



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:57 pm BST

PDB ID : 2MSK
Title : Solution Structure and Chemical Shift Assignments for BeF₃ activated Receiver Domain of Nitrogen Regulatory Protein C (NtrC) at 35C
Authors : Clarkson, M.W.; Pontiggia, F.; Villali, J.; Kern, D.
Deposited on : 2014-08-04

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 ⓘ 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

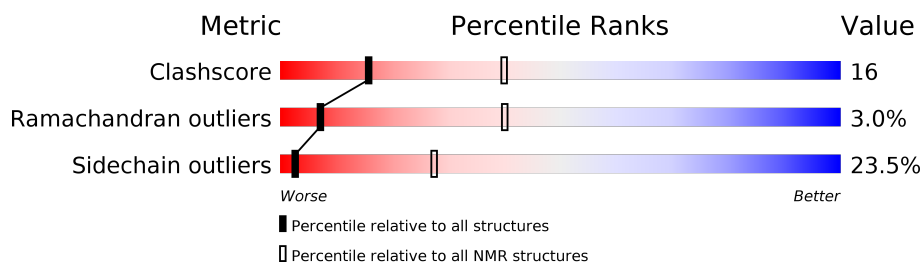
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 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	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	124	

2 Ensemble composition and analysis

This entry contains 25 models. Model 3 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:3-A:121 (119)	0.32	3

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 5 clusters and 1 single-model cluster was found.

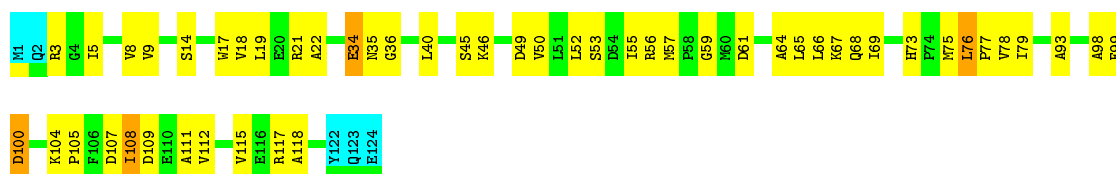
Cluster number	Models
1	1, 2, 3, 8, 11, 14, 15, 20, 21
2	4, 6, 7, 12, 13, 16, 19, 24
3	17, 22, 25
4	9, 18
5	5, 10
Single-model clusters	23

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1910 atoms, of which 955 are hydrogens and 0 are deuteriums.

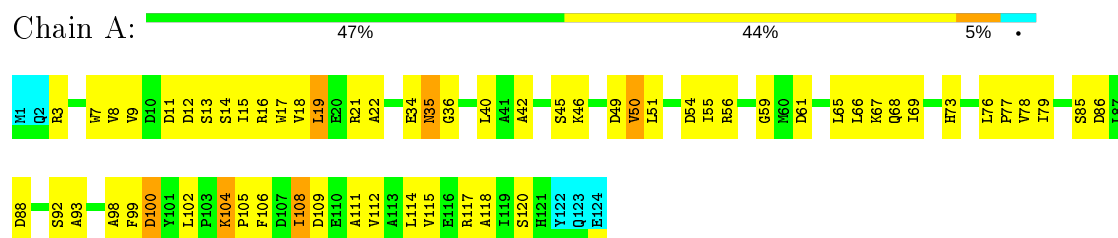
- Molecule 1 is a protein called Nitrogen regulation protein NR(I).

Mol	Chain	Residues	Atoms						Trace
1	A	124	Total	C	H	N	O	S	0
			1910	606	955	162	181	6	



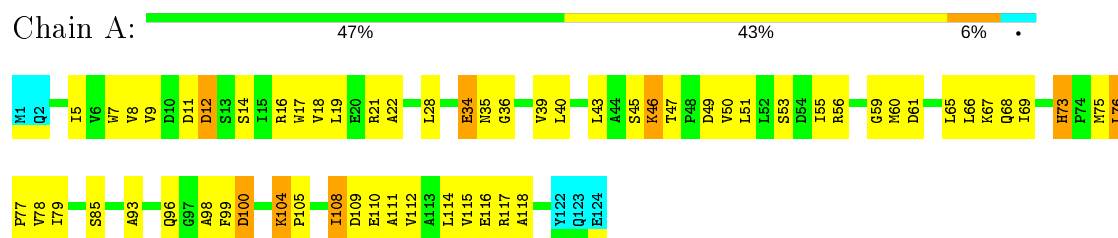
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Nitrogen regulation protein NR(I)



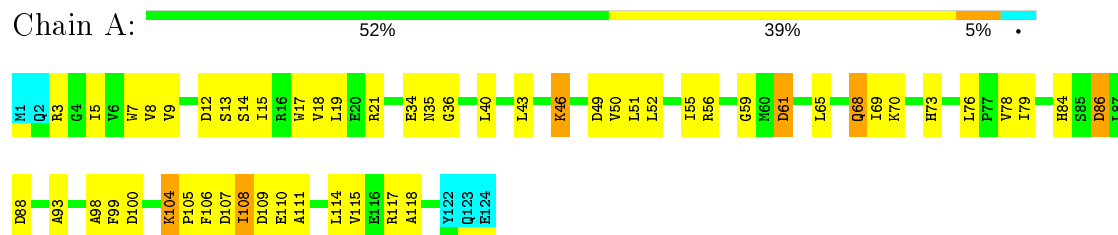
4.2.4 Score per residue for model 4

- Molecule 1: Nitrogen regulation protein NR(I)



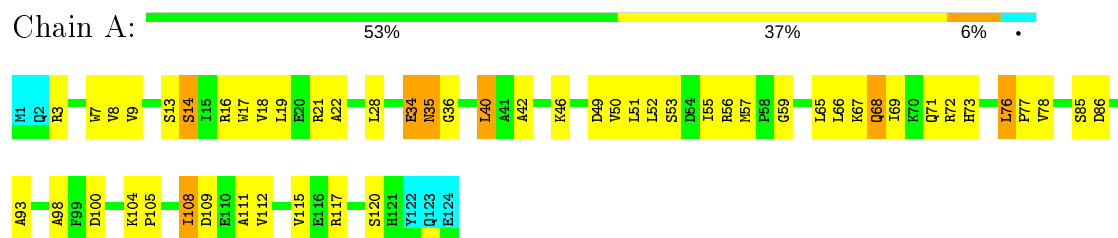
4.2.5 Score per residue for model 5

- Molecule 1: Nitrogen regulation protein NR(I)



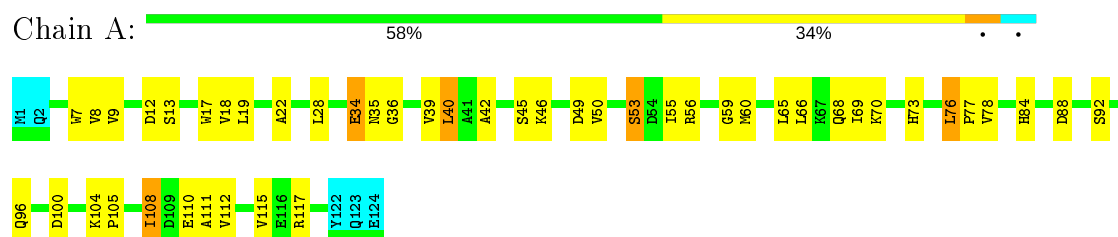
4.2.6 Score per residue for model 6

- Molecule 1: Nitrogen regulation protein NR(I)



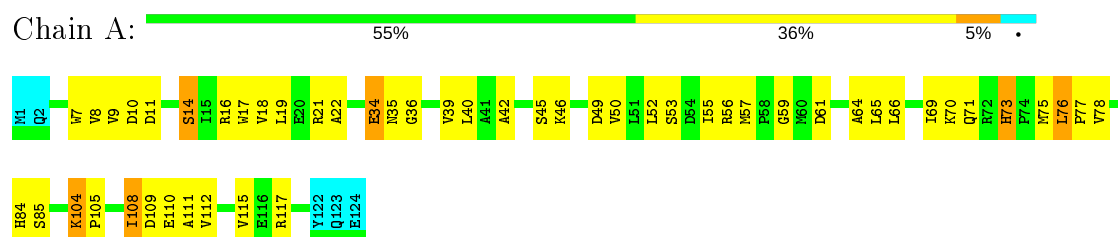
4.2.7 Score per residue for model 7

- Molecule 1: Nitrogen regulation protein NR(I)



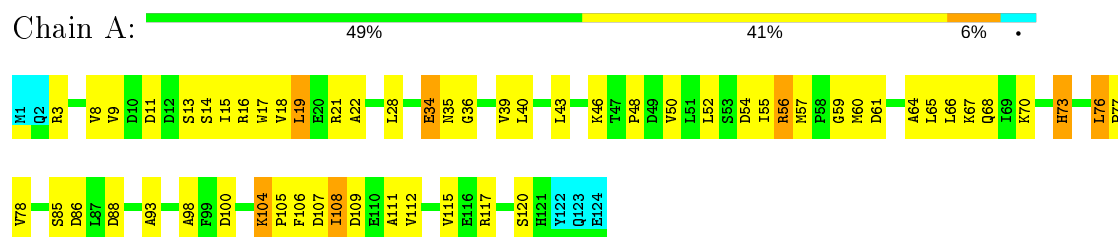
4.2.8 Score per residue for model 8

- Molecule 1: Nitrogen regulation protein NR(I)



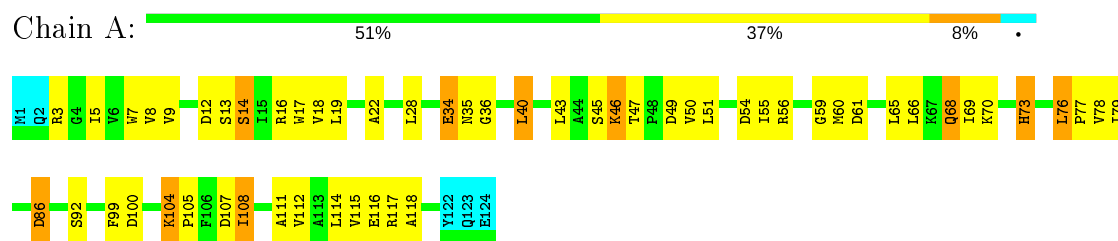
4.2.9 Score per residue for model 9

- Molecule 1: Nitrogen regulation protein NR(I)



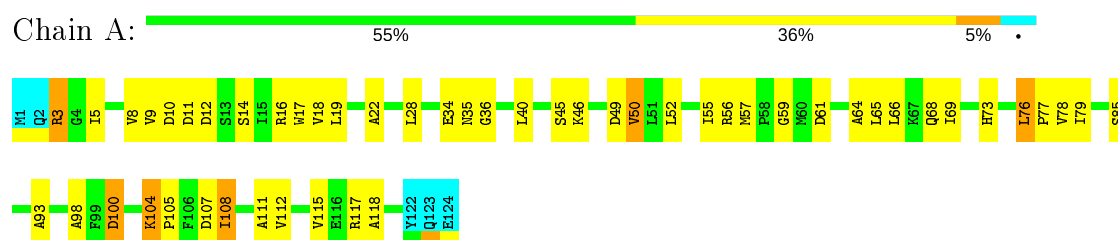
4.2.10 Score per residue for model 10

- Molecule 1: Nitrogen regulation protein NR(I)



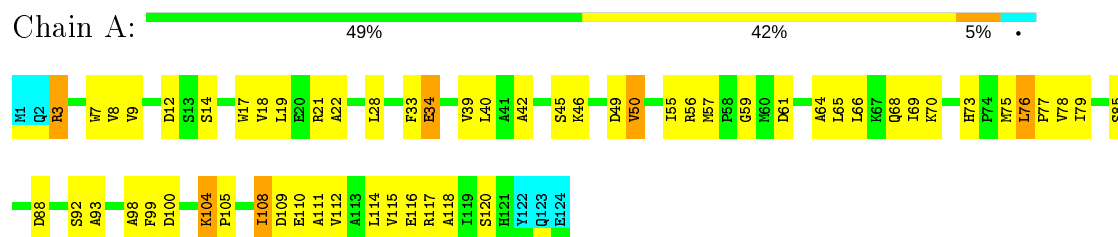
4.2.11 Score per residue for model 11

- Molecule 1: Nitrogen regulation protein NR(I)



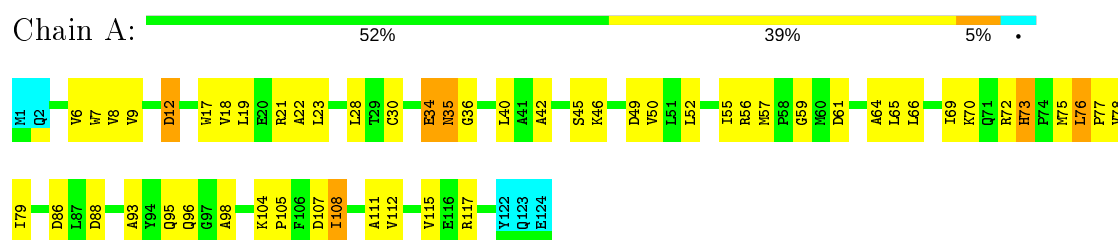
4.2.12 Score per residue for model 12

- Molecule 1: Nitrogen regulation protein NR(I)



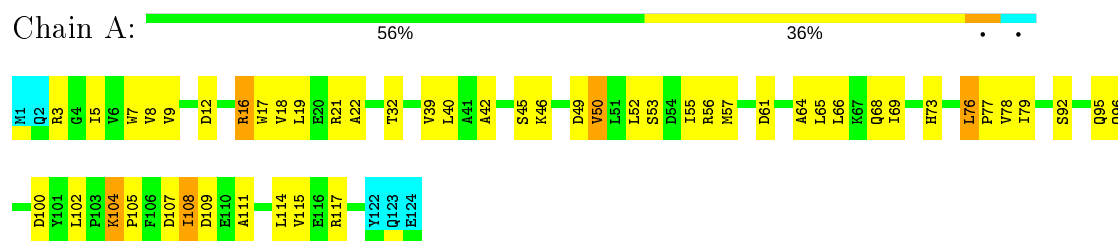
4.2.13 Score per residue for model 13

- Molecule 1: Nitrogen regulation protein NR(I)



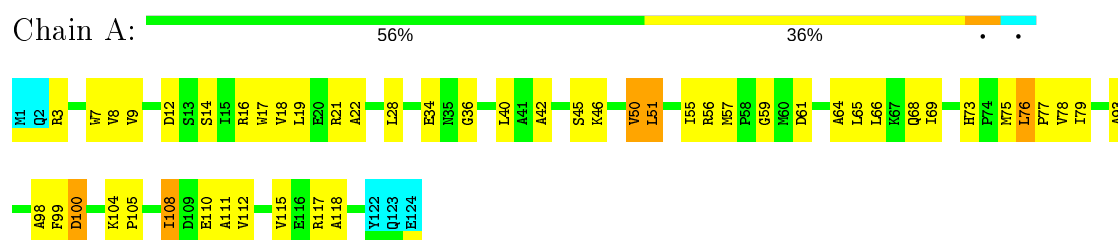
4.2.14 Score per residue for model 14

- Molecule 1: Nitrogen regulation protein NR(I)



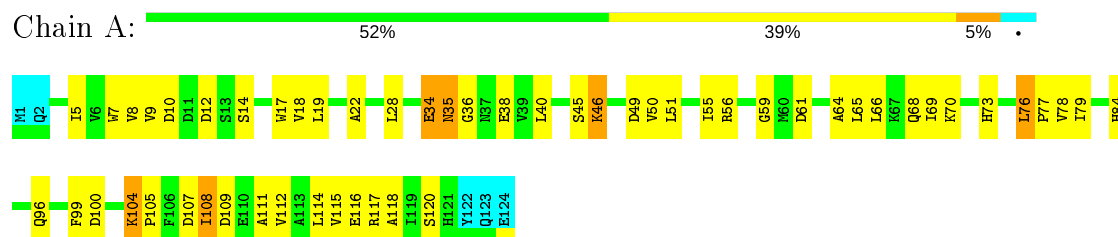
4.2.15 Score per residue for model 15

- Molecule 1: Nitrogen regulation protein NR(I)



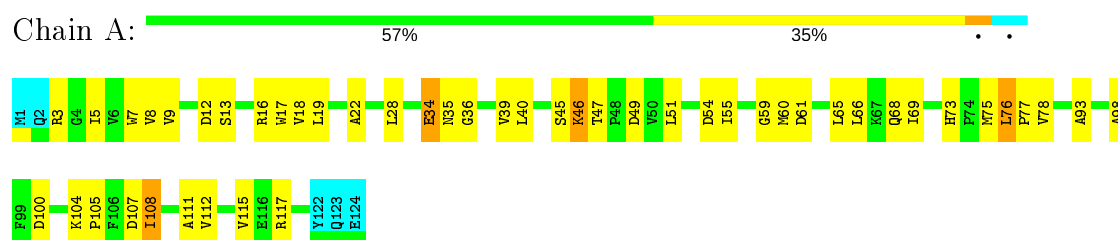
4.2.16 Score per residue for model 16

- Molecule 1: Nitrogen regulation protein NR(I)



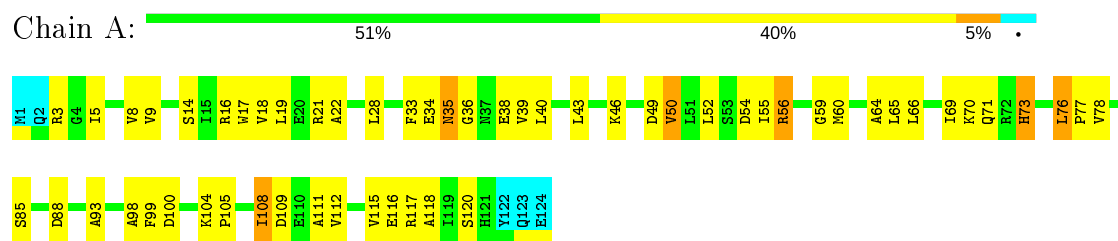
4.2.17 Score per residue for model 17

- Molecule 1: Nitrogen regulation protein NR(I)



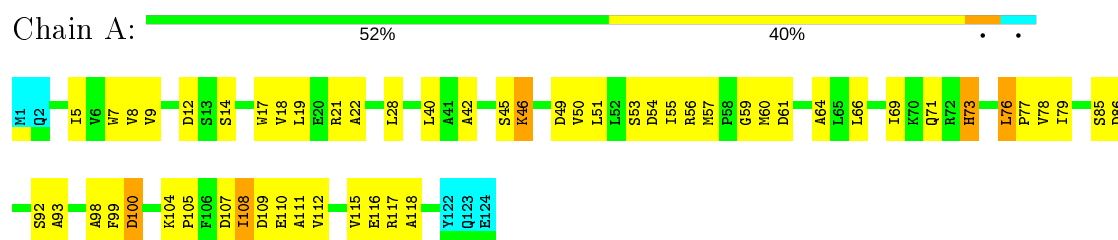
4.2.18 Score per residue for model 18

- Molecule 1: Nitrogen regulation protein NR(I)



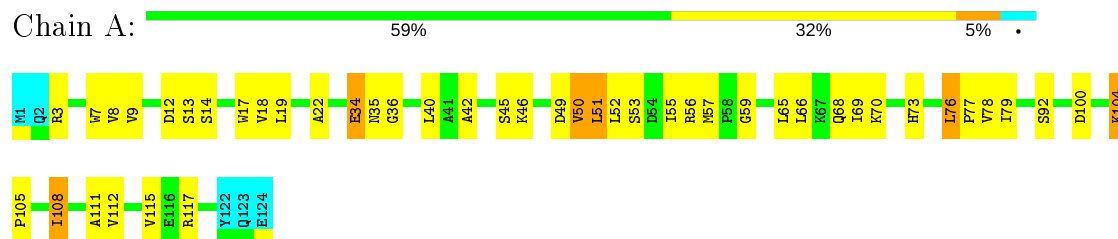
4.2.19 Score per residue for model 19

- Molecule 1: Nitrogen regulation protein NR(I)



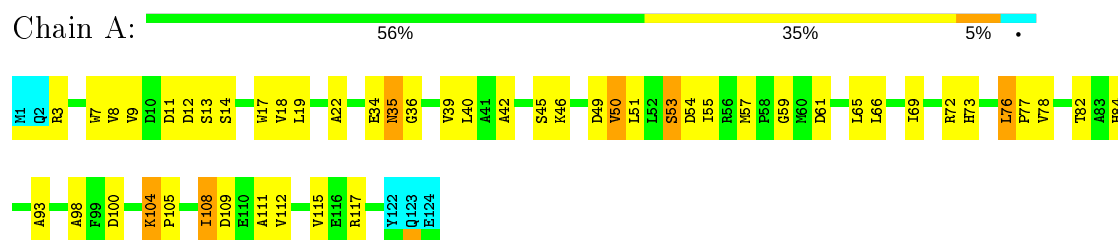
4.2.20 Score per residue for model 20

- Molecule 1: Nitrogen regulation protein NR(I)



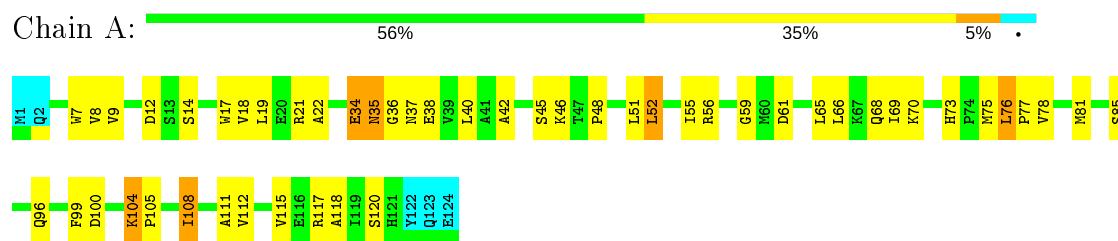
4.2.21 Score per residue for model 21

- Molecule 1: Nitrogen regulation protein NR(I)



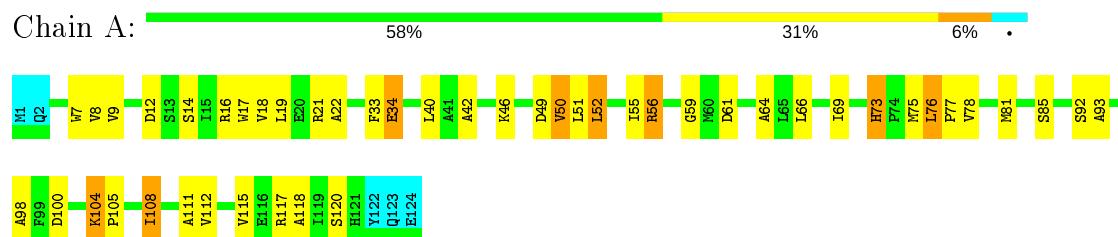
4.2.22 Score per residue for model 22

- Molecule 1: Nitrogen regulation protein NR(I)



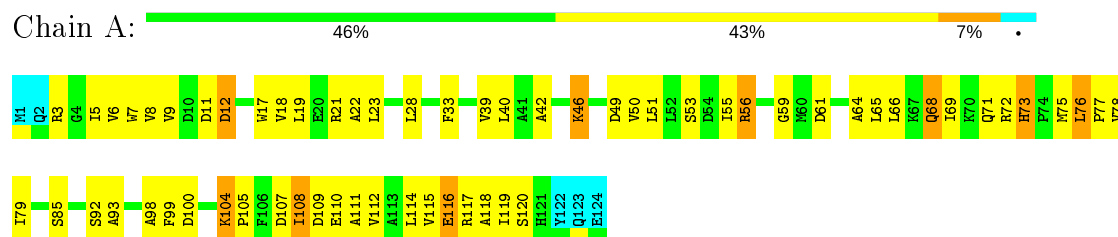
4.2.23 Score per residue for model 23

- Molecule 1: Nitrogen regulation protein NR(I)



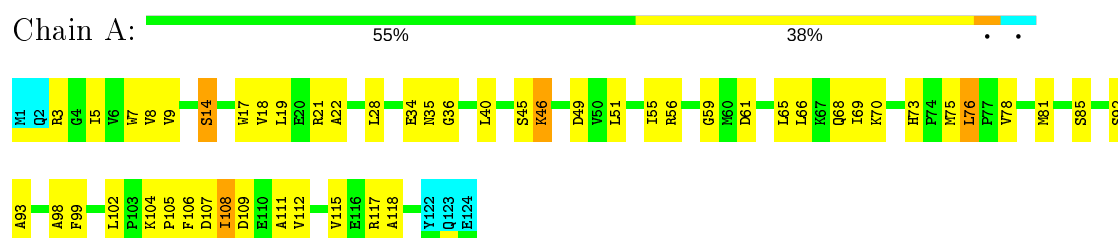
4.2.24 Score per residue for model 24

- Molecule 1: Nitrogen regulation protein NR(I)



4.2.25 Score per residue for model 25

- Molecule 1: Nitrogen regulation protein NR(I)



5 Refinement protocol and experimental data overview

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

Of the 300 calculated structures, 25 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
CYANA	structure solution	
CYANA	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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1565
Number of shifts mapped to atoms	1565
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

6.1 Standard geometry

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

There are no bond-length outliers.

There are no bond-angle outliers.

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	908	915	915	30±3
All	All	22700	22875	22875	738

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 16.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD12	1:A:69:ILE:HD11	1.06	1.27	6	23
1:A:69:ILE:HD12	1:A:78:VAL:HG21	0.93	1.40	3	20
1:A:50:VAL:HG11	1:A:115:VAL:HG13	0.81	1.48	5	13
1:A:8:VAL:HG21	1:A:19:LEU:HD12	0.78	1.56	9	4
1:A:69:ILE:HD13	1:A:78:VAL:HG21	0.76	1.56	16	2
1:A:39:VAL:HG11	1:A:65:LEU:HD21	0.73	1.59	12	5
1:A:8:VAL:HG22	1:A:52:LEU:HD13	0.72	1.59	8	8
1:A:66:LEU:HD13	1:A:78:VAL:HG11	0.71	1.60	9	1
1:A:22:ALA:HB2	1:A:108:ILE:HG13	0.68	1.65	12	22
1:A:8:VAL:HG21	1:A:19:LEU:HD13	0.68	1.65	20	20
1:A:28:LEU:HD11	1:A:112:VAL:HG13	0.67	1.67	17	12
1:A:79:ILE:HD13	1:A:114:LEU:HD21	0.66	1.66	4	7
1:A:19:LEU:HD21	1:A:106:PHE:CZ	0.66	2.26	1	4
1:A:7:TRP:CB	1:A:51:LEU:HD12	0.65	2.22	5	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:69:ILE:HG22	1:A:73:HIS:CE1	0.65	2.26	16	4
1:A:69:ILE:CD1	1:A:78:VAL:HG21	0.64	2.23	12	5
1:A:50:VAL:CG1	1:A:115:VAL:HG13	0.64	2.22	24	13
1:A:18:VAL:O	1:A:108:ILE:HG21	0.64	1.92	3	18
1:A:111:ALA:O	1:A:115:VAL:HG23	0.63	1.93	8	25
1:A:108:ILE:O	1:A:112:VAL:HG23	0.63	1.93	13	20
1:A:14:SER:O	1:A:18:VAL:HG22	0.63	1.93	2	14
1:A:7:TRP:HB3	1:A:51:LEU:HD12	0.63	1.70	3	9
1:A:36:GLY:CA	1:A:65:LEU:HD13	0.63	2.24	4	6
1:A:8:VAL:HG21	1:A:19:LEU:CD1	0.63	2.24	9	20
1:A:8:VAL:HG22	1:A:52:LEU:CD1	0.62	2.25	8	6
1:A:69:ILE:HD12	1:A:78:VAL:CG2	0.62	2.25	14	9
1:A:66:LEU:CD1	1:A:78:VAL:HG11	0.61	2.26	18	8
1:A:22:ALA:HB1	1:A:112:VAL:CG2	0.61	2.24	25	6
1:A:22:ALA:HB2	1:A:108:ILE:CG1	0.61	2.25	9	17
1:A:28:LEU:CD1	1:A:112:VAL:HG13	0.61	2.26	17	3
1:A:8:VAL:HG11	1:A:19:LEU:HD11	0.60	1.71	19	14
1:A:17:TRP:CE3	1:A:18:VAL:HG13	0.60	2.32	1	25
1:A:93:ALA:HB1	1:A:98:ALA:HB2	0.60	1.73	6	17
1:A:8:VAL:HG11	1:A:19:LEU:CD1	0.59	2.28	14	19
1:A:66:LEU:HD12	1:A:69:ILE:CD1	0.59	2.27	15	9
1:A:39:VAL:CG1	1:A:65:LEU:HD21	0.58	2.28	12	1
1:A:36:GLY:HA2	1:A:65:LEU:HD22	0.57	1.77	13	9
1:A:40:LEU:HD21	1:A:68:GLN:OE1	0.57	2.00	7	3
1:A:76:LEU:HD12	1:A:77:PRO:O	0.56	2.00	7	17
1:A:73:HIS:O	1:A:76:LEU:HD22	0.56	2.01	25	1
1:A:47:THR:HG21	1:A:73:HIS:CE1	0.55	2.36	4	1
1:A:55:ILE:HG21	1:A:86:ASP:CB	0.55	2.32	5	2
1:A:55:ILE:HD13	1:A:82:THR:HG21	0.55	1.78	21	1
1:A:40:LEU:HD13	1:A:68:GLN:NE2	0.55	2.16	4	2
1:A:9:VAL:O	1:A:9:VAL:HG13	0.55	2.02	12	12
1:A:5:ILE:HD12	1:A:46:LYS:HE3	0.55	1.79	24	2
1:A:73:HIS:CE1	1:A:76:LEU:HD13	0.55	2.37	25	1
1:A:69:ILE:HB	1:A:76:LEU:HD21	0.54	1.76	23	2
1:A:7:TRP:HB2	1:A:51:LEU:HD12	0.54	1.80	20	6
1:A:5:ILE:HD13	1:A:46:LYS:CE	0.54	2.32	2	3
1:A:99:PHE:CZ	1:A:118:ALA:HB2	0.54	2.38	19	3
1:A:73:HIS:O	1:A:76:LEU:HD23	0.54	2.03	18	8
1:A:19:LEU:HD21	1:A:106:PHE:CE1	0.53	2.38	5	1
1:A:76:LEU:HD12	1:A:77:PRO:HD2	0.53	1.81	12	2
1:A:9:VAL:HG13	1:A:9:VAL:O	0.53	2.03	11	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LEU:HD22	1:A:114:LEU:HD23	0.52	1.80	3	1
1:A:47:THR:HG21	1:A:73:HIS:NE2	0.52	2.19	4	2
1:A:5:ILE:HD12	1:A:46:LYS:HE2	0.52	1.80	17	5
1:A:99:PHE:CE2	1:A:118:ALA:HB2	0.52	2.40	22	2
1:A:7:TRP:CH2	1:A:42:ALA:HB1	0.52	2.40	8	15
1:A:36:GLY:O	1:A:65:LEU:HD13	0.51	2.04	21	14
1:A:9:VAL:HG21	1:A:35:ASN:C	0.51	2.25	18	17
1:A:3:ARG:HA	1:A:28:LEU:HD23	0.51	1.83	11	3
1:A:23:LEU:HD12	1:A:30:CYS:HB2	0.51	1.81	13	1
1:A:99:PHE:CE1	1:A:118:ALA:HB2	0.50	2.41	10	9
1:A:23:LEU:HD12	1:A:30:CYS:CB	0.50	2.36	13	1
1:A:76:LEU:HD12	1:A:77:PRO:CD	0.50	2.37	6	2
1:A:40:LEU:HD13	1:A:68:GLN:OE1	0.50	2.07	24	1
1:A:79:ILE:HD13	1:A:114:LEU:CD2	0.50	2.37	5	2
1:A:50:VAL:HG21	1:A:79:ILE:CD1	0.50	2.37	13	1
1:A:40:LEU:HD13	1:A:68:GLN:HE22	0.49	1.65	9	1
1:A:40:LEU:HA	1:A:43:LEU:HD12	0.49	1.83	18	2
1:A:61:ASP:OD1	1:A:64:ALA:HB3	0.48	2.07	24	12
1:A:15:ILE:O	1:A:19:LEU:HD23	0.48	2.08	5	4
1:A:77:PRO:CB	1:A:118:ALA:HB1	0.48	2.37	23	3
1:A:5:ILE:HD13	1:A:46:LYS:HE2	0.48	1.83	14	2
1:A:66:LEU:CD1	1:A:69:ILE:HD11	0.48	2.35	25	5
1:A:8:VAL:HG12	1:A:10:ASP:OD1	0.48	2.08	8	1
1:A:79:ILE:HG23	1:A:100:ASP:O	0.48	2.09	19	9
1:A:93:ALA:HB1	1:A:98:ALA:CB	0.47	2.38	6	1
1:A:8:VAL:HG12	1:A:10:ASP:OD2	0.47	2.09	16	1
1:A:108:ILE:HD13	1:A:108:ILE:N	0.47	2.25	25	13
1:A:52:LEU:CD2	1:A:102:LEU:HD23	0.47	2.39	14	1
1:A:102:LEU:HD22	1:A:114:LEU:CD2	0.47	2.39	3	1
1:A:6:VAL:HG22	1:A:115:VAL:HG11	0.47	1.85	13	1
1:A:108:ILE:N	1:A:108:ILE:HD13	0.47	2.25	15	11
1:A:102:LEU:HD21	1:A:106:PHE:CD1	0.47	2.45	25	1
1:A:76:LEU:HD23	1:A:77:PRO:HD2	0.47	1.87	16	3
1:A:40:LEU:HD11	1:A:68:GLN:OE1	0.47	2.10	10	2
1:A:50:VAL:HG21	1:A:115:VAL:O	0.46	2.11	12	4
1:A:73:HIS:ND1	1:A:76:LEU:HD13	0.46	2.25	25	1
1:A:40:LEU:HD13	1:A:68:GLN:HE21	0.46	1.70	4	1
1:A:50:VAL:HG21	1:A:79:ILE:HD12	0.46	1.88	13	1
1:A:51:LEU:HD23	1:A:53:SER:N	0.46	2.26	6	1
1:A:66:LEU:HD11	1:A:78:VAL:HG11	0.45	1.88	19	1
1:A:104:LYS:HA	1:A:105:PRO:C	0.45	2.32	13	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:PHE:CD1	1:A:39:VAL:HG22	0.44	2.48	18	2
1:A:22:ALA:HB1	1:A:112:VAL:HG21	0.44	1.88	17	1
1:A:99:PHE:CD2	1:A:118:ALA:HB2	0.44	2.47	25	1
1:A:73:HIS:ND1	1:A:76:LEU:HD23	0.44	2.28	6	1
1:A:39:VAL:HG12	1:A:43:LEU:HG	0.43	1.90	18	3
1:A:8:VAL:HG13	1:A:52:LEU:HD13	0.43	1.89	6	1
1:A:73:HIS:CE1	1:A:76:LEU:HD23	0.43	2.48	12	2
1:A:5:ILE:HD12	1:A:46:LYS:CE	0.43	2.44	19	1
1:A:48:PRO:O	1:A:76:LEU:HD13	0.43	2.14	9	1
1:A:43:LEU:HD12	1:A:65:LEU:HD11	0.43	1.91	10	1
1:A:76:LEU:O	1:A:76:LEU:HD23	0.43	2.14	25	1
1:A:18:VAL:C	1:A:108:ILE:HG21	0.42	2.33	22	5
1:A:36:GLY:CA	1:A:65:LEU:HD22	0.42	2.43	5	1
1:A:48:PRO:O	1:A:76:LEU:HD21	0.42	2.14	22	1
1:A:61:ASP:OD1	1:A:64:ALA:HB2	0.42	2.14	23	1
1:A:60:MET:SD	1:A:64:ALA:HB3	0.42	2.54	18	1
1:A:69:ILE:CD1	1:A:78:VAL:HG11	0.42	2.45	21	1
1:A:43:LEU:HD13	1:A:68:GLN:NE2	0.42	2.29	5	1
1:A:6:VAL:HG21	1:A:23:LEU:HD22	0.42	1.91	24	1
1:A:93:ALA:C	1:A:98:ALA:HB2	0.42	2.35	13	1
1:A:116:GLU:HA	1:A:119:ILE:HD12	0.42	1.90	24	1
1:A:5:ILE:HD13	1:A:46:LYS:HE3	0.42	1.91	2	1
1:A:39:VAL:HG12	1:A:65:LEU:HD11	0.42	1.91	17	2
1:A:16:ARG:NE	1:A:32:THR:HG22	0.41	2.30	14	1
1:A:33:PHE:O	1:A:34:GLU:CB	0.41	2.67	23	2
1:A:40:LEU:CD2	1:A:43:LEU:HD12	0.41	2.45	18	1
1:A:51:LEU:HD23	1:A:52:LEU:N	0.41	2.31	23	1
1:A:9:VAL:HG11	1:A:65:LEU:CD2	0.41	2.46	24	1
1:A:93:ALA:O	1:A:98:ALA:HB2	0.41	2.16	13	1
1:A:77:PRO:HB3	1:A:118:ALA:HB1	0.40	1.92	22	1
1:A:52:LEU:HD21	1:A:102:LEU:HD23	0.40	1.93	14	1
1:A:40:LEU:HD21	1:A:65:LEU:HD12	0.40	1.94	4	1

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	119/124 (96%)	103±2 (86±2%)	13±1 (11±1%)	4±1 (3±1%)	7	40
All	All	2975/3100 (96%)	2567 (86%)	320 (11%)	88 (3%)	7	40

All 8 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	59	GLY	24
1	A	56	ARG	20
1	A	34	GLU	19
1	A	50	VAL	14
1	A	60	MET	4
1	A	12	ASP	4
1	A	53	SER	2
1	A	61	ASP	1

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	97/102 (95%)	74±3 (77±3%)	23±3 (23±3%)	3	27
All	All	2425/2550 (95%)	1856 (77%)	569 (23%)	3	27

All 52 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	76	LEU	25
1	A	108	ILE	25
1	A	117	ARG	25
1	A	55	ILE	22
1	A	49	ASP	22
1	A	40	LEU	21
1	A	46	LYS	21
1	A	73	HIS	20
1	A	100	ASP	20
1	A	45	SER	18

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Mol	Chain	Res	Type	Models (Total)
1	A	12	ASP	18
1	A	21	ARG	17
1	A	104	LYS	16
1	A	68	GLN	16
1	A	34	GLU	16
1	A	109	ASP	15
1	A	3	ARG	15
1	A	85	SER	14
1	A	16	ARG	13
1	A	57	MET	13
1	A	107	ASP	12
1	A	70	LYS	12
1	A	75	MET	12
1	A	92	SER	10
1	A	53	SER	9
1	A	13	SER	9
1	A	120	SER	9
1	A	14	SER	9
1	A	110	GLU	8
1	A	35	ASN	8
1	A	61	ASP	8
1	A	11	ASP	8
1	A	88	ASP	7
1	A	96	GLN	7
1	A	56	ARG	7
1	A	54	ASP	7
1	A	116	GLU	7
1	A	86	ASP	7
1	A	84	HIS	5
1	A	71	GLN	5
1	A	67	LYS	5
1	A	38	GLU	4
1	A	72	ARG	4
1	A	52	LEU	4
1	A	81	MET	3
1	A	95	GLN	2
1	A	60	MET	2
1	A	19	LEU	2
1	A	51	LEU	2
1	A	47	THR	1
1	A	37	ASN	1
1	A	10	ASP	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: input_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	1565
Number of shifts mapped to atoms	1565
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	123	-0.09 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	116	0.01 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}'$	115	0.18 ± 0.18	None needed (< 0.5 ppm)
^{15}N	116	-0.01 ± 0.33	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 93%, i.e. 1310 atoms were assigned a chemical shift out of a possible 1412. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	576/583 (99%)	232/232 (100%)	231/238 (97%)	113/113 (100%)
Sidechain	655/741 (88%)	394/429 (92%)	255/284 (90%)	6/28 (21%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	79/88 (90%)	41/47 (87%)	36/36 (100%)	2/5 (40%)
Overall	1310/1412 (93%)	667/708 (94%)	522/558 (94%)	121/146 (83%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 92%, i.e. 1365 atoms were assigned a chemical shift out of a possible 1483. 24 out of 24 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	594/608 (98%)	240/242 (99%)	238/248 (96%)	116/118 (98%)
Sidechain	684/779 (88%)	413/452 (91%)	263/297 (89%)	8/30 (27%)
Aromatic	87/96 (91%)	45/51 (88%)	40/40 (100%)	2/5 (40%)
Overall	1365/1483 (92%)	698/745 (94%)	541/585 (92%)	126/153 (82%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	48	PRO	HB2	-0.33	3.82 – 0.32	-6.9
1	A	48	PRO	HD3	1.19	5.52 – 1.72	-6.4

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

