wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	7O2K
BMRB ID	:	27877
Title	:	NMR solution structue of cytotoxin 2 from Naja Kaouthia
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Deposited on	:	2021-03-30

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 (i) 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 (i)) were used in the production of this report:

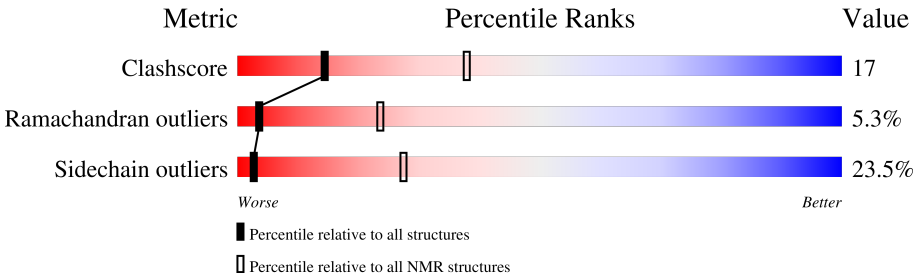
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 84%.

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	60	55% 38% 7%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:1-A:60 (60)	0.63	3

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 870 atoms, of which 406 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytotoxin 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	60	867	294	404	81	78	10	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		
			Total	H	O
2	A	1	3	2	1

4 Residue-property plots (i)

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: Cytotoxin 2

Chain A: 55% 38% 7%

L1 K2 C3 N4 K5 L6 I7 P8 L9 A10 Y11 K12 P15 Y22 K23 M24 F25 M26 V27 K30 V34 K35 R36 I39 K44 L47 L48 Y51 C54 N55 T56 D57 N60

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

The representative model is number 3. Colouring as in section 4.1 above.

- Molecule 1: Cytotoxin 2

Chain A: 55% 35% 10%

L1 N4 I7 P8 L9 K12 P15 Y22 K23 M24 F25 M26 V27 S28 N29 K30 T31 V32 P33 V34 K35 R36 I39 P43 L47 L48 C54 N55 T56 D57 R58 C59 N60

5 Refinement protocol and experimental data overview (i)

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

Of the 200 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
CYANA	refinement	
CYANA	structure calculation	1.0.3

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	3
Total number of shifts	1845
Number of shifts mapped to atoms	1593
Number of unparsed shifts	0
Number of shifts with mapping errors	252
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	463	404	492	16±3
2	A	1	2	0	0±0
All	All	9280	8120	9840	328

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 17.

5 of 137 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ILE:HD12	1:A:41:VAL:O	0.91	1.65	12	3
1:A:39:ILE:HD13	1:A:40:ASP:N	0.81	1.90	6	3
1:A:9:LEU:C	1:A:9:LEU:HD22	0.78	1.99	1	1
1:A:6:LEU:HD12	1:A:36:ARG:NH1	0.69	2.02	10	2
1:A:29:ASN:ND2	1:A:32:VAL:HG23	0.69	2.02	3	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	58/60 (97%)	50±1 (86±2%)	5±1 (9±2%)	3±0 (5±1%)	3 23
All	All	1160/1200 (97%)	996 (86%)	102 (9%)	62 (5%)	3 23

All 5 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	8	PRO	20
1	A	9	LEU	20
1	A	15	PRO	20
1	A	29	ASN	1
1	A	58	ARG	1

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	56/56 (100%)	43±2 (77±3%)	13±2 (23±3%)	3 27
All	All	1120/1120 (100%)	857 (77%)	263 (23%)	3 27

5 of 28 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	22	TYR	20
1	A	27	VAL	20
1	A	34	VAL	18
1	A	56	THR	18
1	A	36	ARG	17

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 monosaccharides 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 (i)

The completeness of assignment taking into account all chemical shift lists is 84% for the well-defined parts and 84% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CT2nk_major_assigned_shifts*

7.1.1 Bookkeeping (i)

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

Total number of shifts	679
Number of shifts mapped to atoms	591
Number of unparsed shifts	0
Number of shifts with mapping errors	88
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 88) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	1	LEU	HB2	1.552	0.020	1
1	A	2	LYS	HB2	1.369	0.020	1
1	A	2	LYS	HG2	1.401	0.020	1
1	A	2	LYS	HD2	1.3	0.020	1
1	A	2	LYS	HE2	2.856	0.020	1
1	A	3	CYS	HB2	2.494	0.020	2
1	A	4	ASN	HB2	2.22	0.020	2
1	A	5	LYS	HB2	1.478	0.020	2
1	A	5	LYS	HG2	1.277	0.020	2
1	A	5	LYS	HD2	1.563	0.020	2
1	A	5	LYS	HE2	2.925	0.020	1
1	A	6	LEU	HB2	1.618	0.020	2
1	A	7	ILE	HG12	1.217	0.020	2
1	A	8	PRO	HB2	1.965	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	8	PRO	HG2	1.994	0.020	2
1	A	8	PRO	HD2	3.688	0.020	2
1	A	9	LEU	HB2	1.667	0.020	2
1	A	11	TYR	HB2	2.627	0.020	2
1	A	12	LYS	HB2	1.73	0.020	1
1	A	12	LYS	HG2	1.228	0.020	2
1	A	12	LYS	HD2	1.719	0.020	2
1	A	12	LYS	HE2	2.957	0.020	2
1	A	14	CYS	HB2	2.802	0.020	2
1	A	15	PRO	HB2	1.964	0.020	2
1	A	15	PRO	HG2	1.875	0.020	2
1	A	15	PRO	HD2	3.441	0.020	2
1	A	18	LYS	HB2	1.341	0.020	2
1	A	18	LYS	HG2	1.064	0.020	2
1	A	18	LYS	HD2	1.378	0.020	1
1	A	18	LYS	HE2	2.941	0.020	1
1	A	19	ASN	HB2	2.616	0.020	2
1	A	20	LEU	HB2	1.362	0.020	2
1	A	21	CYS	HB2	2.954	0.020	2
1	A	22	TYR	HB2	3.006	0.020	2
1	A	23	LYS	HB2	1.547	0.020	2
1	A	23	LYS	HG2	1.408	0.020	2
1	A	23	LYS	HD2	1.662	0.020	2
1	A	23	LYS	HE2	2.718	0.020	1
1	A	24	MET	HB2	1.667	0.020	2
1	A	24	MET	HG2	1.51	0.020	2
1	A	25	PHE	HB2	2.626	0.020	2
1	A	26	MET	HB2	1.954	0.020	2
1	A	26	MET	HG2	2.603	0.020	2
1	A	28	SER	HB2	3.839	0.020	2
1	A	29	ASN	HB2	2.715	0.020	2
1	A	30	LYS	HB2	1.621	0.020	2
1	A	30	LYS	HG2	1.304	0.020	2
1	A	30	LYS	HD2	1.57	0.020	1
1	A	30	LYS	HE2	2.942	0.020	1
1	A	33	PRO	HB2	1.408	0.020	2
1	A	33	PRO	HG2	1.701	0.020	2
1	A	33	PRO	HD2	3.837	0.020	2
1	A	35	LYS	HB2	1.669	0.020	2
1	A	35	LYS	HG2	1.514	0.020	2
1	A	35	LYS	HD2	1.787	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	35	LYS	HE2	3.021	0.020	1
1	A	36	ARG	HB2	1.115	0.020	2
1	A	36	ARG	HG2	1.382	0.020	1
1	A	36	ARG	HD2	2.85	0.020	2
1	A	38	CYS	HB2	2.916	0.020	2
1	A	39	ILE	HG12	1.363	0.020	2
1	A	40	ASP	HB2	2.762	0.020	1
1	A	42	CYS	HB2	2.721	0.020	2
1	A	43	PRO	HB2	0.47	0.020	2
1	A	43	PRO	HG2	0.658	0.020	2
1	A	43	PRO	HD2	2.35	0.020	2
1	A	44	LYS	HB2	1.677	0.020	2
1	A	44	LYS	HG2	1.525	0.020	1
1	A	44	LYS	HD2	1.694	0.020	1
1	A	44	LYS	HE2	3.003	0.020	1
1	A	45	ASN	HB2	2.866	0.020	2
1	A	46	SER	HB2	3.964	0.020	2
1	A	47	LEU	HB2	1.61	0.020	2
1	A	48	LEU	HB2	1.664	0.020	2
1	A	50	LYS	HB2	1.413	0.020	2
1	A	50	LYS	HG2	1.123	0.020	2
1	A	50	LYS	HD2	1.577	0.020	2
1	A	50	LYS	HE2	2.79	0.020	2
1	A	51	TYR	HB2	2.765	0.020	2
1	A	53	CYS	HB2	3.059	0.020	2
1	A	54	CYS	HB2	3.417	0.020	2
1	A	55	ASN	HB2	2.63	0.020	2
1	A	57	ASP	HB2	2.264	0.020	2
1	A	58	ARG	HG2	0.814	0.020	2
1	A	58	ARG	HB2	1.71	0.020	2
1	A	58	ARG	HD2	2.304	0.020	2
1	A	59	CYS	HB2	3.334	0.020	2
1	A	60	ASN	HB2	2.315	0.020	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	57	2.50 ± 0.35	Should be applied
$^{13}C_{\beta}$	55	1.97 ± 0.37	Should be applied

