



# Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 06:29 pm GMT

PDB ID : 1EVC  
Title : NMR structure of CYANOBACTERIAL TOXIN, PHOSPHATASE-1/-2A INHIBITOR  
Authors : Bagu, J.R.; Sykes, B.D.  
Deposited on : 1996-02-14

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	trunk28760
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

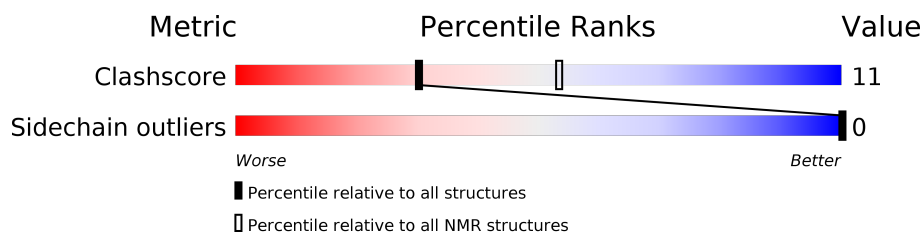
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*SOLUTION NMR*

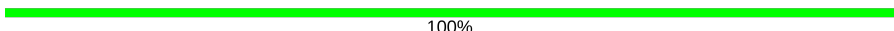
The overall completeness of chemical shifts assignment was not calculated.

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	125131	11601
Sidechain outliers	121581	10367

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  $\geq 3$ , 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	5	 100%

## 2 Ensemble composition and analysis ⓘ

This entry contains 48 models.

Cyrange was unable to find well-defined residues.

Error message: Less than two structures selected.

NmrClust was unable to cluster the ensemble.

Error message: Wrapper check: not enough residues in core to run NmrClust

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 109 atoms, of which 55 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MOTUPORIN.

Mol	Chain	Residues	Atoms					Trace
1	A	5	Total	C	H	N	O	0
			109	40	55	5	9	

## 4 Residue-property plots

### 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: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

#### 4.2.1 Score per residue for model 1

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.2 Score per residue for model 2


- Molecule 1: MOTUPORIN

Chain A:  40% 60%

D1	V2	?3	E4	X5
----	----	----	----	----

#### 4.2.3 Score per residue for model 3

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.4 Score per residue for model 4

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.5 Score per residue for model 5

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.6 Score per residue for model 6


- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.7 Score per residue for model 7

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.8 Score per residue for model 8

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.9 Score per residue for model 9

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.10 Score per residue for model 10

- Molecule 1: MOTUPORIN

Chain A:  80% 20%

D1	V2	?3	E4	X5
----	----	----	----	----

#### 4.2.11 Score per residue for model 11

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.12 Score per residue for model 12

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.13 Score per residue for model 13


- Molecule 1: MOTUPORIN

Chain A:  80% 20%

D1	V2	?3	E4	X5
----	----	----	----	----

#### 4.2.14 Score per residue for model 14

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.15 Score per residue for model 15

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.16 Score per residue for model 16

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.17 Score per residue for model 17

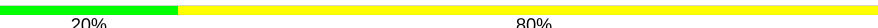
- Molecule 1: MOTUPORIN

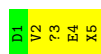
Chain A:  40% 60%



#### 4.2.18 Score per residue for model 18

- Molecule 1: MOTUPORIN

Chain A:  20% 80%





#### 4.2.19 Score per residue for model 19

- Molecule 1: MOTUPORIN

Chain A:  40% 60%



#### 4.2.20 Score per residue for model 20

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.21 Score per residue for model 21

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.22 Score per residue for model 22

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.23 Score per residue for model 23

- Molecule 1: MOTUPORIN

Chain A:  40% 60%



#### 4.2.24 Score per residue for model 24

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.25 Score per residue for model 25

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.26 Score per residue for model 26

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.27 Score per residue for model 27

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.28 Score per residue for model 28

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.29 Score per residue for model 29


- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.30 Score per residue for model 30

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.31 Score per residue for model 31

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.32 Score per residue for model 32

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.33 Score per residue for model 33

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.34 Score per residue for model 34

- Molecule 1: MOTUPORIN

Chain A:  40% 60%



#### 4.2.35 Score per residue for model 35

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.36 Score per residue for model 36

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.37 Score per residue for model 37

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.38 Score per residue for model 38


- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.39 Score per residue for model 39

- Molecule 1: MOTUPORIN

Chain A:  80% 20%



#### 4.2.40 Score per residue for model 40

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.41 Score per residue for model 41

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.42 Score per residue for model 42

- Molecule 1: MOTUPORIN

Chain A:  40% 60%



#### 4.2.43 Score per residue for model 43

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.44 Score per residue for model 44

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.45 Score per residue for model 45

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.46 Score per residue for model 46

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.47 Score per residue for model 47

- Molecule 1: MOTUPORIN

Chain A:  100%

There are no outlier residues in this chain.

#### 4.2.48 Score per residue for model 48

- Molecule 1: MOTUPORIN

Chain A:  60% 40%



## 5 Refinement protocol and experimental data overview

Of the ? calculated structures, 48 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
DGII	refinement	

No chemical shift data was provided. 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACB, MDH, FGA, 1ZN

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	54	55	51	1±2
All	All	2592	2640	2451	57

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 11.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:1ZN:H5	1:A:3:1ZN:H18	1.00	1.29	3	1
1:A:3:1ZN:H18	1:A:3:1ZN:C4	0.93	1.93	16	1
1:A:3:1ZN:H3	1:A:3:1ZN:C5	0.87	1.98	39	1
1:A:3:1ZN:H18	1:A:3:1ZN:H5	0.86	1.46	39	1
1:A:3:1ZN:C3	1:A:3:1ZN:H18	0.78	2.07	3	2
1:A:4:FGA:N	1:A:5:MDH:HM1	0.75	1.97	42	6
1:A:3:1ZN:C14	1:A:3:1ZN:H5	0.69	2.17	39	2
1:A:3:1ZN:C20	1:A:4:FGA:HG3	0.67	2.19	34	6
1:A:3:1ZN:C9	1:A:3:1ZN:H14	0.65	2.22	7	1
1:A:3:1ZN:H14	1:A:3:1ZN:C4	0.65	2.22	7	2
1:A:3:1ZN:C4	1:A:3:1ZN:H15	0.63	2.23	31	1
1:A:3:1ZN:H19	1:A:3:1ZN:H4	0.63	1.70	39	2

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:3:1ZN:H2	1:A:3:1ZN:C9	0.62	2.24	30	1
1:A:3:1ZN:H18	1:A:3:1ZN:C3	0.60	2.23	39	1
1:A:3:1ZN:C9	1:A:3:1ZN:H15	0.58	2.27	31	1
1:A:3:1ZN:C4	1:A:3:1ZN:H3	0.57	2.29	39	2
1:A:3:1ZN:C14	1:A:3:1ZN:C2	0.56	2.83	39	2
1:A:3:1ZN:C4	1:A:3:1ZN:H2	0.56	2.31	30	4
1:A:3:1ZN:H4	1:A:3:1ZN:C14	0.52	2.34	16	1
1:A:3:1ZN:C14	1:A:3:1ZN:H4	0.52	2.34	39	2
1:A:3:1ZN:C9	1:A:3:1ZN:H2	0.51	2.35	14	1
1:A:3:1ZN:C14	1:A:3:1ZN:C3	0.51	2.86	39	1
1:A:3:1ZN:C2	1:A:3:1ZN:C14	0.49	2.90	16	1
1:A:3:1ZN:C11	1:A:3:1ZN:C4	0.49	2.90	7	2
1:A:3:1ZN:C2	1:A:3:1ZN:H18	0.48	2.37	3	2
1:A:3:1ZN:C4	1:A:3:1ZN:C1	0.46	2.93	39	3
1:A:3:1ZN:H14	1:A:3:1ZN:C5	0.45	2.41	34	1
1:A:3:1ZN:H4	1:A:3:1ZN:H18	0.43	1.89	16	1
1:A:3:1ZN:C5	1:A:3:1ZN:H2	0.43	2.44	23	1
1:A:2:VAL:HG13	1:A:2:VAL:O	0.42	2.15	18	1
1:A:4:FGA:HG3	1:A:5:MDH:HM1	0.40	1.75	48	2
1:A:4:FGA:CB	1:A:5:MDH:HM1	0.40	2.46	19	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	0	-	-	-	-
All	All	0	-	-	-	-

There are no Ramachandran outliers.

### 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	1/1 (100%)	1±0 (100±0%)	0±0 (0±0%)	100	100
All	All	48/48 (100%)	48 (100%)	0 (0%)	100	100

There are no protein residues with a non-rotameric sidechain to report.

### 6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
1	ACB	A	1	1	5,8,9	2.47±0.01	0±0 (0±0%)
1	1ZN	A	3	1	22,23,24	1.71±0.01	0±0 (0±0%)
1	FGA	A	4	1	7,7,9	1.85±0.01	0±0 (0±0%)
1	MDH	A	5	1	5,6,7	4.66±0.01	1±0 (20±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	ACB	A	1	1	3,10,12	2.97±0.05	0±0 (0±0%)
1	1ZN	A	3	1	24,29,31	1.69±0.01	0±0 (0±0%)

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
1	FGA	A	4	1	4,7,11	1.47±0.03	0±0 (0±0%)
1	MDH	A	5	1	1,6,8	4.87±0.05	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ACB	A	1	1	-	0±0,6,10,12	0±0,0,0,0
1	1ZN	A	3	1	-	0±0,22,25,27	0±0,1,1,1
1	FGA	A	4	1	-	0±0,3,6,9	0±0,0,0,0
1	MDH	A	5	1	-	0±0,1,6,8	0±0,0,0,0

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	5	MDH	C-CA	8.96	1.54	1.43	20	48

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided