



# Full wwPDB NMR Structure Validation Report ⓘ

Nov 28, 2017 – 05:00 PM EST

PDB ID : 5L82  
Title : NMR Structure of Enterocin K1 in 50%/50% TFE/Water  
Authors : Ovchinnikov, K.; Kristiansen, P.E.; Diep, D.  
Deposited on : unknown

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

Cyrange : Kirchner and Güntert (2011)  
NmrClust : Kelley et al. (1996)  
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
ShiftChecker : rb-20030345  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

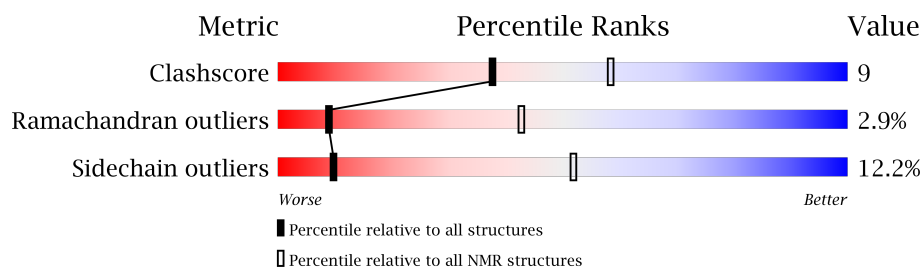
# 1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	37	 76% 14% 5% 5%

## 2 Ensemble composition and analysis ⓘ

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: *lowest energy*.

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:2-A:36 (35)	0.06	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 4 clusters. No single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 647 atoms, of which 324 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Enterococcin K1.

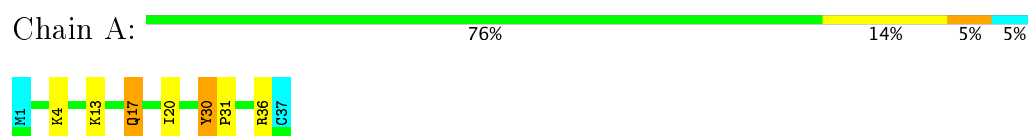
Mol	Chain	Residues	Atoms						Trace
1	A	37	Total	C	H	N	O	S	0
			647	218	324	53	50	2	

## 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: Enterococcin K1

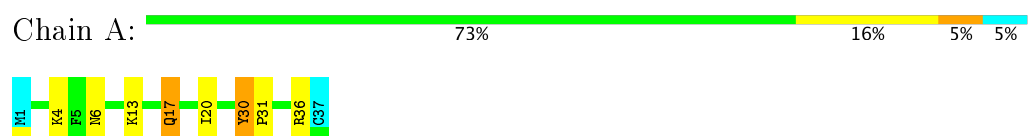


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section [4.1](#) above.

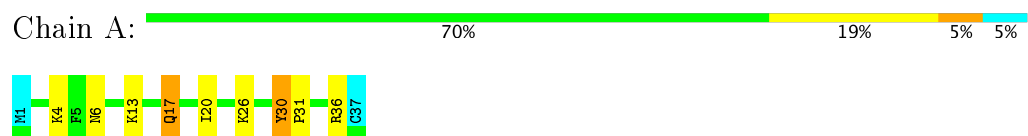
#### 4.2.1 Score per residue for model 1

- Molecule 1: Enterococcin K1



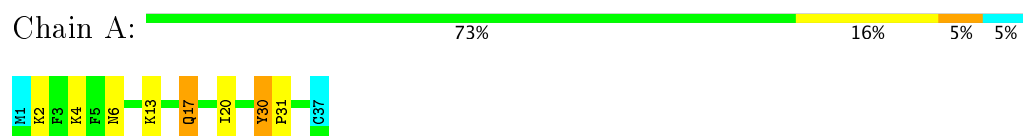
#### 4.2.2 Score per residue for model 2

- Molecule 1: Enterococcin K1



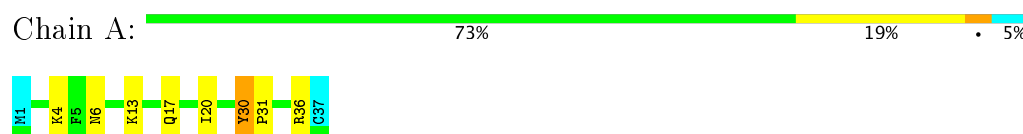
### 4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Enterococcin K1



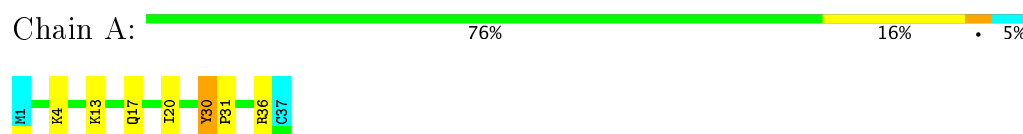
### 4.2.4 Score per residue for model 4

- Molecule 1: Enterococcin K1



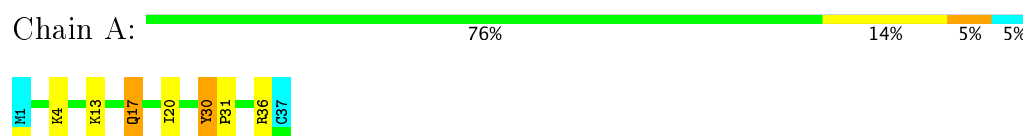
### 4.2.5 Score per residue for model 5

- Molecule 1: Enterococcin K1



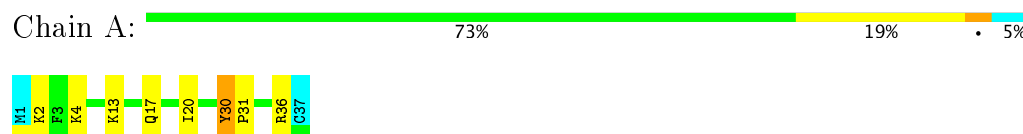
### 4.2.6 Score per residue for model 6

- Molecule 1: Enterococcin K1




### 4.2.7 Score per residue for model 7

- Molecule 1: Enterococcin K1



#### 4.2.8 Score per residue for model 8


- Molecule 1: Enterococcin K1

Chain A:  78% 11% 5% 5%



#### 4.2.9 Score per residue for model 9


- Molecule 1: Enterococcin K1

Chain A:  76% 16% 5%



#### 4.2.10 Score per residue for model 10

- Molecule 1: Enterococcin K1

Chain A:  76% 16% 5%



#### 4.2.11 Score per residue for model 11

- Molecule 1: Enterococcin K1

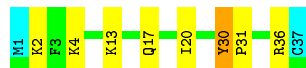
Chain A:  73% 16% 5% 5%



#### 4.2.12 Score per residue for model 12

- Molecule 1: Enterococcin K1

Chain A:  73% 19% 5%



#### 4.2.13 Score per residue for model 13

- Molecule 1: Enterococcin K1

Chain A:  76% 14% 5% 5%



#### 4.2.14 Score per residue for model 14


- Molecule 1: Enterococcin K1

Chain A:  76% 14% 5% 5%



#### 4.2.15 Score per residue for model 15

- Molecule 1: Enterococcin K1

Chain A:  78% 11% 5% 5%



#### 4.2.16 Score per residue for model 16


- Molecule 1: Enterococcin K1

Chain A:  76% 16% 5%



#### 4.2.17 Score per residue for model 17

- Molecule 1: Enterococcin K1

Chain A:  76% 16% 5%





#### 4.2.18 Score per residue for model 18

- Molecule 1: Enterococcin K1

Chain A:  73% 19% • 5%



#### 4.2.19 Score per residue for model 19

- Molecule 1: Enterococcin K1

Chain A:  76% 16% • 5%



#### 4.2.20 Score per residue for model 20

- Molecule 1: Enterococcin K1

Chain A:  73% 16% 5% 5%



## 5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CYANA	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)	5l82_cs.cif
Number of chemical shift lists	1
Total number of shifts	474
Number of shifts mapped to atoms	0
Number of unparsed shifts	474
Number of shifts with mapping errors	0
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](#)

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	309	310	310	6±0
All	All	6180	6200	6200	115

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:TYR:HB2	1:A:31:PRO:HD3	0.61	1.73	7	20
1:A:30:TYR:H	1:A:31:PRO:HD2	0.59	1.56	2	20
1:A:30:TYR:HB2	1:A:31:PRO:CD	0.53	2.33	19	20
1:A:17:GLN:HA	1:A:20:ILE:HD12	0.48	1.84	10	20
1:A:30:TYR:N	1:A:31:PRO:HD2	0.46	2.25	2	20
1:A:30:TYR:CB	1:A:31:PRO:CD	0.42	2.97	15	15

### 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	35/37 (95%)	28±1 (80±2%)	6±1 (17±2%)	1±0 (3±0%)	9	43
All	All	700/740 (95%)	560 (80%)	120 (17%)	20 (3%)	9	43

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
1	A	30	TYR	20

### 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	32/34 (94%)	28±1 (88±3%)	4±1 (12±3%)	10	52
All	All	640/680 (94%)	562 (88%)	78 (12%)	10	52

All 7 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	13	LYS	20
1	A	4	LYS	19
1	A	36	ARG	16
1	A	17	GLN	10
1	A	2	LYS	6
1	A	6	ASN	4
1	A	26	LYS	3

### 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 carbohydrates in this entry.

## 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 6.7 Other polymers [i](#)

There are no such molecules in this entry.

## 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 0% for the well-defined parts and 0% for the entire structure.

### 7.1 Chemical shift list 1

File name: 5l82\_cs.cif

Chemical shift list name: *assigned\_chem\_shift\_list*

#### 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	474
Number of shifts mapped to atoms	0
Number of unparsed shifts	474
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following errors were found when reading this chemical shift list.

- Entity instance (chain) must be specified. All 474 occurrences are reported below.

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	?	4	LYS	HD3	1.708	?	1
2	?	4	LYS	HE3	3.024	?	1
3	?	5	PHE	HB3	3.062	?	1
4	?	1	MET	HB3	2.149	?	1
5	?	12	VAL	H	8.164	?	1
6	?	3	PHE	N	119.628	?	1
7	?	3	PHE	H	8.051	?	1
8	?	3	PHE	HA	4.651	?	1
9	?	3	PHE	CB	39.789	?	1
10	?	3	PHE	HB2	3.119	?	1
11	?	3	PHE	HB3	2.998	?	1
12	?	3	PHE	HD2	7.254	?	1
13	?	3	PHE	HD1	7.254	?	1
14	?	3	PHE	HE2	7.299	?	1
15	?	3	PHE	HE1	7.299	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
16	?	3	PHE	CD2	131.594	?	1
17	?	3	PHE	CD1	131.594	?	1
18	?	4	LYS	N	122.270	?	1
19	?	4	LYS	H	8.001	?	1
20	?	4	LYS	CA	55.958	?	1
21	?	4	LYS	HA	4.338	?	1
22	?	4	LYS	CB	33.266	?	1
23	?	4	LYS	HB2	1.788	?	1
24	?	4	LYS	HB3	1.708	?	1
25	?	4	LYS	CG	24.404	?	1
26	?	4	LYS	HG2	1.360	?	1
27	?	4	LYS	HG3	1.408	?	1
28	?	4	LYS	CD	28.944	?	1
29	?	4	LYS	HD2	1.708	?	1
30	?	4	LYS	CE	41.962	?	1
31	?	4	LYS	HE2	3.024	?	1
32	?	5	PHE	N	120.790	?	1
33	?	5	PHE	H	7.880	?	1
34	?	5	PHE	HA	4.608	?	1
35	?	5	PHE	CB	39.809	?	1
36	?	5	PHE	HB2	3.062	?	1
37	?	5	PHE	HD2	7.247	?	1
38	?	5	PHE	HD1	7.247	?	1
39	?	5	PHE	HE2	7.347	?	1
40	?	5	PHE	HE1	7.347	?	1
41	?	5	PHE	CD2	131.594	?	1
42	?	5	PHE	CD1	131.594	?	1
43	?	5	PHE	CE2	129.551	?	1
44	?	5	PHE	CE1	129.551	?	1
45	?	6	ASN	N	121.225	?	1
46	?	6	ASN	H	8.099	?	1
47	?	6	ASN	CA	50.119	?	1
48	?	6	ASN	HA	4.990	?	1
49	?	6	ASN	CB	38.981	?	1
50	?	6	ASN	HB2	2.710	?	1
51	?	6	ASN	HB3	2.993	?	1
52	?	6	ASN	ND2	110.973	?	1
53	?	6	ASN	HD21	7.622	?	1
54	?	6	ASN	HD22	6.826	?	1
55	?	7	PRO	CD	50.245	?	1
56	?	7	PRO	CA	64.136	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
57	?	7	PRO	HA	4.434	?	1
58	?	7	PRO	CB	31.535	?	1
59	?	7	PRO	HB2	2.254	?	1
60	?	7	PRO	HB3	2.134	?	1
61	?	7	PRO	CG	26.211	?	1
62	?	7	PRO	HG2	1.986	?	1
63	?	7	PRO	HD2	3.808	?	1
64	?	7	PRO	HD3	3.533	?	1
65	?	8	THR	N	113.523	?	1
66	?	8	THR	H	8.007	?	1
67	?	8	THR	CA	65.938	?	1
68	?	8	THR	HA	3.961	?	1
69	?	8	THR	CB	68.834	?	1
70	?	8	THR	HB	4.151	?	1
71	?	8	THR	HG22	1.259	?	1
72	?	8	THR	HG23	1.259	?	1
73	?	8	THR	HG21	1.259	?	1
74	?	8	THR	CG2	20.945	?	1
75	?	9	GLY	N	107.141	?	1
76	?	9	GLY	H	8.211	?	1
77	?	9	GLY	CA	46.893	?	1
78	?	9	GLY	HA2	3.839	?	1
79	?	9	GLY	HA3	3.892	?	1
80	?	10	THR	N	116.285	?	1
81	?	10	THR	H	7.808	?	1
82	?	10	THR	CA	66.134	?	1
83	?	10	THR	HA	4.049	?	1
84	?	10	THR	CB	68.930	?	1
85	?	10	THR	HB	4.339	?	1
86	?	10	THR	HG22	1.340	?	1
87	?	10	THR	HG23	1.340	?	1
88	?	10	THR	HG21	1.340	?	1
89	?	10	THR	CG2	21.188	?	1
90	?	11	ILE	N	122.329	?	1
91	?	11	ILE	H	7.844	?	1
92	?	11	ILE	CA	64.962	?	1
93	?	11	ILE	HA	3.780	?	1
94	?	11	ILE	CB	37.758	?	1
95	?	11	ILE	HB	2.045	?	1
96	?	11	ILE	HG22	0.983	?	1
97	?	11	ILE	HG23	0.983	?	1

