



wwPDB NMR Structure Validation Summary Report ⓘ

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BMRB ID : 34717
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.
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with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

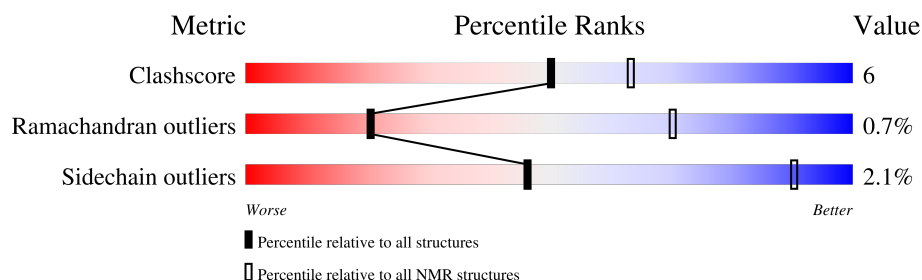
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 81%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	194	

2 Ensemble composition and analysis

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, A:238-A:281 (166)	0.67	2

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

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	A	180	Total	C	H	N	O	S	0
			2860	905	1441	239	271	4	

There are 9 discrepancies between the modelled and reference sequences:

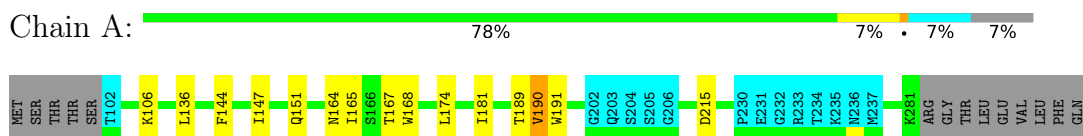
Chain	Residue	Modelled	Actual	Comment	Reference
A	97	MET	-	initiating methionine	UNP Q8GF97
A	283	GLY	-	expression tag	UNP Q8GF97
A	284	THR	-	expression tag	UNP Q8GF97
A	285	LEU	-	expression tag	UNP Q8GF97
A	286	GLU	-	expression tag	UNP Q8GF97
A	287	VAL	-	expression tag	UNP Q8GF97
A	288	LEU	-	expression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

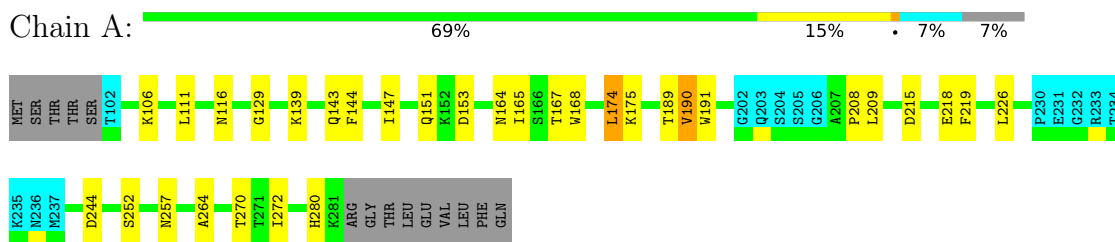
- Molecule 1: TccC3



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



5 Refinement protocol and experimental data overview

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	1956
Number of unparsed shifts	0
Number of shifts with mapping errors	111
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	81%

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	1320	1346	1343	15±3
All	All	13200	13460	13430	148

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 6.

5 of 65 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				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	Percentiles	
1	A	165/194 (85%)	159±2 (96±1%)	5±2 (3±1%)	1±0 (1±0%)	20	70
All	All	1650/1940 (85%)	1590 (96%)	48 (3%)	12 (1%)	20	70

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 ⓘ

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	149/173 (86%)	146±1 (98±1%)	3±1 (2±1%)	46	90
All	All	1490/1730 (86%)	1458 (98%)	32 (2%)	46	90

5 of 15 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	111	LEU	3
1	A	174	LEU	3
1	A	189	THR	3
1	A	274	LEU	2

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides 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 81% for the well-defined parts and 80% 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

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	1956
Number of unparsed shifts	0
Number of shifts with mapping errors	111
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 111) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	282	ARG	H	8.464	0.009	1
1	A	282	ARG	HA	3.979	0.005	1
1	A	282	ARG	HB2	1.629	0.008	2
1	A	282	ARG	HB3	1.505	0.009	2
1	A	282	ARG	HD2	2.973	0.004	2
1	A	282	ARG	HD3	2.974	0.005	2
1	A	282	ARG	HG2	1.452	0.01	2
1	A	282	ARG	HG3	1.462	0.009	2
1	A	282	ARG	CA	56.334	0.043	1
1	A	282	ARG	CB	30.682	0.051	1
1	A	282	ARG	CD	43.144	0.043	1
1	A	282	ARG	CG	27.523	0.077	1
1	A	282	ARG	N	123.928	0.014	1
1	A	283	GLY	H	8.505	0.005	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	283	GLY	HA2	3.748	0.007	2
1	A	283	GLY	HA3	3.751	0.005	2
1	A	283	GLY	CA	44.941	0.065	1
1	A	283	GLY	N	110.159	0.113	1
1	A	284	THR	H	8.056	0.006	1
1	A	284	THR	HA	4.084	0.004	1
1	A	284	THR	HB	3.981	0.006	1
1	A	284	THR	HG21	0.957	0.005	1
1	A	284	THR	HG22	0.957	0.005	1
1	A	284	THR	HG23	0.957	0.005	1
1	A	284	THR	CA	61.74	0.042	1
1	A	284	THR	CB	69.581	0.034	1
1	A	284	THR	CG2	21.459	0.013	1
1	A	284	THR	N	113.895	0.086	1
1	A	285	LEU	H	8.205	0.006	1
1	A	285	LEU	HA	4.132	0.005	1
1	A	285	LEU	HB2	1.402	0.01	2
1	A	285	LEU	HB3	1.391	0.017	2
1	A	285	LEU	HD11	0.696	0.009	2
1	A	285	LEU	HD12	0.696	0.009	2
1	A	285	LEU	HD13	0.696	0.009	2
1	A	285	LEU	HD21	0.633	0.005	2
1	A	285	LEU	HD22	0.633	0.005	2
1	A	285	LEU	HD23	0.633	0.005	2
1	A	285	LEU	HG	1.39	0.006	1
1	A	285	LEU	CA	54.939	0.044	1
1	A	285	LEU	CB	42.079	0.039	1
1	A	285	LEU	CD1	24.626	0.06	2
1	A	285	LEU	CD2	23.399	0.066	2
1	A	285	LEU	CG	26.829	0.053	1
1	A	285	LEU	N	124.317	0.012	1
1	A	286	GLU	H	8.229	0.007	1
1	A	286	GLU	HA	4.022	0.006	1
1	A	286	GLU	HB2	1.766	0.007	2
1	A	286	GLU	HB3	1.683	0.003	2
1	A	286	GLU	HG2	2.018	0.012	2
1	A	286	GLU	HG3	1.958	0.001	2
1	A	286	GLU	CA	56.302	0.038	1
1	A	286	GLU	CB	30.056	0.059	1
1	A	286	GLU	CG	36.19	0.054	1
1	A	286	GLU	N	122.497	0.024	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	287	VAL	H	8.059	0.006	1
1	A	287	VAL	HA	3.78	0.004	1
1	A	287	VAL	HB	1.746	0.005	1
1	A	287	VAL	HG11	0.662	0.004	2
1	A	287	VAL	HG12	0.662	0.004	2
1	A	287	VAL	HG13	0.662	0.004	2
1	A	287	VAL	HG21	0.578	0.006	2
1	A	287	VAL	HG22	0.578	0.006	2
1	A	287	VAL	HG23	0.578	0.006	2
1	A	287	VAL	CA	62.111	0.04	1
1	A	287	VAL	CB	32.494	0.044	1
1	A	287	VAL	CG1	20.473	0.029	2
1	A	287	VAL	CG2	21.133	0.046	2
1	A	287	VAL	N	122.286	0.04	1
1	A	288	LEU	H	8.137	0.006	1
1	A	288	LEU	HA	4.098	0.008	1
1	A	288	LEU	HB2	1.155	0.004	2
1	A	288	LEU	HB3	1.313	0.008	2
1	A	288	LEU	HD11	0.65	0.005	2
1	A	288	LEU	HD12	0.65	0.005	2
1	A	288	LEU	HD13	0.65	0.005	2
1	A	288	LEU	HD21	0.577	0.009	2
1	A	288	LEU	HD22	0.577	0.009	2
1	A	288	LEU	HD23	0.577	0.009	2
1	A	288	LEU	HG	1.277	0.001	1
1	A	288	LEU	CA	54.626	0.031	1
1	A	288	LEU	CB	42.386	0.042	1
1	A	288	LEU	CD1	24.61	0.052	2
1	A	288	LEU	CD2	23.177	0.049	2
1	A	288	LEU	CG	26.819	0.044	1
1	A	288	LEU	N	126.034	0.009	1
1	A	289	PHE	H	8.122	0.005	1
1	A	289	PHE	HA	4.398	0.005	1
1	A	289	PHE	HB2	2.951	0.004	2
1	A	289	PHE	HB3	2.77	0.007	2
1	A	289	PHE	HD1	7.026	0.008	1
1	A	289	PHE	HD2	7.026	0.008	1
1	A	289	PHE	HE1	7.112	0.003	1
1	A	289	PHE	HE2	7.112	0.003	1
1	A	289	PHE	CA	57.435	0.035	1
1	A	289	PHE	CB	39.295	0.043	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	289	PHE	CD1	131.602	0.021	1
1	A	289	PHE	CD2	131.602	0.021	1
1	A	289	PHE	CE1	131.451	0.06	1
1	A	289	PHE	CE2	131.451	0.06	1
1	A	289	PHE	N	121.171	0.03	1
1	A	290	GLN	H	7.691	0.006	1
1	A	290	GLN	HA	3.897	0.006	1
1	A	290	GLN	HB2	1.846	0.004	2
1	A	290	GLN	HB3	1.665	0.003	2
1	A	290	GLN	HG2	2.001	0.011	2
1	A	290	GLN	HG3	2.016	?	2
1	A	290	GLN	CA	57.071	0.059	1
1	A	290	GLN	CB	30.387	0.059	1
1	A	290	GLN	CG	33.946	0.063	1
1	A	290	GLN	N	126.295	0.029	1

7.1.2 Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	187	0.30 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	176	0.03 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	171	0.52 ± 0.24	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 81%, i.e. 1853 atoms were assigned a chemical shift out of a possible 2291. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	640/814 (79%)	324/327 (99%)	165/332 (50%)	151/155 (97%)
Sidechain	1062/1301 (82%)	710/845 (84%)	334/412 (81%)	18/44 (41%)
Aromatic	151/176 (86%)	77/86 (90%)	71/81 (88%)	3/9 (33%)
Overall	1853/2291 (81%)	1111/1258 (88%)	570/825 (69%)	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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	181	ILE	HG13	-2.37	-0.82 – 3.23	-8.8
1	A	176	ASP	HB2	0.64	1.41 – 4.01	-8.0
1	A	106	LYS	HG2	-0.27	0.13 – 2.61	-6.6
1	A	113	ARG	HD2	1.67	1.97 – 4.26	-6.3
1	A	189	THR	HB	2.32	2.57 – 5.77	-5.8
1	A	255	ALA	HB1	-0.02	0.14 – 2.58	-5.7
1	A	255	ALA	HB2	-0.02	0.14 – 2.58	-5.7
1	A	255	ALA	HB3	-0.02	0.14 – 2.58	-5.7
1	A	187	LYS	HE3	1.85	1.92 – 3.89	-5.4
1	A	265	GLU	HB3	0.92	0.95 – 3.05	-5.1
1	A	164	ASN	HB2	1.25	1.27 – 4.34	-5.0
1	A	165	ILE	HA	1.41	1.43 – 6.88	-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. If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:

