



Full wwPDB NMR Structure Validation Report ⓘ

Dec 14, 2016 – 12:47 AM EST

PDB ID : 2NBI
Title : Structure of the PSCD-region of the cell wall protein pleuralin-1
Authors : De Sanctis, S.; Wenzler, M.; Kroeger, N.; Malloni, W.M.; Sumper, M.; Rainer, D.; Zadavec, P.; Brunner, E.; Kremer, W.; Kalbitzer, H.R.
Deposited on : 2016-02-23

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-20028442
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

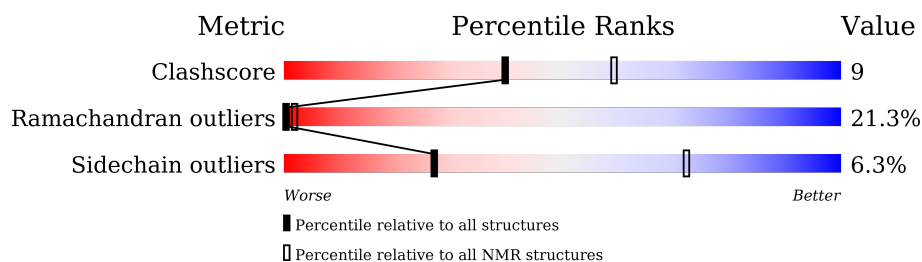
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 18%.

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	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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	494	 65% 28% 6% •

2 Ensemble composition and analysis ⓘ

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 6888 atoms, of which 3287 are hydrogens and 0 are deuteriums.

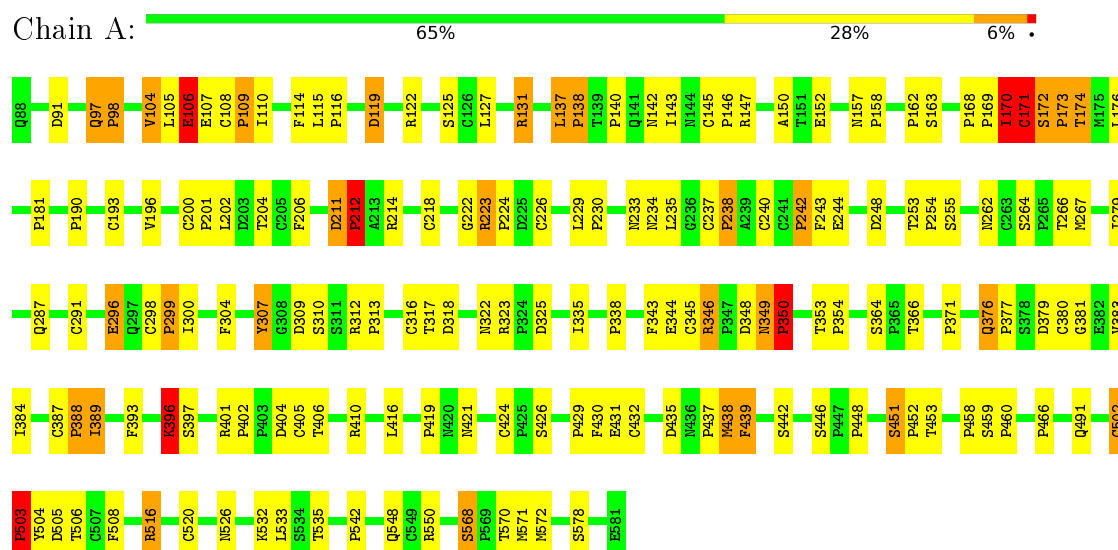
- Molecule 1 is a protein called HEP200 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	494	Total	C	H	N	O	S	0
			6888	2209	3287	576	754	62	

4 Residue-property plots

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: HEP200 protein



5 Refinement protocol and experimental data overview

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

Of the 2000 calculated structures, 1 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	structure solution	1.21
CNS	refinement	
AUREMOL	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)	2nbi_cs.cif
Number of chemical shift lists	1
Total number of shifts	1074
Number of shifts mapped to atoms	1046
Number of unparsed shifts	28
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	18%

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

6 Model quality

6.1 Standard geometry

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	0.89	4/3735 (0.1%)	0.87	1/5181 (0.0%)
All	All	0.89	4/3735 (0.1%)	0.87	1/5181 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	C-O	-6.54	1.10	1.23
1	A	170	ILE	CA-C	6.44	1.69	1.52
1	A	171	CYS	N-CA	6.39	1.59	1.46
1	A	350	PRO	N-CD	-6.11	1.39	1.47

All angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	PRO	N-CA-CB	-5.91	96.10	102.60

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	3601	3287	3284	64
All	All	3601	3287	3284	64

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:98:PRO:HA	1:A:104:VAL:HG11	0.78	1.54
1:A:107:GLU:HG2	1:A:109:PRO:CD	0.76	2.11
1:A:107:GLU:HG2	1:A:109:PRO:HD2	0.71	1.63
1:A:108:CYS:SG	1:A:109:PRO:HD3	0.67	2.29
1:A:107:GLU:CB	1:A:170:ILE:H	0.66	2.03
1:A:106:GLU:HB3	1:A:174:THR:HB	0.65	1.68
1:A:106:GLU:CB	1:A:174:THR:HB	0.62	2.25
1:A:104:VAL:HA	1:A:170:ILE:C	0.61	2.16
1:A:396:LYS:HD2	1:A:397:SER:N	0.60	2.12
1:A:104:VAL:HG12	1:A:170:ILE:HB	0.59	1.73
1:A:325:ASP:OD2	1:A:335:ILE:HB	0.59	1.98
1:A:104:VAL:HA	1:A:170:ILE:CA	0.57	2.29
1:A:106:GLU:C	1:A:171:CYS:H	0.57	2.04
1:A:349:ASN:OD1	1:A:350:PRO:HD3	0.55	2.01
1:A:387:CYS:SG	1:A:388:PRO:HD3	0.55	2.41
1:A:107:GLU:HB2	1:A:170:ILE:H	0.55	1.62
1:A:106:GLU:HG3	1:A:172:SER:N	0.54	2.17
1:A:404:ASP:OD2	1:A:437:PRO:HB3	0.53	2.04
1:A:211:ASP:HB3	1:A:212:PRO:HD3	0.53	1.79
1:A:502:CYS:H	1:A:503:PRO:CD	0.52	2.17
1:A:532:LYS:HG2	1:A:548:GLN:OE1	0.51	2.06
1:A:107:GLU:H	1:A:170:ILE:N	0.51	2.04
1:A:446:SER:O	1:A:448:PRO:HD3	0.50	2.05
1:A:107:GLU:H	1:A:169:PRO:C	0.49	2.11
1:A:222:GLY:O	1:A:224:PRO:HD3	0.48	2.08
1:A:107:GLU:C	1:A:109:PRO:HD2	0.48	2.29
1:A:238:PRO:HD2	1:A:240:CYS:SG	0.48	2.49
1:A:379:ASP:HB3	1:A:383:VAL:HG22	0.48	1.86
1:A:503:PRO:HB2	1:A:568:SER:C	0.48	2.29
1:A:108:CYS:HA	1:A:173:PRO:CD	0.47	2.39
1:A:323:ARG:NE	1:A:323:ARG:HA	0.47	2.24
1:A:226:CYS:O	1:A:242:PRO:HA	0.47	2.09
1:A:438:MET:O	1:A:439:PHE:HB2	0.47	2.09
1:A:119:ASP:O	1:A:162:PRO:HB2	0.46	2.09
1:A:451:SER:HB2	1:A:452:PRO:HD3	0.46	1.87
1:A:410:ARG:NE	1:A:410:ARG:HA	0.46	2.26
1:A:223:ARG:HA	1:A:223:ARG:NE	0.46	2.25
1:A:226:CYS:SG	1:A:237:CYS:N	0.45	2.90
1:A:503:PRO:HA	1:A:571:MET:HB3	0.45	1.89
1:A:317:THR:HB	1:A:343:PHE:CD2	0.43	2.47
1:A:296:GLU:O	1:A:299:PRO:HD2	0.43	2.14
1:A:406:THR:HB	1:A:430:PHE:CD1	0.43	2.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)
1:A:200:CYS:SG	1:A:201:PRO:HD3	0.43	2.54
1:A:229:LEU:HB3	1:A:230:PRO:CD	0.43	2.43
1:A:508:PHE:O	1:A:516:ARG:HB2	0.43	2.14
1:A:383:VAL:HA	1:A:389:ILE:CD1	0.43	2.42
1:A:106:GLU:HG3	1:A:172:SER:H	0.43	1.71
1:A:107:GLU:N	1:A:170:ILE:N	0.42	2.67
1:A:105:LEU:N	1:A:170:ILE:HA	0.42	2.28
1:A:125:SER:CB	1:A:158:PRO:HA	0.42	2.45
1:A:106:GLU:HA	1:A:173:PRO:O	0.42	2.15
1:A:137:LEU:HB3	1:A:138:PRO:HD3	0.42	1.91
1:A:211:ASP:CB	1:A:212:PRO:HD3	0.42	2.45
1:A:131:ARG:NE	1:A:131:ARG:HA	0.42	2.30
1:A:346:ARG:HD2	1:A:346:ARG:N	0.42	2.29
1:A:379:ASP:CB	1:A:383:VAL:HG22	0.41	2.45
1:A:506:THR:O	1:A:572:MET:HG2	0.41	2.15
1:A:107:GLU:CB	1:A:170:ILE:N	0.41	2.80
1:A:104:VAL:HA	1:A:170:ILE:O	0.41	2.15
1:A:376:GLN:H	1:A:377:PRO:HD2	0.41	1.76
1:A:502:CYS:O	1:A:571:MET:HB3	0.40	2.16
1:A:98:PRO:CA	1:A:104:VAL:HG21	0.40	2.47
1:A:97:GLN:OE1	1:A:168:PRO:HB2	0.40	2.16
1:A:152:GLU:O	1:A:157:ASN:HB3	0.40	2.15

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	492/494 (100%)	240 (49%)	147 (30%)	105 (21%)	0	2
All	All	492/494 (100%)	240 (49%)	147 (30%)	105 (21%)	0	2

All 105 Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type
1	A	266	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	466	PRO
1	A	535	THR
1	A	419	PRO
1	A	211	ASP
1	A	173	PRO
1	A	504	TYR
1	A	542	PRO
1	A	366	THR
1	A	138	PRO
1	A	435	ASP
1	A	190	PRO
1	A	426	SER
1	A	307	TYR
1	A	389	ILE
1	A	503	PRO
1	A	364	SER
1	A	114	PHE
1	A	502	CYS
1	A	146	PRO
1	A	163	SER
1	A	298	CYS
1	A	140	PRO
1	A	238	PRO
1	A	526	ASN
1	A	460	PRO
1	A	442	SER
1	A	279	ILE
1	A	106	GLU
1	A	309	ASP
1	A	520	CYS
1	A	119	ASP
1	A	432	CYS
1	A	459	SER
1	A	104	VAL
1	A	255	SER
1	A	338	PRO
1	A	316	CYS
1	A	137	LEU
1	A	345	CYS
1	A	264	SER
1	A	438	MET
1	A	109	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	405	CYS
1	A	380	CYS
1	A	172	SER
1	A	578	SER
1	A	147	ARG
1	A	91	ASP
1	A	212	PRO
1	A	396	LYS
1	A	116	PRO
1	A	193	CYS
1	A	244	GLU
1	A	304	PHE
1	A	206	PHE
1	A	310	SER
1	A	458	PRO
1	A	181	PRO
1	A	371	PRO
1	A	439	PHE
1	A	322	ASN
1	A	145	CYS
1	A	424	CYS
1	A	381	GLY
1	A	550	ARG
1	A	451	SER
1	A	568	SER
1	A	171	CYS
1	A	299	PRO
1	A	254	PRO
1	A	218	CYS
1	A	97	GLN
1	A	150	ALA
1	A	354	PRO
1	A	384	ILE
1	A	393	PHE
1	A	491	GLN
1	A	402	PRO
1	A	431	GLU
1	A	376	GLN
1	A	287	GLN
1	A	202	LEU
1	A	353	THR
1	A	388	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	291	CYS
1	A	570	THR
1	A	318	ASP
1	A	300	ILE
1	A	115	LEU
1	A	242	PRO
1	A	429	PRO
1	A	348	ASP
1	A	110	ILE
1	A	350	PRO
1	A	344	GLU
1	A	313	PRO
1	A	253	THR
1	A	98	PRO
1	A	174	THR
1	A	296	GLU
1	A	453	THR
1	A	505	ASP
1	A	248	ASP
1	A	235	LEU

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	460/460 (100%)	431 (94%)	29 (6%)	27	72
All	All	460/460 (100%)	431 (94%)	29 (6%)	27	72

All 29 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	131	ARG
1	A	533	LEU
1	A	421	ASN
1	A	196	VAL
1	A	170	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	142	ASN
1	A	346	ARG
1	A	401	ARG
1	A	312	ARG
1	A	307	TYR
1	A	122	ARG
1	A	143	ILE
1	A	171	CYS
1	A	349	ASN
1	A	503	PRO
1	A	396	LYS
1	A	267	MET
1	A	204	THR
1	A	223	ARG
1	A	234	ASN
1	A	127	LEU
1	A	262	ASN
1	A	516	ARG
1	A	214	ARG
1	A	233	ASN
1	A	416	LEU
1	A	212	PRO
1	A	243	PHE
1	A	176	LEU

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 18% for the well-defined parts and 18% for the entire structure.

7.1 Chemical shift list 1

File name: 2nbi_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	1074
Number of shifts mapped to atoms	1046
Number of unparsed shifts	28
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. All 28 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	2	TYR	C	175.42	0.20	1
2	?	2	TYR	CA	57.75	0.20	1
3	?	2	TYR	CB	40.12	0.20	1
4	?	3	TYR	H	7.64	0.02	1
5	?	3	TYR	HA	4.77	0.05	1
6	?	3	TYR	C	176.10	0.20	1
7	?	3	TYR	CA	59.30	0.20	1
8	?	3	TYR	N	115.11	0.33	1
9	?	5	HIS	HA	3.97	0.05	1
10	?	5	HIS	HB2	3.11	0.05	2
11	?	5	HIS	HB3	3.20	0.05	2
12	?	5	HIS	C	176.39	0.20	1
13	?	5	HIS	CA	56.70	0.20	1
14	?	5	HIS	CB	30.07	0.20	1
15	?	8	HIS	HA	4.57	0.05	1

Continued on next page...

Continued from previous page...

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	8	HIS	HB2	2.98	0.05	1
17	?	8	HIS	HB3	2.98	0.05	1
18	?	8	HIS	C	173.92	0.20	1
19	?	8	HIS	CA	55.82	0.20	1
20	?	8	HIS	CB	30.60	0.20	1
21	?	9	HIS	H	8.35	0.02	1
22	?	9	HIS	HA	4.65	0.05	1
23	?	9	HIS	HB2	3.08	0.05	1
24	?	9	HIS	HB3	3.08	0.05	1
25	?	9	HIS	C	175.59	0.20	1
26	?	9	HIS	CA	56.17	0.20	1
27	?	9	HIS	CB	30.74	0.20	1
28	?	9	HIS	N	120.44	0.33	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	100	0.35 ± 0.23	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	89	0.27 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	86	0.02 ± 0.25	None needed (< 0.5 ppm)
^{15}N	76	0.15 ± 0.89	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 18%, i.e. 971 atoms were assigned a chemical shift out of a possible 5453. 8 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	437/2242 (19%)	175/874 (20%)	186/988 (19%)	76/380 (20%)
Sidechain	522/3025 (17%)	325/1848 (18%)	189/1095 (17%)	8/82 (10%)
Aromatic	12/186 (6%)	12/102 (12%)	0/84 (0%)	0/0 (—%)
Overall	971/5453 (18%)	512/2824 (18%)	375/2167 (17%)	84/462 (18%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 18%, i.e. 971 atoms were assigned a chemical shift out of a possible 5453. 8 out of 40 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	437/2242 (19%)	175/874 (20%)	186/988 (19%)	76/380 (20%)
Sidechain	522/3025 (17%)	325/1848 (18%)	189/1095 (17%)	8/82 (10%)
Aromatic	12/186 (6%)	12/102 (12%)	0/84 (0%)	0/0 (—%)
Overall	971/5453 (18%)	512/2824 (18%)	375/2167 (17%)	84/462 (18%)

7.1.4 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
1	A	401	ARG	NE	127.48	92.63 – 76.73	26.9
1	A	410	ARG	NE	124.58	92.63 – 76.73	25.1

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:

