

wwPDB NMR Structure Validation Summary Report (i)

Jun 22, 2022 – 01:13 pm BST

PDB ID : 7ZBQ

Title : Structure of the ADP-ribosyltransferase TccC3HVR from Photorhabdus

Luminescens

Authors: Lindemann, F.; Belyy, A.; Friedrich, D.; Schmieder, P.; Bardiaux, B.; Roderer,

D.; Funk, J.; Protze, J.; Bieling, P.; Oschkinat, H.; Raunser, S.

Deposited on : 2022-03-24

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 types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

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 : 2.29

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

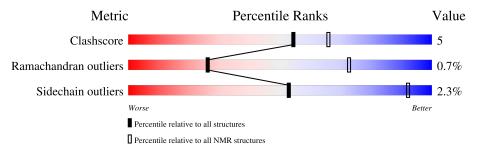
Validation Pipeline (wwPDB-VP) : 2.29

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 79%.

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	NMR archive
Metric	$(\# \mathrm{Entries})$	$(\# \mathrm{Entries})$
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	194	78%	7% •	7%	7%		



2 Ensemble composition and analysis (i)

This entry contains 10 models. Model 2 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:103-A:201, A:207-A:229,	0.39	2			
	A:238-A:281 (166)					

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 2 single-model clusters were found.

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



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2860 atoms, of which 1441 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called TccC3.

Mol	Chain	Residues	Atoms					Trace	
1	Λ	190	Total	С	Н	N	О	S	0
1 A	A 180	2860	905	1441	239	271	4	U	

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	initiating methionine	UNP Q8GF97
A	283	GLY	-	expression tag	UNP Q8GF97
A	284	THR	-	expression tag	UNP Q8GF97
A	285	LEU	-	expression tag	UNP Q8GF97
A	286	GLU	_	expression tag	UNP Q8GF97
A	287	VAL	-	expression tag	UNP Q8GF97
A	288	LEU	-	expression tag	UNP Q8GF97
A	289	PHE	-	expression tag	UNP Q8GF97
A	290	GLN	_	expression tag	UNP Q8GF97

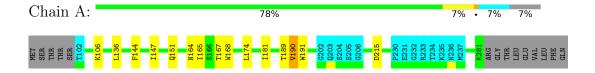


4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide 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.

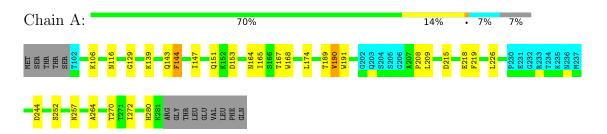
• Molecule 1: TccC3



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

The representative model is number 2. Colouring as in section 4.1 above.

• Molecule 1: TccC3





Refinement protocol and experimental data overview (i) 5



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

Of the 400 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
ARIA	structure calculation	2.3.2
CNS	refinement	1.21

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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	2067
Number of shifts mapped to atoms	2067
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	79%



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		I	Bond lengths	Bond angles		
		RMSZ	#Z>5	RMSZ	#Z>5	
1	A	0.36 ± 0.04	$1\pm1/1351~(~0.0\pm~0.1\%)$	0.42 ± 0.01	$0\pm0/1832~(~0.0\pm~0.0\%)$	
All	All	0.36	6/13510 (0.0%)	0.42	0/18320 (0.0%)	

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

Mal	Chain	Dec	Tuno	Atoms	Z	Observed(Å)	Ideal(Å)	Mod	dels
MIOI	Chain	nes	туре	Atoms		Observed(A)	Ideal(A)	Worst	Total
1	A	180	TYR	CE1-CZ	-6.66	1.29	1.38	7	3
1	A	180	TYR	CE2-CZ	6.52	1.47	1.38	7	3

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	1320	1346	1343	14±2
All	All	13200	13460	13430	143

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 5.

5 of 61 unique clashes are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
Atom-1	Atom-2	Clash(A)	Distance(A)	Worst	Total
1:A:147:ILE:HA	1:A:151:GLN:O	0.68	1.88	7	8
1:A:181:ILE:HA	1:A:191:TRP:CZ2	0.65	2.27	7	7
1:A:116:ASN:O	1:A:117:ARG:HD2	0.63	1.93	7	1
1:A:136:LEU:HB2	1:A:269:LEU:O	0.60	1.97	9	4
1:A:164:ASN:O	1:A:167:THR:HG22	0.55	2.00	9	7

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	Perce	ntiles
1	A	165/194 (85%)	159±2 (96±1%)	5±2 (3±1%)	1±0 (1±0%)	26	73
All	All	1650/1940 (85%)	1590 (96%)	48 (3%)	12 (1%)	26	73

All 3 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	190	VAL	10
1	A	259	GLY	1
1	A	260	PRO	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	Perce	ntiles
1	A	149/173 (86%)	146±1 (98±0%)	4±1 (2±0%)	53	92
All	All	1490/1730 (86%)	1455 (98%)	35 (2%)	53	92

5 of 16 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	190	VAL	9
1	A	144	PHE	5
1	A	175	LYS	3
1	A	189	THR	3
1	A	179	ASN	2

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 monosaccharides 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 79% for the well-defined parts and 78% for the entire structure.

7.1 Chemical shift list 1

File name: working cs.cif

Chemical shift list name: assigned_chem_shift_list

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	2067
Number of shifts mapped to atoms	2067
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

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
$^{13}\mathrm{C}_{\alpha}$	187	0.30 ± 0.11	None needed ($< 0.5 \text{ ppm}$)
$^{13}C_{\beta}$	176	0.03 ± 0.10	None needed ($< 0.5 \text{ ppm}$)
¹³ C′	0		None (insufficient data)
^{15}N	171	0.54 ± 0.18	Should be applied

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 79%, i.e. 1647 atoms were assigned a chemical shift out of a possible 2081. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	$^{1}\mathbf{H}$	$^{13}\mathbf{C}$	$^{15}{ m N}$
Backbone	634/808 (78%)	318/321 (99%)	165/332 (50%)	151/155 (97%)
Sidechain	867/1109 (78%)	529/653 (81%)	320/412 (78%)	18/44 (41%)

Continued on next page...



Continued from previous page...

	Total	$^{1}\mathrm{H}$	$^{13}\mathbf{C}$	$^{15}\mathbf{N}$
Aromatic	146/164 (89%)	77/86 (90%)	66/69 (96%)	3/9 (33%)
Overall	1647/2081 (79%)	924/1060 (87%)	551/813 (68%)	172/208 (83%)

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	181	ILE	HG13	-2.37	3.260.84	-8.7
1	A	176	ASP	HB2	0.64	4.07 - 1.37	-7.7
1	A	113	ARG	HD2	1.67	4.27 - 1.97	-6.3
1	A	106	LYS	HG2	-0.27	2.67 - 0.07	-6.3
1	A	189	THR	НВ	2.32	5.82 - 2.52	-5.6
1	A	187	LYS	HE3	1.85	3.86 - 1.96	-5.6
1	A	255	ALA	HB2	-0.02	2.61 - 0.11	-5.5
1	A	255	ALA	HB3	-0.02	2.61 - 0.11	-5.5
1	A	255	ALA	HB1	-0.02	2.61 - 0.11	-5.5
1	A	164	ASN	HB2	1.25	4.36 - 1.26	-5.0

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:

