Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 04:38 PM BST

PDB ID	:	1NWD
Title	:	Solution Structure of Ca2+/Calmodulin bound to the C-terminal Domain of Petunia Glutamate Decarboxylase
Authors	:	Yap, K.L.; Yuan, T.; Mal, T.K.; Vogel, H.J.; Ikura, M.
Deposited on	:	2003-02-06

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:

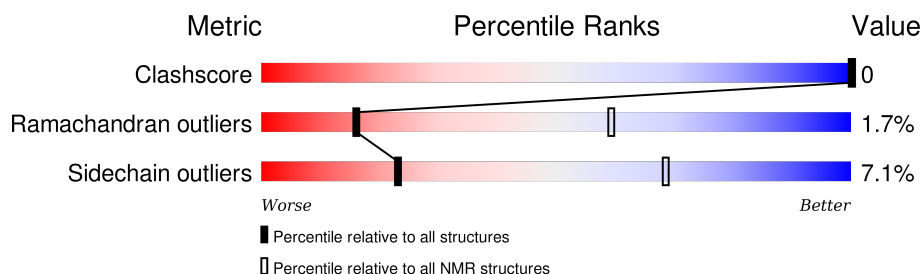|		
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
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 93%.

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	Percentile Ranks	Value
Clashscore		0
Ramachandran outliers		1.7%
Sidechain outliers		7.1%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all NMR structures

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	148	90% • 7%
2	B	28	71% • 25%
2	C	28	75% 25%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 12 is the overall representative, medoid model (most similar to other models). The authors have identified model 4 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:7-A:75, A:80-A:148, B:6-B:26, C:6-C:26 (180)	0.56	12

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 1 single-model cluster was found.

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

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3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3235 atoms, of which 1597 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	148	2263	714	1097	188	255	9	0

- Molecule 2 is a protein called Glutamate decarboxylase.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	28	484	149	250	40	44	1	0
2	C	28	Total	C	H	N	O	S	0
			484	149	250	40	44	1	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLY	-	CLONING ARTIFACT	UNP Q07346
B	2	SER	-	CLONING ARTIFACT	UNP Q07346
C	1	GLY	-	CLONING ARTIFACT	UNP Q07346
C	2	SER	-	CLONING ARTIFACT	UNP Q07346

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

Mol	Chain	Residues	Atoms	
			Total	Ca
3	A	4	4	4

# 4 Residue-property plots ⓘ

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.
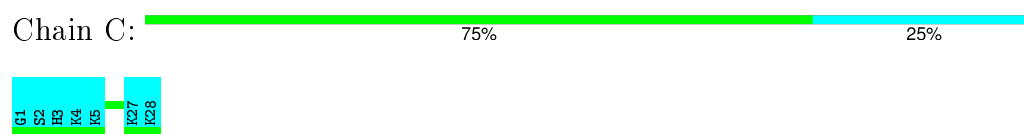
- Molecule 1: Calmodulin
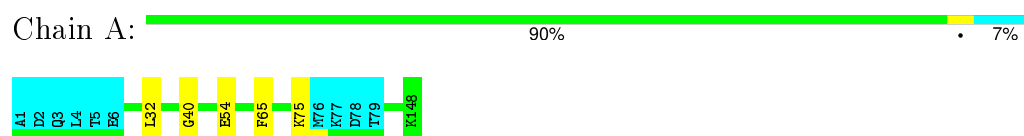
Chain A:

- Molecule 2: Glutamate decarboxylase

Chain B:

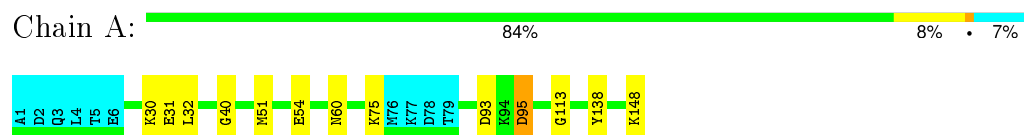- Molecule 2: Glutamate decarboxylase

Chain C:
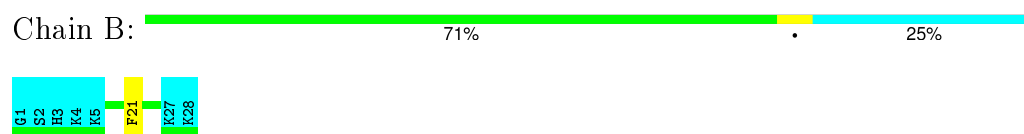
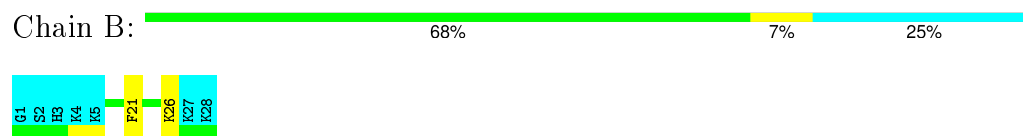## 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

- Molecule 1: Calmodulin

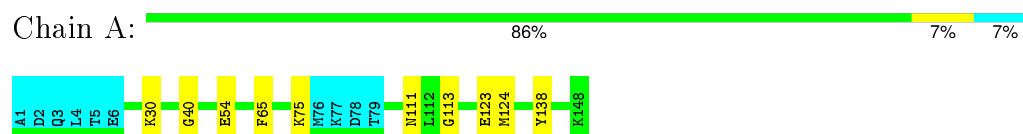Chain A:

• Molecule 2: Glutamate decarboxylase

Chain B:

• Molecule 2: Glutamate decarboxylase

Chain C:

4.2.2 Score per residue for model 2

• Molecule 1: Calmodulin

Chain A:

• Molecule 2: Glutamate decarboxylase

Chain B:

• Molecule 2: Glutamate decarboxylase

Chain C:
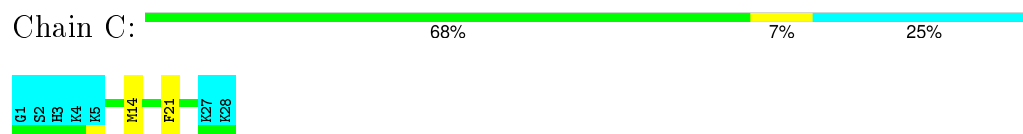
4.2.3 Score per residue for model 3

• Molecule 1: Calmodulin
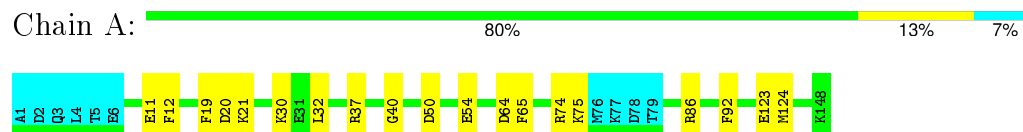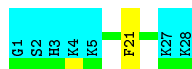
Chain A:

• Molecule 2: Glutamate decarboxylase

Chain B:

G1 S2 H3 K4 K5 F21 K27 K28

• Molecule 2: Glutamate decarboxylase

Chain C: 64% 11% 25%

G1 S2 H3 K4 K5 Q11 F21 K25 K26 K27 K28

4.2.4 Score per residue for model 4

• Molecule 1: Calmodulin
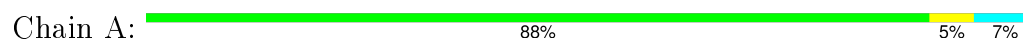
Chain A: 88% 5% 7%

A1 D2 Q3 L4 T5 E6 K21 R37 G40 F65 K75 M76 K77 D78 T79 E87 R106 G113 K148

• Molecule 2: Glutamate decarboxylase

Chain B: 71% . 25%

G1 S2 H3 K4 K5 F21 K27 K28

• Molecule 2: Glutamate decarboxylase

Chain C: 68% 7% 25%

G1 S2 H3 K4 K5 K20 F21 K27 K28

4.2.5 Score per residue for model 5

• Molecule 1: Calmodulin
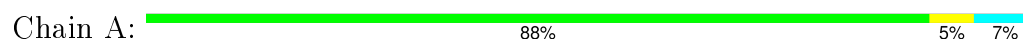
Chain A: 88% 5% 7%

A1 D2 Q3 L4 T5 E6 E14 R37 G40 R74 K75 M76 K77 D78 T79 D95 G113 K148

• Molecule 2: Glutamate decarboxylase

Chain B: 71% . 25%

G1 S2 H3 K4 K5 F21 K27 K28

• Molecule 2: Glutamate decarboxylase

Chain C:

75%   25%

G1 S2 H3 K4 K5   K27 K28
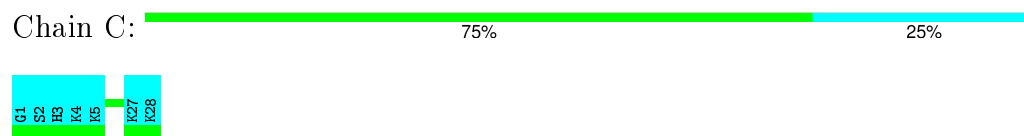
4.2.6 Score per residue for model 6

• Molecule 1: Calmodulin
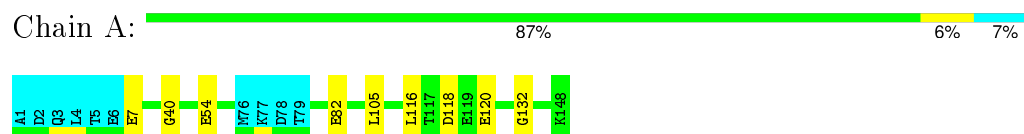
Chain A:

87%   6%   7%

A1 D2 Q3 L4 T5 E6 E7   G40   E54   M76 K77 D78 T79   E82   L105   L116 T117 D118 E119 E120   G132   K148

• Molecule 2: Glutamate decarboxylase

Chain B:

68%   7%   25%

G1 S2 H3 K4 K5   W18   F21   K27 K28

• Molecule 2: Glutamate decarboxylase

Chain C:

68%   7%   25%

G1 S2 H3 K4 K5   Q11   K26 K27 K28
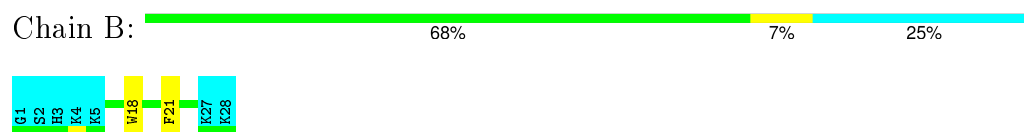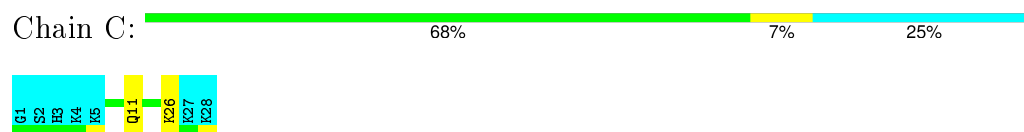
4.2.7 Score per residue for model 7

• Molecule 1: Calmodulin
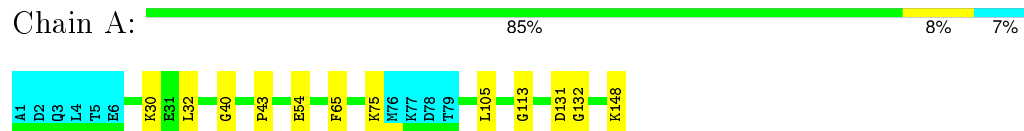
Chain A:

85%   8%   7%

A1 D2 Q3 L4 T5 E6   K30 E31 L32   G40 P43   E54   F65   K75 M76 K77 D78 T79   L105   G113   D131 G132   K148

• Molecule 2: Glutamate decarboxylase

Chain B:

64%   11%   25%

G1 S2 H3 K4 K5   I15   K20 F21   K27 K28

• Molecule 2: Glutamate decarboxylase

Chain C:

68%   7%   25%

G1 S2 H3 K4 K5 E13 K26 K27 K28

4.2.8 Score per residue for model 8

- Molecule 1: Calmodulin

Chain A:

86% 6% • 7%

A1 D2 Q3 L4 T5 E6 L32 R37 G40 E54 F65 M76 K77 D78 T79 Y99 L105 G113 N137 E140 K148

- Molecule 2: Glutamate decarboxylase

Chain B:

68% • • 25%

G1 S2 H3 K4 K5 F21 V22 E23 K27 K28

- Molecule 2: Glutamate decarboxylase

Chain C:

68% 7% 25%

G1 S2 H3 K4 K5 M14 K20 K27 K28

4.2.9 Score per residue for model 9

- Molecule 1: Calmodulin

Chain A:

86% 7% 7%

A1 D2 Q3 L4 T5 E6 E14 R37 G40 E54 K75 M76 K77 D78 T79 R86 R90 K94 G113 E114 K115 Y138 K148

- Molecule 2: Glutamate decarboxylase

Chain B:

61% 14% 25%

G1 S2 H3 K4 K5 I15 K20 F21 K26 K27 K28

- Molecule 2: Glutamate decarboxylase

Chain C:

71% • 25%

G1 S2 H3 K4 K5 F21 K27 K28

4.2.10 Score per residue for model 10

• Molecule 1: Calmodulin

• Molecule 2: Glutamate decarboxylase

• Molecule 2: Glutamate decarboxylase

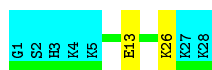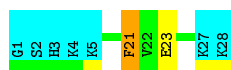### 4.2.11 Score per residue for model 11

• Molecule 1: Calmodulin

• Molecule 2: Glutamate decarboxylase
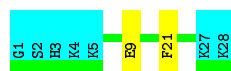
• Molecule 2: Glutamate decarboxylase
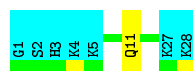
4.2.12 Score per residue for model 12 (medoid)
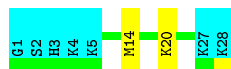
• Molecule 1: Calmodulin

Chain A: 84%   9%   7%

A1 D2 Q3 L4 T5 E6 K21 L32 G40 E54 N60 F65 M71 K75 M76 K77 D78 T79 F89 D95 L105 E123 K148

- Molecule 2: Glutamate decarboxylase

Chain B: 64%   11%   25%

G1 S2 H3 K4 K5 I15 F21 K25 K26 K28

- Molecule 2: Glutamate decarboxylase

Chain C: 64%   11%   25%

G1 S2 H3 K4 K5 E9 K20 F21 K27 K28

4.2.13   Score per residue for model 13

- Molecule 1: Calmodulin

Chain A: 87%   6%   7%

A1 D2 Q3 L4 T5 E6 F19 L32 G40 M76 K77 D78 T79 D80 S81 E84 R90 K94 K115 Y138 K148

- Molecule 2: Glutamate decarboxylase

Chain B: 71%   .   25%

G1 S2 H3 K4 K5 F21 K27 K28

- Molecule 2: Glutamate decarboxylase

Chain C: 68%   7%   25%

G1 S2 H3 K4 K5 K19 K20 F21 K27 K28
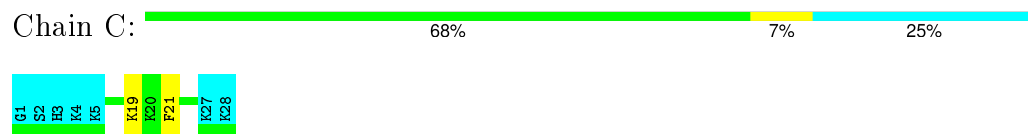
4.2.14   Score per residue for model 14

- Molecule 1: Calmodulin
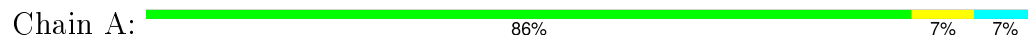
Chain A: 86%   7%   7%

A1 D2 Q3 L4 T5 E6 L32 G40 E54 R74 K75 M76 K77 D78 T79 F89 L105 R106 H107 Q143 K148

• Molecule 2: Glutamate decarboxylase

Chain B: 68% 7% 25%

G1 S2 H3 K4 K5 M14 F21 K27 K28

• Molecule 2: Glutamate decarboxylase

Chain C: 71% • 25%

G1 S2 H3 K4 K5 K26 K27 K28

4.2.15 Score per residue for model 15

• Molecule 1: Calmodulin
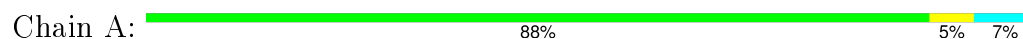
Chain A: 88% 5% 7%

A1 D2 Q3 L4 T5 E6 L32 R37 G40 D50 F65 M76 K77 D78 T79 L112 E119 D133 K148

• Molecule 2: Glutamate decarboxylase

Chain B: 68% 7% 25%

G1 S2 H3 K4 K5 F21 K26 K27 K28

• Molecule 2: Glutamate decarboxylase

Chain C: 68% 7% 25%

G1 S2 H3 K4 K5 M14 K19 K27 K28

4.2.16 Score per residue for model 16

• Molecule 1: Calmodulin
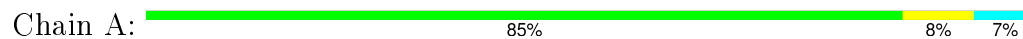
Chain A: 85% 8% 7%

A1 D2 Q3 L4 T5 E6 L18 F19 L32 G40 Q41 E54 N60 K75 M76 K77 D78 T79 R90 G113 E114 K115 K148
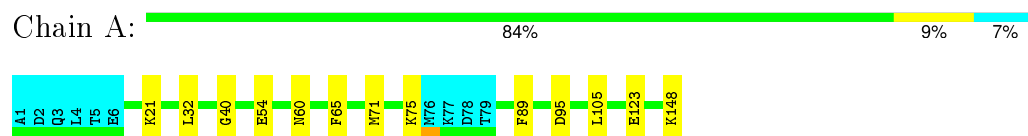
• Molecule 2: Glutamate decarboxylase

Chain B:

• Molecule 2: Glutamate decarboxylase

Chain C:
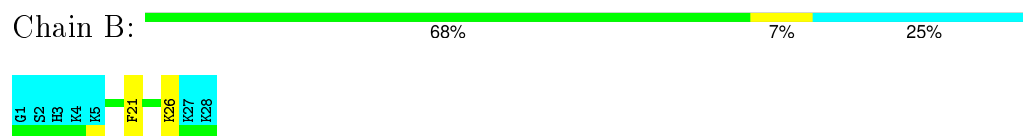
4.2.17 Score per residue for model 17

• Molecule 1: Calmodulin
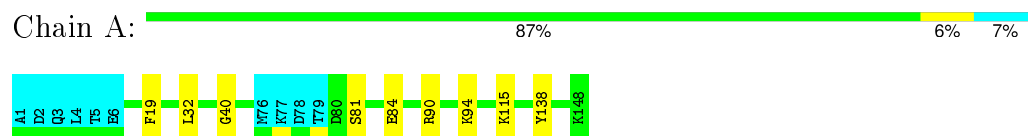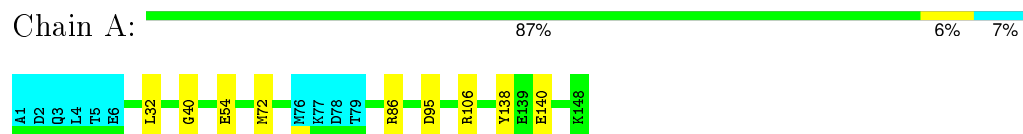
Chain A:

• Molecule 2: Glutamate decarboxylase
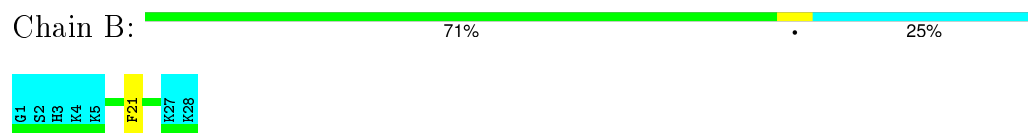
Chain B:

• Molecule 2: Glutamate decarboxylase

Chain C:
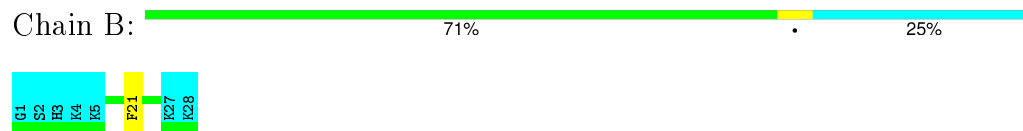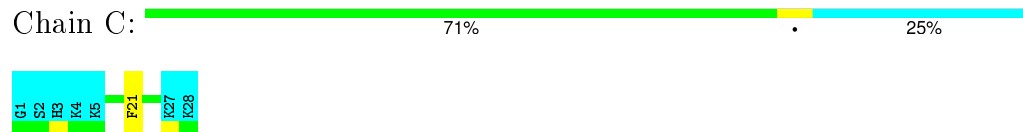
4.2.18 Score per residue for model 18

• Molecule 1: Calmodulin
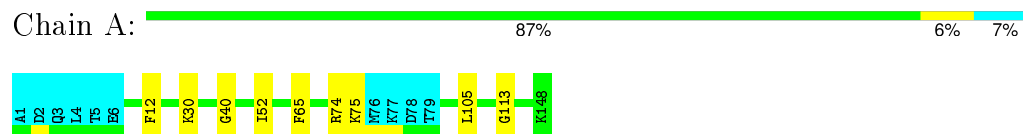
Chain A:

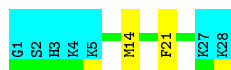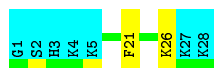• Molecule 2: Glutamate decarboxylase

Chain B:

G1 S2 H3 K4 K5 I15 K20 F21 K27 K28

● Molecule 2: Glutamate decarboxylase

Chain C: 71% · 25%

G1 S2 H3 K4 K5 Q11 K27 K28
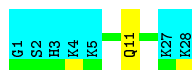
4.2.19 Score per residue for model 19

● Molecule 1: Calmodulin
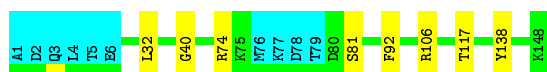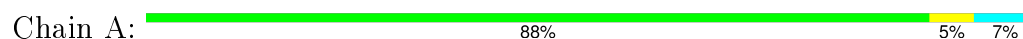
Chain A: 88% 5% 7%

A1 D2 Q3 L4 T5 E6 L32 G40 R74 K75 M76 K77 D78 T79 D80 S81 F92 R106 T117 Y138 K148

● Molecule 2: Glutamate decarboxylase

Chain B: 61% 14% 25%

G1 S2 H3 K4 K5 E9 W18 F21 K26 K27 K28

● Molecule 2: Glutamate decarboxylase

Chain C: 68% 7% 25%

G1 S2 H3 K4 K5 F21 K25 K26 K27 K28
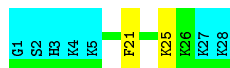
4.2.20 Score per residue for model 20

● Molecule 1: Calmodulin
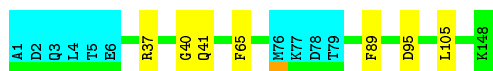
Chain A: 89% 5% 7%

A1 D2 Q3 L4 T5 E6 R37 G40 Q41 F65 M76 K77 D78 T79 F89 D95 L105 K148

● Molecule 2: Glutamate decarboxylase

Chain B: 68% 7% 25%

G1 S2 H3 K4 K5 E9 F21 K27 K28

• **Molecule 2: Glutamate decarboxylase**

Chain C:

5 Refinement protocol and experimental data overview ⓘ

The models were refined using the following method: *simulated annealing and torsion angle dynamics*.

Of the 200 calculated structures, 20 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
CNS	refinement	1.1
DYANA	structure solution	1.5

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 5770
Number of chemical shift lists	3
Total number of shifts	3282
Number of shifts mapped to atoms	3282
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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: CA

There are no covalent bond-length or bond-angle outliers.

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	0.3±0.5
2	B	0.0±0.0	0.1±0.2
All	All	0	8

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	138	TYR	Sidechain	2
1	A	99	TYR	Sidechain	2
1	A	12	PHE	Sidechain	1
1	A	68	PHE	Sidechain	1
2	B	21	PHE	Sidechain	1
1	A	89	PHE	Sidechain	1

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
All	All	28920	27620	27600	-

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.

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	137/148 (93%)	114±3 (83±2%)	20±3 (14±2%)	3±1 (2±1%)	13	52
2	B	21/28 (75%)	20±1 (94±5%)	1±1 (6±5%)	0±0 (0±1%)	38	79
2	C	21/28 (75%)	21±0 (98±2%)	0±0 (2±2%)	0±0 (0±0%)	100	100
All	All	3580/4080 (88%)	3090 (86%)	429 (12%)	61 (2%)	16	59

All 15 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	40	GLY	20
1	A	75	LYS	11
1	A	113	GLY	10
1	A	95	ASP	5
1	A	132	GLY	3
2	B	26	LYS	2
1	A	43	PRO	2
1	A	133	ASP	1
1	A	137	ASN	1
1	A	140	GLU	1
1	A	92	PHE	1
1	A	74	ARG	1
1	A	131	ASP	1
1	A	54	GLU	1
1	A	115	LYS	1

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	117/126 (93%)	110±3 (94±2%)	7±3 (6±2%)	27	73
2	B	20/26 (77%)	18±1 (89±5%)	2±1 (11±5%)	12	56
2	C	20/26 (77%)	18±1 (91±4%)	2±1 (9±4%)	17	62
All	All	3140/3560 (88%)	2917 (93%)	223 (7%)	23	68

All 77 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	21	PHE	20
1	A	32	LEU	12
1	A	65	PHE	11
1	A	54	GLU	11
2	C	21	PHE	9
1	A	37	ARG	7
1	A	105	LEU	7
2	C	26	LYS	6
2	B	15	ILE	6
1	A	148	LYS	6
1	A	74	ARG	5
1	A	30	LYS	5
2	C	11	GLN	4
2	B	20	LYS	4
1	A	138	TYR	4
1	A	106	ARG	4
1	A	19	PHE	4
2	C	14	MET	4
2	B	9	GLU	3
1	A	115	LYS	3
1	A	90	ARG	3
1	A	86	ARG	3
2	C	20	LYS	3
1	A	123	GLU	3
1	A	124	MET	3
1	A	60	ASN	3

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Mol	Chain	Res	Type	Models (Total)
2	C	19	LYS	3
1	A	21	LYS	3
2	B	26	LYS	3
2	C	25	LYS	2
1	A	89	PHE	2
2	B	23	GLU	2
1	A	81	SER	2
1	A	41	GLN	2
1	A	75	LYS	2
1	A	14	GLU	2
1	A	50	ASP	2
1	A	94	LYS	2
2	B	18	TRP	2
2	C	13	GLU	2
1	A	140	GLU	2
1	A	112	LEU	2
2	C	9	GLU	1
1	A	118	ASP	1
1	A	51	MET	1
1	A	92	PHE	1
1	A	72	MET	1
1	A	95	ASP	1
1	A	116	LEU	1
1	A	145	MET	1
1	A	111	ASN	1
2	C	12	LEU	1
2	B	14	MET	1
1	A	31	GLU	1
1	A	7	GLU	1
2	B	25	LYS	1
1	A	135	GLN	1
1	A	12	PHE	1
1	A	71	MET	1
2	B	11	GLN	1
1	A	117	THR	1
1	A	52	ILE	1
1	A	107	HIS	1
1	A	87	GLU	1
2	B	12	LEU	1
1	A	84	GLU	1
1	A	18	LEU	1
1	A	137	ASN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	82	GLU	1
1	A	93	ASP	1
1	A	83	GLU	1
1	A	20	ASP	1
1	A	119	GLU	1
1	A	143	GLN	1
1	A	120	GLU	1
1	A	11	GLU	1
1	A	64	ASP	1

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 carbohydrates 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 93% for the well-defined parts and 91% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5770

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	1828
Number of shifts mapped to atoms	1828
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
$^{13}C_{\alpha}$	148	-0.32 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	137	0.09 ± 0.07	None needed (< 0.5 ppm)
$^{13}C'$	144	-0.51 ± 0.07	Should be applied
^{15}N	144	0.45 ± 0.17	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 69%, i.e. 1523 atoms were assigned a chemical shift out of a possible 2200. 15 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	683/896 (76%)	274/358 (77%)	273/360 (76%)	136/178 (76%)
Sidechain	748/1166 (64%)	459/675 (68%)	278/445 (62%)	11/46 (24%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	92/138 (67%)	50/74 (68%)	42/60 (70%)	0/4 (0%)
Overall	1523/2200 (69%)	783/1107 (71%)	593/865 (69%)	147/228 (64%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 65%, i.e. 1625 atoms were assigned a chemical shift out of a possible 2517. 16 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

|	Total	^{1}H	^{13}C	^{15}N
Backbone	728/1016 (72%)	292/406 (72%)	292/408 (72%)	144/202 (71%)
Sidechain	805/1347 (60%)	494/784 (63%)	299/507 (59%)	12/56 (21%)
Aromatic	92/154 (60%)	50/82 (61%)	42/64 (66%)	0/8 (0%)
Overall	1625/2517 (65%)	836/1272 (66%)	633/979 (65%)	156/266 (59%)

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.

Random coil index (RCI) for chain A:
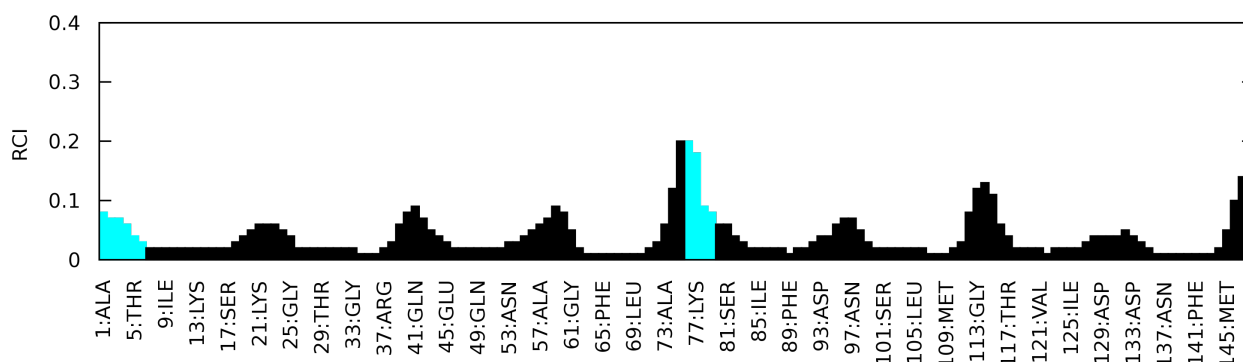
7.2 Chemical shift list 2

File name: BMRB entry 5770

Chemical shift list name: *assigned_ chem_ shift_ list_ 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	728
Number of shifts mapped to atoms	728
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)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	52	-0.35 ± 0.21	None needed (< 0.5 ppm)
$^{13}C_\beta$	52	0.02 ± 0.17	None needed (< 0.5 ppm)
$^{13}C'$	48	-0.62 ± 0.15	Should be applied
^{15}N	50	-0.27 ± 0.42	None needed (< 0.5 ppm)

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 24%, i.e. 524 atoms were assigned a chemical shift out of a possible 2200. 6 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	210/896 (23%)	84/358 (23%)	84/360 (23%)	42/178 (24%)
Sidechain	276/1166 (24%)	172/675 (25%)	102/445 (23%)	2/46 (4%)
Aromatic	38/138 (28%)	22/74 (30%)	14/60 (23%)	2/4 (50%)
Overall	524/2200 (24%)	278/1107 (25%)	200/865 (23%)	46/228 (20%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 672 atoms were assigned a chemical shift out of a possible 2517. 6 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	252/1016 (25%)	102/406 (25%)	100/408 (25%)	50/202 (25%)

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	Total	**¹H**	**¹³C**	**¹⁵N**
Sidechain	378/1347 (28%)	240/784 (31%)	136/507 (27%)	2/56 (4%)
Aromatic	42/154 (27%)	24/82 (29%)	16/64 (25%)	2/8 (25%)
Overall	672/2517 (27%)	366/1272 (29%)	252/979 (26%)	54/266 (20%)

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 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 B:

Random coil index (RCI) for chain C:
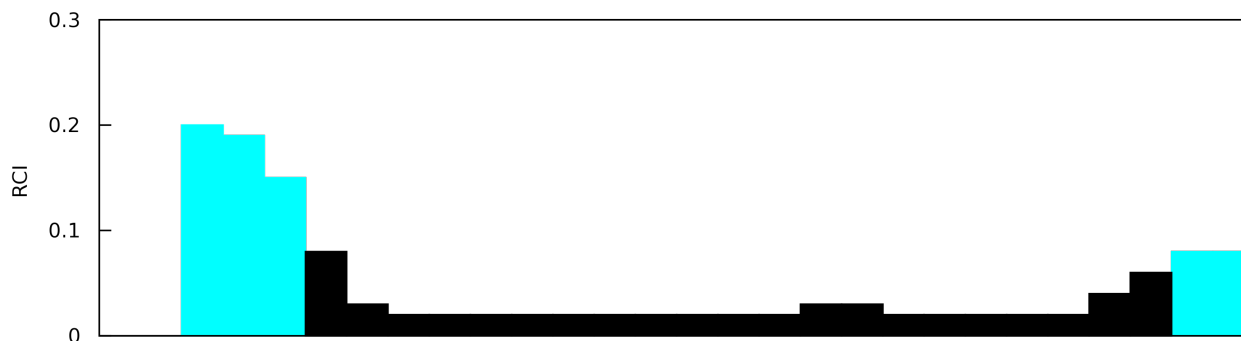
7.3 Chemical shift list 3

File name: BMRB entry 5770

Chemical shift list name: *assigned_chem_shift_list_3*

7.3.1 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	726
Number of shifts mapped to atoms	726
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

7.3.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	52	-0.40 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_\beta$	52	-0.04 ± 0.14	None needed (< 0.5 ppm)
$^{13}C'$	48	-0.67 ± 0.10	Should be applied
^{15}N	50	-0.07 ± 0.34	None needed (< 0.5 ppm)

7.3.3 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 24%, i.e. 522 atoms were assigned a chemical shift out of a possible 2200. 6 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	210/896 (23%)	84/358 (23%)	84/360 (23%)	42/178 (24%)
Sidechain	276/1166 (24%)	172/675 (25%)	102/445 (23%)	2/46 (4%)
Aromatic	36/138 (26%)	22/74 (30%)	12/60 (20%)	2/4 (50%)
Overall	522/2200 (24%)	278/1107 (25%)	198/865 (23%)	46/228 (20%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 27%, i.e. 670 atoms were assigned a chemical shift out of a possible 2517. 6 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

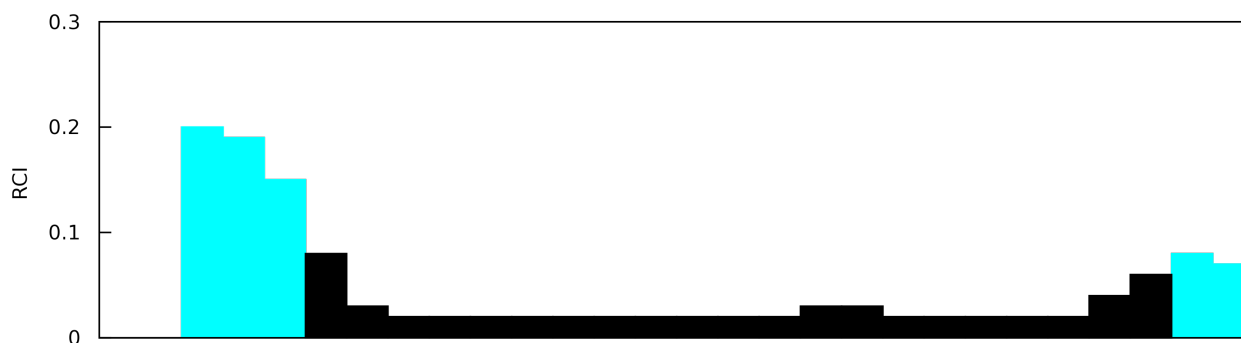|	Total	^{1}H	^{13}C	^{15}N
Backbone	252/1016 (25%)	102/406 (25%)	100/408 (25%)	50/202 (25%)
Sidechain	378/1347 (28%)	240/784 (31%)	136/507 (27%)	2/56 (4%)
Aromatic	40/154 (26%)	24/82 (29%)	14/64 (22%)	2/8 (25%)
Overall	670/2517 (27%)	366/1272 (29%)	250/979 (26%)	54/266 (20%)

7.3.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.3.5 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 B:

Random coil index (RCI) for chain C: