



Full wwPDB NMR Structure Validation Report ⓘ

Mar 25, 2026 – 02:18 AM UTC

PDB ID : 2IUE / pdb_00002iue
BMRB ID : 7313
Title : Pactolus I-domain: Functional Switching of the Rossmann Fold
Authors : Sen, M.; Legge, G.B.
Deposited on : 2006-06-02

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

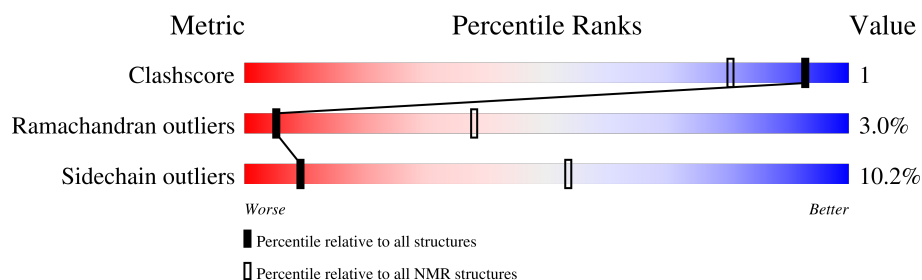
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 25%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	212	

2 Ensemble composition and analysis

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 20 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:3-A:13, A:40-A:60, A:75-A:194 (152)	0.38	20

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 2 clusters and 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2813 atoms, of which 1168 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called INTEGRIN BETA-2-LIKE PROTEIN.

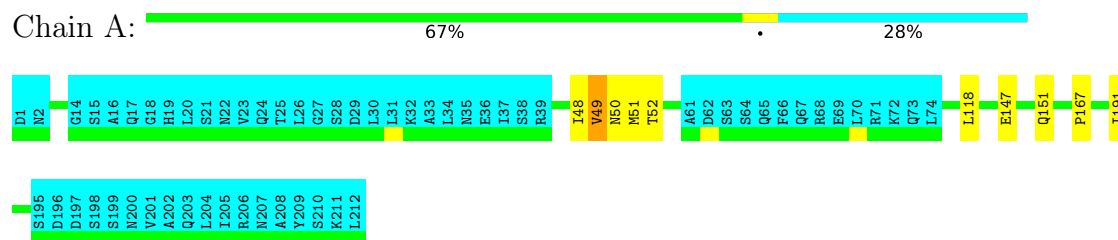
Mol	Chain	Residues	Atoms						Trace
1	A	212	Total	C	H	N	O	S	0
			2813	1029	1168	293	317	6	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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: INTEGRIN BETA-2-LIKE PROTEIN

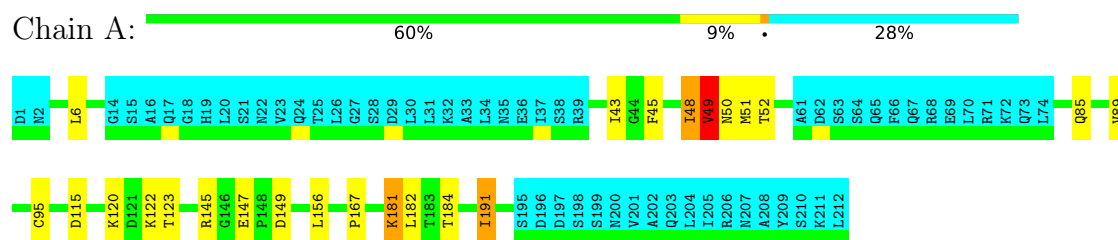


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

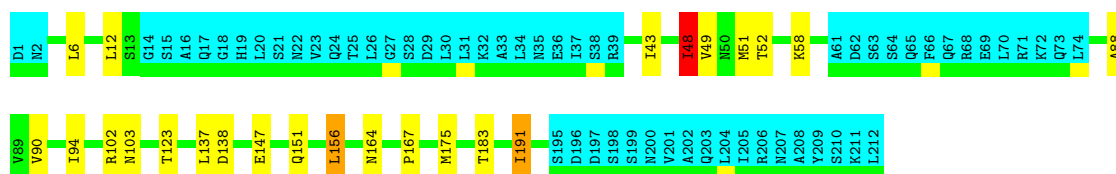
- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



4.2.2 Score per residue for model 2

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN





4.2.3 Score per residue for model 3

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN

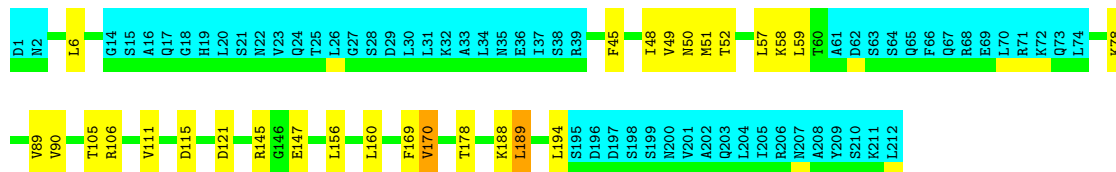
Chain A: 59% 9% 28%



4.2.4 Score per residue for model 4

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN

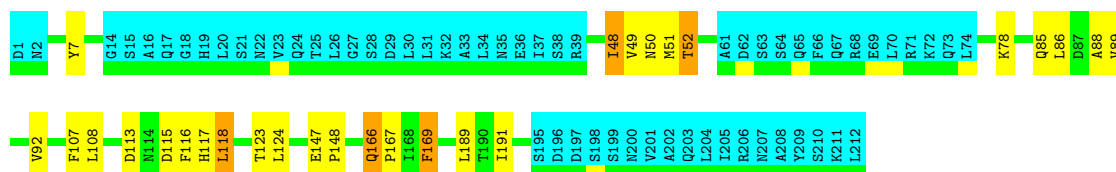
Chain A: 58% 12% 28%



4.2.5 Score per residue for model 5

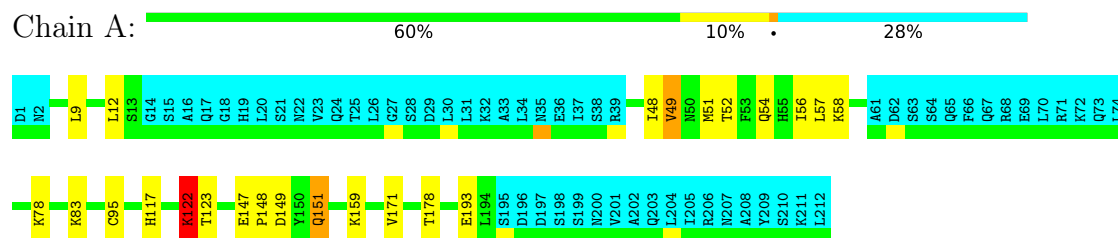
- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN

Chain A: 58% 11% 28%



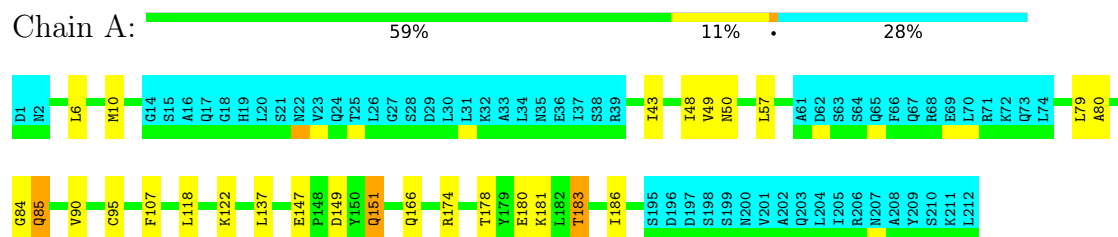
4.2.6 Score per residue for model 6

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



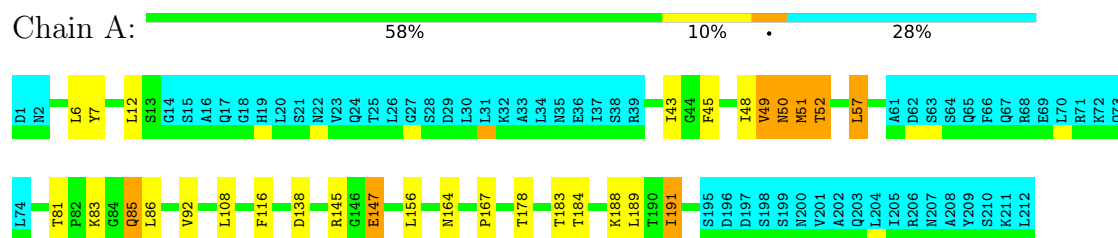
4.2.7 Score per residue for model 7

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



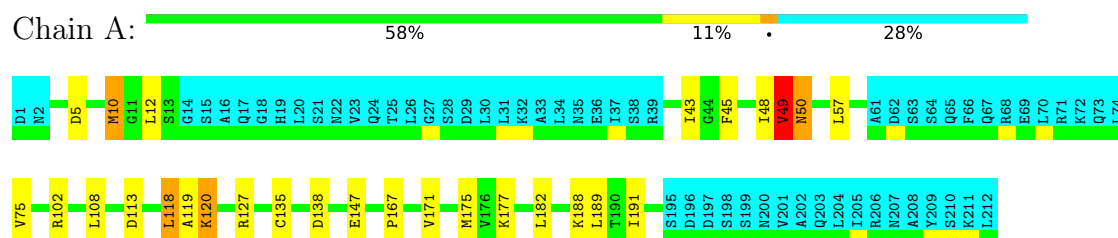
4.2.8 Score per residue for model 8

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



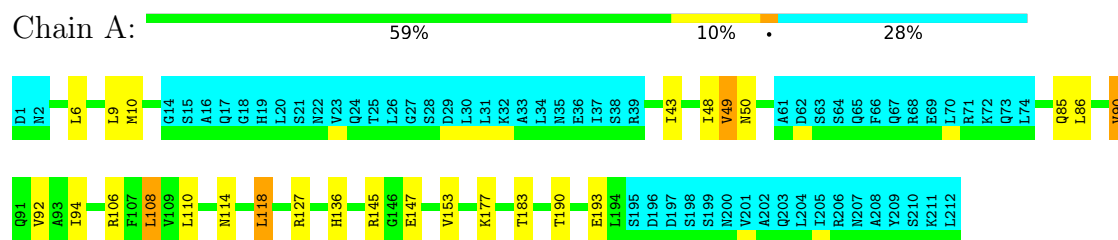
4.2.9 Score per residue for model 9

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



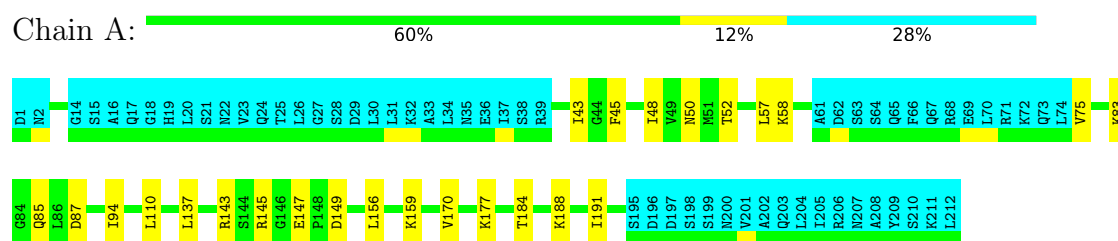
4.2.10 Score per residue for model 10

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



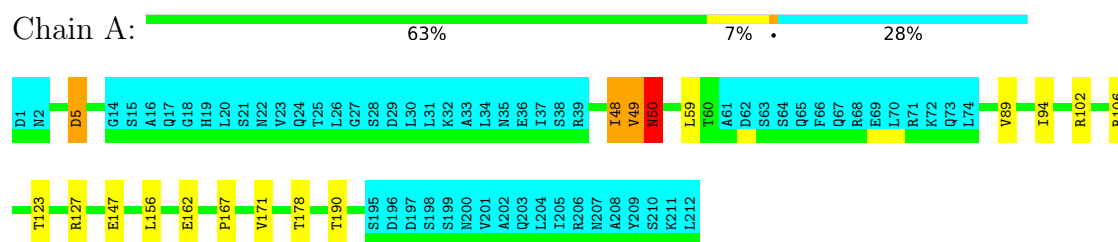
4.2.11 Score per residue for model 11

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



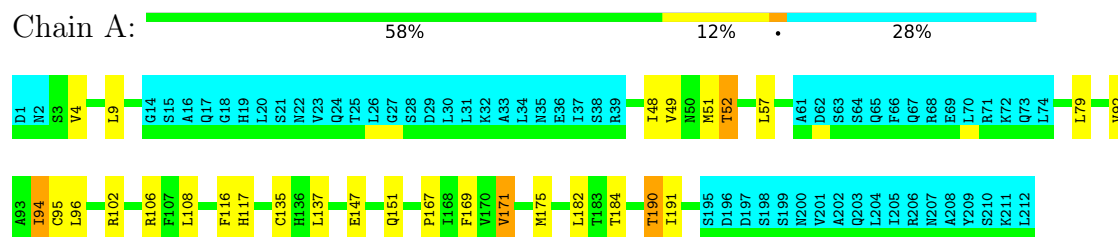
4.2.12 Score per residue for model 12

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



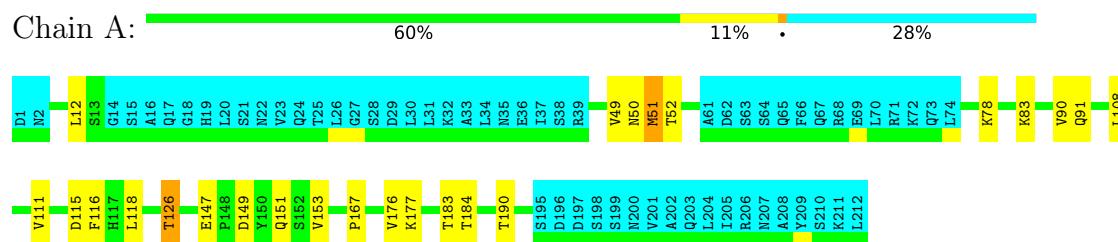
4.2.13 Score per residue for model 13

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



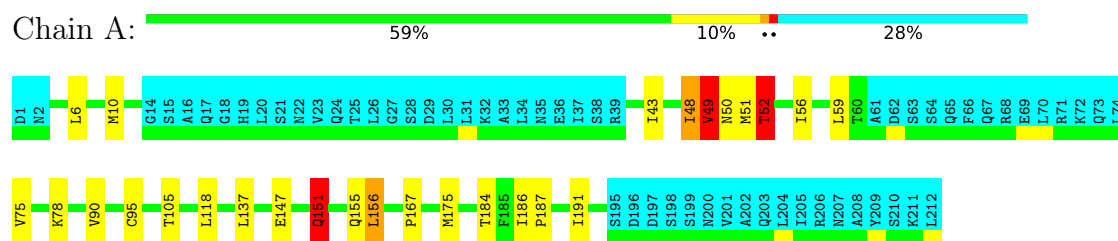
4.2.14 Score per residue for model 14

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



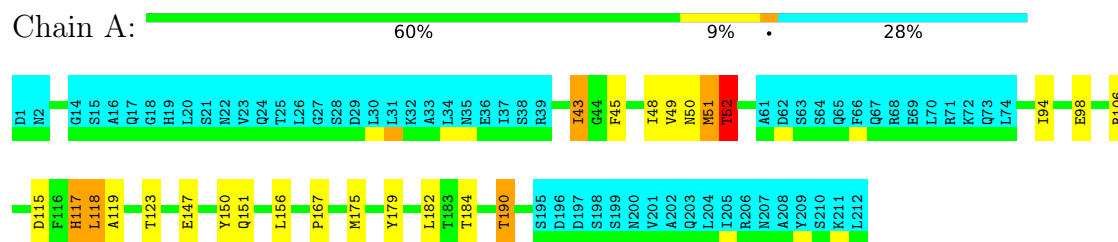
4.2.15 Score per residue for model 15

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



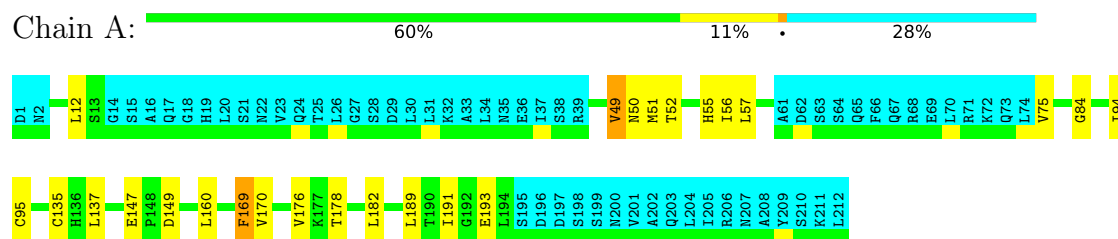
4.2.16 Score per residue for model 16

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



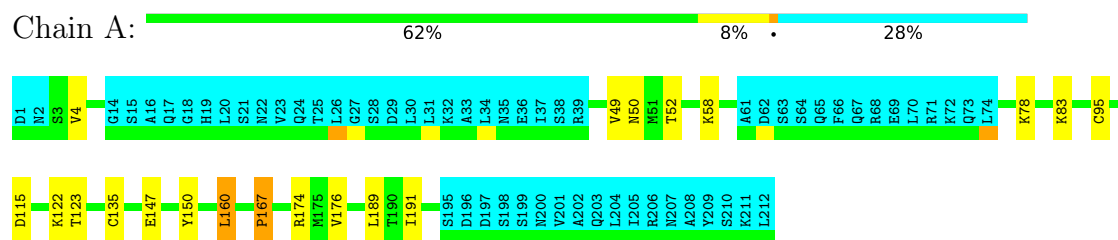
4.2.17 Score per residue for model 17

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



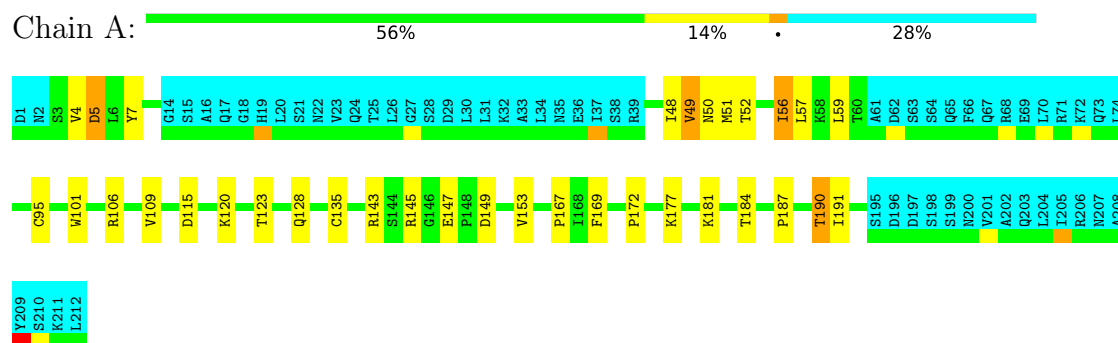
4.2.18 Score per residue for model 18

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



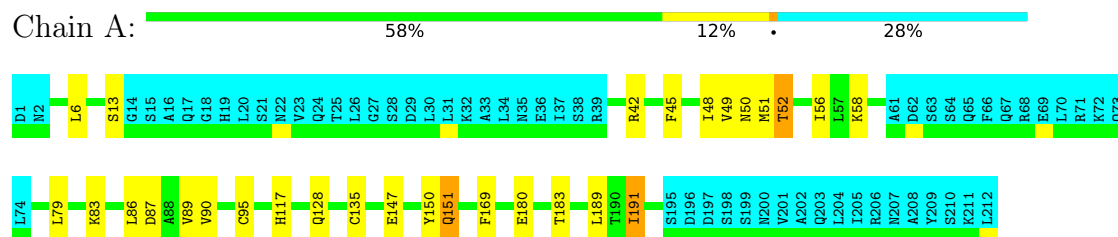
4.2.19 Score per residue for model 19

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



4.2.20 Score per residue for model 20 (medoid)

- Molecule 1: INTEGRIN BETA-2-LIKE PROTEIN



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DYANA AMBER 8.0 AND MODELLER8V2*.

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *LOWEST POTENTIAL ENERGY ENSEMBLES*.

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

Software name	Classification	Version
Amber	refinement	8.0
NMRPipe	structure solution	
NMRView	structure solution	
DYANA	structure solution	
Amber	structure solution	8.0
MOLMOL	structure solution	
MODELLER	structure solution	

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	804
Number of shifts mapped to atoms	798
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

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±0.01	0±0/1203 (0.0± 0.0%)	1.54±0.04	9±4/1627 (0.5± 0.2%)
All	All	0.89	1/24060 (0.0%)	1.54	176/32540 (0.5%)

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	1.1±1.0
All	All	0	22

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	138	ASP	CA-C	5.65	1.55	1.52	8	1

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	51	MET	N-CA-C	-10.09	98.99	112.72	15	3
1	A	149	ASP	CA-CB-CG	9.90	122.50	112.60	7	8
1	A	5	ASP	CA-CB-CG	9.72	122.32	112.60	12	3
1	A	166	GLN	CB-CA-C	9.26	119.34	110.17	5	1
1	A	169	PHE	CA-CB-CG	8.68	122.48	113.80	5	5
1	A	51	MET	CA-C-N	8.26	137.32	121.54	15	13
1	A	51	MET	C-N-CA	8.26	137.32	121.54	15	13
1	A	148	PRO	CA-C-N	8.15	133.08	121.42	6	2
1	A	148	PRO	C-N-CA	8.15	133.08	121.42	6	2
1	A	43	ILE	CA-C-N	8.15	127.88	121.61	16	5

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	43	ILE	C-N-CA	8.15	127.88	121.61	16	5
1	A	85	GLN	N-CA-C	6.65	119.35	111.71	5	2
1	A	49	VAL	CA-C-N	6.55	134.05	121.54	20	6
1	A	49	VAL	C-N-CA	6.55	134.05	121.54	20	6
1	A	149	ASP	N-CA-CB	-6.49	100.26	110.06	6	1
1	A	167	PRO	N-CA-CB	6.32	109.22	103.34	16	10
1	A	116	PHE	CA-CB-CG	6.30	120.10	113.80	13	1
1	A	126	THR	CB-CA-C	6.30	121.40	111.95	14	1
1	A	50	ASN	CB-CA-C	6.28	118.78	109.29	4	1
1	A	183	THR	CA-CB-CG2	6.27	121.15	110.50	7	1
1	A	190	THR	CA-C-N	6.25	130.33	121.96	12	5
1	A	190	THR	C-N-CA	6.25	130.33	121.96	12	5
1	A	87	ASP	CA-CB-CG	6.22	118.82	112.60	11	1
1	A	117	HIS	CA-CB-CG	6.22	120.02	113.80	16	1
1	A	95	CYS	CA-C-N	6.20	128.91	120.54	6	3
1	A	95	CYS	C-N-CA	6.20	128.91	120.54	6	3
1	A	78	LYS	CA-C-N	6.08	128.68	120.65	18	2
1	A	78	LYS	C-N-CA	6.08	128.68	120.65	18	2
1	A	75	VAL	N-CA-C	5.94	116.53	110.05	15	1
1	A	185	PHE	CA-CB-CG	5.94	119.74	113.80	3	1
1	A	171	VAL	CA-C-N	5.85	125.81	119.78	6	4
1	A	171	VAL	C-N-CA	5.85	125.81	119.78	6	4
1	A	151	GLN	CA-CB-CG	5.75	125.60	114.10	15	1
1	A	50	ASN	CA-CB-CG	5.75	118.35	112.60	12	1
1	A	10	MET	N-CA-C	5.73	118.82	109.59	15	1
1	A	5	ASP	CB-CA-C	5.72	118.97	110.62	9	1
1	A	181	LYS	N-CA-CB	5.61	119.20	110.44	1	1
1	A	123	THR	N-CA-C	5.61	118.16	111.71	3	1
1	A	117	HIS	CB-CG-CD2	-5.61	123.91	131.20	20	5
1	A	105	THR	CB-CA-C	5.59	119.61	109.37	15	1
1	A	87	ASP	N-CA-C	-5.58	104.59	111.40	20	1
1	A	186	ILE	N-CA-C	5.56	113.66	108.15	7	1
1	A	94	ILE	CA-CB-CG1	5.53	119.81	110.40	13	1
1	A	56	ILE	CB-CA-C	5.53	120.36	111.29	19	1
1	A	55	HIS	CB-CG-CD2	-5.53	124.01	131.20	17	1
1	A	128	GLN	N-CA-CB	-5.52	103.25	110.59	20	1
1	A	48	ILE	N-CA-C	5.51	116.29	108.42	2	1
1	A	151	GLN	OE1-CD-NE2	-5.50	117.10	122.60	13	1
1	A	111	VAL	N-CA-C	5.50	115.81	108.11	14	1
1	A	172	PRO	N-CA-CB	5.48	107.93	103.32	19	1
1	A	52	THR	CB-CA-C	5.46	121.29	110.42	15	1

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	190	THR	CB-CA-C	5.43	124.69	111.65	13	1
1	A	49	VAL	CB-CA-C	5.42	120.17	111.29	6	1
1	A	122	LYS	N-CA-C	5.39	119.34	112.87	6	1
1	A	86	LEU	CB-CA-C	5.35	120.26	110.36	20	1
1	A	168	ILE	CB-CA-C	5.34	116.49	110.41	3	1
1	A	190	THR	CA-CB-CG2	5.31	119.53	110.50	19	1
1	A	187	PRO	CA-C-N	5.29	131.64	121.54	19	2
1	A	187	PRO	C-N-CA	5.29	131.64	121.54	19	2
1	A	52	THR	CA-CB-CG2	5.24	119.41	110.50	16	1
1	A	91	GLN	OE1-CD-NE2	-5.21	117.39	122.60	14	1
1	A	52	THR	CA-CB-OG1	-5.21	101.79	109.60	15	1
1	A	80	ALA	CA-C-N	5.19	126.21	119.78	7	1
1	A	80	ALA	C-N-CA	5.19	126.21	119.78	7	1
1	A	85	GLN	CA-C-N	5.17	127.92	120.38	7	1
1	A	85	GLN	C-N-CA	5.17	127.92	120.38	7	1
1	A	85	GLN	OE1-CD-NE2	-5.15	117.45	122.60	10	2
1	A	164	ASN	CA-CB-CG	5.14	117.74	112.60	2	1
1	A	122	LYS	CA-C-N	5.09	127.61	120.28	3	1
1	A	122	LYS	C-N-CA	5.09	127.61	120.28	3	1
1	A	182	LEU	N-CA-C	-5.08	107.21	113.41	9	1
1	A	52	THR	CA-C-N	5.07	130.29	122.93	13	1
1	A	52	THR	C-N-CA	5.07	130.29	122.93	13	1
1	A	84	GLY	CA-C-N	5.06	131.20	121.54	7	2
1	A	84	GLY	C-N-CA	5.06	131.20	121.54	7	2
1	A	119	ALA	CA-C-N	5.02	131.13	121.54	16	1
1	A	119	ALA	C-N-CA	5.02	131.13	121.54	16	1
1	A	136	HIS	CB-CG-CD2	-5.00	124.70	131.20	10	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	45	PHE	Sidechain	6
1	A	145	ARG	Sidechain	4
1	A	116	PHE	Sidechain	2
1	A	7	TYR	Sidechain	2
1	A	106	ARG	Sidechain	2
1	A	174	ARG	Sidechain	1
1	A	169	PHE	Sidechain	1
1	A	127	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	102	ARG	Sidechain	1
1	A	42	ARG	Sidechain	1
1	A	150	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	1182	856	1210	3±2
All	All	23640	17123	24200	66

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 1.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:HG12	1:A:170:VAL:HG22	0.70	1.63	4	1
1:A:10:MET:HE2	1:A:45:PHE:CZ	0.70	2.21	9	1
1:A:90:VAL:HG21	1:A:156:LEU:HD22	0.65	1.69	15	1
1:A:86:LEU:HD23	1:A:156:LEU:HD21	0.62	1.72	8	1
1:A:151:GLN:H	1:A:151:GLN:CD	0.58	2.05	14	5
1:A:10:MET:HE1	1:A:12:LEU:HD21	0.57	1.75	9	1
1:A:85:GLN:CG	1:A:110:LEU:HD21	0.55	2.32	11	1
1:A:181:LYS:O	1:A:184:THR:HG22	0.54	2.02	19	1
1:A:51:MET:O	1:A:52:THR:HG23	0.52	2.05	8	2
1:A:90:VAL:O	1:A:94:ILE:HD12	0.52	2.05	10	2
1:A:151:GLN:NE2	1:A:151:GLN:H	0.51	2.02	15	1
1:A:48:ILE:HD13	1:A:49:VAL:N	0.50	2.21	1	3
1:A:50:ASN:C	1:A:52:THR:H	0.50	2.14	15	2
1:A:160:LEU:HD22	1:A:167:PRO:HG3	0.48	1.84	18	1
1:A:92:VAL:HG11	1:A:108:LEU:HD13	0.48	1.85	3	2
1:A:90:VAL:CG1	1:A:156:LEU:HD22	0.47	2.39	2	1
1:A:171:VAL:HB	1:A:175:MET:HE3	0.47	1.86	13	1
1:A:118:LEU:HD22	1:A:119:ALA:H	0.47	1.70	9	1
1:A:49:VAL:CG2	1:A:50:ASN:H	0.47	2.22	15	1
1:A:170:VAL:HG23	1:A:194:LEU:HB2	0.46	1.86	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:59:LEU:HD11	1:A:101:TRP:CE3	0.46	2.46	19	1
1:A:169:PHE:CD2	1:A:189:LEU:HD21	0.46	2.45	17	2
1:A:49:VAL:HG23	1:A:50:ASN:H	0.46	1.70	15	1
1:A:169:PHE:CD2	1:A:189:LEU:HD11	0.46	2.46	20	1
1:A:167:PRO:HG2	1:A:189:LEU:HG	0.45	1.88	5	2
1:A:122:LYS:HE3	1:A:150:TYR:CZ	0.45	2.47	18	1
1:A:122:LYS:HE2	1:A:127:ARG:CG	0.45	2.42	3	1
1:A:118:LEU:HD23	1:A:118:LEU:H	0.45	1.71	16	1
1:A:10:MET:CE	1:A:45:PHE:CZ	0.44	2.98	9	1
1:A:50:ASN:C	1:A:52:THR:N	0.44	2.75	15	1
1:A:90:VAL:HG21	1:A:151:GLN:CG	0.44	2.43	20	1
1:A:180:GLU:O	1:A:183:THR:HG22	0.44	2.11	7	1
1:A:107:PHE:CD2	1:A:166:GLN:HB2	0.44	2.48	7	1
1:A:9:LEU:HD12	1:A:92:VAL:HG21	0.43	1.89	10	1
1:A:48:ILE:HD13	1:A:88:ALA:HB2	0.43	1.89	5	1
1:A:5:ASP:HB2	1:A:59:LEU:HD13	0.43	1.90	19	1
1:A:122:LYS:N	1:A:122:LYS:HE2	0.43	2.29	6	1
1:A:117:HIS:HB3	1:A:150:TYR:CE2	0.43	2.49	16	1
1:A:118:LEU:HD21	1:A:153:VAL:HG23	0.43	1.90	10	1
1:A:118:LEU:H	1:A:118:LEU:CD2	0.43	2.27	16	1
1:A:7:TYR:CD1	1:A:92:VAL:HG21	0.42	2.49	5	1
1:A:86:LEU:HB2	1:A:116:PHE:CZ	0.42	2.49	8	2
1:A:120:LYS:O	1:A:123:THR:HG22	0.42	2.15	19	1
1:A:118:LEU:H	1:A:118:LEU:HD13	0.42	1.75	5	1
1:A:175:MET:CE	1:A:179:TYR:CE1	0.42	3.02	16	1
1:A:108:LEU:HD13	1:A:110:LEU:HD13	0.41	1.91	10	1
1:A:92:VAL:HG11	1:A:108:LEU:HD23	0.41	1.93	8	1
1:A:90:VAL:HG21	1:A:151:GLN:HG3	0.41	1.91	20	1
1:A:13:SER:OG	1:A:83:LYS:HE2	0.41	2.15	20	1
1:A:151:GLN:H	1:A:151:GLN:NE2	0.41	2.13	20	1
1:A:86:LEU:HD22	1:A:116:PHE:CE2	0.40	2.51	5	1
1:A:48:ILE:HG21	1:A:88:ALA:HB2	0.40	1.92	2	1
1:A:107:PHE:CE1	1:A:166:GLN:HG3	0.40	2.52	5	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	152/212 (72%)	133±2 (87±1%)	15±2 (10±1%)	5±2 (3±1%)	5	38
All	All	3040/4240 (72%)	2655 (87%)	294 (10%)	91 (3%)	5	38

All 15 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	147	GLU	19
1	A	49	VAL	14
1	A	52	THR	14
1	A	50	ASN	13
1	A	191	ILE	7
1	A	115	ASP	6
1	A	57	LEU	6
1	A	188	LYS	3
1	A	120	LYS	2
1	A	138	ASP	2
1	A	103	ASN	1
1	A	79	LEU	1
1	A	85	GLN	1
1	A	174	ARG	1
1	A	59	LEU	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	132/184 (72%)	119±2 (90±2%)	13±2 (10±2%)	9	53
All	All	2640/3680 (72%)	2372 (90%)	268 (10%)	9	53

All 79 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	48	ILE	17
1	A	191	ILE	9

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Mol	Chain	Res	Type	Models (Total)
1	A	6	LEU	8
1	A	123	THR	7
1	A	156	LEU	7
1	A	184	THR	7
1	A	58	LYS	7
1	A	151	GLN	7
1	A	118	LEU	7
1	A	49	VAL	6
1	A	89	VAL	6
1	A	12	LEU	6
1	A	137	LEU	6
1	A	178	THR	6
1	A	95	CYS	6
1	A	135	CYS	6
1	A	183	THR	5
1	A	56	ILE	5
1	A	83	LYS	5
1	A	177	LYS	5
1	A	94	ILE	5
1	A	43	ILE	4
1	A	182	LEU	4
1	A	78	LYS	4
1	A	90	VAL	4
1	A	106	ARG	4
1	A	108	LEU	4
1	A	50	ASN	4
1	A	57	LEU	4
1	A	85	GLN	3
1	A	122	LYS	3
1	A	102	ARG	3
1	A	175	MET	3
1	A	10	MET	3
1	A	52	THR	3
1	A	127	ARG	3
1	A	147	GLU	3
1	A	160	LEU	3
1	A	189	LEU	3
1	A	193	GLU	3
1	A	75	VAL	3
1	A	145	ARG	3
1	A	4	VAL	3
1	A	190	THR	3

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Mol	Chain	Res	Type	Models (Total)
1	A	176	VAL	3
1	A	181	LYS	2
1	A	96	LEU	2
1	A	124	LEU	2
1	A	59	LEU	2
1	A	170	VAL	2
1	A	113	ASP	2
1	A	9	LEU	2
1	A	159	LYS	2
1	A	143	ARG	2
1	A	79	LEU	2
1	A	153	VAL	2
1	A	92	VAL	1
1	A	148	PRO	1
1	A	168	ILE	1
1	A	105	THR	1
1	A	121	ASP	1
1	A	54	GLN	1
1	A	81	THR	1
1	A	164	ASN	1
1	A	188	LYS	1
1	A	120	LYS	1
1	A	86	LEU	1
1	A	114	ASN	1
1	A	5	ASP	1
1	A	162	GLU	1
1	A	51	MET	1
1	A	126	THR	1
1	A	155	GLN	1
1	A	186	ILE	1
1	A	98	GLU	1
1	A	174	ARG	1
1	A	115	ASP	1
1	A	128	GLN	1
1	A	180	GLU	1

6.3.3 RNA ⓘ

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 oligosaccharides 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 25% for the well-defined parts and 28% 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	804
Number of shifts mapped to atoms	798
Number of unparsed shifts	0
Number of shifts with mapping errors	6
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 6 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	ASP	H	8.2	0.02	1
1	A	212	SER	H	7.6	0.02	1
1	A	212	SER	C	175.5	0.1	1
1	A	212	SER	CA	59.6	0.1	1
1	A	212	SER	CB	64.8	0.1	1
1	A	212	SER	N	121.6	0.02	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
$^{13}\text{C}_\alpha$	167	0.19 ± 0.15	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	152	0.84 ± 0.13	Should be checked

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Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}'$	163	2.98 ± 0.12	Should be applied
^{15}N	161	-0.90 ± 0.37	Should be applied

7.1.3 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 25%, i.e. 516 atoms were assigned a chemical shift out of a possible 2090. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	420/764 (55%)	104/313 (33%)	212/304 (70%)	104/147 (71%)
Sidechain	96/1187 (8%)	0/776 (0%)	96/365 (26%)	0/46 (0%)
Aromatic	0/139 (0%)	0/69 (0%)	0/66 (0%)	0/4 (0%)
Overall	516/2090 (25%)	104/1158 (9%)	308/735 (42%)	104/197 (53%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 28%, i.e. 799 atoms were assigned a chemical shift out of a possible 2887. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	648/1067 (61%)	160/436 (37%)	328/424 (77%)	160/207 (77%)
Sidechain	151/1655 (9%)	0/1076 (0%)	151/507 (30%)	0/72 (0%)
Aromatic	0/165 (0%)	0/82 (0%)	0/78 (0%)	0/5 (0%)
Overall	799/2887 (28%)	160/1594 (10%)	479/1009 (47%)	160/284 (56%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