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C'$	0	—	None (insufficient data)
^{15}N	51	1.34 ± 0.63	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 82%, i.e. 676 atoms were assigned a chemical shift out of a possible 822. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	225/294 (77%)	117/118 (99%)	57/120 (48%)	51/56 (91%)
Sidechain	434/491 (88%)	306/320 (96%)	127/150 (85%)	1/21 (5%)
Aromatic	17/37 (46%)	17/17 (100%)	0/20 (0%)	0/0 (—%)
Overall	676/822 (82%)	440/455 (97%)	184/290 (63%)	52/77 (68%)

7.1.4 Statistically unusual chemical shifts (i)

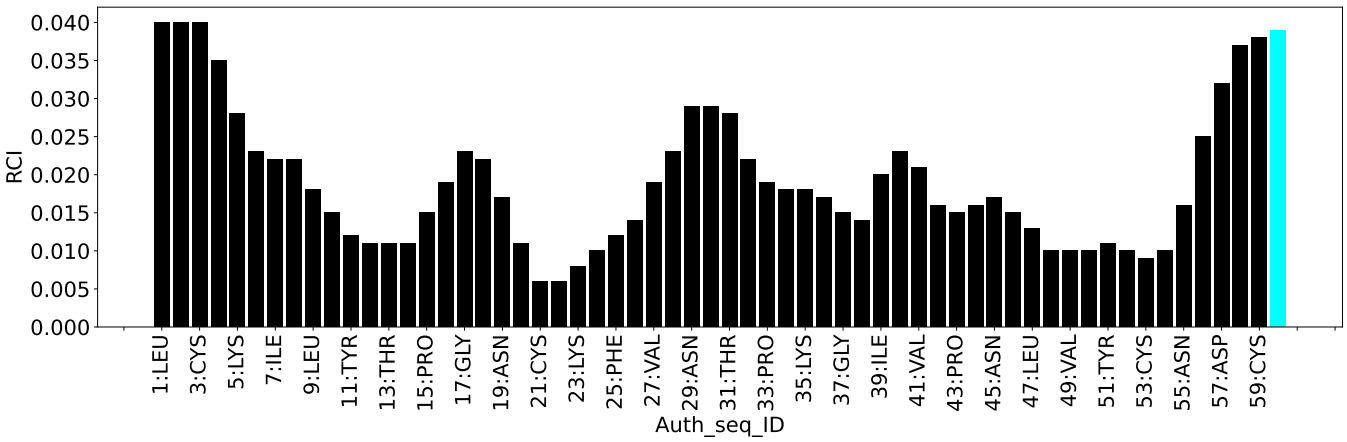
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	36	ARG	CG	33.37	21.24 – 33.19	5.2

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *CT2nk_minor_assigned_shifts*

7.2.1 Bookkeeping (i)

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

Total number of shifts	575
Number of shifts mapped to atoms	493
Number of unparsed shifts	0
Number of shifts with mapping errors	82
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. First 5 (of 82) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	1	LEU	HB2	1.552	0.020	1
2	A	2	LYS	HB2	1.364	0.020	1
2	A	2	LYS	HG2	1.405	0.020	1
2	A	2	LYS	HD2	1.301	0.020	1
2	A	2	LYS	HE2	2.872	0.020	1
2	A	3	CYS	HB2	2.578	0.020	2
2	A	4	ASN	HB2	2.195	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	5	LYS	HB2	1.821	0.020	2
2	A	5	LYS	HG2	1.397	0.020	1
2	A	5	LYS	HD2	1.443	0.020	1
2	A	6	LEU	HB2	1.557	0.020	2
2	A	7	ILE	HG12	1.261	0.020	1
2	A	8	PRO	HB2	2.071	0.020	2
2	A	8	PRO	HG2	1.633	0.020	2
2	A	8	PRO	HD2	3.398	0.020	2
2	A	9	LEU	HB2	1.442	0.020	2
2	A	11	TYR	HB2	2.668	0.020	2
2	A	12	LYS	HB2	1.44	0.020	2
2	A	12	LYS	HG2	1.315	0.020	1
2	A	12	LYS	HD2	1.742	0.020	1
2	A	14	CYS	HB2	2.799	0.020	2
2	A	15	PRO	HB2	1.964	0.020	2
2	A	15	PRO	HG2	1.875	0.020	2
2	A	15	PRO	HD2	3.441	0.020	2
2	A	18	LYS	HB2	1.341	0.020	2
2	A	18	LYS	HG2	1.064	0.020	2
2	A	18	LYS	HD2	1.378	0.020	1
2	A	18	LYS	HE2	2.941	0.020	1
2	A	19	ASN	HB2	2.616	0.020	2
2	A	20	LEU	HB2	1.362	0.020	2
2	A	21	CYS	HB2	2.954	0.020	2
2	A	22	TYR	HB2	3.018	0.020	2
2	A	23	LYS	HB2	1.548	0.020	2
2	A	23	LYS	HG2	1.407	0.020	2
2	A	23	LYS	HD2	1.662	0.020	2
2	A	25	PHE	HB2	2.547	0.020	2
2	A	26	MET	HB2	1.955	0.020	2
2	A	26	MET	HG2	2.605	0.020	2
2	A	28	SER	HB2	3.839	0.020	2
2	A	29	ASN	HB2	2.715	0.020	2
2	A	30	LYS	HB2	1.621	0.020	2
2	A	30	LYS	HG2	1.304	0.020	2
2	A	30	LYS	HD2	1.57	0.020	1
2	A	30	LYS	HE2	2.942	0.020	1
2	A	33	PRO	HB2	1.418	0.020	2
2	A	33	PRO	HG2	1.737	0.020	2
2	A	33	PRO	HD2	3.828	0.020	2
2	A	35	LYS	HB2	1.668	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
2	A	35	LYS	HG2	1.517	0.020	2
2	A	35	LYS	HD2	1.796	0.020	2
2	A	35	LYS	HE2	3.018	0.020	1
2	A	36	ARG	HB2	1.344	0.020	2
2	A	36	ARG	HG2	1.406	0.020	1
2	A	36	ARG	HD2	2.725	0.020	1
2	A	38	CYS	HB2	2.916	0.020	2
2	A	39	ILE	HG12	1.363	0.020	2
2	A	40	ASP	HB2	2.762	0.020	1
2	A	42	CYS	HB2	2.721	0.020	2
2	A	43	PRO	HB2	0.47	0.020	2
2	A	43	PRO	HG2	0.658	0.020	2
2	A	43	PRO	HD2	2.35	0.020	2
2	A	44	LYS	HB2	1.682	0.020	2
2	A	44	LYS	HG2	1.507	0.020	1
2	A	44	LYS	HE2	2.999	0.020	1
2	A	45	ASN	HB2	2.866	0.020	2
2	A	46	SER	HB2	3.964	0.020	2
2	A	47	LEU	HB2	1.61	0.020	2
2	A	48	LEU	HB2	1.664	0.020	2
2	A	50	LYS	HB2	1.413	0.020	2
2	A	50	LYS	HG2	1.123	0.020	2
2	A	50	LYS	HD2	1.577	0.020	2
2	A	50	LYS	HE2	2.79	0.020	2
2	A	51	TYR	HB2	2.765	0.020	2
2	A	53	CYS	HB2	3.059	0.020	2
2	A	54	CYS	HB2	3.419	0.020	2
2	A	55	ASN	HB2	2.63	0.020	2
2	A	57	ASP	HB2	2.264	0.020	2
2	A	58	ARG	HG2	0.81	0.020	2
2	A	58	ARG	HB2	1.639	0.020	2
2	A	58	ARG	HD2	2.184	0.020	2
2	A	59	CYS	HB2	3.335	0.020	2
2	A	60	ASN	HB2	2.3	0.020	2

7.2.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	37	2.50 ± 0.18	Should be applied

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\beta}$	35	2.00 ± 0.30	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	32	0.92 ± 0.39	Should be applied

7.2.3 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 70%, i.e. 575 atoms were assigned a chemical shift out of a possible 822. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	186/294 (63%)	117/118 (99%)	37/120 (31%)	32/56 (57%)
Sidechain	377/491 (77%)	293/320 (92%)	83/150 (55%)	1/21 (5%)
Aromatic	12/37 (32%)	12/17 (71%)	0/20 (0%)	0/0 (—%)
Overall	575/822 (70%)	422/455 (93%)	120/290 (41%)	33/77 (43%)

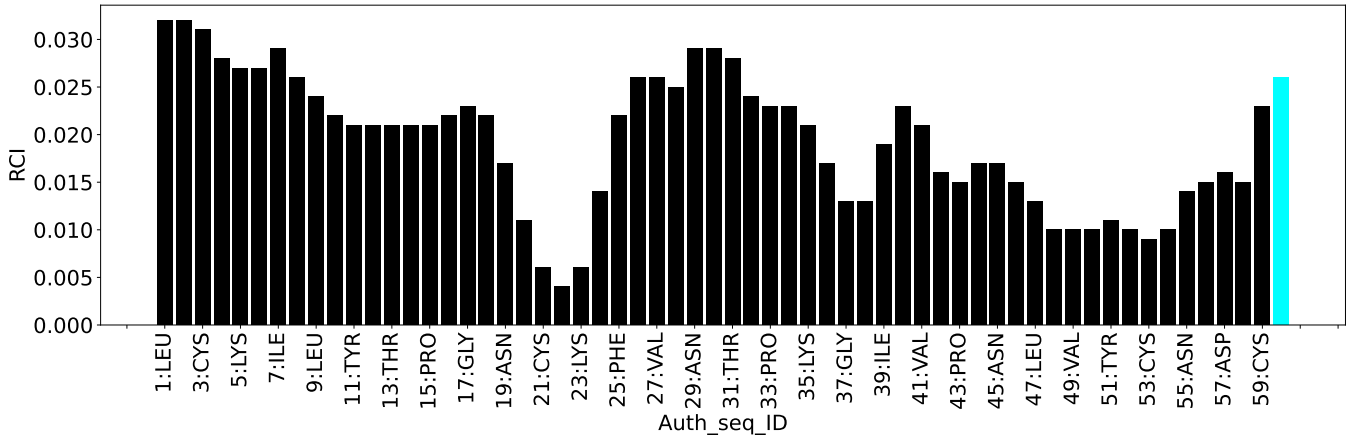
7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 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:



7.3 Chemical shift list 3

File name: working_cs.cif

Chemical shift list name: *CT3nk_minor_assigned_shifts*

7.3.1 Bookkeeping (i)

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

Total number of shifts	591
Number of shifts mapped to atoms	509
Number of unparsed shifts	0
Number of shifts with mapping errors	82
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

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

- No matching atom found in the structure. First 5 (of 82) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3	A	1	LEU	HB2	1.552	0.020	1
3	A	2	LYS	HB2	1.364	0.020	1
3	A	2	LYS	HG2	1.405	0.020	1
3	A	2	LYS	HD2	1.301	0.020	1
3	A	2	LYS	HE2	2.872	0.020	1
3	A	3	CYS	HB2	2.578	0.020	2
3	A	4	ASN	HB2	2.195	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3	A	5	LYS	HB2	1.821	0.020	2
3	A	5	LYS	HG2	1.397	0.020	1
3	A	5	LYS	HD2	1.443	0.020	1
3	A	6	LEU	HB2	1.557	0.020	2
3	A	7	ILE	HG12	1.261	0.020	1
3	A	8	PRO	HB2	2.071	0.020	2
3	A	8	PRO	HG2	1.633	0.020	2
3	A	8	PRO	HD2	3.398	0.020	2
3	A	9	LEU	HB2	1.442	0.020	2
3	A	11	TYR	HB2	2.668	0.020	2
3	A	12	LYS	HB2	1.44	0.020	2
3	A	12	LYS	HG2	1.315	0.020	1
3	A	12	LYS	HD2	1.742	0.020	1
3	A	14	CYS	HB2	2.799	0.020	2
3	A	15	PRO	HB2	1.964	0.020	2
3	A	15	PRO	HG2	1.875	0.020	2
3	A	15	PRO	HD2	3.441	0.020	2
3	A	18	LYS	HB2	1.341	0.020	2
3	A	18	LYS	HG2	1.064	0.020	2
3	A	18	LYS	HD2	1.378	0.020	1
3	A	18	LYS	HE2	2.941	0.020	1
3	A	19	ASN	HB2	2.619	0.020	2
3	A	20	LEU	HB2	1.409	0.020	2
3	A	21	CYS	HB2	2.96	0.020	2
3	A	22	TYR	HB2	3.018	0.020	2
3	A	23	LYS	HB2	1.548	0.020	2
3	A	23	LYS	HG2	1.407	0.020	2
3	A	23	LYS	HD2	1.662	0.020	2
3	A	25	PHE	HB2	2.547	0.020	2
3	A	26	MET	HB2	1.955	0.020	2
3	A	26	MET	HG2	2.605	0.020	2
3	A	28	SER	HB2	3.839	0.020	2
3	A	29	ASN	HB2	2.715	0.020	2
3	A	30	LYS	HB2	1.621	0.020	2
3	A	30	LYS	HG2	1.304	0.020	2
3	A	30	LYS	HD2	1.57	0.020	1
3	A	30	LYS	HE2	2.942	0.020	1
3	A	33	PRO	HB2	1.418	0.020	2
3	A	33	PRO	HG2	1.737	0.020	2
3	A	33	PRO	HD2	3.828	0.020	2
3	A	35	LYS	HB2	1.668	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
3	A	35	LYS	HG2	1.517	0.020	2
3	A	35	LYS	HD2	1.796	0.020	2
3	A	35	LYS	HE2	3.018	0.020	1
3	A	36	ARG	HB2	1.344	0.020	2
3	A	36	ARG	HG2	1.406	0.020	1
3	A	36	ARG	HD2	2.725	0.020	1
3	A	38	CYS	HB2	2.916	0.020	2
3	A	39	ILE	HG12	1.379	0.020	2
3	A	40	ASP	HB2	2.703	0.020	2
3	A	42	CYS	HB2	2.724	0.020	2
3	A	43	PRO	HB2	0.559	0.020	2
3	A	43	PRO	HG2	0.683	0.020	2
3	A	43	PRO	HD2	2.323	0.020	2
3	A	44	LYS	HB2	1.692	0.020	2
3	A	44	LYS	HG2	1.534	0.020	1
3	A	44	LYS	HE2	3.003	0.020	1
3	A	45	ASN	HB2	2.866	0.020	2
3	A	46	SER	HB2	3.964	0.020	2
3	A	47	LEU	HB2	1.61	0.020	2
3	A	48	LEU	HB2	1.667	0.020	2
3	A	50	LYS	HB2	1.413	0.020	2
3	A	50	LYS	HG2	1.123	0.020	2
3	A	50	LYS	HD2	1.577	0.020	2
3	A	50	LYS	HE2	2.79	0.020	2
3	A	51	TYR	HB2	2.765	0.020	2
3	A	53	CYS	HB2	3.063	0.020	2
3	A	54	CYS	HB2	3.419	0.020	2
3	A	55	ASN	HB2	2.63	0.020	2
3	A	57	ASP	HB2	2.264	0.020	2
3	A	58	ARG	HG2	0.81	0.020	2
3	A	58	ARG	HB2	1.639	0.020	2
3	A	58	ARG	HD2	2.184	0.020	2
3	A	59	CYS	HB2	3.335	0.020	2
3	A	60	ASN	HB2	2.3	0.020	2

7.3.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	43	2.39 ± 0.20	Should be applied

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\beta}$	40	1.98 ± 0.29	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	37	0.71 ± 0.48	None needed (imprecise)

7.3.3 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 72%, i.e. 591 atoms were assigned a chemical shift out of a possible 822. 0 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	197/294 (67%)	117/118 (99%)	43/120 (36%)	37/56 (66%)
Sidechain	382/491 (78%)	287/320 (90%)	94/150 (63%)	1/21 (5%)
Aromatic	12/37 (32%)	12/17 (71%)	0/20 (0%)	0/0 (—%)
Overall	591/822 (72%)	416/455 (91%)	137/290 (47%)	38/77 (49%)

7.3.4 Statistically unusual chemical shifts (i)

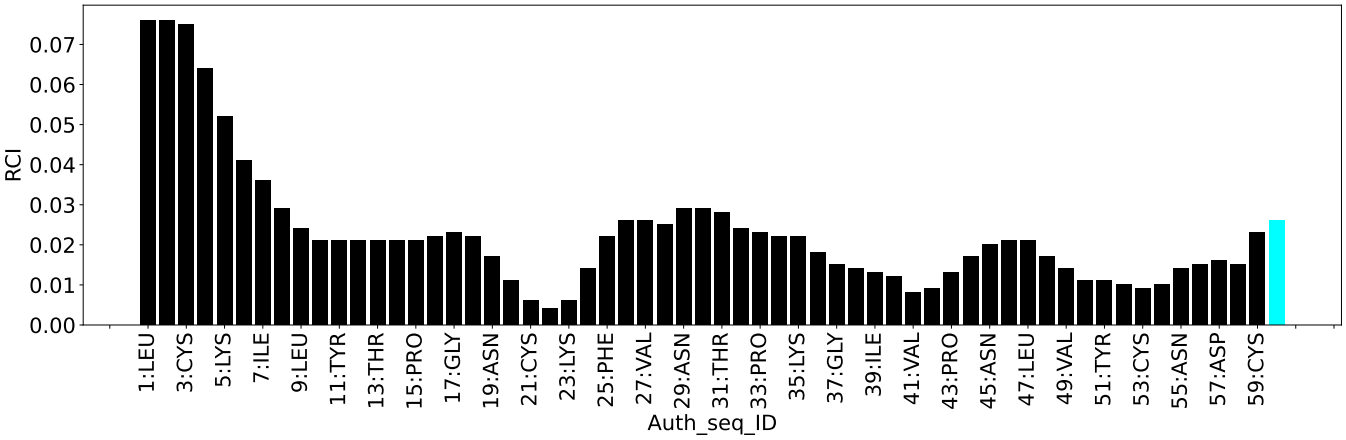
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
3	A	41	VAL	CB	18.30	23.86 – 41.50	-8.2

7.3.5 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:


RCI
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
1:LEU
3:CYS
5:LYS
7:ILE
9:LEU
11:TYR
13:THR
15:PRO
17:GLY
19:ASN
21:CYS
23:LYS
25:PHE
27:VAL
29:ASN
31:THR
33:PRO
35:LYS
37:GLY
39:ILE
41:VAL
43:PRO
45:ASN
47:LEU
49:VAL
51:TYR
53:CYS
55:ASN
57:ASP
59:CYS
Auth_seq_ID