wwPDB NMR Structure Validation Summary Report (i)

May 29, 2020 – 07:37 am BST

PDB ID	:	5LXK
Title	:	NMR structure of the C-terminal domain of the Bacteriophage T5 decoration protein pb10.
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Deposited on	:	2016-09-22

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
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

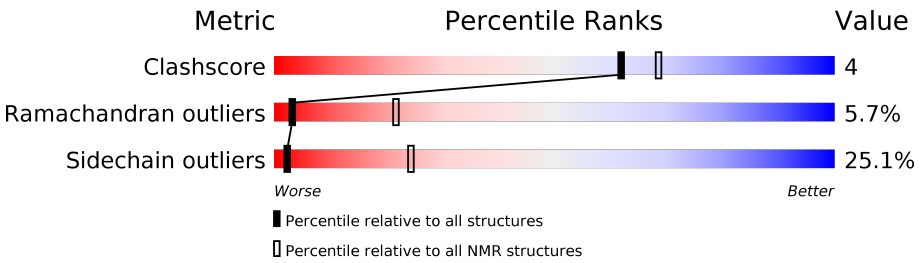
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 91%.

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	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

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	101	50% 21% 5% • 18% 5%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 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:79-A:156 (78)	0.29	7

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 3 clusters and 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1334 atoms, of which 659 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Decoration protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	96	1334	417	659	107	149	2	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	ALA	-	expression tag	UNP Q6QGD6
A	165	LEU	-	expression tag	UNP Q6QGD6
A	166	GLU	-	expression tag	UNP Q6QGD6
A	167	HIS	-	expression tag	UNP Q6QGD6
A	168	HIS	-	expression tag	UNP Q6QGD6
A	169	HIS	-	expression tag	UNP Q6QGD6
A	170	HIS	-	expression tag	UNP Q6QGD6
A	171	HIS	-	expression tag	UNP Q6QGD6
A	172	HIS	-	expression tag	UNP Q6QGD6

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: Decoration protein

Chain A: 50% 21% 5% • 18% 5%

A72 L73 T74 L75 S76 K77 D78 L79 E87 G88 L91 T92 Y104 T105 Y106 T109 K110 D111 I115 A118 S119 G120 A121 T122 Y123 T124 K125 P126 T127 Y136 K137 V140 T141 D142 S143 S147 K148 D149 S150 C153 V157 N158 P159 T160 V161 P162 G163 G164 L165

E166 H167 HIS HIS HIS HIS HIS

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

The representative model is number 7. Colouring as in section 4.1 above.

- Molecule 1: Decoration protein

Chain A: 51% 21% • • 18% 5%

A72 L73 T74 L75 S76 K77 D78 L79 M83 G88 T92 L93 A97 Y106 T109 K110 D111 I115 S119 G120 A121 T122 Y123 T124 K125 P126 T127 A128 D132 K137 V140 T141 D142 S143 S147 S150 C153 V157 N158 P159 T160 V161 P162 G163 G164

L165 E166 H167 HIS HIS HIS HIS HIS

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 200 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
INCA	structure calculation	
CNS	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 6 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1054
Number of shifts mapped to atoms	1054
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	91%

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

COVALENT-GEOMETRY INFOmissingINFO

5.1 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	546	528	528	5±2
All	All	10920	10560	10560	96

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 4.

5 of 43 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:LEU:HD21	1:A:136:TYR:CZ	0.68	2.23	8	1
1:A:110:LYS:HG2	1:A:115:ILE:HG22	0.67	1.66	17	1
1:A:91:LEU:HD21	1:A:128:ALA:HB2	0.65	1.68	19	1
1:A:128:ALA:HB1	1:A:132:ASP:CB	0.57	2.27	15	8
1:A:110:LYS:HZ1	1:A:132:ASP:HA	0.57	1.60	9	2

5.2 Torsion angles (i)

5.2.1 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	78/101 (77%)	63±1 (81±2%)	10±2 (13±2%)	4±1 (6±1%)	3	22
All	All	1560/2020 (77%)	1268 (81%)	203 (13%)	89 (6%)	3	22

5 of 8 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	121	ALA	20
1	A	143	SER	20
1	A	120	GLY	14
1	A	88	GLY	14
1	A	119	SER	7

5.2.2 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	59/79 (75%)	44±1 (75±2%)	15±1 (25±2%)	2	24
All	All	1180/1580 (75%)	884 (75%)	296 (25%)	2	24

5 of 34 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	137	LYS	20
1	A	106	TYR	20
1	A	140	VAL	20
1	A	115	ILE	20
1	A	109	THR	19

5.2.3 RNA (i)

There are no RNA molecules in this entry.

5.3 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.4 Carbohydrates (i)

There are no carbohydrates in this entry.

5.5 Ligand geometry (i)

There are no ligands in this entry.

5.6 Other polymers (i)

There are no such molecules in this entry.

5.7 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 91% for the well-defined parts and 91% for the entire structure.

6.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *c72_depchim_renum.bmrb*

6.1.1 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	1054
Number of shifts mapped to atoms	1054
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

6.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	96	0.21 ± 0.13	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	87	0.07 ± 0.19	None needed (< 0.5 ppm)
$^{13}C'$	94	0.48 ± 0.15	None needed (< 0.5 ppm)
^{15}N	88	-1.23 ± 0.31	Should be applied

6.1.3 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 91%, i.e. 717 atoms were assigned a chemical shift out of a possible 787. 1 out of 9 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	379/382 (99%)	150/152 (99%)	155/156 (99%)	74/74 (100%)
Sidechain	294/361 (81%)	176/207 (85%)	117/148 (79%)	1/6 (17%)

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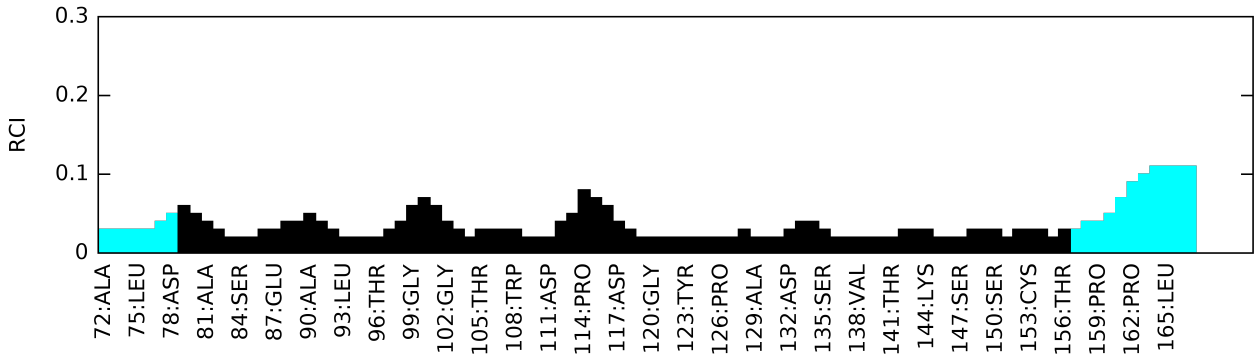
	Total	^{1}H	^{13}C	^{15}N
Aromatic	44/44 (100%)	22/22 (100%)	21/21 (100%)	1/1 (100%)
Overall	717/787 (91%)	348/381 (91%)	293/325 (90%)	76/81 (94%)

6.1.4 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	123	TYR	HB3	0.59	4.75 – 0.95	-5.9

6.1.5 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: