wwPDB NMR Structure Validation Summary Report (i)

Apr 27, 2016 – 12:30 AM BST

PDB ID	:	2L4W
Title	:	NMR structure of the Xanthomonas VirB7
Authors	:	Souza, D.P.; Farah, C.S.; Salinas, R.K.
Deposited on	:	2010-10-15

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:

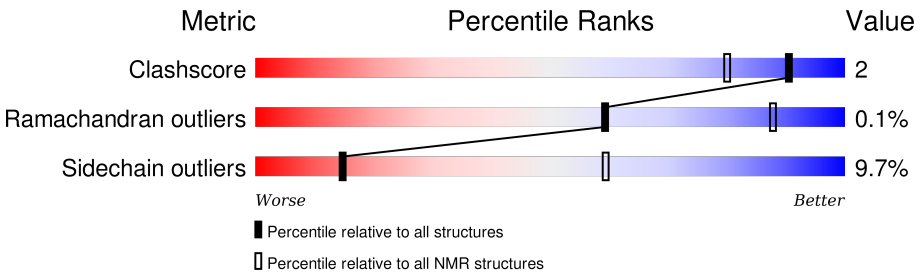
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	rb-20027457
Ideal 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 96%.

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	61% 5% 34%

2 Ensemble composition and analysis (i)

This entry contains 20 models. 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: *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:53-A:131 (79)	0.22	9

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 6 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1795 atoms, of which 890 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	120	1795	572	890	149	180	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	EXPRESSION TAG	UNP Q8PJB3
A	21	SER	-	EXPRESSION TAG	UNP Q8PJB3
A	22	HIS	-	EXPRESSION TAG	UNP Q8PJB3
A	23	MET	-	EXPRESSION TAG	UNP Q8PJB3

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: Uncharacterized protein

Chain A: 61% 5% 34%

G20 S21 H22 M23 T24 K25 P26 A27 P28 D29 F30 G31 G32 R33 W34 K35 H36 V37 N38 H39 F40 D41 E42 A43 P44 T45 E46 I47 P48 L49 Y50 T51 S52 T66 S80 T88 L89 S94 T99 P132 V133 S134 S135 G136 A137 K138 L139

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: Uncharacterized protein

Chain A: 54% 12% 34%

G20 S21 H22 M23 T24 K25 P26 A27 P28 D29 F30 G31 G32 R33 W34 K35 H36 V37 N38 H39 F40 D41 E42 A43 P44 T45 E46 I47 P48 L49 Y50 T51 S52 Y55 L64 K65 T66 Y81 N82 L83 T88 L89 T99 S100 V101 Y112 S120 L127 V128 P132 V133

S134 S135 G136 A137 K138 L139

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics, simulated annealing cartesian dynamics.*

Of the 300 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 solution	2.1
HADDOCK	refinement	2.0
CNS	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 17257
Number of chemical shift lists	1
Total number of shifts	1444
Number of shifts mapped to atoms	1444
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	96%

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	589	586	586	2±1
All	All	11780	11720	11720	50

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 2.

5 of 25 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:ALA:HB3	1:A:94:SER:HA	0.65	1.69	7	5
1:A:81:TYR:CE2	1:A:83:LEU:HB2	0.53	2.39	19	7
1:A:80:SER:OG	1:A:125:LYS:HE2	0.51	2.05	14	3
1:A:81:TYR:OH	1:A:86:ASP:HA	0.51	2.05	11	3
1:A:61:ASP:HA	1:A:70:ARG:NH1	0.49	2.22	11	1

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	79/120 (66%)	77±1 (97±2%)	2±1 (3±2%)	0±0 (0±0%)	59 88
All	All	1580/2400 (66%)	1533 (97%)	45 (3%)	2 (0%)	59 88

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	90	ILE	1
1	A	123	ALA	1

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	66/100 (66%)	60±2 (90±3%)	6±2 (10±3%)	15 59
All	All	1320/2000 (66%)	1192 (90%)	128 (10%)	15 59

5 of 24 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	89	LEU	19
1	A	99	THR	19
1	A	88	THR	14
1	A	66	THR	10
1	A	94	SER	9

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 96% for the well-defined parts and 92% for the entire structure.

7.1 Chemical shift list 1

File name: BMRB entry 17257

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	1444
Number of shifts mapped to atoms	1444
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

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	118	-0.21 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	111	0.27 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	110	0.11 ± 0.12	None needed (< 0.5 ppm)
^{15}N	108	-0.18 ± 0.27	None needed (< 0.5 ppm)

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 96%, i.e. 852 atoms were assigned a chemical shift out of a possible 888. 0 out of 16 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	384/387 (99%)	154/154 (100%)	155/158 (98%)	75/75 (100%)
Sidechain	418/449 (93%)	247/260 (95%)	161/175 (92%)	10/14 (71%)

Continued on next page...

Continued from previous page...

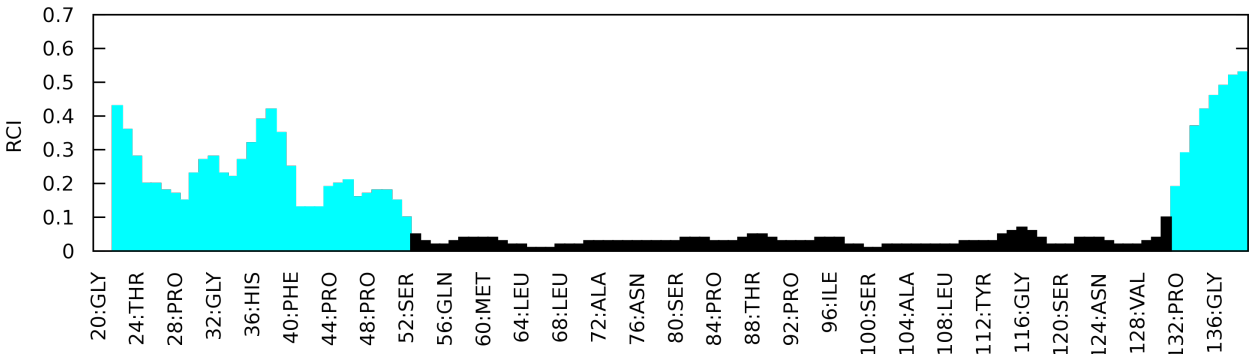
	Total	^{1}H	^{13}C	^{15}N
Aromatic	50/52 (96%)	25/26 (96%)	24/25 (96%)	1/1 (100%)
Overall	852/888 (96%)	426/440 (97%)	340/358 (95%)	86/90 (96%)

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	55	TYR	HB2	0.74	4.76 – 1.06	-5.9

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: