WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report (i)

Apr 26, 2016 – 09:16 PM BST

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PDB ID	:	2IGZ
Title	:	NMR structure of the sterol-dependent antifungal antibiotic bacillomycin Lc
Authors	:	Volpon, L.; Tsan, P.; Besson, F.; Lancelin, J.M.
Deposited on	:	2006-09-25

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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 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.
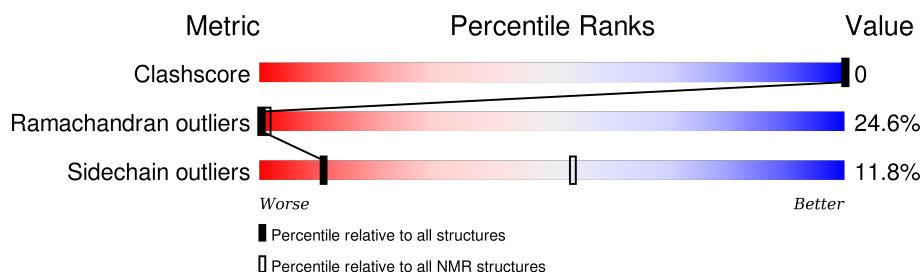
Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	114402	11133
Ramachandran outliers	111179	9975
Sidechain outliers	111093	9958

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	8	63% 38%

2 Ensemble composition and analysis (i)

This entry contains 19 models.

Cyrange was unable to find well-defined residues.

Error message: The number of core atoms (4) was below the domain threshold value (8).

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 147 atoms, of which 74 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BACILLOMYCIN L-3.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	8	147	47	74	10	16	0

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: BACILLOMYCIN L-3

Chain A:

63%   38%

?1 N2 S5 T8

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: BACILLOMYCIN L-3

Chain A:

50%   50%

?1 N2 S5 T8

4.2.2 Score per residue for model 2

• Molecule 1: BACILLOMYCIN L-3

Chain A:

75%   25%

?1 N2 T8

4.2.3   Score per residue for model 3

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.4   Score per residue for model 4

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.5   Score per residue for model 5

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.6   Score per residue for model 6

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.7   Score per residue for model 7

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.8 Score per residue for model 8

• Molecule 1: BACILLOMYCIN L-3

Chain A:

75%   13%   13%

?1 N2 T7 T8

4.2.9 Score per residue for model 9

• Molecule 1: BACILLOMYCIN L-3

Chain A:

75%   25%

?1 N2 T8

4.2.10 Score per residue for model 10

• Molecule 1: BACILLOMYCIN L-3

Chain A:

50%   38%   13%

?1 N2 E6 S7 T8

4.2.11 Score per residue for model 11

• Molecule 1: BACILLOMYCIN L-3

Chain A:

63%   25%   13%

?1 N2 S5 T8

4.2.12 Score per residue for model 12

• Molecule 1: BACILLOMYCIN L-3

Chain A:

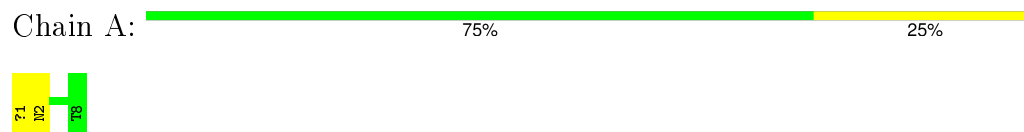63%   25%   13%

?1 N2 S5 T8

4.2.13 Score per residue for model 13

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.14 Score per residue for model 14

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.15 Score per residue for model 15

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.16 Score per residue for model 16

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.17 Score per residue for model 17

• Molecule 1: BACILLOMYCIN L-3

Chain A:

4.2.18   Score per residue for model 18

• Molecule 1: BACILLOMYCIN L-3

Chain A:

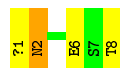#### 4.2.19   Score per residue for model 19

• Molecule 1: BACILLOMYCIN L-3

Chain A:

5   Refinement protocol and experimental data overview ⓘ

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

Of the 50 calculated structures, 19 were deposited, based on the following criterion: *STRUCTURES WITH THE LEAST RESTRAINT VIOLATIONS, STRUCTURES WITH THE LOWEST ENERGY*.

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

Software name	Classification	Version
CHARMM 22	refinement	
X-PLOR 3.851	structure solution	
XWINNMR	structure solution	
GIFA 4.0	structure solution	
MOLMOL	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 7294, BMRB entry 7295
Number of chemical shift lists	2
Total number of shifts	144
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	144
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: DSN, DSG, DTY, AFC

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	0.95±0.05	0±0/27 (0.0±0.0%)	1.62±0.28	1±0/32 (2.0±1.5%)
All	All	0.95	0/513 (0.0%)	1.64	12/608 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	1.6±1.1
All	All	0	30

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	2	ASN	N-CA-C	-6.03	94.72	111.00	7	12

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	1	AFC	Mainchain,Peptide	13
1	A	5	SER	Peptide	3
1	A	6	GLU	Peptide	1

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
All	All	1387	1406	1318	-

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 -.

There are no clashes.

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	3/8 (38%)	1±1 (30±18%)	1±1 (46±25%)	1±1 (25±24%)	0　1
All	All	57/152 (38%)	17 (30%)	26 (46%)	14 (25%)	0　1

All 2 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	2	ASN	7
1	A	5	SER	7

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	4/4 (100%)	4±1 (88±15%)	0±1 (12±15%)	11	53
All	All	76/76 (100%)	67 (88%)	9 (12%)	11	53

All 2 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	8	THR	8
1	A	2	ASN	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	AFC	A	1	1	16,16,17	0.81±0.04	0±0 (0±0%)
1	DTY	A	3	1	10,12,13	1.00±0.02	0±0 (0±0%)
1	DSG	A	4	1	5,7,8	0.93±0.06	0±0 (0±0%)
1	DSN	A	7	1	3,5,6	0.63±0.08	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	AFC	A	1	1	15,17,19	0.70±0.15	0±0 (0±0%)
1	DTY	A	3	1	13,15,17	0.73±0.09	0±0 (0±0%)
1	DSG	A	4	1	6,8,10	0.97±0.12	0±0 (0±0%)
1	DSN	A	7	1	3,5,7	1.52±0.40	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	AFC	A	1	1	-	0±0,16,16,17	0±0,0,0,0
1	DTY	A	3	1	-	0±0,4,6,8	0±0,1,1,1
1	DSG	A	4	1	-	0±0,4,6,8	0±0,0,0,0
1	DSN	A	7	1	-	0±0,2,4,6	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 (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: BMRB entry 7294

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	96
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	96
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 96 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	DTY	HB3	2.95	0.02	1
UNMAPPED	7	THR	H	7.7	0.02	1
UNMAPPED	7	THR	HA	4.05	0.02	1
UNMAPPED	8	AFC	HM2	0.85	0.02	2
UNMAPPED	7	THR	HB	4.07	0.02	1
UNMAPPED	8	AFC	HH3	1.19	0.07	4
UNMAPPED	2	DTY	HA	4.21	0.02	1
UNMAPPED	8	AFC	HC2	1.35	0.02	2
UNMAPPED	8	AFC	HA3	2.27	0.02	2
UNMAPPED	2	DTY	HH	9.18	0.02	1
UNMAPPED	4	SER	HG	4.92	0.02	1
UNMAPPED	6	DSN	H	8.14	0.02	1
UNMAPPED	5	GLU	H	7.97	0.02	1
UNMAPPED	8	AFC	HL2	1.19	0.07	4

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	3	DSG	HB3	2.52	0.02	2
UNMAPPED	2	DTY	CD1	129.5	0.2	1
UNMAPPED	3	DSG	CB	36.7	0.2	1
UNMAPPED	2	DTY	CD2	129.5	0.2	1
UNMAPPED	8	AFC	HF2	1.19	0.07	4
UNMAPPED	5	GLU	HE2	11.96	0.02	1
UNMAPPED	1	ASN	H	7.9	0.02	1
UNMAPPED	8	AFC	HG3	1.19	0.07	4
UNMAPPED	8	AFC	HI3	1.19	0.07	4
UNMAPPED	3	DSG	HA	4.47	0.02	1
UNMAPPED	7	THR	HG23	1.01	0.02	1
UNMAPPED	8	AFC	HJ3	1.19	0.07	4
UNMAPPED	8	AFC	CE	29.1	0.2	1
UNMAPPED	8	AFC	HD3	1.19	0.07	4
UNMAPPED	8	AFC	CC	33.7	0.2	1
UNMAPPED	4	SER	CB	61.1	0.2	1
UNMAPPED	8	AFC	HE2	1.19	0.07	4
UNMAPPED	2	DTY	CB	35.4	0.2	1
UNMAPPED	2	DTY	HB2	2.68	0.02	1
UNMAPPED	2	DTY	CA	55.5	0.2	1
UNMAPPED	6	DSN	HA	4.34	0.02	1
UNMAPPED	6	DSN	HG	4.87	0.02	1
UNMAPPED	8	AFC	HA2	2.27	0.02	2
UNMAPPED	6	DSN	HB3	3.57	0.02	2
UNMAPPED	2	DTY	HE1	6.63	0.02	3
UNMAPPED	8	AFC	HB	3.97	0.02	1
UNMAPPED	2	DTY	HE2	6.64	0.02	3
UNMAPPED	1	ASN	HA	4.39	0.02	1
UNMAPPED	5	GLU	HG2	2.26	0.02	1
UNMAPPED	8	AFC	H	7.3	0.02	1
UNMAPPED	1	ASN	HD21	6.93	0.02	2
UNMAPPED	8	AFC	HL3	1.19	0.07	4
UNMAPPED	3	DSG	HB2	2.5	0.02	2
UNMAPPED	3	DSG	CA	50.4	0.2	1
UNMAPPED	7	THR	CB	69.7	0.2	1
UNMAPPED	8	AFC	HF3	1.19	0.07	4
UNMAPPED	2	DTY	CE2	114.9	0.2	1
UNMAPPED	2	DTY	CE1	114.9	0.2	1
UNMAPPED	8	AFC	HG2	1.19	0.07	4
UNMAPPED	7	THR	HG1	4.82	0.02	1
UNMAPPED	8	AFC	HI2	1.19	0.07	4

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	7	THR	HG22	1.01	0.02	1
UNMAPPED	7	THR	HG21	1.01	0.02	1
UNMAPPED	5	GLU	HA	4.19	0.02	1
UNMAPPED	1	ASN	HB3	2.18	0.02	1
UNMAPPED	8	AFC	CM	13.6	0.2	1
UNMAPPED	5	GLU	HB3	1.93	0.02	1
UNMAPPED	6	DSN	CB	61.1	0.2	1
UNMAPPED	5	GLU	CG	29.9	0.2	1
UNMAPPED	5	GLU	CB	26.6	0.2	1
UNMAPPED	4	SER	HB2	3.58	0.02	2
UNMAPPED	3	DSG	H	8.01	0.02	1
UNMAPPED	8	AFC	HH2	1.19	0.07	4
UNMAPPED	1	ASN	CB	36.5	0.2	1
UNMAPPED	1	ASN	CA	50.0	0.2	1
UNMAPPED	5	GLU	HG3	2.32	0.02	1
UNMAPPED	8	AFC	HC3	1.37	0.02	2
UNMAPPED	6	DSN	HB2	3.62	0.02	2
UNMAPPED	8	AFC	HK3	1.19	0.07	4
UNMAPPED	4	SER	CA	54.8	0.2	1
UNMAPPED	8	AFC	HK2	1.19	0.07	4
UNMAPPED	1	ASN	HD22	7.24	0.02	2
UNMAPPED	4	SER	HA	4.24	0.02	1
UNMAPPED	4	SER	H	7.55	0.02	1
UNMAPPED	2	DTY	HD2	7.01	0.02	3
UNMAPPED	2	DTY	H	8.29	0.02	1
UNMAPPED	2	DTY	HD1	7.0	0.02	3
UNMAPPED	7	THR	CA	58.6	0.2	1
UNMAPPED	3	DSG	HD21	6.93	0.02	2
UNMAPPED	7	THR	CG2	19.7	0.2	1
UNMAPPED	3	DSG	HD22	7.29	0.02	2
UNMAPPED	8	AFC	HJ2	1.19	0.07	4
UNMAPPED	8	AFC	CD	31.3	0.2	1
UNMAPPED	1	ASN	HB2	2.29	0.02	1
UNMAPPED	8	AFC	CA	40.8	0.2	1
UNMAPPED	8	AFC	HD2	1.19	0.07	4
UNMAPPED	8	AFC	CB	46.1	0.2	1
UNMAPPED	5	GLU	HB2	1.83	0.02	1
UNMAPPED	6	DSN	CA	55.0	0.2	1
UNMAPPED	5	GLU	CA	52.5	0.2	1
UNMAPPED	8	AFC	HE3	1.19	0.07	4
UNMAPPED	4	SER	HB3	3.59	0.02	2

7.1.2   Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	8	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	8	0.00 ± 0.00	None needed (< 0.5 ppm)
$^{13}C'$	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 41. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)
Sidechain	0/21 (0%)	0/12 (0%)	0/8 (0%)	0/1 (0%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/41 (0%)	0/20 (0%)	0/16 (0%)	0/5 (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 41. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)
Sidechain	0/21 (0%)	0/12 (0%)	0/8 (0%)	0/1 (0%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/41 (0%)	0/20 (0%)	0/16 (0%)	0/5 (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	5	GLU	CG	29.90	$42.24 - 29.94$	-5.0

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_1). RCI is only applicable to proteins.

7.2   Chemical shift list 2

File name: BMRB entry 7295

Chemical shift list name: *assigned_ chem_ shift_ list_ 1*

7.2.1   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	48
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	48
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.

- Chain not found in structure. All 48 occurences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	DTY	HB3	2.69	0.02	1
UNMAPPED	1	ASP	HB2	2.32	0.02	2
UNMAPPED	7	THR	H	7.75	0.02	1
UNMAPPED	6	DSN	HB2	3.56	0.02	1
UNMAPPED	1	ASP	HD2	12.3	0.02	1
UNMAPPED	5	GLN	HE21	6.84	0.02	2
UNMAPPED	7	THR	HB	4.23	0.02	1
UNMAPPED	5	GLN	HE22	7.3	0.02	2
UNMAPPED	4	SER	HA	4.1	0.02	1
UNMAPPED	4	SER	H	7.76	0.02	1
UNMAPPED	7	THR	HG1	4.87	0.02	1
UNMAPPED	5	GLN	HG3	2.16	0.02	2
UNMAPPED	5	GLN	HB2	1.87	0.02	1
UNMAPPED	2	DTY	HD2	7.06	0.02	3
UNMAPPED	2	DTY	HA	4.31	0.02	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	2	DTY	H	8.56	0.02	1
UNMAPPED	2	DTY	HD1	7.0	0.02	3
UNMAPPED	2	DTY	HB2	3.0	0.02	1
UNMAPPED	7	THR	HA	4.01	0.02	1
UNMAPPED	7	THR	HG21	1.04	0.02	1
UNMAPPED	2	DTY	HH	9.19	0.02	1
UNMAPPED	1	ASP	H	8.28	0.02	1
UNMAPPED	1	ASP	HA	4.43	0.02	1
UNMAPPED	3	DSG	HD21	6.97	0.02	2
UNMAPPED	5	GLN	HG2	2.12	0.02	2
UNMAPPED	5	GLN	HB3	1.96	0.02	1
UNMAPPED	3	DSG	HD22	7.37	0.02	2
UNMAPPED	6	DSN	H	7.81	0.02	1
UNMAPPED	8	BAL	HB3	3.4	0.02	2
UNMAPPED	6	DSN	HA	4.36	0.02	1
UNMAPPED	8	BAL	H	7.16	0.02	1
UNMAPPED	3	DSG	HB3	2.64	0.02	2
UNMAPPED	4	SER	HB2	3.64	0.02	1
UNMAPPED	3	DSG	H	8.03	0.02	1
UNMAPPED	1	ASP	HB3	2.38	0.02	2
UNMAPPED	6	DSN	HB3	3.56	0.02	1
UNMAPPED	5	GLN	H	7.91	0.02	1
UNMAPPED	5	GLN	HA	4.16	0.02	1
UNMAPPED	2	DTY	HE1	6.65	0.02	3
UNMAPPED	8	BAL	HA2	2.32	0.02	2
UNMAPPED	2	DTY	HE2	6.66	0.02	3
UNMAPPED	7	THR	HG22	1.04	0.02	1
UNMAPPED	8	BAL	HA1	2.32	0.02	2
UNMAPPED	8	BAL	HB2	3.29	0.02	2
UNMAPPED	3	DSG	HA	4.51	0.02	1
UNMAPPED	3	DSG	HB2	2.51	0.02	2
UNMAPPED	4	SER	HB3	3.64	0.02	1
UNMAPPED	7	THR	HG23	1.04	0.02	1

7.2.2   Chemical shift referencing (i)

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

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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 41. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)
Sidechain	0/21 (0%)	0/12 (0%)	0/8 (0%)	0/1 (0%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/41 (0%)	0/20 (0%)	0/16 (0%)	0/5 (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 41. 0 out of 0 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	0/20 (0%)	0/8 (0%)	0/8 (0%)	0/4 (0%)
Sidechain	0/21 (0%)	0/12 (0%)	0/8 (0%)	0/1 (0%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	0/41 (0%)	0/20 (0%)	0/16 (0%)	0/5 (0%)

7.2.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

7.2.5 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.