



wwPDB NMR Structure Validation Summary Report

Jun 3, 2020 – 12:53 pm BST

PDB ID : 6CM1
Title : MT1-MMP HPX Domain with Blade 2 Loop Bound to Nanodiscs
Authors : Marcink, T.C.; Van Doren, S.R.
Deposited on : 2018-03-02

This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>
with specific help available everywhere you see the  symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
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

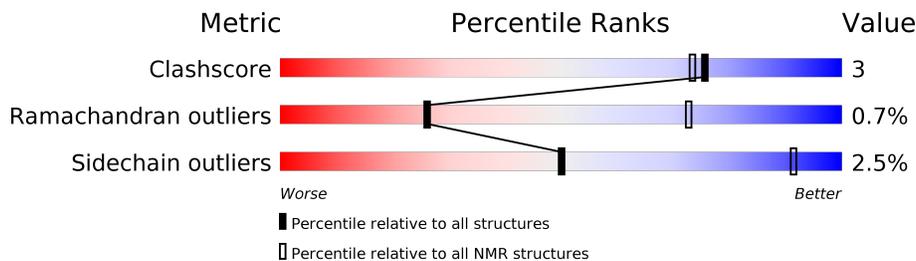
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 3%.

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	196	
2	B	211	
2	C	211	

2 Ensemble composition and analysis

This entry contains 15 models. Model 10 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:316-A:511, B:55-B:265, C:55-C:262 (615)	0.89	10

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 4 clusters. No single-model clusters were found.

Cluster number	Models
1	5, 6, 7, 8
2	9, 10, 11, 12
3	1, 2, 3, 4
4	13, 14, 15

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 35924 atoms, of which 20751 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrix metalloproteinase-14.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	196	3202	1067	1565	277	284	9	0

- Molecule 2 is a protein called Apolipoprotein A-I.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	211	3498	1101	1745	308	340	4	0
2	C	211	3498	1101	1745	308	340	4	0

There are 44 discrepancies between the modelled and reference sequences:

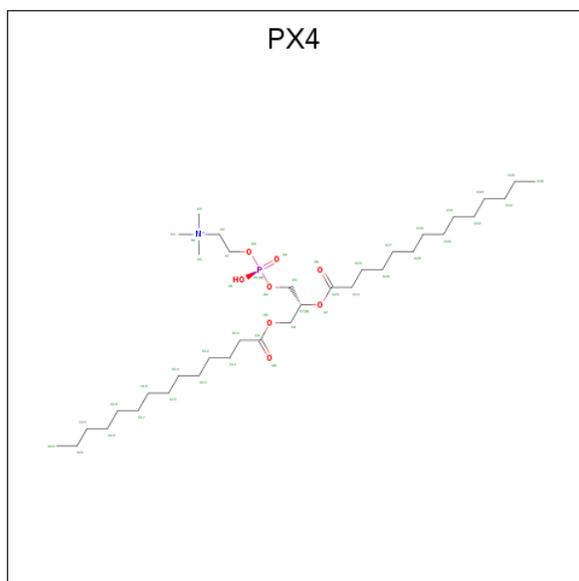
Chain	Residue	Modelled	Actual	Comment	Reference
B	99	PRO	-	insertion	UNP P02647
B	100	TYR	-	insertion	UNP P02647
B	101	LEU	-	insertion	UNP P02647
B	102	ASP	-	insertion	UNP P02647
B	103	ASP	-	insertion	UNP P02647
B	104	PHE	-	insertion	UNP P02647
B	105	GLN	-	insertion	UNP P02647
B	106	LYS	-	insertion	UNP P02647
B	107	LYS	-	insertion	UNP P02647
B	108	TRP	-	insertion	UNP P02647
B	109	GLN	-	insertion	UNP P02647
B	110	GLU	-	insertion	UNP P02647
B	111	GLU	-	insertion	UNP P02647
B	112	MET	-	insertion	UNP P02647
B	113	GLU	-	insertion	UNP P02647
B	114	LEU	-	insertion	UNP P02647
B	115	TYR	-	insertion	UNP P02647
B	116	ARG	-	insertion	UNP P02647
B	117	GLN	-	insertion	UNP P02647
B	118	LYS	-	insertion	UNP P02647
B	119	VAL	-	insertion	UNP P02647
B	120	GLU	-	insertion	UNP P02647
C	99	PRO	-	insertion	UNP P02647

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	TYR	-	insertion	UNP P02647
C	101	LEU	-	insertion	UNP P02647
C	102	ASP	-	insertion	UNP P02647
C	103	ASP	-	insertion	UNP P02647
C	104	PHE	-	insertion	UNP P02647
C	105	GLN	-	insertion	UNP P02647
C	106	LYS	-	insertion	UNP P02647
C	107	LYS	-	insertion	UNP P02647
C	108	TRP	-	insertion	UNP P02647
C	109	GLN	-	insertion	UNP P02647
C	110	GLU	-	insertion	UNP P02647
C	111	GLU	-	insertion	UNP P02647
C	112	MET	-	insertion	UNP P02647
C	113	GLU	-	insertion	UNP P02647
C	114	LEU	-	insertion	UNP P02647
C	115	TYR	-	insertion	UNP P02647
C	116	ARG	-	insertion	UNP P02647
C	117	GLN	-	insertion	UNP P02647
C	118	LYS	-	insertion	UNP P02647
C	119	VAL	-	insertion	UNP P02647
C	120	GLU	-	insertion	UNP P02647

- Molecule 3 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula: C₃₆H₇₃NO₈P).



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Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	A	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1

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Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	B	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1
3	C	1	Total 118	C 36	H 72	N 1	O 8	P 1

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Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	P
3	C	1	118	36	72	1	8	1
3	C	1	118	36	72	1	8	1
3	C	1	118	36	72	1	8	1
3	C	1	118	36	72	1	8	1
3	C	1	118	36	72	1	8	1
3	C	1	118	36	72	1	8	1
3	C	1	118	36	72	1	8	1

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	
4	A	1	Total	Na
			1	1

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	
5	A	1	Total	Cl
			1	1

4 Residue-property plots [i](#)

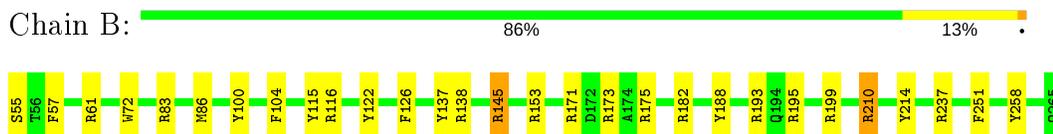
4.1 Average score per residue in the NMR ensemble

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.

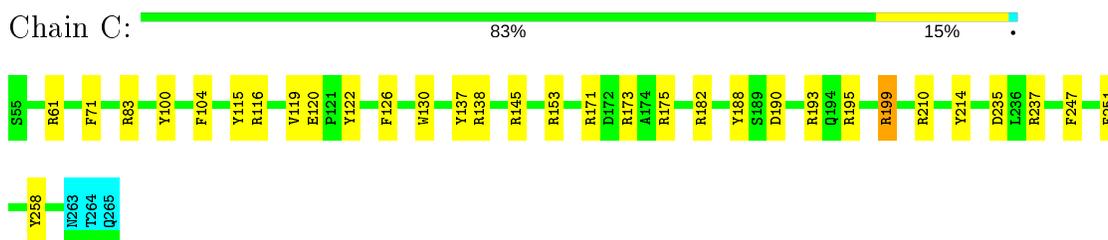
- Molecule 1: Matrix metalloproteinase-14



- Molecule 2: Apolipoprotein A-I



- Molecule 2: Apolipoprotein A-I

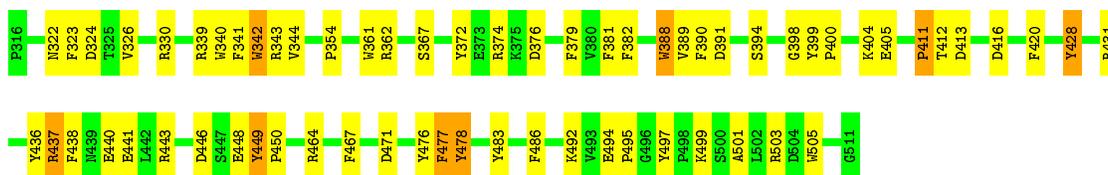


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 10. Colouring as in section 4.1 above.

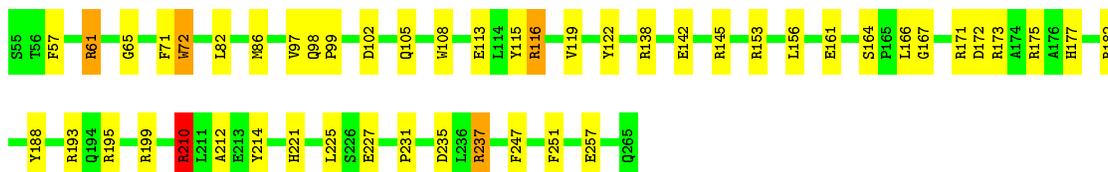
- Molecule 1: Matrix metalloproteinase-14





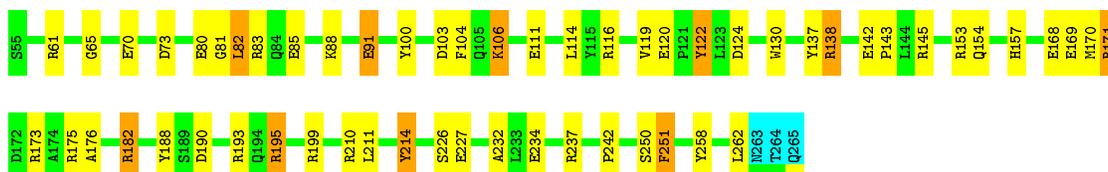
- Molecule 2: Apolipoprotein A-I

Chain B: 77% 21%



- Molecule 2: Apolipoprotein A-I

Chain C: 72% 22% 5%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *molecular dynamics*.

Of the 15 calculated structures, 15 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
HADDOCK	structure calculation	HADDOCK2.1
NAMD	refinement	NAMD2.1 with CUDA GPU processing
NAMD	structure calculation	NAMD2.1 with CUDA GPU processing

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	324
Number of shifts mapped to atoms	324
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	3%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1637	1565	1562	4±2
2	B	1753	1745	1742	3±2
2	C	1728	1724	1721	2±2
3	A	2484	3888	3888	35±5
3	B	4600	7200	7200	53±7
3	C	2944	4608	4608	29±5
All	All	227220	310950	310821	1642

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 3.

5 of 1309 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:402:HIS:CE1	3:A:649:PX4:H12	0.90	2.00	7	5
3:B:338:PX4:H4	3:B:343:PX4:O3	0.74	1.82	2	1
3:C:358:PX4:H9	3:C:361:PX4:O3	0.72	1.85	6	1
3:B:326:PX4:O3	3:B:355:PX4:H3	0.71	1.84	5	3
3:C:351:PX4:O4	3:C:351:PX4:H4	0.70	1.86	13	2

5.2 Torsion angles [i](#)

5.2.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	194/196 (99%)	176±3 (91±1%)	15±3 (8±1%)	3±1 (2±1%)	13	57
2	B	209/211 (99%)	205±2 (98±1%)	4±2 (2±1%)	0±0 (0±0%)	50	82
2	C	207/211 (98%)	202±2 (98±1%)	4±2 (2±1%)	1±1 (0±0%)	44	80
All	All	9150/9270 (99%)	8751 (96%)	338 (4%)	61 (1%)	26	73

5 of 34 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	448	GLU	5
1	A	411	PRO	4
1	A	367	SER	4
1	A	491	LEU	3
2	C	65	GLY	3

5.2.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation

was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	169/169 (100%)	163±3 (97±2%)	6±3 (3±2%)	39 86
2	B	187/187 (100%)	182±1 (97±1%)	5±1 (3±1%)	49 91
2	C	184/187 (98%)	181±1 (98±1%)	3±1 (2±1%)	66 95
All	All	8100/8145 (99%)	7897 (97%)	203 (3%)	50 91

5 of 92 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	210	ARG	15
2	B	145	ARG	15
1	A	361	TRP	14
1	A	492	LYS	14
1	A	368	ILE	7

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no carbohydrates in this entry.

LIGAND-GEOMETRY INFOmissingINFO

5.5 Other polymers [i](#)

There are no such molecules in this entry.

5.6 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Chemical shift validation [i](#)

The completeness of assignment taking into account all chemical shift lists is 3% for the well-defined parts and 3% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *Deposition_nmr_coordinates_6Aug18.txt*

6.1.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	324
Number of shifts mapped to atoms	324
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

6.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	92	1.12 \pm 0.47	Should be applied

6.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 3%, i.e. 262 atoms were assigned a chemical shift out of a possible 8120. 0 out of 99 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	184/3015 (6%)	92/1200 (8%)	0/1230 (0%)	92/585 (16%)
Sidechain	78/4392 (2%)	35/2603 (1%)	43/1554 (3%)	0/235 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	0/713 (0%)	0/377 (0%)	0/310 (0%)	0/26 (0%)
Overall	262/8120 (3%)	127/4180 (3%)	43/3094 (1%)	92/846 (11%)

6.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

6.1.5 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:

