chemical shift referencing

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	144	0.12 ± 0.40	None needed (< 0.5 ppm)

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 12%, i.e. 288 atoms were assigned a chemical shift out of a possible 2321. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	288/878 (33%)	144/358 (40%)	0/348 (0%)	144/172 (84%)
Sidechain	0/1304 (0%)	0/835 (0%)	0/416 (0%)	0/53 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/139 (0%)	0/69 (0%)	0/67 (0%)	0/3 (0%)
Overall	288/2321 (12%)	144/1262 (11%)	0/831 (0%)	144/228 (63%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 12%, i.e. 288 atoms were assigned a chemical shift out of a possible 2321. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	288/878 (33%)	144/358 (40%)	0/348 (0%)	144/172 (84%)
Sidechain	0/1304 (0%)	0/835 (0%)	0/416 (0%)	0/53 (0%)
Aromatic	0/139 (0%)	0/69 (0%)	0/67 (0%)	0/3 (0%)
Overall	288/2321 (12%)	144/1262 (11%)	0/831 (0%)	144/228 (63%)

7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: