



wwPDB NMR Structure Validation Summary Report ⓘ

Aug 7, 2020 – 01:58 AM BST

PDB ID : 5UE2
Title : proMMP-7 with heparin octasaccharide bridging between domains
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Deposited on : 2016-12-29

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:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
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 : 2.13.1
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

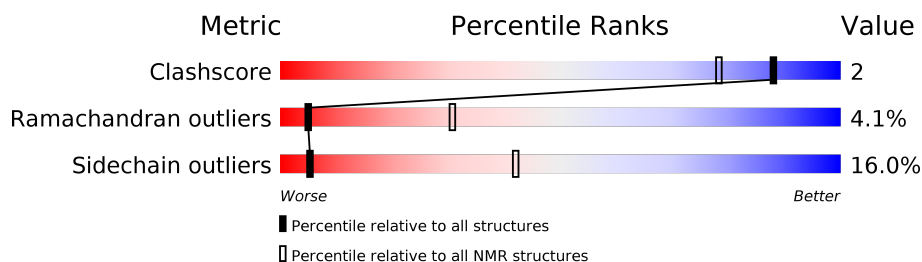
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 85%.

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	247	
2	B	8	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	B	IDS	6	1	-

2 Ensemble composition and analysis

This entry contains 16 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:15-A:22, A:34-A:71, A:83-A:216, A:224-A:239 (196)	0.41	1

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 3 single-model clusters were found.

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

3 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4032 atoms, of which 1945 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Matrilysin.

Mol	Chain	Residues	Atoms						Trace
1	A	247	Total	C	H	N	O	S	0
			3828	1234	1885	338	362	9	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	GLU	engineered mutation	UNP P09237

- Molecule 2 is an oligosaccharide called 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose.



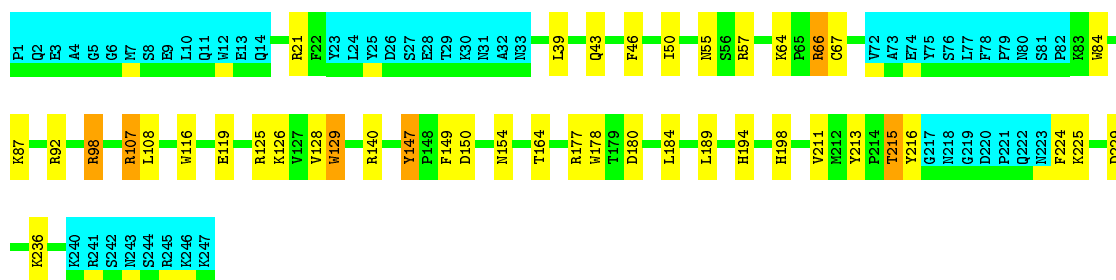
Mol	Chain	Residues	Atoms						Trace
2	B	8	Total	C	H	N	O	S	0
			200	48	60	4	76	12	

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

Mol	Chain	Residues	Atoms	
3	A	2	Total	Ca
			2	2

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
4	A	2	Total	Zn
			2	2



- Molecule 2: 2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose-(1-4)-2-O-sulfo-alpha-L-idopyranuronic acid-(1-4)-2-deoxy-6-O-sulfo-2-(sulfoamino)-alpha-D-glucopyranose

Chain B: 100%

SGN1
IDS2
SGN3
IDS4
SGN5
IDS6
SGN7
IDS8

5 Refinement protocol and experimental data overview

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

Of the 120 calculated structures, 16 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	Classification	Version
CYANA	refinement	2.1
SYBYL-X	refinement	2.1.1
CYANA	structure calculation	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2746
Number of shifts mapped to atoms	2746
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	85%

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: ZN, IDS, CA, SGN

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	0.99±0.01	0±0/1582 (0.0± 0.0%)	1.17±0.02	13±1/2141 (0.6± 0.1%)
All	All	0.99	0/25312 (0.0%)	1.17	204/34256 (0.6%)

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	1.2±1.2
All	All	0	19

There are no bond-length outliers.

5 of 23 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	107	ARG	NE-CZ-NH1	8.23	124.41	120.30	6	13
1	A	140	ARG	NE-CZ-NH1	7.97	124.28	120.30	14	15
1	A	21	ARG	NE-CZ-NH1	7.69	124.14	120.30	14	14
1	A	125	ARG	NE-CZ-NH1	7.60	124.10	120.30	9	15
1	A	66	ARG	NE-CZ-NH1	7.22	123.91	120.30	10	10

There are no chirality outliers.

5 of 11 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	216	TYR	Sidechain	5

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	46	PHE	Sidechain	3
1	A	224	PHE	Sidechain	2
1	A	147	TYR	Sidechain	2
1	A	149	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
1	A	1538	1512	1511	6±2
2	B	140	60	45	0±0
All	All	26912	25152	24897	96

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 2.

5 of 53 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:PHE:CD1	1:A:61:ILE:HD12	0.62	2.29	14	3
1:A:158:HIS:NE2	1:A:171:HIS:ND1	0.58	2.46	16	8
1:A:46:PHE:CD2	1:A:61:ILE:HD12	0.57	2.34	11	2
1:A:46:PHE:CE1	1:A:61:ILE:HD12	0.56	2.36	15	2
1:A:194:HIS:CD2	1:A:198:HIS:NE2	0.55	2.73	14	5

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	196/247 (79%)	170±3 (87±2%)	18±3 (9±1%)	8±2 (4±1%)	5	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3136/3952 (79%)	2716 (87%)	291 (9%)	129 (4%)	5	31

5 of 23 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	154	ASN	16
1	A	55	ASN	16
1	A	147	TYR	15
1	A	144	GLY	11
1	A	66	ARG	10

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	161/205 (79%)	135±5 (84±3%)	26±5 (16±3%)	5	42
All	All	2576/3280 (79%)	2165 (84%)	411 (16%)	5	42

5 of 86 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	236	LYS	16
1	A	128	VAL	16
1	A	108	LEU	16
1	A	129	TRP	16
1	A	224	PHE	15

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 ⓘ

8 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	SGN	B	1	2	18,19,20	3.66±0.00	1±0 (5±0%)
2	IDS	B	2	2	13,16,17	1.25±0.00	0±0 (0±0%)
2	SGN	B	3	2	18,19,20	3.70±0.00	1±0 (5±0%)
2	IDS	B	4	2	13,16,17	1.26±0.00	0±0 (0±0%)
2	SGN	B	5	2	18,19,20	3.71±0.00	1±0 (5±0%)
2	IDS	B	6	2	13,16,17	1.25±0.00	0±0 (0±0%)
2	SGN	B	7	2	18,19,20	3.68±0.00	1±0 (5±0%)
2	IDS	B	8	2	13,16,17	1.21±0.00	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	SGN	B	1	2	22,29,31	1.55±0.00	0±0 (0±0%)
2	IDS	B	2	2	15,24,26	1.14±0.00	0±0 (0±0%)
2	SGN	B	3	2	22,29,31	1.56±0.00	0±0 (0±0%)
2	IDS	B	4	2	15,24,26	0.99±0.00	0±0 (0±0%)
2	SGN	B	5	2	22,29,31	1.71±0.00	0±0 (0±0%)
2	IDS	B	6	2	15,24,26	1.12±0.00	0±0 (0±0%)
2	SGN	B	7	2	22,29,31	1.43±0.00	0±0 (0±0%)
2	IDS	B	8	2	15,24,26	1.06±0.00	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SGN	B	1	2	-	0±0,11,28,31	0±0,1,1,1
2	IDS	B	2	2	-	0±0,5,26,29	0±0,1,1,1
2	SGN	B	3	2	-	0±0,11,28,31	0±0,1,1,1
2	IDS	B	4	2	-	0±0,5,26,29	0±0,1,1,1
2	SGN	B	5	2	-	0±0,11,28,31	0±0,1,1,1
2	IDS	B	6	2	-	0±0,5,26,29	0±0,1,1,1
2	SGN	B	7	2	-	0±0,11,28,31	0±0,1,1,1
2	IDS	B	8	2	-	0±0,5,26,29	0±0,1,1,1

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	5	SGN	S1-N2	14.49	1.79	1.59	10	16
2	B	3	SGN	S1-N2	14.43	1.79	1.59	12	16
2	B	1	SGN	S1-N2	14.39	1.78	1.59	14	16
2	B	7	SGN	S1-N2	14.33	1.78	1.59	5	16

There are no bond-angle outliers.

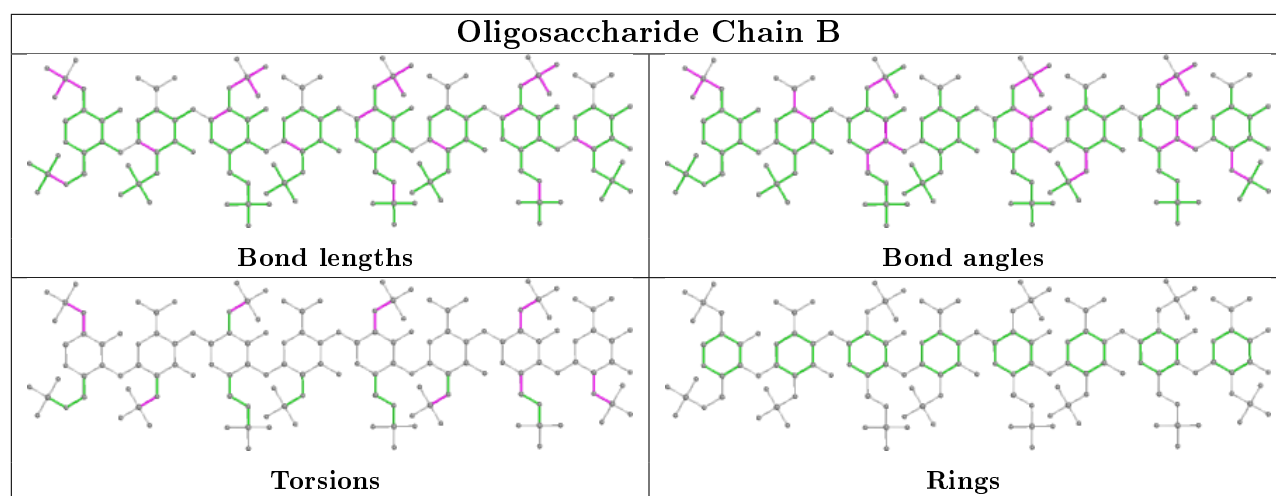
All unique chiral outliers are listed below.

Mol	Chain	Res	Type	Atoms	Models (Total)
2	B	6	IDS	C1	1

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



6.6 Ligand geometry [i](#)

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

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 85% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2746
Number of shifts mapped to atoms	2746
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	236	-0.28 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	212	0.28 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	232	0.04 ± 0.14	None needed (< 0.5 ppm)
^{15}N	220	-0.11 ± 0.42	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 85%, i.e. 2041 atoms were assigned a chemical shift out of a possible 2391. 24 out of 27 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	931/960 (97%)	367/382 (96%)	383/392 (98%)	181/186 (97%)
Sidechain	942/1173 (80%)	574/692 (83%)	358/431 (83%)	10/50 (20%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	168/258 (65%)	87/138 (63%)	77/108 (71%)	4/12 (33%)
Overall	2041/2391 (85%)	1028/1212 (85%)	818/931 (88%)	195/248 (79%)

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	107	ARG	NE	116.85	92.63 – 76.73	20.2
1	A	57	ARG	NE	115.24	92.63 – 76.73	19.2
1	A	92	ARG	NE	114.04	92.63 – 76.73	18.5
1	A	66	ARG	NE	112.31	92.63 – 76.73	17.4
1	A	247	LYS	CE	36.10	46.00 – 37.80	-7.1
1	A	162	PRO	HB2	-0.32	3.82 – 0.32	-6.8
1	A	60	GLU	HB2	0.60	3.08 – 0.98	-6.8
1	A	60	GLU	CG	43.68	42.24 – 29.94	6.2
1	A	60	GLU	HB3	0.64	3.10 – 0.90	-6.2
1	A	65	PRO	HA	2.44	6.05 – 2.75	-6.0
1	A	3	GLU	CG	43.11	42.24 – 29.94	5.7
1	A	62	MET	HG2	0.38	4.23 – 0.63	-5.7
1	A	242	SER	N	135.65	134.24 – 98.34	5.4

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:

