wwPDB NMR Structure Validation Summary Report (i)

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PDB ID	:	1OVY
Title	:	Solution Structure of Ribosomal Protein L18 from Bacillus stearothermophilus
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This is a wwPDB NMR Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

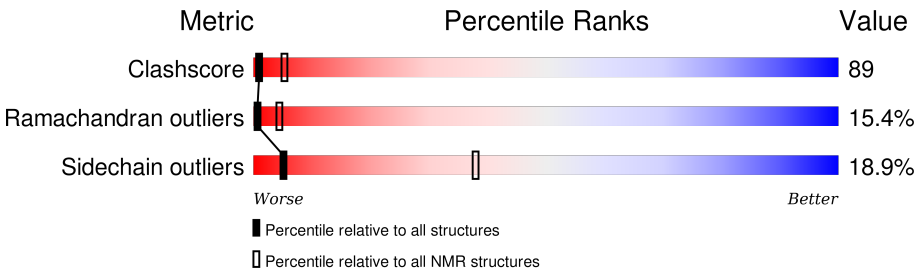
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 (i)

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

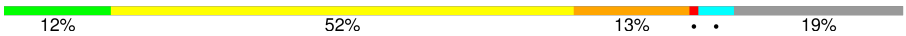
The overall completeness of chemical shifts assignment is 61%.

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	120	

2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:29-A:120 (92)	0.77	1

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 6 single-model clusters were found.

Cluster number	Models
1	1, 10
2	4, 9
Single-model clusters	2; 3; 5; 6; 7; 8

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1517 atoms, of which 767 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 50S Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
1	A	97	1517	470	767	136	144	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: 50S Ribosomal Protein L18

Chain A: 12% 52% 13% • • 19%

MET ILE THR LYS VAL ASP ARG ASN ALA VAL ARG LYS LYS ARG HIS ALA ARG ILE ARG LYS LYS ILE PHE G24 T25 T26 E27 R28 P29 R30 L31 S32 V33 F34 R35 S36 N37 K38 H39 I40 Y41 A42 Q43 I44 I45 D46 D47 T48 K49 S50 A51 T52 I53 V54 S55 A56 S57 T58 L59 D60

F63 G64 L65 D66 S67 T68 N69 N70 I71 E72 A73 A74 K75 K76 V77 G78 E79 L80 V81 A82 A85 L86 E87 K88 G89 I90 K91 Q92 V93 V94 F95 D96 R97 G98 G99 Y100 L101 Y102 H103 G104 R105 V106 K107 A108 L109 A110 D111 A112 A113 R114 E115 A116 G117 L118 E119 F120

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

The representative model is number 1. Colouring as in section 4.1 above.

- Molecule 1: 50S Ribosomal Protein L18

Chain A: 19% 43% 13% • • 19%

MET ILE THR LYS VAL ASP ARG ASN ALA VAL ARG LYS LYS ARG HIS ALA ARG ILE ARG LYS LYS ILE PHE G24 T25 T26 E27 R28 P29 R30 L31 S32 V33 F34 R35 S36 N37 K38 H39 I40 Y41 A42 Q43 I44 I45 D46 D47 S50 A51 T52 I53 V54 S55 A56 S57 T58 L59 D60 K61

E62 F63 D66 S67 T68 I71 E72 A73 A74 K75 K76 V77 G78 E79 L80 V81 A82 K83 R84 A85 L86 E87 K88 G89 I90 K91 Q92 V93 V94 F95 D96 R97 G98 G99 Y100 L101 Y102 H103 G104 K107 A108 L109 A110 D111 A112 A113 R114 L118 E119 F120

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *Aria was used to select and assign peak lists from NOESY experiments. CNS as modified for use with ARIA was used for structure calculation using torsion angle simulated annealing..*

Of the 150 calculated structures, 10 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	1.0
ARIA	structure solution	1.2
CNS	refinement	1.0
ARIA	refinement	1.2

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 5970
Number of chemical shift lists	1
Total number of shifts	956
Number of shifts mapped to atoms	956
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	61%

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	A	0.42±0.13	1±2/721 (0.1±0.2%)	0.52±0.05	0±0/965 (0.0±0.0%)
All	All	0.44	8/7210 (0.1%)	0.52	0/9650 (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
1	A	0.0±0.0	0.2±0.4
All	All	0	2

All 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
1	A	100	TYR	CE2-CZ	-11.36	1.23	1.38	9	2
1	A	100	TYR	CE1-CZ	11.32	1.53	1.38	9	2
1	A	102	TYR	CE1-CZ	-5.87	1.30	1.38	8	2
1	A	102	TYR	CE2-CZ	5.63	1.45	1.38	8	2

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	41	TYR	Sidechain	2

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	712	731	729	128±21
All	All	7120	7310	7290	1280

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 89.

5 of 843 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:VAL:HG11	1:A:113:ALA:HB3	1.08	1.25	9	1
1:A:113:ALA:HB1	1:A:118:LEU:HD22	1.08	1.13	9	1
1:A:31:LEU:HD12	1:A:44:ILE:HG23	1.03	1.05	9	1
1:A:45:ILE:HD13	1:A:53:ILE:HG23	1.01	1.26	7	3
1:A:68:THR:HG23	1:A:74:ALA:HB2	1.00	1.29	9	4

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	91/120 (76%)	58±4 (63±5%)	19±4 (21±5%)	14±2 (15±3%)	1 4
All	All	910/1200 (76%)	576 (63%)	194 (21%)	140 (15%)	1 4

5 of 35 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	37	ASN	10
1	A	102	TYR	9
1	A	54	VAL	8

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Mol	Chain	Res	Type	Models (Total)
1	A	55	SER	8
1	A	51	ALA	8

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	73/98 (74%)	59±4 (81±5%)	14±4 (19±5%)	5 38
All	All	730/980 (74%)	592 (81%)	138 (19%)	5 38

5 of 50 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	120	PHE	8
1	A	107	LYS	8
1	A	41	TYR	7
1	A	100	TYR	6
1	A	39	HIS	5

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 (i)

The completeness of assignment taking into account all chemical shift lists is 61% for the well-defined parts and 61% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 5970

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

7.1.1 Bookkeeping (i)

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

Total number of shifts	956
Number of shifts mapped to atoms	956
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	114	1.05 ± 0.10	Should be applied
$^{13}C_{\beta}$	107	1.05 ± 0.11	Should be applied
$^{13}C'$	0	—	—
^{15}N	109	-0.61 ± 0.36	None needed (imprecise)

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 61%, i.e. 691 atoms were assigned a chemical shift out of a possible 1128. 1 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	349/458 (76%)	172/183 (94%)	91/184 (49%)	86/91 (95%)
Sidechain	321/594 (54%)	210/345 (61%)	107/217 (49%)	4/32 (12%)

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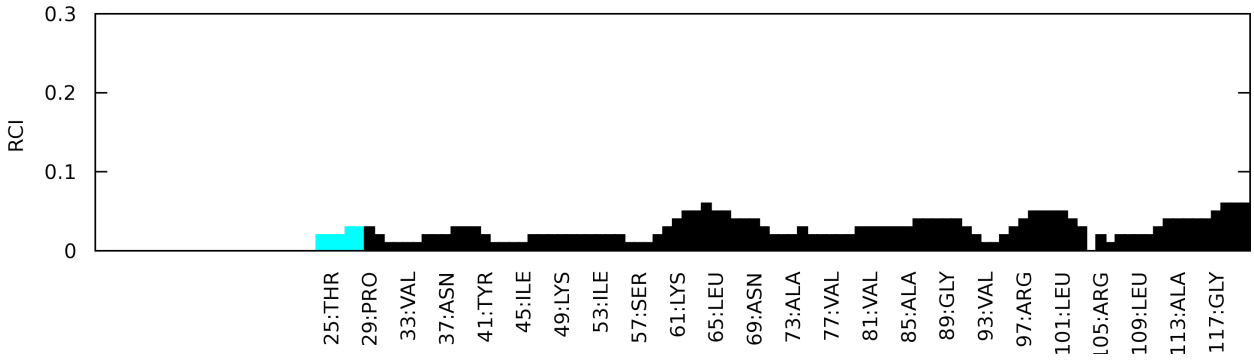
	Total	^{1}H	^{13}C	^{15}N
Aromatic	21/76 (28%)	21/40 (52%)	0/32 (0%)	0/4 (0%)
Overall	691/1128 (61%)	403/568 (71%)	198/433 (46%)	90/127 (71%)

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
1	A	118	LEU	CD1	10.95	32.77 – 16.57	-8.5
1	A	31	LEU	CD1	12.38	32.77 – 16.57	-7.6
1	A	84	ARG	HD2	1.90	4.27 – 1.97	-5.3

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A: