



Full wwPDB NMR Structure Validation Report ⓘ

Apr 26, 2016 – 11:59 PM BST

PDB ID : 2KTN
Title : Spatial structure of Lch-alpha peptide from two-component lantibiotic system
Lichenicidin VK21
Authors : Mineev, K.S.; Shenkarev, Z.O.; Ovchinnikova, T.V.; Arseniev, A.S.
Deposited on : 2010-02-05

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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20027457
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

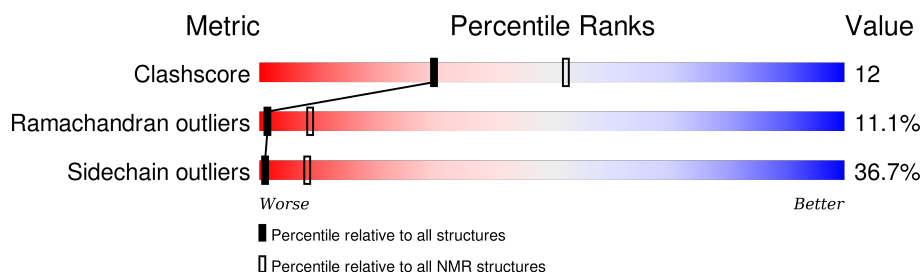
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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	32	

2 Ensemble composition and analysis

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative.

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:21-A:21, A:23-A:23, A:25-A:31 (9)	0.05	2

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 5 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 447 atoms, of which 224 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LICHENICIDIN VK21 A1.

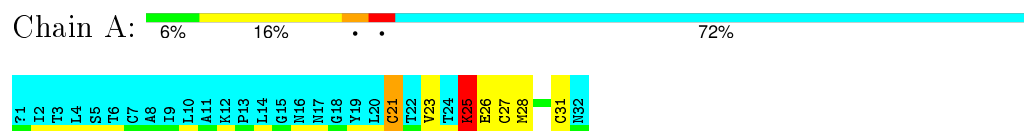
Mol	Chain	Residues	Atoms						Trace
1	A	32	Total	C	H	N	O	S	0
			447	142	224	36	40	5	

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: LICHENICIDIN VK21 A1

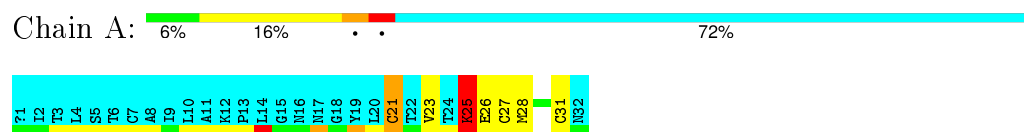


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

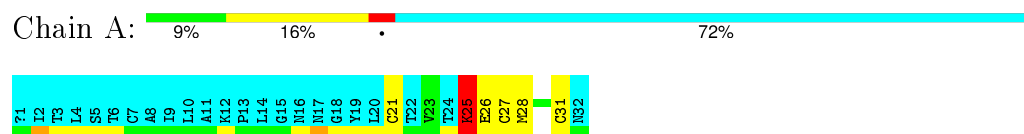
4.2.1 Score per residue for model 1

- Molecule 1: LICHENICIDIN VK21 A1



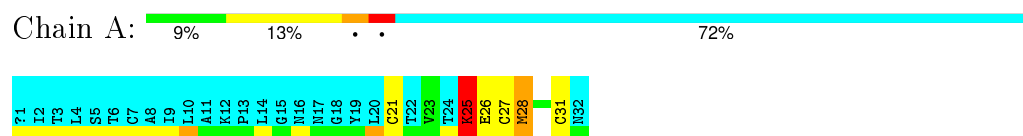
4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: LICHENICIDIN VK21 A1



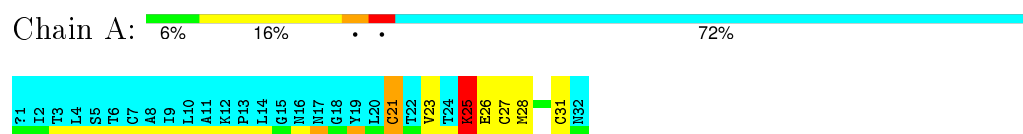
4.2.3 Score per residue for model 3

- Molecule 1: LICHENICIDIN VK21 A1



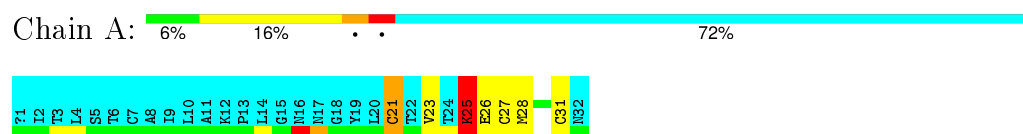
4.2.4 Score per residue for model 4

- Molecule 1: LICHENICIDIN VK21 A1



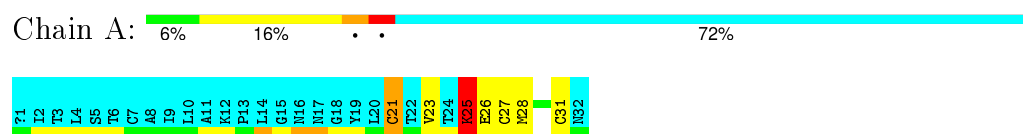
4.2.5 Score per residue for model 5

- Molecule 1: LICHENICIDIN VK21 A1



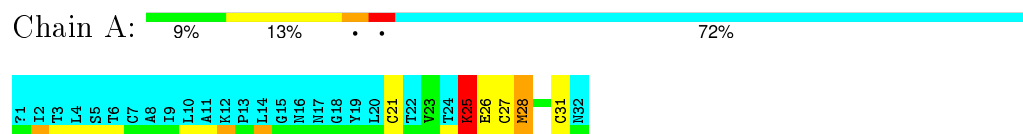
4.2.6 Score per residue for model 6

- Molecule 1: LICHENICIDIN VK21 A1



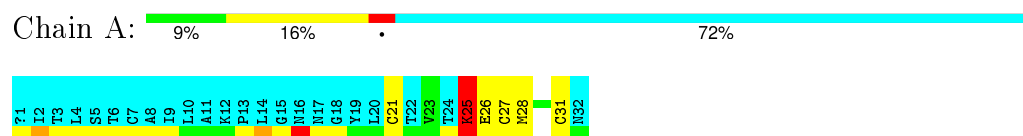
4.2.7 Score per residue for model 7

- Molecule 1: LICHENICIDIN VK21 A1



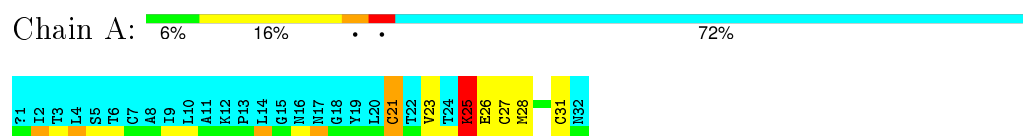
4.2.8 Score per residue for model 8

- Molecule 1: LICHENICIDIN VK21 A1



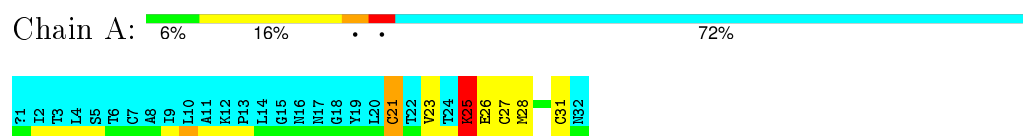
4.2.9 Score per residue for model 9

- Molecule 1: LICHENICIDIN VK21 A1



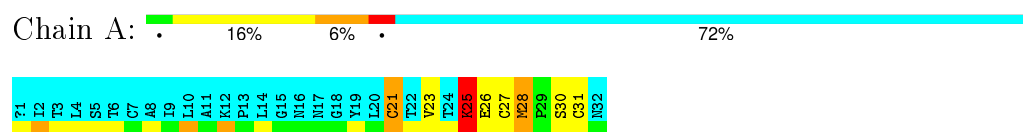
4.2.10 Score per residue for model 10

- Molecule 1: LICHENICIDIN VK21 A1



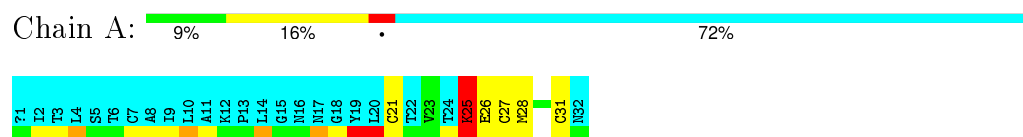
4.2.11 Score per residue for model 11

- Molecule 1: LICHENICIDIN VK21 A1



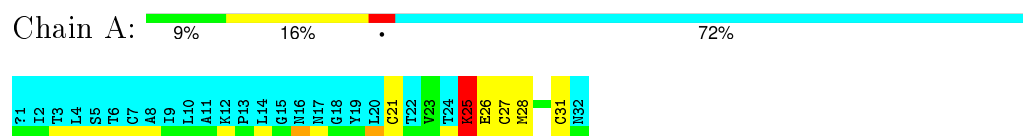
4.2.12 Score per residue for model 12

- Molecule 1: LICHENICIDIN VK21 A1



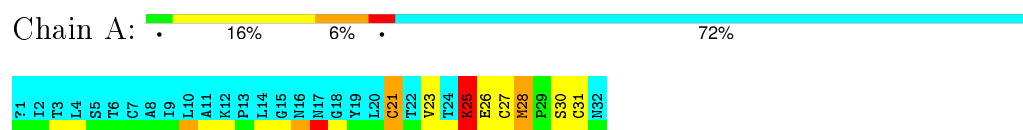
4.2.13 Score per residue for model 13

- Molecule 1: LICHENICIDIN VK21 A1



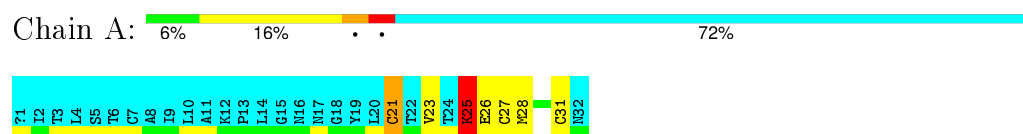
4.2.14 Score per residue for model 14

- Molecule 1: LICHENICIDIN VK21 A1



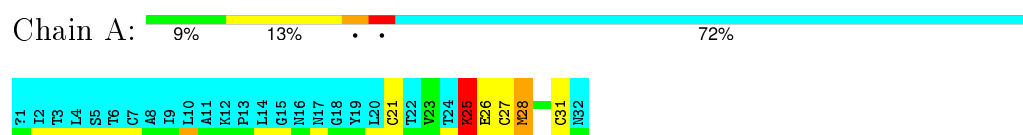
4.2.15 Score per residue for model 15

- Molecule 1: LICHENICIDIN VK21 A1



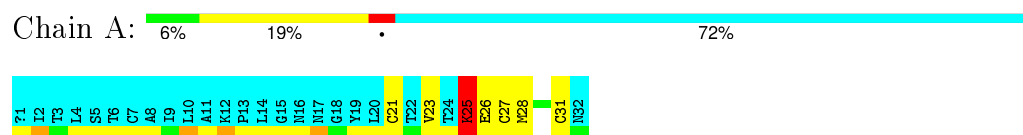
4.2.16 Score per residue for model 16

- Molecule 1: LICHENICIDIN VK21 A1



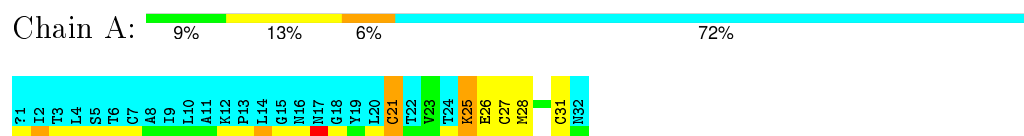
4.2.17 Score per residue for model 17

- Molecule 1: LICHENICIDIN VK21 A1



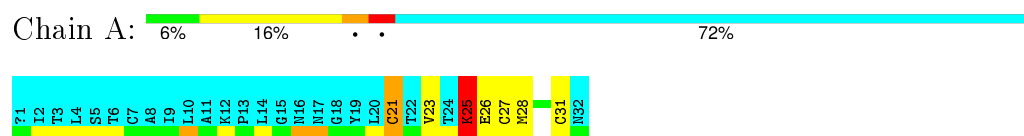
4.2.18 Score per residue for model 18

- Molecule 1: LICHENICIDIN VK21 A1



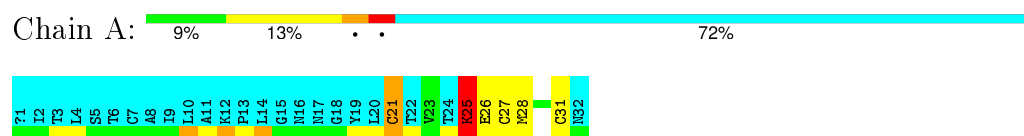
4.2.19 Score per residue for model 19

- Molecule 1: LICHENICIDIN VK21 A1



4.2.20 Score per residue for model 20

- Molecule 1: LICHENICIDIN VK21 A1



5 Refinement protocol and experimental data overview

The models were refined using the following method: *SIMULATED ANNEALING*.

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 2.1	refinement	
CARA 1.5.3	structure solution	
TOPSPIN 2.1	structure solution	
CYANA 2.1	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)	BMRB entry 16709
Number of chemical shift lists	1
Total number of shifts	254
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	254
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	0%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2KT, DAL, DBB, DBU, DHA

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	64	61	61	2±1
All	All	1280	1220	1220	30

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:CYS:O	1:A:23:VAL:HG23	0.81	1.74	19	9
1:A:28:MET:SD	1:A:30:SER:CB	0.46	3.03	11	1
1:A:25:LYS:HA	1:A:28:MET:O	0.43	2.14	13	19
1:A:25:LYS:O	1:A:25:LYS:NZ	0.40	2.50	17	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	9/32 (28%)	6±0 (68±5%)	2±0 (21±5%)	1±0 (11±0%)	1	9
All	All	180/640 (28%)	122 (68%)	38 (21%)	20 (11%)	1	9

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	25	LYS	20

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	9/22 (41%)	6±1 (63±7%)	3±1 (37±7%)	1	8
All	All	180/440 (41%)	114 (63%)	66 (37%)	1	8

All 5 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	31	CYS	20
1	A	21	CYS	20
1	A	25	LYS	19
1	A	28	MET	6
1	A	30	SER	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](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics

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

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	DAL	A	11	1	1,4,5	0.83±0.01	0±0 (0±0%)
1	DBB	A	22	1	3,5,6	0.66±0.01	0±0 (0±0%)
1	DBB	A	24	1	3,5,6	0.67±0.01	0±0 (0±0%)
1	DBB	A	3	1	3,5,6	0.67±0.01	0±0 (0±0%)
1	DHA	A	5	1	4,4,5	1.21±0.01	0±0 (0±0%)
1	DBU	A	6	1	5,5,6	2.07±0.01	0±0 (0±0%)

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

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	DAL	A	11	1	1,4,6	0.50±0.00	0±0 (0±0%)
1	DBB	A	22	1	3,5,7	1.50±0.00	0±0 (0±0%)
1	DBB	A	24	1	3,5,7	1.49±0.01	0±0 (0±0%)
1	DBB	A	3	1	3,5,7	1.50±0.01	0±0 (0±0%)
1	DHA	A	5	1	3,4,6	1.92±0.01	0±0 (0±0%)
1	DBU	A	6	1	2,5,7	4.04±0.01	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	DAL	A	11	1	-	0±0,0,2,4	0±0,0,0,0
1	DBB	A	22	1	-	0±0,2,4,6	0±0,0,0,0
1	DBB	A	24	1	-	0±0,2,4,6	0±0,0,0,0
1	DBB	A	3	1	-	0±0,2,4,6	0±0,0,0,0
1	DHA	A	5	1	-	0±0,0,2,4	0±0,0,0,0
1	DBU	A	6	1	-	0±0,1,4,6	0±0,0,0,0

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates ⓘ

There are no carbohydrates 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 0% for the well-defined parts and 0% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 16709

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	254
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	254
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.

- Chain not found in structure. All 254 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	12	ILE	CG2	14.012	0.4	1
UNMAPPED	22	LEU	HB2	1.694	0.02	2
UNMAPPED	3	PRO	HB3	1.963	0.02	2
UNMAPPED	17	DBU	HB	6.339	0.02	1
UNMAPPED	9	TRP	HD1	7.203	0.02	1
UNMAPPED	9	TRP	HB2	3.351	0.02	2
UNMAPPED	12	ILE	CB	34.926	0.4	1
UNMAPPED	22	LEU	HD11	0.917	0.02	2
UNMAPPED	22	LEU	HD12	0.917	0.02	2
UNMAPPED	6	DBU	CG	11.798	0.4	1
UNMAPPED	27	LYS	CE	39.558	0.4	1
UNMAPPED	1	2KT	H33	2.817	0.02	2
UNMAPPED	6	DBU	CB	131.251	0.4	1
UNMAPPED	27	LYS	CB	29.79	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	22	LEU	HD13	0.917	0.02	2
UNMAPPED	28	CYS	HA	4.433	0.02	1
UNMAPPED	30	SER	CA	59.776	0.4	1
UNMAPPED	3	PRO	HA	4.426	0.02	1
UNMAPPED	4	ALA	CA	50.503	0.4	1
UNMAPPED	30	SER	CB	60.422	0.4	1
UNMAPPED	16	VAL	HA	3.775	0.02	1
UNMAPPED	4	ALA	CB	15.66	0.4	1
UNMAPPED	26	DBU	QG	1.825	0.02	1
UNMAPPED	13	DBU	H	9.576	0.02	1
UNMAPPED	16	VAL	HG21	0.989	0.02	2
UNMAPPED	12	ILE	HG23	0.863	0.02	1
UNMAPPED	26	DBU	H	9.684	0.02	1
UNMAPPED	27	LYS	HZ3	7.813	0.02	1
UNMAPPED	8	DHA	H	9.432	0.02	1
UNMAPPED	12	ILE	H	8.197	0.02	1
UNMAPPED	13	DBU	CG	10.993	0.4	1
UNMAPPED	9	TRP	HE1	10.396	0.02	1
UNMAPPED	9	TRP	CB	27.084	0.4	1
UNMAPPED	4	ALA	HA	4.326	0.02	1
UNMAPPED	28	CYS	HB3	3.184	0.02	2
UNMAPPED	9	TRP	CA	58.172	0.4	1
UNMAPPED	26	DBU	HB	6.473	0.02	1
UNMAPPED	12	ILE	HD11	0.643	0.02	1
UNMAPPED	15	GLY	HA2	3.89	0.02	2
UNMAPPED	1	2KT	C4	5.852	0.4	1
UNMAPPED	3	PRO	HD2	3.638	0.02	2
UNMAPPED	20	ALA	HA	4.051	0.02	1
UNMAPPED	15	GLY	CA	44.078	0.4	1
UNMAPPED	12	ILE	CD1	9.322	0.4	1
UNMAPPED	27	LYS	HG3	1.514	0.02	2
UNMAPPED	24	PRO	HD2	3.994	0.02	2
UNMAPPED	3	PRO	HG3	1.963	0.02	2
UNMAPPED	14	ALA	HB3	1.483	0.02	1
UNMAPPED	28	CYS	HB2	3.512	0.02	2
UNMAPPED	27	LYS	HD2	1.822	0.02	2
UNMAPPED	12	ILE	HB	1.993	0.02	1
UNMAPPED	22	LEU	HG	1.723	0.02	1
UNMAPPED	12	ILE	HA	3.673	0.02	1
UNMAPPED	21	SER	H	7.458	0.02	1
UNMAPPED	23	CYS	HA	4.605	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	20	ALA	HB3	1.41	0.02	1
UNMAPPED	18	VAL	CG2	18.475	0.4	1
UNMAPPED	10	THR	HG21	1.27	0.02	1
UNMAPPED	18	VAL	CG1	19.532	0.4	1
UNMAPPED	27	LYS	HE2	3.021	0.02	2
UNMAPPED	22	LEU	CG	23.905	0.4	1
UNMAPPED	10	THR	HG22	1.27	0.02	1
UNMAPPED	16	VAL	HG13	1.002	0.02	2
UNMAPPED	9	TRP	HZ2	7.366	0.02	1
UNMAPPED	22	LEU	CD2	20.221	0.4	1
UNMAPPED	17	DBU	CB	128.295	0.4	1
UNMAPPED	18	VAL	HG11	1.114	0.02	2
UNMAPPED	11	CYS	H	8.018	0.02	1
UNMAPPED	17	DBU	CG	11.411	0.4	1
UNMAPPED	16	VAL	CG1	19.313	0.4	1
UNMAPPED	18	VAL	CB	28.97	0.4	1
UNMAPPED	23	CYS	CA	58.289	0.4	1
UNMAPPED	31	ARG	HA	4.652	0.02	1
UNMAPPED	8	DHA	HB2	5.441	0.02	2
UNMAPPED	4	ALA	HB1	1.492	0.02	1
UNMAPPED	28	CYS	H	8.049	0.02	1
UNMAPPED	3	PRO	CB	24.549	0.4	1
UNMAPPED	25	ABA	HB	3.661	0.02	1
UNMAPPED	2	DBU	CG	11.162	0.4	1
UNMAPPED	24	PRO	CD	47.316	0.4	1
UNMAPPED	3	PRO	CG	29.446	0.4	1
UNMAPPED	25	ABA	HA	5.003	0.02	1
UNMAPPED	3	PRO	CD	49.638	0.4	1
UNMAPPED	21	SER	HA	4.583	0.02	1
UNMAPPED	20	ALA	CB	15.298	0.4	1
UNMAPPED	14	ALA	H	7.931	0.02	1
UNMAPPED	14	ALA	HA	4.139	0.02	1
UNMAPPED	1	2KT	H32	2.817	0.02	2
UNMAPPED	6	DBU	HB	6.672	0.02	1
UNMAPPED	22	LEU	CB	42.388	0.4	1
UNMAPPED	22	LEU	HD22	0.901	0.02	2
UNMAPPED	21	SER	CA	57.58	0.4	1
UNMAPPED	9	TRP	HA	4.468	0.02	1
UNMAPPED	30	SER	HA	4.179	0.02	1
UNMAPPED	10	THR	H	8.03	0.02	1
UNMAPPED	25	ABA	H	8.393	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	5	DBU	HB	6.391	0.02	1
UNMAPPED	31	ARG	HB3	1.638	0.02	2
UNMAPPED	16	VAL	HB	2.301	0.02	1
UNMAPPED	15	GLY	HA3	3.862	0.02	2
UNMAPPED	7	DAL	HB3	3.078	0.02	2
UNMAPPED	25	ABA	CG	19.949	0.4	1
UNMAPPED	16	VAL	HG23	0.989	0.02	2
UNMAPPED	9	TRP	CZ2	111.398	0.4	1
UNMAPPED	11	CYS	CA	57.844	0.4	1
UNMAPPED	11	CYS	HB2	3.167	0.02	2
UNMAPPED	22	LEU	HD21	0.901	0.02	2
UNMAPPED	31	ARG	HD3	3.314	0.02	2
UNMAPPED	11	CYS	HA	3.858	0.02	1
UNMAPPED	23	CYS	H	9.022	0.02	1
UNMAPPED	13	DBU	QG	1.43	0.02	1
UNMAPPED	31	ARG	HG2	1.72	0.02	2
UNMAPPED	24	PRO	HG2	2.251	0.02	2
UNMAPPED	9	TRP	HE3	7.567	0.02	1
UNMAPPED	5	DBU	H	9.04	0.02	1
UNMAPPED	1	2KT	C3	30.078	0.4	1
UNMAPPED	7	DAL	H	8.014	0.02	1
UNMAPPED	28	CYS	CA	53.448	0.4	1
UNMAPPED	7	DAL	HA	4.433	0.02	1
UNMAPPED	24	PRO	HG3	2.092	0.02	2
UNMAPPED	12	ILE	HD12	0.643	0.02	1
UNMAPPED	3	PRO	HD3	3.566	0.02	2
UNMAPPED	12	ILE	CG1	26.088	0.4	1
UNMAPPED	27	LYS	HG2	1.558	0.02	2
UNMAPPED	21	SER	HB2	3.934	0.02	2
UNMAPPED	24	PRO	HD3	3.657	0.02	2
UNMAPPED	3	PRO	HG2	2.379	0.02	2
UNMAPPED	9	TRP	CE3	117.416	0.4	1
UNMAPPED	27	LYS	HD3	1.695	0.02	2
UNMAPPED	14	ALA	HB1	1.483	0.02	1
UNMAPPED	12	ILE	HG13	1.054	0.02	2
UNMAPPED	18	VAL	HG21	0.996	0.02	2
UNMAPPED	24	PRO	CA	61.493	0.4	1
UNMAPPED	27	LYS	HA	4.838	0.02	1
UNMAPPED	6	DBU	H	9.458	0.02	1
UNMAPPED	27	LYS	H	8.138	0.02	1
UNMAPPED	24	PRO	CB	28.987	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	24	PRO	HA	4.32	0.02	1
UNMAPPED	20	ALA	HB2	1.41	0.02	1
UNMAPPED	10	THR	CG2	19.256	0.4	1
UNMAPPED	24	PRO	CG	25.178	0.4	1
UNMAPPED	20	ALA	HB1	1.41	0.02	1
UNMAPPED	31	ARG	H	7.992	0.02	1
UNMAPPED	30	SER	H	8.213	0.02	1
UNMAPPED	10	THR	HG23	1.27	0.02	1
UNMAPPED	4	ALA	H	8.115	0.02	1
UNMAPPED	18	VAL	HG23	0.996	0.02	2
UNMAPPED	32	CYS	HA	4.167	0.02	1
UNMAPPED	17	DBU	H	9.439	0.02	1
UNMAPPED	18	VAL	HG12	1.114	0.02	2
UNMAPPED	18	VAL	HA	3.804	0.02	1
UNMAPPED	9	TRP	CH2	121.133	0.4	1
UNMAPPED	10	THR	CA	64.229	0.4	1
UNMAPPED	18	VAL	HB	2.27	0.02	1
UNMAPPED	26	DBU	CB	130.767	0.4	1
UNMAPPED	18	VAL	CA	63.83	0.4	1
UNMAPPED	19	DAL	H	8.62	0.02	1
UNMAPPED	23	CYS	HB3	2.605	0.02	2
UNMAPPED	9	TRP	HH2	7.127	0.02	1
UNMAPPED	27	LYS	HZ2	7.813	0.02	1
UNMAPPED	32	CYS	H	7.477	0.02	1
UNMAPPED	4	ALA	HB2	1.492	0.02	1
UNMAPPED	9	TRP	H	9.103	0.02	1
UNMAPPED	32	CYS	HB3	2.949	0.02	2
UNMAPPED	6	DBU	QG	1.846	0.02	1
UNMAPPED	13	DBU	HB	6.213	0.02	1
UNMAPPED	19	DAL	HB3	2.555	0.02	2
UNMAPPED	15	GLY	H	7.931	0.02	1
UNMAPPED	32	CYS	CA	59.68	0.4	1
UNMAPPED	31	ARG	CG	24.751	0.4	1
UNMAPPED	24	PRO	HB2	2.318	0.02	2
UNMAPPED	17	DBU	QG	1.813	0.02	1
UNMAPPED	27	LYS	HB3	1.593	0.02	2
UNMAPPED	22	LEU	HB3	1.641	0.02	2
UNMAPPED	27	LYS	HZ1	7.813	0.02	1
UNMAPPED	3	PRO	HB2	1.963	0.02	2
UNMAPPED	20	ALA	CA	52.605	0.4	1
UNMAPPED	31	ARG	CD	40.625	0.4	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	9	TRP	HB3	3.351	0.02	2
UNMAPPED	12	ILE	CA	62.744	0.4	1
UNMAPPED	16	VAL	CA	63.893	0.4	1
UNMAPPED	22	LEU	CA	52.007	0.4	1
UNMAPPED	27	LYS	CD	26.606	0.4	1
UNMAPPED	22	LEU	HD23	0.901	0.02	2
UNMAPPED	21	SER	CB	62.393	0.4	1
UNMAPPED	27	LYS	CG	22.362	0.4	1
UNMAPPED	32	CYS	CB	36.982	0.4	1
UNMAPPED	5	DBU	QG	1.81	0.02	1
UNMAPPED	2	DBU	QG	1.822	0.02	1
UNMAPPED	32	CYS	HB2	3.704	0.02	2
UNMAPPED	30	SER	HB3	3.74	0.02	2
UNMAPPED	31	ARG	HB2	2.179	0.02	2
UNMAPPED	26	DBU	CG	12.874	0.4	1
UNMAPPED	7	DAL	HB2	3.309	0.02	2
UNMAPPED	31	ARG	HE	7.476	0.02	1
UNMAPPED	12	ILE	HG21	0.863	0.02	1
UNMAPPED	16	VAL	HG22	0.989	0.02	2
UNMAPPED	9	TRP	CZ3	118.508	0.4	1
UNMAPPED	12	ILE	HG22	0.863	0.02	1
UNMAPPED	11	CYS	CB	32.19	0.4	1
UNMAPPED	11	CYS	HB3	2.847	0.02	2
UNMAPPED	31	ARG	HD2	3.314	0.02	2
UNMAPPED	18	VAL	H	7.935	0.02	1
UNMAPPED	25	ABA	QG	1.342	0.02	1
UNMAPPED	31	ARG	HG3	1.637	0.02	2
UNMAPPED	2	DBU	HB	5.957	0.02	1
UNMAPPED	4	ALA	HB3	1.492	0.02	1
UNMAPPED	28	CYS	CB	33.091	0.4	1
UNMAPPED	12	ILE	HD13	0.643	0.02	1
UNMAPPED	27	LYS	HB2	2.231	0.02	2
UNMAPPED	13	DBU	CB	127.948	0.4	1
UNMAPPED	2	DBU	H	10.195	0.02	1
UNMAPPED	21	SER	HB3	3.84	0.02	2
UNMAPPED	14	ALA	CA	52.007	0.4	1
UNMAPPED	20	ALA	H	8.671	0.02	1
UNMAPPED	14	ALA	HB2	1.483	0.02	1
UNMAPPED	14	ALA	CB	15.126	0.4	1
UNMAPPED	12	ILE	HG12	1.672	0.02	2
UNMAPPED	22	LEU	H	8.19	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	2KT	Q4	0.98	0.02	1
UNMAPPED	22	LEU	HA	4.568	0.02	1
UNMAPPED	30	SER	HB2	3.871	0.02	2
UNMAPPED	19	DAL	CB	29.094	0.4	1
UNMAPPED	25	ABA	CB	42.627	0.4	1
UNMAPPED	16	VAL	HG11	1.002	0.02	2
UNMAPPED	27	LYS	HE3	3.021	0.02	2
UNMAPPED	18	VAL	HG22	0.996	0.02	2
UNMAPPED	16	VAL	HG12	1.002	0.02	2
UNMAPPED	10	THR	HB	4.383	0.02	1
UNMAPPED	9	TRP	HZ3	7.035	0.02	1
UNMAPPED	22	LEU	CD1	22.478	0.4	1
UNMAPPED	18	VAL	HG13	1.114	0.02	2
UNMAPPED	10	THR	HA	3.819	0.02	1
UNMAPPED	10	THR	CB	65.645	0.4	1
UNMAPPED	31	ARG	CA	51.611	0.4	1
UNMAPPED	19	DAL	CA	57.703	0.4	1
UNMAPPED	8	DHA	CA	107.652	0.4	1
UNMAPPED	19	DAL	HB2	3.987	0.02	2
UNMAPPED	16	VAL	CG2	18.09	0.4	1
UNMAPPED	23	CYS	HB2	3.747	0.02	2
UNMAPPED	19	DAL	HA	4.05	0.02	1
UNMAPPED	23	CYS	CB	29.621	0.4	1
UNMAPPED	16	VAL	H	8.27	0.02	1
UNMAPPED	16	VAL	CB	28.673	0.4	1
UNMAPPED	8	DHA	HB3	5.097	0.02	2
UNMAPPED	7	DAL	CA	55.325	0.4	1
UNMAPPED	2	DBU	CB	124.946	0.4	1
UNMAPPED	5	DBU	CB	127.731	0.4	1
UNMAPPED	9	TRP	CD1	123.317	0.4	1
UNMAPPED	7	DAL	CB	32.223	0.4	1
UNMAPPED	5	DBU	CG	11.681	0.4	1
UNMAPPED	3	PRO	CA	61.703	0.4	1
UNMAPPED	31	ARG	CB	26.941	0.4	1
UNMAPPED	24	PRO	HB3	2.022	0.02	2

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	22	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	28	0.00 \pm 0.00	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	—
^{15}N	0	—	—

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 98. 0 out of 1 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/43 (0%)	0/17 (0%)	0/18 (0%)	0/8 (0%)
Sidechain	0/55 (0%)	0/34 (0%)	0/20 (0%)	0/1 (0%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/98 (0%)	0/51 (0%)	0/38 (0%)	0/9 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 289. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	0/121 (0%)	0/48 (0%)	0/50 (0%)	0/23 (0%)
Sidechain	0/160 (0%)	0/95 (0%)	0/60 (0%)	0/5 (0%)
Aromatic	0/8 (0%)	0/4 (0%)	0/4 (0%)	0/0 (—%)
Overall	0/289 (0%)	0/147 (0%)	0/114 (0%)	0/28 (0%)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
???	UNMAPPED	3	PRO	CB	24.55	37.79 – 25.89	-6.1

7.1.5 Random Coil Index (RCI) plots [i](#)

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chem_shift_list_1). RCI is only applicable to proteins.