



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 11:51 pm GMT

PDB ID : 2LA3
Title : The NMR structure of the protein NP_344798.1 reveals a CCA-adding enzyme head domain
Authors : Mohanty, B.; Serrano, P.; Geralt, M.; Horst, R.; Wuthrich, K.; Joint Center for Structural Genomics (JCSG)
Deposited on : 2011-03-01

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
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

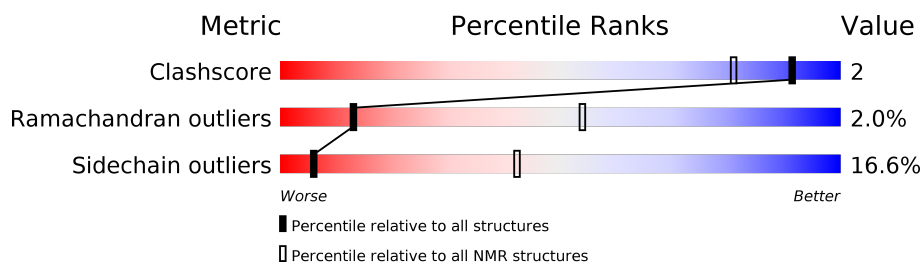
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 88%.

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	191	<div> <div style="width: 78%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 6%; background-color: cyan;"></div> </div> <div>78% 16% 6%</div>

2 Ensemble composition and analysis

This entry contains 20 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:4-A:107, A:113-A:174, A:178-A:191 (180)	0.42	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 1 single-model cluster was found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3164 atoms, of which 1555 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms							Trace
1	A	191	Total	C	H	N	O	S		0
			3164	1030	1555	268	304	7		

There is a discrepancy between the modelled and reference sequences:

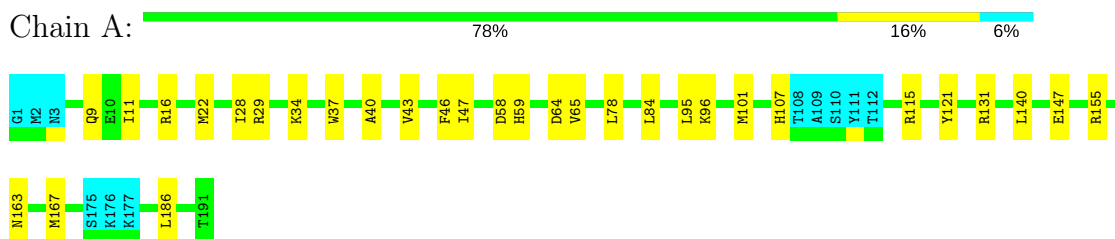
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	leader sequence	UNP Q97SR5

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: Uncharacterized protein

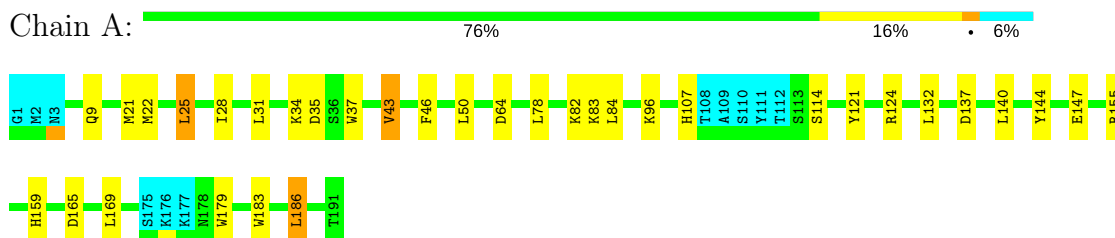


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

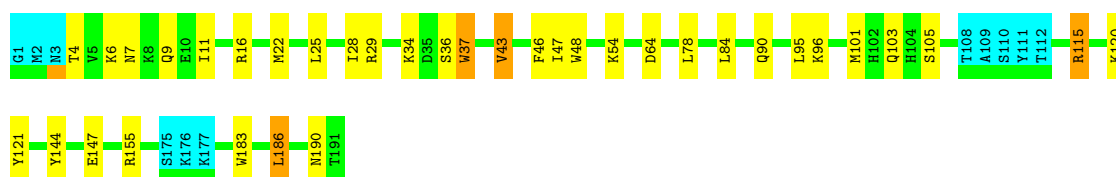
- Molecule 1: Uncharacterized protein



4.2.2 Score per residue for model 2

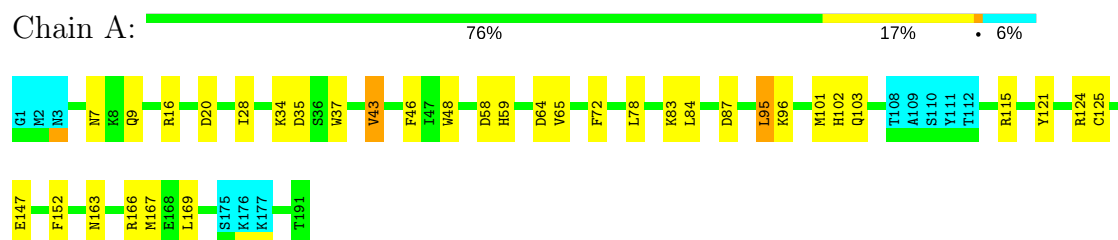
- Molecule 1: Uncharacterized protein





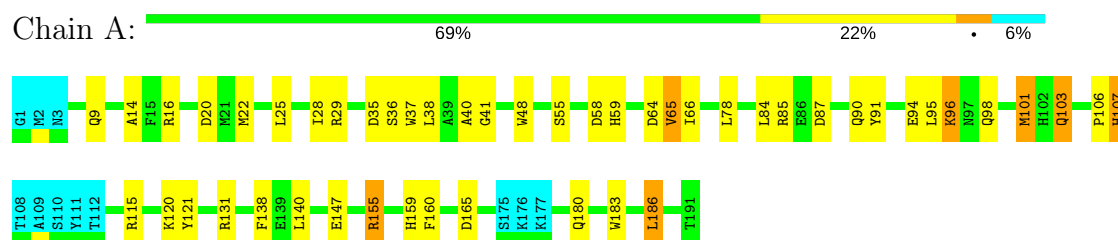
4.2.3 Score per residue for model 3

- Molecule 1: Uncharacterized protein



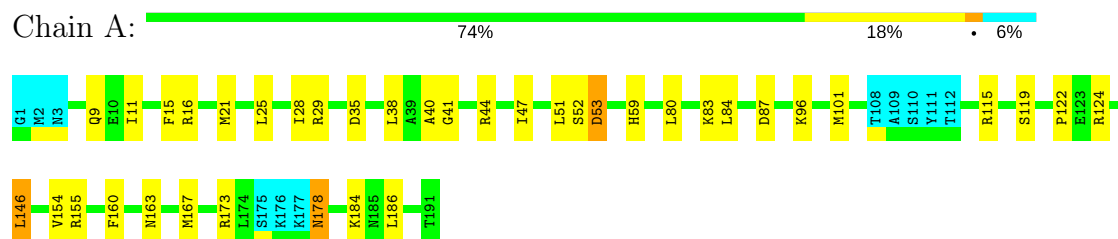
4.2.4 Score per residue for model 4

- Molecule 1: Uncharacterized protein



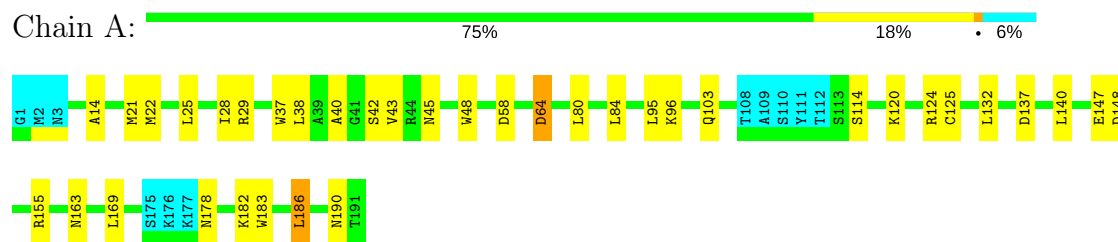
4.2.5 Score per residue for model 5

- Molecule 1: Uncharacterized protein



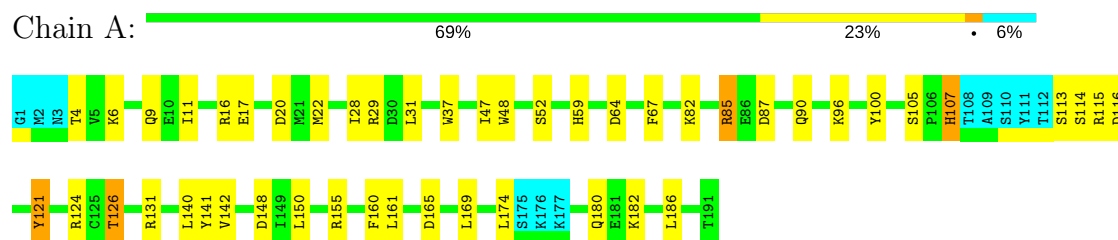
4.2.6 Score per residue for model 6

- Molecule 1: Uncharacterized protein



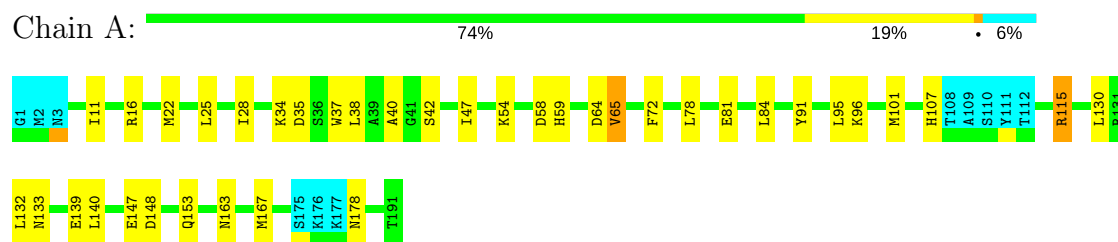
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized protein



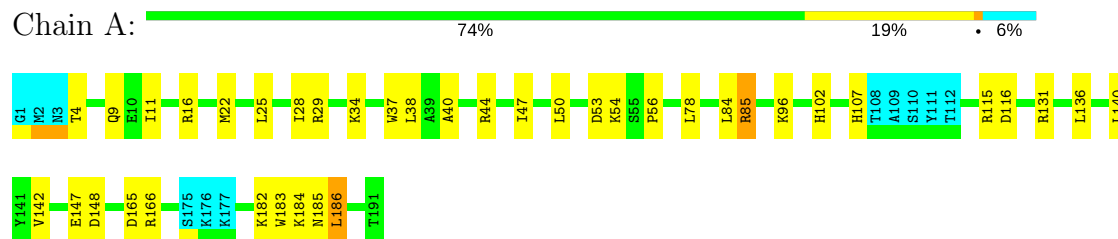
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized protein



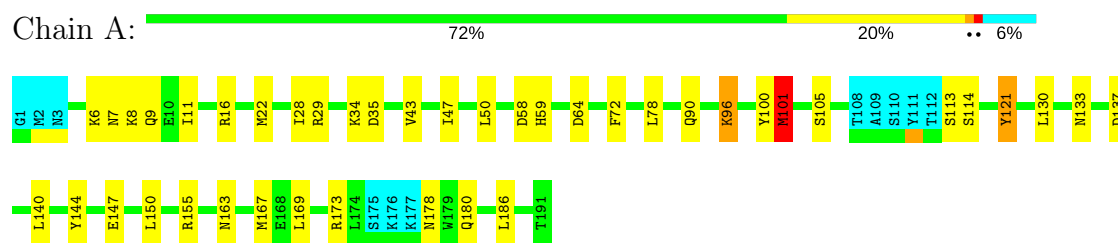
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized protein



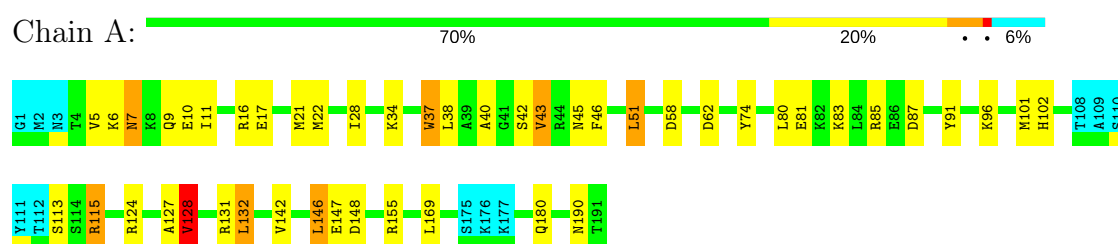
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized protein



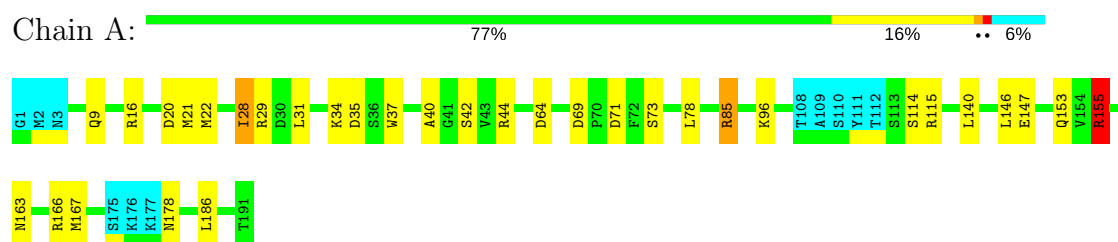
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized protein



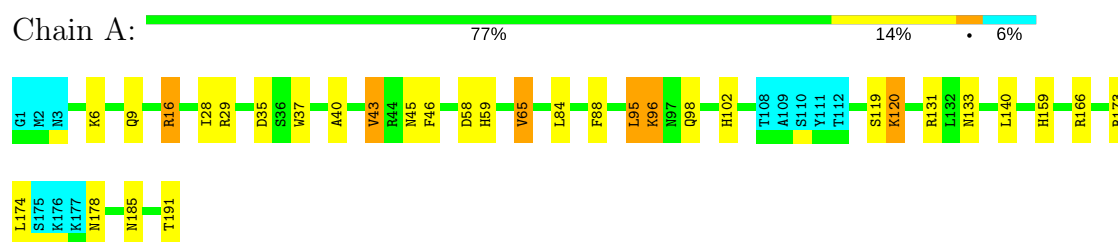
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized protein



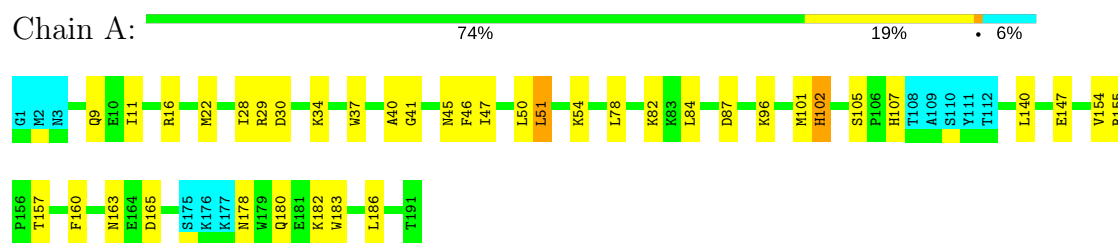
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized protein



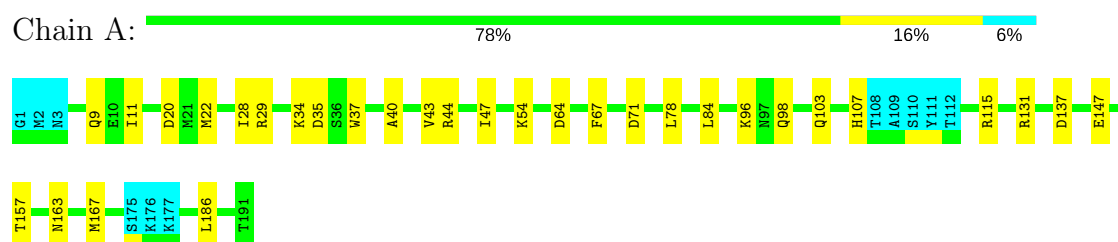
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized protein



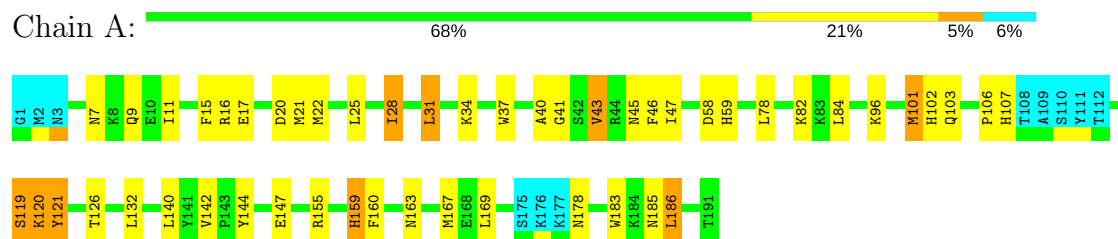
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized protein



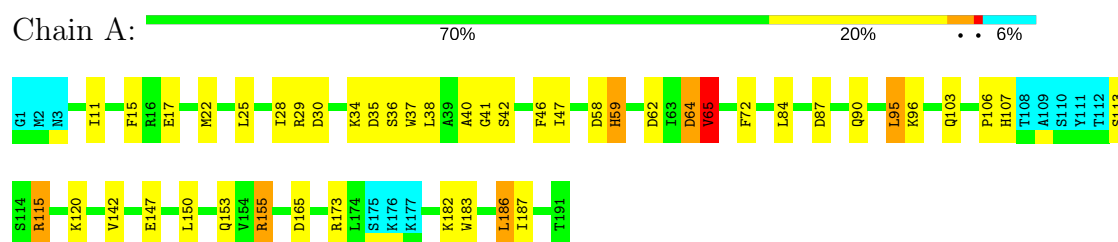
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized protein



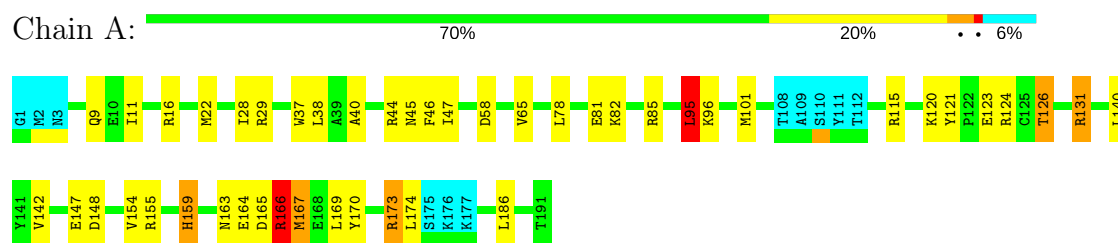
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized protein



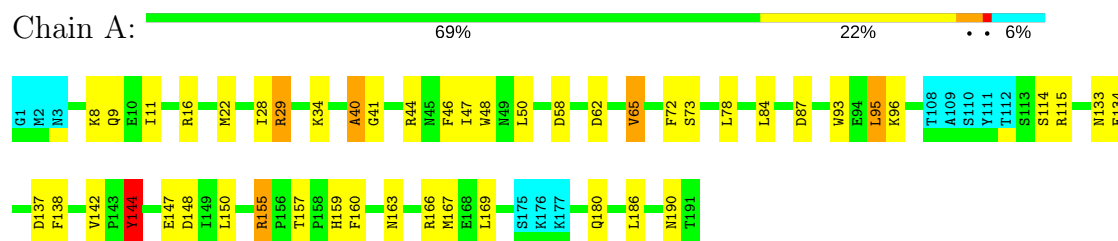
4.2.18 Score per residue for model 18

- Molecule 1: Uncharacterized protein



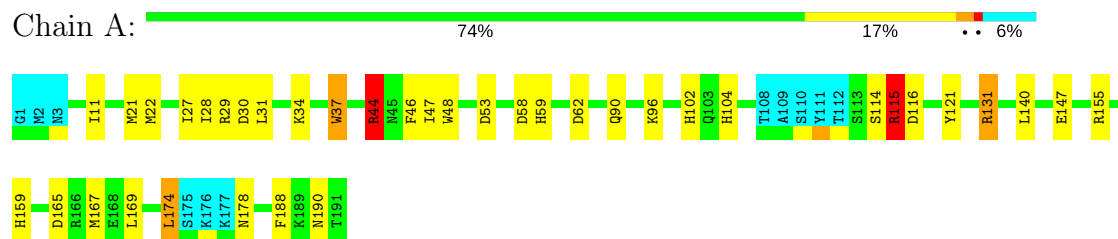
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized protein



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized protein



5 Refinement protocol and experimental data overview

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
UNIO	structure solution	2.0.0
OPALp	refinement	1.2

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)	2la3_cs.str
Number of chemical shift lists	1
Total number of shifts	2435
Number of shifts mapped to atoms	2435
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

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

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	0.63±0.01	0±0/1569 (0.0±0.0%)	1.09±0.03	3±2/2125 (0.1±0.1%)
All	All	0.63	0/31380 (0.0%)	1.09	62/42500 (0.1%)

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	2.6±1.5
All	All	0	53

There are no bond-length outliers.

All 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	144	TYR	CB-CG-CD2	-10.91	114.46	121.00	19	1
1	A	43	VAL	CA-CB-CG2	9.27	124.81	110.90	2	9
1	A	131	ARG	NE-CZ-NH2	-7.69	116.46	120.30	15	3
1	A	85	ARG	NE-CZ-NH1	7.51	124.05	120.30	9	3
1	A	144	TYR	CB-CG-CD1	6.93	125.16	121.00	19	1
1	A	43	VAL	CG1-CB-CG2	6.92	121.97	110.90	11	8
1	A	91	TYR	CB-CG-CD2	-6.87	116.88	121.00	11	1
1	A	85	ARG	NE-CZ-NH2	-6.70	116.95	120.30	12	5
1	A	155	ARG	NE-CZ-NH2	-6.60	117.00	120.30	4	1
1	A	155	ARG	CD-NE-CZ	6.54	132.75	123.60	12	1
1	A	128	VAL	CA-CB-CG2	6.20	120.20	110.90	11	1
1	A	100	TYR	CB-CG-CD2	-6.17	117.30	121.00	10	1
1	A	166	ARG	NE-CZ-NH2	-6.12	117.24	120.30	19	1
1	A	136	LEU	CB-CG-CD1	6.10	121.38	111.00	9	1
1	A	124	ARG	NE-CZ-NH2	-6.08	117.26	120.30	6	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	29	ARG	NE-CZ-NH2	-6.04	117.28	120.30	15	1
1	A	155	ARG	NE-CZ-NH1	5.55	123.07	120.30	12	2
1	A	166	ARG	NE-CZ-NH1	5.43	123.02	120.30	18	1
1	A	121	TYR	CB-CG-CD2	-5.42	117.75	121.00	10	1
1	A	29	ARG	CD-NE-CZ	5.40	131.16	123.60	12	2
1	A	40	ALA	CB-CA-C	5.37	118.15	110.10	9	1
1	A	16	ARG	NE-CZ-NH2	-5.30	117.65	120.30	13	1
1	A	53	ASP	CB-CG-OD1	5.28	123.06	118.30	5	2
1	A	131	ARG	NE-CZ-NH1	5.16	122.88	120.30	15	1
1	A	44	ARG	NE-CZ-NH2	-5.14	117.73	120.30	20	2
1	A	138	PHE	CB-CG-CD1	5.14	124.40	120.80	19	1
1	A	115	ARG	NE-CZ-NH1	5.13	122.86	120.30	2	1
1	A	124	ARG	NE-CZ-NH1	5.11	122.85	120.30	11	1
1	A	132	LEU	CB-CG-CD1	5.10	119.68	111.00	11	1
1	A	115	ARG	NE-CZ-NH2	-5.08	117.76	120.30	8	1
1	A	37	TRP	CA-CB-CG	5.06	123.31	113.70	11	2
1	A	166	ARG	CD-NE-CZ	5.05	130.67	123.60	18	2
1	A	152	PHE	CB-CG-CD1	-5.04	117.27	120.80	3	1

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	44	ARG	Sidechain	6
1	A	40	ALA	Peptide	6
1	A	144	TYR	Sidechain	5
1	A	115	ARG	Sidechain	5
1	A	155	ARG	Sidechain	4
1	A	166	ARG	Sidechain	3
1	A	85	ARG	Sidechain	3
1	A	29	ARG	Sidechain	3
1	A	131	ARG	Sidechain	2
1	A	124	ARG	Sidechain	2
1	A	173	ARG	Sidechain	2
1	A	91	TYR	Sidechain	2
1	A	170	TYR	Sidechain	1
1	A	38	LEU	Peptide	1
1	A	16	ARG	Sidechain	1
1	A	141	TYR	Sidechain	1
1	A	15	PHE	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	62	ASP	Peptide	1
1	A	104	HIS	Sidechain	1
1	A	36	SER	Peptide	1
1	A	74	TYR	Sidechain	1
1	A	121	TYR	Sidechain	1

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	1528	1473	1473	6±3
All	All	30560	29460	29460	110

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:11:ILE:HG21	1:A:47:ILE:HG12	0.68	1.65	18	13
1:A:38:LEU:HD22	1:A:42:SER:CB	0.67	2.19	6	2
1:A:121:TYR:CD2	1:A:126:THR:HG23	0.62	2.29	7	2
1:A:15:PHE:CZ	1:A:25:LEU:HD22	0.62	2.29	17	2
1:A:166:ARG:CZ	1:A:167:MET:HG3	0.60	2.26	18	1
1:A:146:LEU:C	1:A:146:LEU:HD12	0.59	2.18	11	1
1:A:146:LEU:HD12	1:A:146:LEU:C	0.58	2.19	5	1
1:A:65:VAL:HG23	1:A:95:LEU:HA	0.58	1.76	3	7
1:A:183:TRP:HB2	1:A:186:LEU:HD23	0.58	1.75	2	7
1:A:25:LEU:HD23	1:A:132:LEU:HD13	0.57	1.75	16	3
1:A:11:ILE:HG22	1:A:46:PHE:CE2	0.56	2.36	14	4
1:A:182:LYS:HE2	1:A:183:TRP:CH2	0.55	2.36	6	4
1:A:11:ILE:HG21	1:A:47:ILE:CG1	0.54	2.33	18	2
1:A:166:ARG:HG2	1:A:167:MET:N	0.53	2.18	18	1
1:A:120:LYS:HE2	1:A:159:HIS:CD2	0.53	2.38	13	2
1:A:11:ILE:HG22	1:A:46:PHE:CE1	0.52	2.40	2	2
1:A:155:ARG:HH22	1:A:187:ILE:CG2	0.51	2.19	17	1
1:A:51:LEU:H	1:A:51:LEU:HD22	0.51	1.66	14	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:TRP:CZ3	1:A:186:LEU:HD21	0.50	2.41	4	3
1:A:5:VAL:HG23	1:A:10:GLU:CB	0.49	2.37	11	1
1:A:28:ILE:HA	1:A:31:LEU:HD23	0.49	1.83	12	1
1:A:5:VAL:HG23	1:A:10:GLU:HB2	0.48	1.84	11	1
1:A:182:LYS:HE2	1:A:183:TRP:CZ2	0.48	2.44	6	1
1:A:37:TRP:CZ2	1:A:115:ARG:HD2	0.47	2.44	20	1
1:A:66:ILE:HG22	1:A:98:GLN:NE2	0.47	2.24	4	1
1:A:5:VAL:HG22	1:A:7:ASN:H	0.47	1.69	11	1
1:A:43:VAL:O	1:A:46:PHE:CD2	0.47	2.67	16	5
1:A:132:LEU:HD12	1:A:137:ASP:O	0.47	2.10	1	1
1:A:38:LEU:HD23	1:A:64:ASP:O	0.47	2.10	6	1
1:A:80:LEU:HD23	1:A:80:LEU:O	0.46	2.10	11	1
1:A:154:VAL:CG2	1:A:186:LEU:HD12	0.46	2.40	5	1
1:A:96:LYS:HE3	1:A:101:MET:CE	0.46	2.40	4	2
1:A:38:LEU:HD12	1:A:64:ASP:O	0.46	2.09	17	1
1:A:182:LYS:HG3	1:A:183:TRP:CD2	0.45	2.47	17	1
1:A:50:LEU:HD23	1:A:56:PRO:HG3	0.45	1.88	9	1
1:A:120:LYS:HE3	1:A:159:HIS:CD2	0.45	2.46	16	1
1:A:174:LEU:HD22	1:A:188:PHE:CE2	0.45	2.47	20	1
1:A:5:VAL:HG21	1:A:11:ILE:CD1	0.44	2.43	11	1
1:A:127:ALA:O	1:A:128:VAL:HG13	0.44	2.12	11	1
1:A:128:VAL:HG12	1:A:142:VAL:HG12	0.44	1.89	11	1
1:A:122:PRO:HA	1:A:160:PHE:CE1	0.43	2.48	5	1
1:A:153:GLN:NE2	1:A:155:ARG:HH21	0.43	2.11	17	2
1:A:164:GLU:HA	1:A:166:ARG:CZ	0.43	2.42	18	1
1:A:182:LYS:HG3	1:A:183:TRP:CE3	0.43	2.49	17	1
1:A:182:LYS:CE	1:A:183:TRP:CH2	0.43	3.00	6	1
1:A:121:TYR:CD2	1:A:126:THR:CG2	0.43	3.02	18	1
1:A:130:LEU:HD12	1:A:139:GLU:O	0.42	2.14	8	1
1:A:121:TYR:CD2	1:A:126:THR:HG22	0.42	2.50	16	1
1:A:25:LEU:HD22	1:A:132:LEU:HG	0.42	1.91	8	1
1:A:169:LEU:HD23	1:A:169:LEU:C	0.41	2.34	10	1
1:A:183:TRP:CB	1:A:186:LEU:HD23	0.41	2.45	6	1
1:A:48:TRP:CH2	1:A:186:LEU:HD21	0.41	2.50	7	1
1:A:154:VAL:HG21	1:A:186:LEU:HD11	0.41	1.91	14	2
1:A:166:ARG:CG	1:A:167:MET:N	0.41	2.83	18	1
1:A:25:LEU:CD2	1:A:132:LEU:HD13	0.41	2.45	1	1
1:A:28:ILE:HA	1:A:31:LEU:HD22	0.41	1.92	16	1
1:A:96:LYS:HE2	1:A:98:GLN:NE2	0.41	2.30	13	1
1:A:43:VAL:O	1:A:46:PHE:CD1	0.41	2.74	11	1
1:A:186:LEU:C	1:A:186:LEU:HD13	0.40	2.36	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:LEU:HD11	1:A:38:LEU:HD22	0.40	1.92	4	1
1:A:186:LEU:HD13	1:A:186:LEU:C	0.40	2.37	10	1

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	179/191 (94%)	156±3 (87±2%)	19±3 (11±2%)	4±2 (2±1%)	13	54
All	All	3580/3820 (94%)	3128 (87%)	380 (11%)	72 (2%)	13	54

All 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	107	HIS	8
1	A	40	ALA	8
1	A	59	HIS	8
1	A	102	HIS	6
1	A	41	GLY	6
1	A	178	ASN	6
1	A	101	MET	5
1	A	103	GLN	4
1	A	4	THR	3
1	A	95	LEU	3
1	A	106	PRO	3
1	A	184	LYS	1
1	A	27	ILE	1
1	A	35	ASP	1
1	A	119	SER	1
1	A	128	VAL	1
1	A	94	GLU	1
1	A	174	LEU	1
1	A	179	TRP	1
1	A	50	LEU	1

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Mol	Chain	Res	Type	Models (Total)
1	A	93	TRP	1
1	A	65	VAL	1
1	A	100	TYR	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	170/179 (95%)	142±5 (83±3%)	28±5 (17±3%)	6	42
All	All	3400/3580 (95%)	2837 (83%)	563 (17%)	6	42

All 104 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	28	ILE	20
1	A	96	LYS	20
1	A	147	GLU	17
1	A	37	TRP	17
1	A	22	MET	17
1	A	9	GLN	16
1	A	34	LYS	14
1	A	16	ARG	14
1	A	84	LEU	14
1	A	78	LEU	13
1	A	140	LEU	13
1	A	155	ARG	12
1	A	115	ARG	12
1	A	58	ASP	12
1	A	163	ASN	11
1	A	64	ASP	11
1	A	167	MET	10
1	A	29	ARG	10
1	A	169	LEU	9
1	A	186	LEU	9
1	A	35	ASP	9
1	A	87	ASP	8

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Mol	Chain	Res	Type	Models (Total)
1	A	165	ASP	8
1	A	21	MET	7
1	A	148	ASP	7
1	A	114	SER	7
1	A	101	MET	7
1	A	121	TYR	7
1	A	20	ASP	6
1	A	120	LYS	6
1	A	159	HIS	6
1	A	142	VAL	6
1	A	45	ASN	6
1	A	180	GLN	6
1	A	90	GLN	6
1	A	95	LEU	5
1	A	6	LYS	5
1	A	54	LYS	5
1	A	160	PHE	5
1	A	82	LYS	5
1	A	65	VAL	5
1	A	7	ASN	5
1	A	190	ASN	5
1	A	131	ARG	5
1	A	72	PHE	5
1	A	137	ASP	4
1	A	105	SER	4
1	A	150	LEU	4
1	A	133	ASN	4
1	A	173	ARG	4
1	A	31	LEU	4
1	A	17	GLU	4
1	A	103	GLN	4
1	A	83	LYS	4
1	A	25	LEU	4
1	A	113	SER	4
1	A	178	ASN	4
1	A	116	ASP	3
1	A	107	HIS	3
1	A	62	ASP	3
1	A	157	THR	3
1	A	48	TRP	3
1	A	185	ASN	3
1	A	50	LEU	3

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Mol	Chain	Res	Type	Models (Total)
1	A	174	LEU	3
1	A	146	LEU	3
1	A	30	ASP	3
1	A	124	ARG	3
1	A	81	GLU	3
1	A	119	SER	3
1	A	59	HIS	3
1	A	42	SER	3
1	A	38	LEU	3
1	A	80	LEU	2
1	A	166	ARG	2
1	A	51	LEU	2
1	A	36	SER	2
1	A	53	ASP	2
1	A	71	ASP	2
1	A	125	CYS	2
1	A	67	PHE	2
1	A	52	SER	2
1	A	126	THR	2
1	A	73	SER	2
1	A	102	HIS	2
1	A	8	LYS	2
1	A	184	LYS	1
1	A	128	VAL	1
1	A	55	SER	1
1	A	123	GLU	1
1	A	88	PHE	1
1	A	153	GLN	1
1	A	144	TYR	1
1	A	85	ARG	1
1	A	138	PHE	1
1	A	132	LEU	1
1	A	44	ARG	1
1	A	161	LEU	1
1	A	191	THR	1
1	A	69	ASP	1
1	A	98	GLN	1
1	A	182	LYS	1
1	A	130	LEU	1
1	A	134	GLU	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 88% for the well-defined parts and 88% for the entire structure.

7.1 Chemical shift list 1

File name: 2la3_cs.str

Chemical shift list name: *PS_June022010_BM5_CarbonylsShifts.str*

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	2435
Number of shifts mapped to atoms	2435
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	189	-0.32 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	184	0.18 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	129	-0.40 ± 0.12	None needed (< 0.5 ppm)
^{15}N	177	0.40 ± 0.23	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 88%, i.e. 2106 atoms were assigned a chemical shift out of a possible 2390. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	814/882 (92%)	346/351 (99%)	300/360 (83%)	168/171 (98%)
Sidechain	1079/1258 (86%)	671/741 (91%)	383/458 (84%)	25/59 (42%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	213/250 (85%)	110/133 (83%)	98/107 (92%)	5/10 (50%)
Overall	2106/2390 (88%)	1127/1225 (92%)	781/925 (84%)	198/240 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 88%, i.e. 2211 atoms were assigned a chemical shift out of a possible 2513. 0 out of 29 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	861/937 (92%)	366/373 (98%)	318/382 (83%)	177/182 (97%)
Sidechain	1129/1318 (86%)	703/777 (90%)	400/479 (84%)	26/62 (42%)
Aromatic	221/258 (86%)	114/137 (83%)	102/111 (92%)	5/10 (50%)
Overall	2211/2513 (88%)	1183/1287 (92%)	820/972 (84%)	208/254 (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	44	ARG	HG3	-1.30	3.00 – 0.10	-9.8
1	A	115	ARG	HG2	-0.84	2.92 – 0.22	-8.9
1	A	131	ARG	HD3	1.32	4.36 – 1.86	-7.2
1	A	143	PRO	HD3	1.06	5.52 – 1.72	-6.7
1	A	20	ASP	HB2	1.24	4.07 – 1.37	-5.5
1	A	44	ARG	HD2	1.86	4.27 – 1.97	-5.5
1	A	182	LYS	HB3	0.33	3.10 – 0.40	-5.3
1	A	44	ARG	HD3	1.81	4.36 – 1.86	-5.2
1	A	20	ASP	HB3	1.24	4.07 – 1.27	-5.1

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:

