



# wwPDB NMR Structure Validation Summary Report ⓘ

Apr 26, 2016 – 04:39 PM BST

PDB ID : 1OSL  
Title : Solution structure of a dimeric lactose DNA-binding domain complexed to a nonspecific DNA sequence  
Authors : Kalodimos, C.G.; Bonvin, A.M.J.J.; Boelens, R.; Kaptein, R.  
Deposited on : 2003-03-20

This is a wwPDB NMR Structure Validation Summary 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.

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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 : unknown  
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

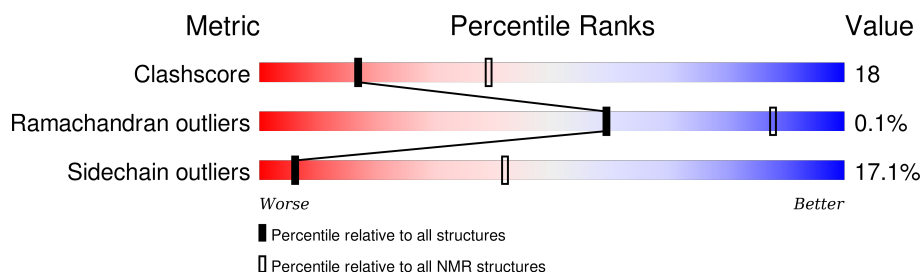
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

The overall completeness of chemical shifts assignment is 38%.

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  $\geq 3$ , 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	C	18	94% (green) 6% (yellow)
1	D	18	94% (green) 6% (yellow)
2	A	62	23% (green) 29% (yellow) . (orange) 47% (cyan)
2	B	62	19% (green) 26% (yellow) 5% (orange) 50% (cyan)

## 2 Ensemble composition and analysis ⓘ

This entry contains 20 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 9 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:5-A:24, A:34-A:46 (33)	0.08	9
2	B:5-B:24, B:35-B:45 (31)	0.09	15

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models in file

### 3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3061 atoms, of which 1376 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(\*CP\*GP\*AP\*TP\*AP\*AP\*GP\*AP\*TP\*AP\*TP\*CP\*TP\*TP\*AP\*TP\*CP\*G)-3'.

Mol	Chain	Residues	Atoms						Trace
1	C	18	Total	C	H	N	O	P	0
			572	177	206	66	106	17	
1	D	18	Total	C	H	N	O	P	0
			572	177	206	66	106	17	

- Molecule 2 is a protein called Lactose operon repressor.

Mol	Chain	Residues	Atoms						Trace
2	A	62	Total	C	H	N	O	S	0
			959	296	483	85	92	3	
2	B	62	Total	C	H	N	O	S	0
			958	296	481	85	93	3	

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	CYS	VAL	ENGINEERED	UNP P03023
B	52	CYS	VAL	ENGINEERED	UNP P03023

## 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: 5'-D(\*CP\*GP\*AP\*TP\*AP\*AP\*GP\*AP\*TP\*AP\*TP\*CP\*TP\*TP\*AP\*TP\*CP\*G)-3'

Chain C: 

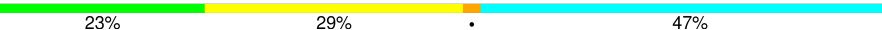


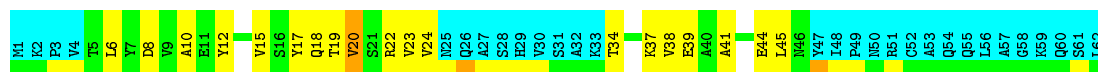
- Molecule 1: 5'-D(\*CP\*GP\*AP\*TP\*AP\*AP\*GP\*AP\*TP\*AP\*TP\*CP\*TP\*TP\*AP\*TP\*CP\*G)-3'

Chain D: 



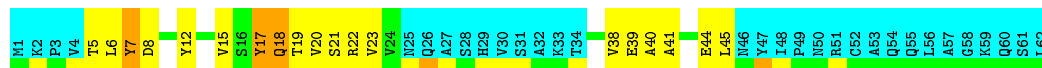
- Molecule 2: Lactose operon repressor

Chain A: 



- Molecule 2: Lactose operon repressor

Chain B: 



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


The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: 5'-D(\*CP\*GP\*AP\*TP\*AP\*AP\*GP\*AP\*TP\*AP\*TP\*CP\*TP\*TP\*AP\*TP\*CP\*G)-3'

Chain C:  94% 6%



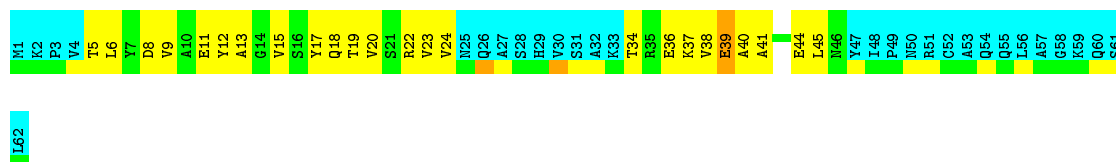
- Molecule 1: 5'-D(\*CP\*GP\*AP\*TP\*AP\*AP\*GP\*AP\*TP\*AP\*TP\*CP\*TP\*TP\*AP\*TP\*CP\*G)-3'

Chain D:  89% 11%



- Molecule 2: Lactose operon repressor

Chain A:  15% 37% 47%



- Molecule 2: Lactose operon repressor

Chain B:  21% 21% 6% 50%



## 5 Refinement protocol and experimental data overview

The models were refined using the following method: *THE STRUCTURE OF THE COMPLEX WAS CALCULATED AS FOLLOWS. FIRST THE STRUCTURE OF THE DIMERIC LACHP62-V52C WAS CALCULATED USING ONLY PROTEIN NMR RESTRAINTS. THE 100 BEST STRUCTURES WERE SELECTED AND DOCKED ONTO THE NONSPECIFIC LAC OPERATOR B-DNA USING SIMULATED ANNEALING. DISTANCE AND PLANARITY RESTRAINTS FOR THE DNA WERE INCORPORATED IN ORDER TO KEEP DNA CLOSE TO B-DNA CONFORMATION..*

Of the 400 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
CNS	structure solution	1.1
CNS	refinement	1.1

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 5791
Number of chemical shift lists	3
Total number of shifts	1367
Number of shifts mapped to atoms	1212
Number of unparsed shifts	0
Number of shifts with mapping errors	155
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	38%

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

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	C	0.35±0.01	0±0/410 (0.0±0.0%)	0.77±0.01	0±0/631 (0.0±0.0%)
1	D	0.35±0.01	0±0/410 (0.0±0.0%)	0.77±0.01	0±0/631 (0.0±0.0%)
2	A	0.68±0.15	1±1/259 (0.4±0.5%)	0.59±0.02	0±0/353 (0.0±0.0%)
2	B	1.15±0.45	2±2/244 (1.0±0.7%)	0.89±0.10	1±1/332 (0.2±0.4%)
All	All	0.67	71/26460 (0.3%)	0.76	15/38940 (0.0%)

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
2	B	0.0±0.0	0.3±0.6
All	All	0	6

5 of 10 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	7	TYR	CE1-CZ	16.96	1.60	1.38	6	13
2	B	7	TYR	CE2-CZ	-16.36	1.17	1.38	9	13
2	B	17	TYR	CE1-CZ	-14.12	1.20	1.38	9	8
2	B	17	TYR	CE2-CZ	13.82	1.56	1.38	9	8
2	B	12	TYR	CE2-CZ	-7.28	1.29	1.38	14	3

5 of 6 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	7	TYR	CE1-CZ-OH	-6.35	102.95	120.10	6	4
2	B	19	THR	N-CA-CB	6.15	121.99	110.30	19	2

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	B	7	TYR	CD1-CE1-CZ	-6.02	114.38	119.80	6	3
2	B	17	TYR	OH-CZ-CE2	-5.79	104.47	120.10	16	3
2	B	7	TYR	CZ-CE2-CD2	5.73	124.96	119.80	9	2

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)
2	B	7	TYR	Sidechain	4
2	B	17	TYR	Sidechain	2

## 6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	C	366	206	206	2±1
1	D	366	206	206	1±1
2	A	256	252	252	16±3
2	B	241	239	239	21±2
All	All	24580	18060	18060	775

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 18.

5 of 106 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:23:VAL:HG11	2:A:38:VAL:HG21	0.92	1.39	12	20
2:B:20:VAL:HB	2:B:38:VAL:HB	0.87	1.44	8	20
2:A:34:THR:HA	2:A:37:LYS:HD2	0.87	1.42	9	2
2:B:18:GLN:HA	2:B:21:SER:HB3	0.84	1.50	15	10
2:B:6:LEU:HB3	2:B:17:TYR:CE1	0.81	2.10	9	20

## 6.3 Torsion angles

### 6.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	33/62 (53%)	31±0 (95±1%)	2±0 (5±1%)	0±0 (0±0%)	100	100
2	B	31/62 (50%)	29±1 (93±3%)	2±1 (7±3%)	0±0 (0±1%)	56	85
All	All	1280/2480 (52%)	1200 (94%)	79 (6%)	1 (0%)	59	88

All 1 unique Ramachandran outliers are listed below.

Mol	Chain	Res	Type	Models (Total)
2	B	18	GLN	1

### 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	
2	A	27/51 (53%)	23±1 (84±5%)	4±1 (16±5%)	6	43
2	B	25/51 (49%)	21±1 (82±4%)	5±1 (18±4%)	5	40
All	All	1040/2040 (51%)	862 (83%)	178 (17%)	6	42

5 of 25 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)
2	B	7	TYR	20
2	B	18	GLN	17
2	A	20	VAL	16
2	A	18	GLN	15
2	A	22	ARG	14

### 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 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 38% for the well-defined parts and 48% for the entire structure.

### 7.1 Chemical shift list 1

File name: BMRB entry 5791

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	1212
Number of shifts mapped to atoms	1212
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

#### 7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	116	$-0.07 \pm 0.16$	None needed ( $< 0.5$ ppm)
$^{13}\text{C}_\beta$	0	—	—
$^{13}\text{C}'$	114	$0.05 \pm 0.20$	None needed ( $< 0.5$ ppm)
$^{15}\text{N}$	116	$0.73 \pm 0.18$	Should be applied

#### 7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 38%, i.e. 550 atoms were assigned a chemical shift out of a possible 1453. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^1\text{H}$	$^{13}\text{C}$	$^{15}\text{N}$
Backbone	318/320 (99%)	128/128 (100%)	126/128 (98%)	64/64 (100%)
Sidechain	208/383 (54%)	197/218 (90%)	4/148 (3%)	7/17 (41%)

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	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Aromatic	24/48 (50%)	24/24 (100%)	0/24 (0%)	0/0 (—%)
Overall	550/1453 (38%)	349/784 (45%)	130/546 (24%)	71/123 (58%)

#### 7.1.4 Statistically unusual chemical shifts ⓘ

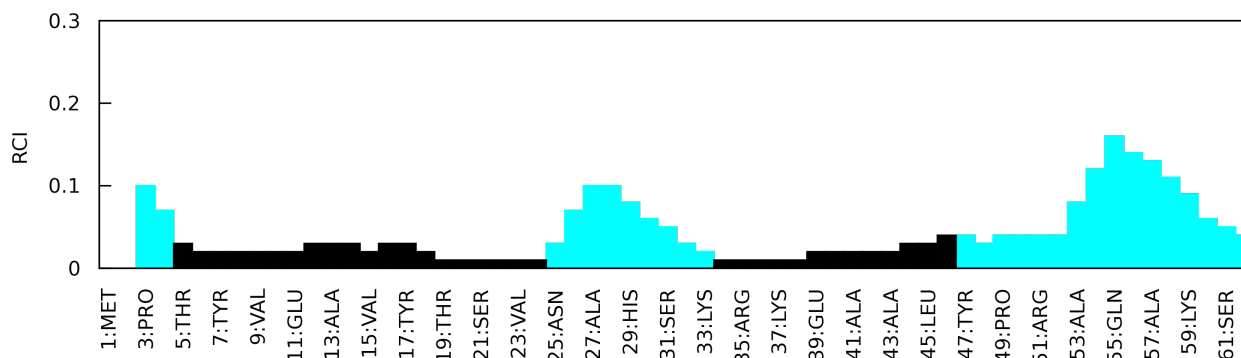
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	B	20	VAL	CG1	42.40	28.40 – 14.60	15.1
1	A	20	VAL	CG1	42.40	28.40 – 14.60	15.1
1	B	6	LEU	CD2	41.77	32.60 – 15.60	10.4
1	A	6	LEU	CD2	41.77	32.60 – 15.60	10.4
1	B	36	GLU	HG3	4.31	3.31 – 1.21	9.8
1	A	36	GLU	HG3	4.31	3.31 – 1.21	9.8

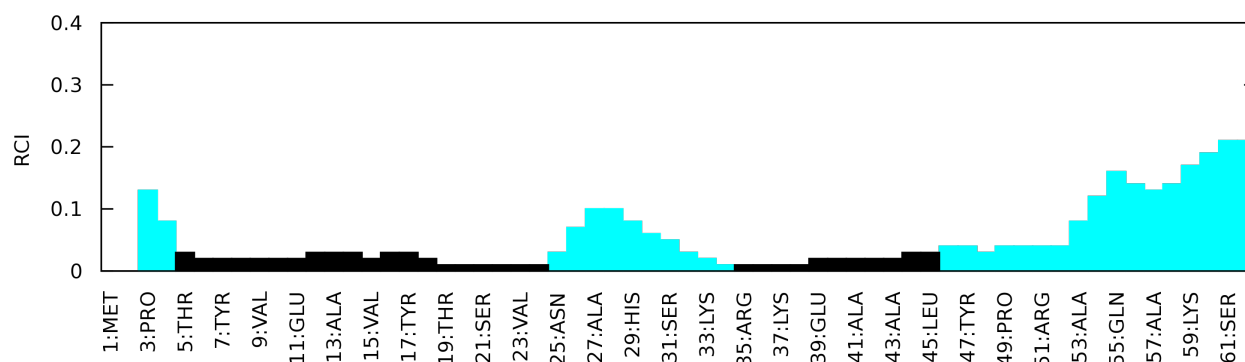
#### 7.1.5 Random Coil Index (RCI) plots ⓘ

The images below report *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.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain B:



## 7.2 Chemical shift list 2

File name: BMRB entry 5791

Chemical shift list name: *assigned\_chem\_shift\_list\_2*

### 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	80
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	80
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. First 5 (of 80) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	1	DC	H5'	3.726	-1.0	1
UNMAPPED	4	DT	H5''	4.268	-1.0	1
UNMAPPED	2	DG	H1'	5.527	-1.0	1
UNMAPPED	5	DA	H3'	5.051	-1.0	1
UNMAPPED	4	DT	H2''	2.235	-1.0	1

### 7.2.2 Chemical shift referencing ⓘ

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 1453. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	<b>Total</b>	<b><sup>1</sup>H</b>	<b><sup>13</sup>C</b>	<b><sup>15</sup>N</b>
Backbone	0/320 (0%)	0/128 (0%)	0/128 (0%)	0/64 (0%)
Sidechain	0/383 (0%)	0/218 (0%)	0/148 (0%)	0/17 (0%)
Aromatic	0/48 (0%)	0/24 (0%)	0/24 (0%)	0/0 (—%)
Overall	0/1453 (0%)	0/784 (0%)	0/546 (0%)	0/123 (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\_2). RCI is only applicable to proteins.

## 7.3 Chemical shift list 3

File name: BMRB entry 5791

Chemical shift list name: *assigned\_chem\_shift\_list\_3*

### 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	75
Number of shifts mapped to atoms	0
Number of unparsed shifts	0
Number of shifts with mapping errors	75
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. First 5 (of 75) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
UNMAPPED	7	DT	H71	1.401	-1.0	2
UNMAPPED	7	DT	H6	7.187	-1.0	3
UNMAPPED	7	DT	H5'	3.951	-1.0	1
UNMAPPED	8	DC	H2''	2.372	-1.0	1
UNMAPPED	4	DT	H2''	2.24	-1.0	1

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

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

### 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 0%, i.e. 0 atoms were assigned a chemical shift out of a possible 1453. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	<sup>1</sup> H	<sup>13</sup> C	<sup>15</sup> N
Backbone	0/320 (0%)	0/128 (0%)	0/128 (0%)	0/64 (0%)
Sidechain	0/383 (0%)	0/218 (0%)	0/148 (0%)	0/17 (0%)
Aromatic	0/48 (0%)	0/24 (0%)	0/24 (0%)	0/0 (—%)
Overall	0/1453 (0%)	0/784 (0%)	0/546 (0%)	0/123 (0%)

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

There are no statistically unusual chemical shifts.

### 7.3.5 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\_3). RCI is only applicable to proteins.