*Continued on next page...*



*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
98	?	11	ILE	HG21	0.983	?	1
99	?	11	ILE	CG2	16.322	?	1
100	?	11	ILE	CG1	28.517	?	1
101	?	11	ILE	HG12	1.708	?	1
102	?	12	VAL	CA	66.785	?	1
103	?	12	VAL	HA	3.699	?	1
104	?	12	VAL	CB	32.507	?	1
105	?	12	VAL	HB	2.165	?	1
106	?	12	VAL	HG12	0.985	?	1
107	?	12	VAL	HG13	0.985	?	1
108	?	12	VAL	HG11	0.985	?	1
109	?	12	VAL	HG23	1.100	?	1
110	?	12	VAL	HG22	1.100	?	1
111	?	12	VAL	HG21	1.100	?	1
112	?	12	VAL	CG1	20.298	?	1
113	?	12	VAL	CG2	21.961	?	1
114	?	13	LYS	N	121.835	?	1
115	?	13	LYS	H	8.034	?	1
116	?	13	LYS	CA	58.497	?	1
117	?	13	LYS	HA	4.039	?	1
118	?	13	LYS	CB	32.143	?	1
119	?	13	LYS	HB2	2.013	?	1
120	?	13	LYS	CG	25.132	?	1
121	?	13	LYS	HG2	1.457	?	1
122	?	13	LYS	HG3	1.655	?	1
123	?	13	LYS	CD	28.780	?	1
124	?	13	LYS	HD2	1.738	?	1
125	?	13	LYS	CE	41.979	?	1
126	?	13	LYS	HE2	2.986	?	1
127	?	14	LYS	N	120.586	?	1
128	?	14	LYS	H	8.049	?	1
129	?	14	LYS	CA	55.400	?	1
130	?	14	LYS	HA	4.144	?	1
131	?	14	LYS	CB	31.820	?	1
132	?	14	LYS	HB2	2.074	?	1
133	?	14	LYS	HB3	1.981	?	1
134	?	14	LYS	CG	24.737	?	1
135	?	14	LYS	HG2	1.560	?	1
136	?	14	LYS	HG3	1.653	?	1
137	?	14	LYS	CD	29.248	?	1
138	?	14	LYS	HD2	1.741	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
139	?	14	LYS	CE	41.989	?	1
140	?	14	LYS	HE2	2.996	?	1
141	?	15	LEU	N	119.632	?	1
142	?	15	LEU	H	8.824	?	1
143	?	15	LEU	CA	58.089	?	1
144	?	15	LEU	HA	4.265	?	1
145	?	15	LEU	CB	41.617	?	1
146	?	15	LEU	HB2	1.923	?	1
147	?	15	LEU	HB3	1.691	?	1
148	?	15	LEU	CG	26.568	?	1
149	?	15	LEU	HG	1.920	?	1
150	?	15	LEU	HD11	0.933	?	1
151	?	15	LEU	HD12	0.933	?	1
152	?	15	LEU	HD13	0.933	?	1
153	?	15	LEU	HD22	0.902	?	1
154	?	15	LEU	HD23	0.902	?	1
155	?	15	LEU	HD21	0.902	?	1
156	?	15	LEU	CD1	24.073	?	1
157	?	15	LEU	CD2	22.217	?	1
158	?	16	THR	N	114.837	?	1
159	?	16	THR	H	8.340	?	1
160	?	16	THR	CA	67.225	?	1
161	?	16	THR	HA	4.060	?	1
162	?	16	THR	CB	68.738	?	1
163	?	16	THR	HB	4.433	?	1
164	?	16	THR	HG22	1.356	?	1
165	?	16	THR	HG23	1.356	?	1
166	?	16	THR	HG21	1.356	?	1
167	?	16	THR	CG2	20.303	?	1
168	?	17	GLN	N	119.628	?	1
169	?	17	GLN	H	8.140	?	1
170	?	17	GLN	CA	59.657	?	1
171	?	17	GLN	HA	4.063	?	1
172	?	17	GLN	CB	28.141	?	1
173	?	17	GLN	HB2	2.229	?	1
174	?	17	GLN	HB3	2.389	?	1
175	?	17	GLN	CG	34.247	?	1
176	?	17	GLN	HG2	2.406	?	1
177	?	17	GLN	HG3	2.714	?	1
178	?	17	GLN	NE2	108.716	?	1
179	?	17	GLN	HE21	6.685	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
180	?	17	GLN	HE22	7.082	?	1
181	?	18	TYR	N	119.657	?	1
182	?	18	TYR	H	8.224	?	1
183	?	18	TYR	CA	56.285	?	1
184	?	18	TYR	HA	4.361	?	1
185	?	18	TYR	CB	37.648	?	1
186	?	18	TYR	HB2	3.269	?	1
187	?	18	TYR	HD2	7.157	?	1
188	?	18	TYR	HD1	7.157	?	1
189	?	18	TYR	HE2	6.792	?	1
190	?	18	TYR	HE1	6.792	?	1
191	?	18	TYR	CD2	132.614	?	1
192	?	18	TYR	CD1	132.614	?	1
193	?	18	TYR	CE1	117.571	?	1
194	?	18	TYR	CE2	117.571	?	1
195	?	19	GLU	N	118.769	?	1
196	?	19	GLU	H	8.595	?	1
197	?	19	GLU	CA	59.368	?	1
198	?	19	GLU	HA	4.176	?	1
199	?	19	GLU	CB	27.857	?	1
200	?	19	GLU	HB2	2.338	?	1
201	?	19	GLU	HB3	2.507	?	1
202	?	19	GLU	CG	32.904	?	1
203	?	19	GLU	HG2	2.829	?	1
204	?	19	GLU	HG3	2.621	?	1
205	?	20	ILE	N	119.831	?	1
206	?	20	ILE	H	8.520	?	1
207	?	20	ILE	CA	65.645	?	1
208	?	20	ILE	HA	3.843	?	1
209	?	20	ILE	CB	37.978	?	1
210	?	20	ILE	HB	2.129	?	1
211	?	20	ILE	HG22	1.166	?	1
212	?	20	ILE	HG23	1.166	?	1
213	?	20	ILE	HG21	1.166	?	1
214	?	20	ILE	CG2	17.693	?	1
215	?	20	ILE	CG1	29.195	?	1
216	?	20	ILE	HG12	2.082	?	1
217	?	20	ILE	HG13	1.246	?	1
218	?	20	ILE	HD11	1.021	?	1
219	?	20	ILE	HD12	1.021	?	1
220	?	20	ILE	HD13	1.021	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
221	?	20	ILE	CD1	12.840	?	1
222	?	21	ALA	N	122.532	?	1
223	?	21	ALA	H	8.232	?	1
224	?	21	ALA	CA	55.033	?	1
225	?	21	ALA	HA	4.144	?	1
226	?	21	ALA	HB2	1.595	?	1
227	?	21	ALA	HB3	1.595	?	1
228	?	21	ALA	HB1	1.595	?	1
229	?	21	ALA	CB	17.515	?	1
230	?	22	TRP	N	120.488	?	1
231	?	22	TRP	H	8.877	?	1
232	?	22	TRP	CA	60.979	?	1
233	?	22	TRP	HA	4.174	?	1
234	?	22	TRP	CB	28.488	?	1
235	?	22	TRP	HB2	3.142	?	1
236	?	22	TRP	HB3	3.444	?	1
237	?	22	TRP	CD1	126.599	?	1
238	?	22	TRP	CE3	120.616	?	1
239	?	22	TRP	NE1	127.061	?	1
240	?	22	TRP	HD1	7.051	?	1
241	?	22	TRP	HE3	7.593	?	1
242	?	22	TRP	CZ3	121.315	?	1
243	?	22	TRP	CZ2	114.096	?	1
244	?	22	TRP	HE1	9.726	?	1
245	?	22	TRP	HZ3	7.147	?	1
246	?	22	TRP	CH2	123.994	?	1
247	?	22	TRP	HZ2	7.445	?	1
248	?	22	TRP	HH2	7.220	?	1
249	?	23	PHE	H	8.780	?	1
250	?	23	PHE	HA	3.926	?	1
251	?	23	PHE	CB	39.138	?	1
252	?	23	PHE	HB2	3.459	?	1
253	?	23	PHE	HB3	3.425	?	1
254	?	23	PHE	HD2	7.360	?	1
255	?	23	PHE	HD1	7.360	?	1
256	?	23	PHE	HE2	7.070	?	1
257	?	23	PHE	HE1	7.070	?	1
258	?	23	PHE	CD2	131.023	?	1
259	?	23	PHE	CD1	131.023	?	1
260	?	23	PHE	CE2	131.233	?	1
261	?	23	PHE	CE1	131.233	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
262	?	24	LYS	H	8.787	?	1
263	?	24	LYS	CA	60.331	?	1
264	?	24	LYS	HA	4.036	?	1
265	?	24	LYS	CB	31.580	?	1
266	?	24	LYS	HB2	1.930	?	1
267	?	24	LYS	CG	24.577	?	1
268	?	24	LYS	HG2	1.180	?	1
269	?	24	LYS	CD	28.383	?	1
270	?	24	LYS	HD2	0.925	?	1
271	?	24	LYS	HD3	1.204	?	1
272	?	24	LYS	CE	42.131	?	1
273	?	24	LYS	HE2	2.751	?	1
274	?	25	ASN	N	118.351	?	1
275	?	25	ASN	H	8.307	?	1
276	?	25	ASN	CA	55.642	?	1
277	?	25	ASN	HA	4.390	?	1
278	?	25	ASN	CB	38.694	?	1
279	?	25	ASN	HB2	2.802	?	1
280	?	25	ASN	HB3	2.661	?	1
281	?	25	ASN	ND2	110.390	?	1
282	?	25	ASN	HD21	7.153	?	1
283	?	25	ASN	HD22	6.614	?	1
284	?	26	LYS	N	116.666	?	1
285	?	26	LYS	H	7.825	?	1
286	?	26	LYS	CA	56.275	?	1
287	?	26	LYS	HA	3.961	?	1
288	?	26	LYS	CB	31.875	?	1
289	?	26	LYS	HB2	1.222	?	1
290	?	26	LYS	HB3	1.239	?	1
291	?	26	LYS	CG	23.431	?	1
292	?	26	LYS	HG2	0.882	?	1
293	?	26	LYS	HG3	0.750	?	1
294	?	26	LYS	CD	27.745	?	1
295	?	26	LYS	HD2	1.316	?	1
296	?	26	LYS	CE	41.890	?	1
297	?	26	LYS	HE2	2.644	?	1
298	?	26	LYS	HE3	2.731	?	1
299	?	27	HIS	N	121.283	?	1
300	?	27	HIS	H	7.972	?	1
301	?	27	HIS	CA	55.538	?	1
302	?	27	HIS	HA	4.448	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
303	?	27	HIS	CB	28.592	?	1
304	?	27	HIS	HB2	2.767	?	1
305	?	27	HIS	HB3	2.465	?	1
306	?	27	HIS	CD2	119.698	?	1
307	?	27	HIS	CE1	135.109	?	1
308	?	27	HIS	HD2	6.482	?	1
309	?	27	HIS	HE1	8.127	?	1
310	?	28	GLY	N	107.141	?	1
311	?	28	GLY	H	8.194	?	1
312	?	28	GLY	CA	44.810	?	1
313	?	28	GLY	HA2	3.712	?	1
314	?	28	GLY	HA3	4.093	?	1
315	?	29	TYR	H	7.136	?	1
316	?	29	TYR	CA	55.614	?	1
317	?	29	TYR	HA	4.567	?	1
318	?	29	TYR	CB	39.469	?	1
319	?	29	TYR	HB2	2.966	?	1
320	?	29	TYR	HB3	2.847	?	1
321	?	29	TYR	HD2	7.010	?	1
322	?	29	TYR	HD1	7.010	?	1
323	?	29	TYR	HE2	6.793	?	1
324	?	29	TYR	HE1	6.793	?	1
325	?	29	TYR	CD2	133.817	?	1
326	?	29	TYR	CD1	133.817	?	1
327	?	29	TYR	CE1	117.535	?	1
328	?	29	TYR	CE2	117.535	?	1
329	?	30	TYR	N	121.254	?	1
330	?	30	TYR	H	8.092	?	1
331	?	30	TYR	CA	61.203	?	1
332	?	30	TYR	HA	4.363	?	1
333	?	30	TYR	CB	39.146	?	1
334	?	30	TYR	HB2	3.429	?	1
335	?	30	TYR	HD2	6.941	?	1
336	?	30	TYR	HD1	6.941	?	1
337	?	30	TYR	HE2	6.872	?	1
338	?	30	TYR	HE1	6.872	?	1
339	?	30	TYR	CD2	132.825	?	1
340	?	30	TYR	CD1	132.825	?	1
341	?	30	TYR	CE1	117.775	?	1
342	?	30	TYR	CE2	117.775	?	1
343	?	31	PRO	CD	49.628	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
344	?	31	PRO	CA	65.148	?	1
345	?	31	PRO	HA	3.909	?	1
346	?	31	PRO	CB	30.883	?	1
347	?	31	PRO	HB2	1.836	?	1
348	?	31	PRO	HB3	1.749	?	1
349	?	31	PRO	CG	26.675	?	1
350	?	31	PRO	HG2	1.508	?	1
351	?	31	PRO	HG3	1.953	?	1
352	?	31	PRO	HD2	3.241	?	1
353	?	31	PRO	HD3	3.457	?	1
354	?	32	TRP	H	6.354	?	1
355	?	32	TRP	HA	4.757	?	1
356	?	32	TRP	CB	26.825	?	1
357	?	32	TRP	HB2	3.222	?	1
358	?	32	TRP	HB3	3.541	?	1
359	?	32	TRP	CD1	126.806	?	1
360	?	32	TRP	CE3	118.891	?	1
361	?	32	TRP	NE1	130.226	?	1
362	?	32	TRP	HD1	7.133	?	1
363	?	32	TRP	HE3	7.544	?	1
364	?	32	TRP	CZ3	121.970	?	1
365	?	32	TRP	CZ2	115.169	?	1
366	?	32	TRP	HE1	10.022	?	1
367	?	32	TRP	HZ3	7.143	?	1
368	?	32	TRP	CH2	124.677	?	1
369	?	32	TRP	HZ2	6.903	?	1
370	?	32	TRP	HH2	6.965	?	1
371	?	33	GLU	N	120.682	?	1
372	?	33	GLU	H	7.663	?	1
373	?	33	GLU	CA	56.203	?	1
374	?	33	GLU	HA	4.447	?	1
375	?	33	GLU	CB	29.852	?	1
376	?	33	GLU	HB2	2.204	?	1
377	?	33	GLU	HB3	2.187	?	1
378	?	33	GLU	CG	35.178	?	1
379	?	33	GLU	HG2	2.062	?	1
380	?	33	GLU	HG3	2.395	?	1
381	?	34	ILE	N	120.216	?	1
382	?	34	ILE	H	7.372	?	1
383	?	34	ILE	CA	58.705	?	1
384	?	34	ILE	HA	4.284	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
385	?	34	ILE	CB	38.639	?	1
386	?	34	ILE	HB	1.867	?	1
387	?	34	ILE	HG22	0.959	?	1
388	?	34	ILE	HG23	0.959	?	1
389	?	34	ILE	HG21	0.959	?	1
390	?	34	ILE	CG2	16.314	?	1
391	?	34	ILE	CG1	27.087	?	1
392	?	34	ILE	HG12	1.575	?	1
393	?	34	ILE	HG13	1.189	?	1
394	?	34	ILE	HD11	0.891	?	1
395	?	34	ILE	HD12	0.891	?	1
396	?	34	ILE	HD13	0.891	?	1
397	?	34	ILE	CD1	12.077	?	1
398	?	35	PRO	CD	50.437	?	1
399	?	35	PRO	CA	63.107	?	1
400	?	35	PRO	HA	4.257	?	1
401	?	35	PRO	CB	31.547	?	1
402	?	35	PRO	HB2	1.941	?	1
403	?	35	PRO	HB3	2.170	?	1
404	?	35	PRO	CG	26.958	?	1
405	?	35	PRO	HG2	2.011	?	1
406	?	35	PRO	HG3	1.863	?	1
407	?	35	PRO	HD2	3.718	?	1
408	?	35	PRO	HD3	3.545	?	1
409	?	36	ARG	N	120.035	?	1
410	?	36	ARG	H	7.935	?	1
411	?	36	ARG	HA	4.448	?	1
412	?	36	ARG	CB	30.911	?	1
413	?	36	ARG	HB2	1.939	?	1
414	?	36	ARG	HB3	1.819	?	1
415	?	36	ARG	CG	26.739	?	1
416	?	36	ARG	HG2	1.724	?	1
417	?	36	ARG	CD	43.095	?	1
418	?	36	ARG	HD2	3.247	?	1
419	?	36	ARG	NE	120.439	?	1
420	?	36	ARG	HE	7.203	?	1
421	?	37	CYS	N	120.819	?	1
422	?	37	CYS	H	7.919	?	1
423	?	37	CYS	CA	58.179	?	1
424	?	37	CYS	HA	4.530	?	1
425	?	37	CYS	CB	28.383	?	1

*Continued on next page...*



*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
426	?	37	CYS	HB2	2.996	?	1
427	?	2	LYS	HD3	1.716	?	1
428	?	2	LYS	HE3	3.014	?	1
429	?	7	PRO	HG3	1.986	?	1
430	?	13	LYS	HB3	2.013	?	1
431	?	13	LYS	HE3	2.986	?	1
432	?	13	LYS	HD3	1.738	?	1
433	?	14	LYS	HD3	1.741	?	1
434	?	14	LYS	HE3	2.996	?	1
435	?	18	TYR	HB3	3.269	?	1
436	?	24	LYS	HB3	1.930	?	1
437	?	24	LYS	HE3	2.751	?	1
438	?	24	LYS	HG3	1.180	?	1
439	?	26	LYS	HD3	1.316	?	1
440	?	30	TYR	HB3	3.429	?	1
441	?	36	ARG	HD3	3.247	?	1
442	?	36	ARG	HG3	1.724	?	1
443	?	37	CYS	HB3	2.996	?	1
444	?	12	VAL	N	118.503	?	1
445	?	11	ILE	CD1	12.026	?	1
446	?	11	ILE	HD11	0.900	?	1
447	?	11	ILE	HD12	0.900	?	1
448	?	11	ILE	HD13	0.900	?	1
449	?	11	ILE	HG13	1.211	?	1
450	?	1	MET	CG	30.741	?	1
451	?	1	MET	CA	59.332	?	1
452	?	1	MET	HG2	2.515	?	1
453	?	1	MET	HG3	2.570	?	1
454	?	1	MET	HA	4.155	?	1
455	?	1	MET	HB2	2.149	?	1
456	?	1	MET	CB	32.522	?	1
457	?	1	MET	HE1	2.121	?	1
458	?	1	MET	HE3	2.121	?	1
459	?	1	MET	HE2	2.121	?	1
460	?	1	MET	CE	16.164	?	1
461	?	2	LYS	N	123.484	?	1
462	?	2	LYS	H	8.506	?	1
463	?	2	LYS	CA	56.248	?	1
464	?	2	LYS	HA	4.405	?	1
465	?	2	LYS	CB	33.334	?	1
466	?	2	LYS	HB2	1.721	?	1

*Continued on next page...*

*Continued from previous page...*

Shift ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
467	?	2	LYS	HB3	1.774	?	1
468	?	2	LYS	CG	24.424	?	1
469	?	2	LYS	HG2	1.445	?	1
470	?	2	LYS	HG3	1.385	?	1
471	?	2	LYS	CD	28.761	?	1
472	?	2	LYS	HD2	1.716	?	1
473	?	2	LYS	CE	42.039	?	1
474	?	2	LYS	HE2	3.014	?	1

### 7.1.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

### 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 495. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/169 (0%)	0/67 (0%)	0/70 (0%)	0/32 (0%)
Sidechain	0/244 (0%)	0/147 (0%)	0/85 (0%)	0/12 (0%)
Aromatic	0/82 (0%)	0/43 (0%)	0/36 (0%)	0/3 (0%)
Overall	0/495 (0%)	0/257 (0%)	0/191 (0%)	0/47 (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 516. 0 out of 2 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/179 (0%)	0/71 (0%)	0/74 (0%)	0/34 (0%)
Sidechain	0/255 (0%)	0/154 (0%)	0/89 (0%)	0/12 (0%)
Aromatic	0/82 (0%)	0/43 (0%)	0/36 (0%)	0/3 (0%)
Overall	0/516 (0%)	0/268 (0%)	0/199 (0%)	0/49 (0%)

### 7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

### 7.1.5 Random Coil Index (RCI) plots

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