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P R O T E I N   D A T A   B A N K

wwPDB NMR Structure Validation Summary Report ⓘ

Jun 22, 2024 – 03:48 PM EDT

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PDB ID	:	5LVY
BMRB ID	:	34042
Title	:	Structural studies of the Aggregative Adherence Fimbriae of Enteroaggregative Escherichia coli
Authors	:	Liu, B.; Matthews, S.
Deposited on	:	2016-09-14

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	Percentile Ranks	Value
Clashscore		12
Ramachandran outliers		4.5%
Sidechain outliers		9.7%

Worse   *Better*

▮ Percentile relative to all structures

🮒 Percentile relative to all NMR structures
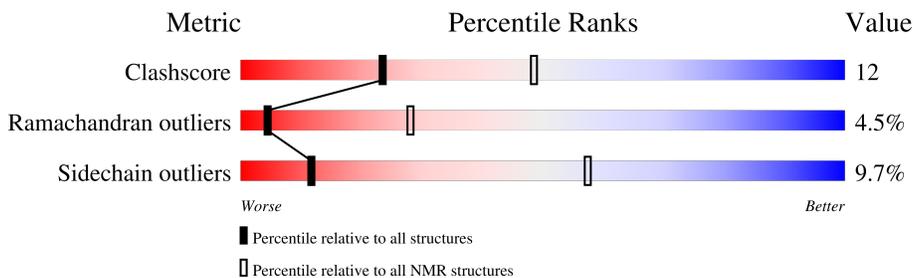
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	154	60% 25% · 11%

2   Ensemble composition and analysis ⓘ

This entry contains 10 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:11-A:79, A:89-A:144, A:151-A:162 (137)	0.50	6

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 1 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 10

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 2311 atoms, of which 1151 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Adhesin protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	154	2311	732	1151	192	232	4	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	VAL	ALA	conflict	UNP C9K5V2
A	132	ASP	-	expression tag	UNP C9K5V2
A	133	ASN	-	expression tag	UNP C9K5V2
A	134	LYS	-	expression tag	UNP C9K5V2
A	135	GLN	-	expression tag	UNP C9K5V2
A	136	ALA	-	expression tag	UNP C9K5V2
A	137	ASN	-	expression tag	UNP C9K5V2
A	138	PRO	-	expression tag	UNP C9K5V2
A	139	THR	-	expression tag	UNP C9K5V2
A	140	PRO	-	expression tag	UNP C9K5V2
A	141	SER	-	expression tag	UNP C9K5V2
A	142	SER	-	expression tag	UNP C9K5V2
A	143	LEU	-	expression tag	UNP C9K5V2
A	144	THR	-	expression tag	UNP C9K5V2
A	145	SER	-	expression tag	UNP C9K5V2
A	146	LYS	-	expression tag	UNP C9K5V2
A	147	ALA	-	expression tag	UNP C9K5V2
A	148	ALA	-	expression tag	UNP C9K5V2
A	149	GLY	-	expression tag	UNP C9K5V2
A	150	LYS	-	expression tag	UNP C9K5V2
A	151	ASN	-	expression tag	UNP C9K5V2
A	152	ILE	-	expression tag	UNP C9K5V2
A	153	VAL	-	expression tag	UNP C9K5V2
A	154	SER	-	expression tag	UNP C9K5V2
A	155	SER	-	expression tag	UNP C9K5V2
A	156	THR	-	expression tag	UNP C9K5V2
A	157	GLY	-	expression tag	UNP C9K5V2
A	158	THR	-	expression tag	UNP C9K5V2
A	159	ILE	-	expression tag	UNP C9K5V2
A	160	THR	-	expression tag	UNP C9K5V2
A	161	ILE	-	expression tag	UNP C9K5V2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	162	SER	-	expression tag	UNP C9K5V2

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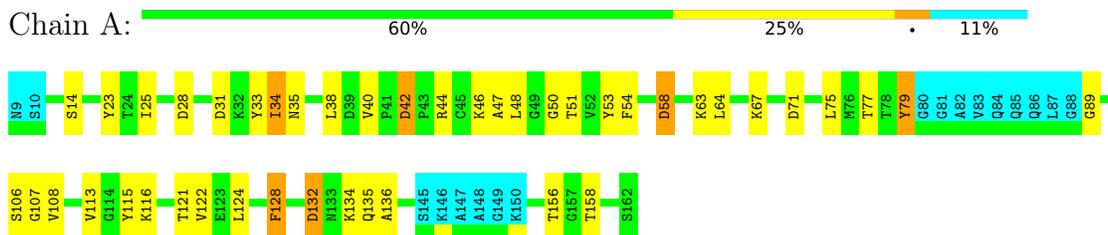
4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 6. Colouring as in section 4.1 above.

• Molecule 1: Adhesin protein
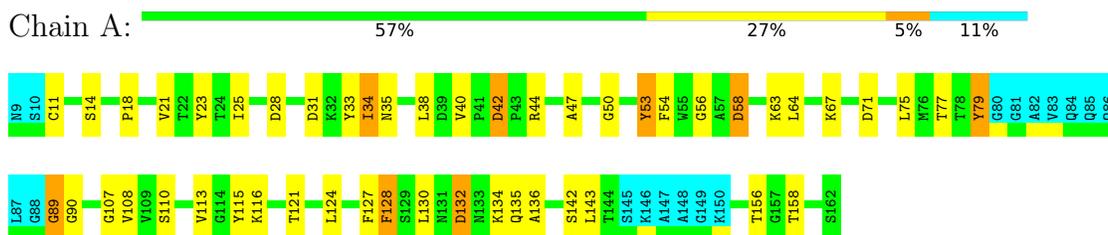
5 Refinement protocol and experimental data overview ⓘ

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

Of the 10 calculated structures, 10 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
ARIA	structure calculation	

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	1661
Number of shifts mapped to atoms	1661
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%

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	0.52±0.08	3±1/1075 (0.2± 0.1%)	0.49±0.02	0±0/1462 (0.0± 0.0%)
All	All	0.53	26/10750 (0.2%)	0.49	0/14620 (0.0%)

5 of 6 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
1	A	79	TYR	CE1-CZ	-9.08	1.26	1.38	9	5
1	A	23	TYR	CE2-CZ	-8.48	1.27	1.38	9	1
1	A	79	TYR	CE2-CZ	8.47	1.49	1.38	9	5
1	A	53	TYR	CE2-CZ	-8.03	1.28	1.38	6	7
1	A	23	TYR	CE1-CZ	7.92	1.48	1.38	9	1

There are no bond-angle outliers.

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	1049	1036	1035	26±4
All	All	10490	10360	10350	255

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 12.

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5 of 88 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Models Total
1:A:128:PHE:CZ	1:A:130:LEU:HG	0.71	2.19	10	2
1:A:14:SER:O	1:A:38:LEU:HA	0.70	1.87	1	10
1:A:50:GLY:HA2	1:A:128:PHE:CD2	0.62	2.30	10	9
1:A:67:LYS:HA	1:A:71:ASP:O	0.61	1.95	10	10
1:A:58:ASP:HB3	1:A:63:LYS:H	0.61	1.56	4	10

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	136/154 (88%)	112±2 (82±2%)	18±2 (13±1%)	6±1 (4±1%)	4	28
All	All	1360/1540 (88%)	1118 (82%)	181 (13%)	61 (4%)	4	28

5 of 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	132	ASP	9
1	A	134	LYS	9
1	A	42	ASP	8
1	A	136	ALA	8
1	A	31	ASP	5

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	120/130 (92%)	108±2 (90±2%)	12±2 (10±2%)	12	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1200/1300 (92%)	1084 (90%)	116 (10%)	12 57

5 of 27 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	34	ILE	10
1	A	79	TYR	10
1	A	116	LYS	10
1	A	128	PHE	10
1	A	158	THR	10

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

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 85% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *agg3.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	1661
Number of shifts mapped to atoms	1661
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	134

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	144	0.11 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_\beta$	127	-0.13 ± 0.20	None needed (< 0.5 ppm)
$^{13}C'$	139	0.30 ± 0.12	None needed (< 0.5 ppm)
^{15}N	129	-0.52 ± 0.42	None needed (imprecise)

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. 1553 atoms were assigned a chemical shift out of a possible 1768. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	642/679 (95%)	264/278 (95%)	259/274 (95%)	119/127 (94%)
Sidechain	799/939 (85%)	540/612 (88%)	259/298 (87%)	0/29 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	112/150 (75%)	56/70 (80%)	55/77 (71%)	1/3 (33%)
Overall	1553/1768 (88%)	860/960 (90%)	573/649 (88%)	120/159 (75%)

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.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	128	PHE	CE2	89.97	124.80 – 136.72	-34.2
1	A	127	PHE	CE2	90.47	124.80 – 136.72	-33.8
1	A	53	TYR	CE2	75.75	111.68 – 124.17	-33.8
1	A	36	PHE	CE2	90.58	124.80 – 136.72	-33.7
1	A	128	PHE	CD2	91.39	125.53 – 137.61	-33.3
1	A	127	PHE	CD2	91.57	125.53 – 137.61	-33.1
1	A	54	PHE	CD2	91.66	125.53 – 137.61	-33.0
1	A	36	PHE	CD2	91.83	125.53 – 137.61	-32.9
1	A	93	TYR	CE2	76.92	111.68 – 124.17	-32.8
1	A	120	TYR	CE2	76.93	111.68 – 124.17	-32.8
1	A	33	TYR	CE2	77.38	111.68 – 124.17	-32.5
1	A	79	TYR	CE2	77.47	111.68 – 124.17	-32.4
1	A	23	TYR	CE2	77.56	111.68 – 124.17	-32.3
1	A	128	PHE	CD1	91.39	125.33 – 137.83	-32.1
1	A	15	ILE	CG2	59.91	10.93 – 24.12	32.1
1	A	105	ILE	CG2	59.80	10.93 – 24.12	32.1
1	A	73	TYR	CE2	77.92	111.68 – 124.17	-32.0
1	A	127	PHE	CD1	91.57	125.33 – 137.83	-32.0
1	A	54	PHE	CD1	91.66	125.33 – 137.83	-31.9
1	A	152	ILE	CG2	59.58	10.93 – 24.12	31.9
1	A	115	TYR	CE2	78.19	111.68 – 124.17	-31.8
1	A	36	PHE	CD1	91.83	125.33 – 137.83	-31.8
1	A	53	TYR	CE1	75.75	111.24 – 124.66	-31.4
1	A	128	PHE	CE1	89.97	124.17 – 137.29	-31.1
1	A	159	ILE	CG2	58.17	10.93 – 24.12	30.8
1	A	127	PHE	CE1	90.47	124.17 – 137.29	-30.7
1	A	161	ILE	CG2	57.92	10.93 – 24.12	30.6
1	A	36	PHE	CE1	90.58	124.17 – 137.29	-30.6
1	A	93	TYR	CE1	76.92	111.24 – 124.66	-30.6
1	A	120	TYR	CE1	76.93	111.24 – 124.66	-30.6
1	A	25	ILE	CG2	57.84	10.93 – 24.12	30.6
1	A	23	TYR	CD1	90.78	125.84 – 139.60	-30.5

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	33	TYR	CE1	77.38	111.24 – 124.66	-30.2
1	A	79	TYR	CE1	77.47	111.24 – 124.66	-30.2
1	A	23	TYR	CE1	77.56	111.24 – 124.66	-30.1
1	A	73	TYR	CE1	77.92	111.24 – 124.66	-29.8
1	A	115	TYR	CD1	91.67	125.84 – 139.60	-29.8
1	A	115	TYR	CE1	78.19	111.24 – 124.66	-29.6
1	A	34	ILE	CG2	56.34	10.93 – 24.12	29.4
1	A	93	TYR	CD1	92.29	125.84 – 139.60	-29.4
1	A	33	TYR	CD1	92.47	125.84 – 139.60	-29.2
1	A	94	TYR	CD1	92.97	125.84 – 139.60	-28.9
1	A	79	TYR	CD1	93.01	125.84 – 139.60	-28.9
1	A	153	VAL	CG1	60.57	14.71 – 28.29	28.8
1	A	91	TYR	CD1	93.58	125.84 – 139.60	-28.4
1	A	73	TYR	CD1	93.64	125.84 – 139.60	-28.4
1	A	53	TYR	CD1	93.72	125.84 – 139.60	-28.3
1	A	120	TYR	CD1	93.88	125.84 – 139.60	-28.2
1	A	23	TYR	CD2	90.78	125.28 – 140.14	-28.2
1	A	55	TRP	CH2	80.97	116.19 – 131.43	-28.1
1	A	55	TRP	CZ2	74.59	107.20 – 121.33	-28.1
1	A	138	PRO	CA	21.88	55.85 – 70.84	-27.7
1	A	141	SER	CB	22.21	56.28 – 71.32	-27.7
1	A	145	SER	CB	22.21	56.28 – 71.32	-27.7
1	A	115	TYR	CD2	91.67	125.28 – 140.14	-27.6
1	A	16	SER	CB	22.39	56.28 – 71.32	-27.5
1	A	102	PRO	CA	22.11	55.85 – 70.84	-27.5
1	A	17	SER	CB	22.47	56.28 – 71.32	-27.5
1	A	20	PRO	CA	22.29	55.85 – 70.84	-27.4
1	A	10	SER	CB	22.68	56.28 – 71.32	-27.4
1	A	142	SER	CB	22.73	56.28 – 71.32	-27.3
1	A	93	TYR	CD2	92.29	125.28 – 140.14	-27.2
1	A	117	PRO	CA	22.64	55.85 – 70.84	-27.2
1	A	33	TYR	CD2	92.47	125.28 – 140.14	-27.1
1	A	127	PHE	CZ	89.23	121.82 – 136.66	-27.0
1	A	94	TYR	CD2	92.97	125.28 – 140.14	-26.7
1	A	79	TYR	CD2	93.01	125.28 – 140.14	-26.7
1	A	110	SER	CB	23.76	56.28 – 71.32	-26.6
1	A	129	SER	CB	23.84	56.28 – 71.32	-26.6
1	A	140	PRO	CA	23.65	55.85 – 70.84	-26.5
1	A	14	SER	CB	24.00	56.28 – 71.32	-26.5
1	A	12	SER	CB	24.18	56.28 – 71.32	-26.4
1	A	91	TYR	CD2	93.58	125.28 – 140.14	-26.3
1	A	43	PRO	CA	23.88	55.85 – 70.84	-26.3

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	106	SER	CB	24.21	56.28 – 71.32	-26.3
1	A	159	ILE	CD1	56.60	5.18 – 21.60	26.3
1	A	73	TYR	CD2	93.64	125.28 – 140.14	-26.3
1	A	53	TYR	CD2	93.72	125.28 – 140.14	-26.2
1	A	162	SER	CB	24.34	56.28 – 71.32	-26.2
1	A	120	TYR	CD2	93.88	125.28 – 140.14	-26.1
1	A	26	PRO	CA	24.18	55.85 – 70.84	-26.1
1	A	97	SER	CB	24.55	56.28 – 71.32	-26.1
1	A	153	VAL	CG2	60.57	13.71 – 28.88	25.9
1	A	34	ILE	CD1	55.33	5.18 – 21.60	25.5
1	A	155	SER	CB	25.62	56.28 – 71.32	-25.4
1	A	25	ILE	CD1	54.95	5.18 – 21.60	25.3
1	A	154	SER	CB	25.77	56.28 – 71.32	-25.3
1	A	15	ILE	CD1	54.58	5.18 – 21.60	25.1
1	A	152	ILE	CD1	53.83	5.18 – 21.60	24.6
1	A	105	ILE	CD1	53.63	5.18 – 21.60	24.5
1	A	74	THR	CB	27.77	61.12 – 78.27	-24.4
1	A	59	THR	CB	27.88	61.12 – 78.27	-24.4
1	A	144	THR	CB	27.88	61.12 – 78.27	-24.4
1	A	139	THR	CB	28.26	61.12 – 78.27	-24.2
1	A	104	THR	CB	28.48	61.12 – 78.27	-24.0
1	A	147	ALA	CB	61.02	10.19 – 27.75	23.9
1	A	160	THR	CB	28.67	61.12 – 78.27	-23.9
1	A	24	THR	CB	29.00	61.12 – 78.27	-23.7
1	A	57	ALA	CB	60.55	10.19 – 27.75	23.7
1	A	100	THR	CB	29.14	61.12 – 78.27	-23.6
1	A	136	ALA	CB	60.44	10.19 – 27.75	23.6
1	A	27	THR	CB	29.22	61.12 – 78.27	-23.6
1	A	22	THR	CB	29.63	61.12 – 78.27	-23.4
1	A	161	ILE	CD1	51.73	5.18 – 21.60	23.4
1	A	125	THR	CB	29.84	61.12 – 78.27	-23.2
1	A	82	ALA	CB	59.60	10.19 – 27.75	23.1
1	A	148	ALA	CB	59.16	10.19 – 27.75	22.9
1	A	121	THR	CB	30.45	61.12 – 78.27	-22.9
1	A	47	ALA	CB	59.08	10.19 – 27.75	22.8
1	A	77	THR	CB	30.64	61.12 – 78.27	-22.8
1	A	78	THR	CB	30.89	61.12 – 78.27	-22.6
1	A	156	THR	CB	30.94	61.12 – 78.27	-22.6
1	A	158	THR	CB	30.97	61.12 – 78.27	-22.6
1	A	51	THR	CB	31.07	61.12 – 78.27	-22.5
1	A	55	TRP	CD1	88.08	117.34 – 135.80	-20.9
1	A	158	THR	CA	20.30	49.41 – 75.05	-16.4

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	77	THR	CA	20.77	49.41 − 75.05	-16.2
1	A	51	THR	CA	20.98	49.41 − 75.05	-16.1
1	A	104	THR	CA	20.98	49.41 − 75.05	-16.1
1	A	27	THR	CA	21.02	49.41 − 75.05	-16.1
1	A	160	THR	CA	21.30	49.41 − 75.05	-16.0
1	A	100	THR	CA	21.87	49.41 − 75.05	-15.7
1	A	59	THR	CA	22.28	49.41 − 75.05	-15.6
1	A	144	THR	CA	22.29	49.41 − 75.05	-15.6
1	A	74	THR	CA	22.65	49.41 − 75.05	-15.4
1	A	152	ILE	CA	20.88	48.30 − 75.08	-15.2
1	A	96	VAL	CA	20.67	48.38 − 76.73	-14.8
1	A	52	VAL	CA	20.80	48.38 − 76.73	-14.7
1	A	109	VAL	CA	20.98	48.38 − 76.73	-14.7
1	A	83	VAL	CA	21.16	48.38 − 76.73	-14.6
1	A	113	VAL	CA	21.37	48.38 − 76.73	-14.5
1	A	108	VAL	CA	21.44	48.38 − 76.73	-14.5
1	A	95	HIS	CD2	79.80	103.95 − 136.66	-12.4
1	A	125	THR	HB	2.51	2.57 − 5.77	-5.2

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.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: