

Full wwPDB NMR Structure Validation Report (i)

Jun 14, 2020 - 06:50 am BST

:	1DLZ
:	SOLUTION STRUCTURE OF THE CHANNEL-FORMER ZERVAMICIN
	IIB (PEPTAIBOL ANTIBIOTIC)
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:	1999-12-13
	:

This is a Full wwPDB NMR Structure Validation 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:

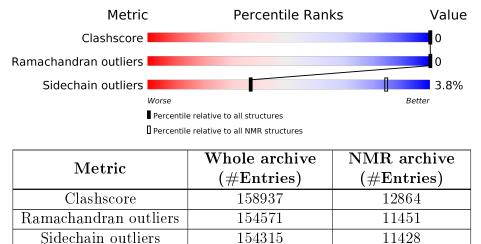
Cyrange	:	Kirchner and Güntert (2011)
$\operatorname{NmrClust}$:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
Percentile statistics		
RCI	:	$v_1n_11_5_13_A$ (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
${ m ShiftChecker}$:	2.11
Ideal geometry (proteins)	:	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 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.



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	А	17	94%	6%	



2 Ensemble composition and analysis (i)

This entry contains 20 models.

Cyrange was unable to find well-defined residues.

Error message: Only domains with < 8 residues could be identified.

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 270 atoms, of which 139 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called ZERVAMICIN IIB.

Mol	Chain	Residues	Atoms			Trace		
1	Λ	17	Total	С	Η	Ν	Ο	0
	А	17	270	90	139	19	22	0

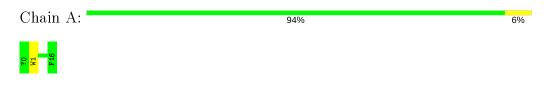


4 Residue-property plots (i)

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.

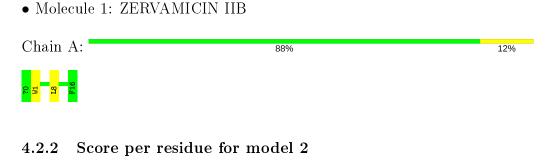
• Molecule 1: ZERVAMICIN IIB



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: ZERVAMICIN IIB

Chain A:

94%





6%

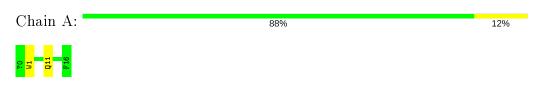
4.2.3 Score per residue for model 3

• Molecule 1: ZERVAMICIN IIB

Chain A:	94%	6%
70 110 110		
424 Seens man posid	us fan weddel 4	
4.2.4 Score per resid	ue for model 4	
• Molecule 1: ZERVAMIC	CIN IIB	
Chain A:	94%	6%
50 FM		
4.2.5 Score per resid	ue for model 5	
• Molecule 1: ZERVAMIC	CIN IIB	
Chain A:	94%	6%
70 11 F16		
4.2.6 Score per resid	ue for model 6	
• Molecule 1: ZERVAMIC	CIN IIB	
Chain A:	88%	12%

4.2.7 Score per residue for model 7

• Molecule 1: ZERVAMICIN IIB





4.2.8 Score per residue for model 8

• Molecule 1: ZERVAMICIN IIB

Chain A:	94%	6%
10 11 10 10 10 10 10 10 10 10 10 10 10 1		
4.2.9 Score per	r residue for model 9	
• Molecule 1: ZEF	RVAMICIN IIB	
Chain A:	94%	6%
10 M1 F16		
4.2.10 Score p	er residue for model 10	
• Molecule 1: ZEF	RVAMICIN IIB	
• Molecule 1: ZEF Chain A:	RVAMICIN IIB 88%	12%
		12%
Chain A: ខ្ល <u>ុដ្ឋ</u> ព្រ <mark>ដ្ឋ</mark>		12%
Chain A: ខ្ល <u>ុដ្ឋ</u> ព្រ <mark>ដ្ឋ</mark>	^{88%} er residue for model 11	12%

70 W1 F16

4.2.12 Score per residue for model 12

• Molecule 1: ZERVAMICIN IIB

Chain A:	94%	6%



4.2.13 Score per residue for model 13

• Molecule 1: ZERVAMICIN IIB

Chain A: 94%	6%
 4.2.14 Score per residue for model 14 Molecule 1: ZERVAMICIN IIB 	
Chain A: 94%	6%
 4.2.15 Score per residue for model 15 Molecule 1: ZERVAMICIN IIB 	
Chain A: 94%	6%
4.2.16 Score per residue for model 16Molecule 1: ZERVAMICIN IIB	

Chain A:

70 W1 F16

4.2.17 Score per residue for model 17

• Molecule 1: ZERVAMICIN IIB

Chain A:	94%	6%

94%

6%



4.2.18 Score per residue for model 18

• Molecule 1: ZERVAMICIN IIB

Chain A:	94%	6%
4.2.19 Score per resiMolecule 1: ZERVAMI	due for model 19 CIN IIB	
Chain A:	88%	12%
-	due for model 20	
• Molecule 1: ZERVAMI Chain A:	CIN IIB 88%	12%





5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *BEST 20* OUT OF 100 WITH CA BACKBONE RMSD NO LESS THAN 0.05 ANGSTROMS.

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

Software name	Classification	Version
DISCOVER 3.1	refinement	
DYANA 1.5	structure solution	

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: HYP, DIV, PHL, ACE, AIB

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	B	ond lengths	E	Bond angles
	Cham	RMSZ	$\#Z{>}5$	RMSZ	$\#Z{>}5$
1	А	1.21 ± 0.01	$0{\pm}0/71~(~0.0{\pm}~0.0\%)$	$1.34{\pm}0.05$	$1{\pm}0/95~(~1.1{\pm}~0.0\%)$
All	All	1.21	0/1420 ($0.0%$)	1.34	20/1900 ($1.1%$)

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	7	Observed(°)	$Ideal(^{o})$	Moo	lels
		1165	Type	Atoms		Observeu()	Iueai()	Worst	Total
1	А	1	TRP	CD1-NE1-CE2	-5.71	103.86	109.00	17	20

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.

M	ol	Chain	Non-H	H(model)	H(added)	Clashes
A	.11	All	2620	2780	2740	-

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 -.

There are no clashes.



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	\mathbf{ntiles}
1	А	8/17~(47%)	7 ± 0 (88±0%)	1±0 (12±0%)	0±0 (0±0%)	100	100
All	All	160/340~(47%)	140 (88%)	20 (12%)	0 (0%)	100	100

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	А	8/8~(100%)	8±0 (96±6%)	0±0 (4±6%)	36 84
All	All	160/160~(100%)	154 (96%)	6 (4%)	36 84

All 4 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	А	11	GLN	2
1	А	2	ILE	2
1	А	8	LEU	1
1	А	5	ILE	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.



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

8 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	Chain	Res	Link		Bond leng	ths
WIOI	туре	Ullalli		Counts	RMSZ	$\#Z{>}2$		
1	PHL	А	16	1	11, 11, 11	$0.96 {\pm} 0.02$	0±0 (0±0%)	
1	HYP	А	13	1	$6,\!8,\!9$	0.47 ± 0.01	0±0 (0±0%)	
1	HYP	А	10	1	6, 8, 9	$0.47{\pm}0.01$	0±0 (0±0%)	
1	AIB	А	9	1	$1,\!5,\!6$	$1.32{\pm}0.03$	0±0 (0±0%)	
1	DIV	А	4	1	$2,\!6,\!7$	$0.99 {\pm} 0.02$	0±0 (0±0%)	
1	AIB	А	14	1	$1,\!5,\!6$	1.29 ± 0.02	0±0 (0±0%)	
1	AIB	А	12	1	$1,\!5,\!6$	1.27 ± 0.02	0±0 (0±0%)	
1	AIB	А	7	1	$1,\!5,\!6$	1.26 ± 0.02	0±0 (0±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	lol Type Chain		Res	Res Link		Bond ang	jles
	туре	Ullain	nes		Counts	RMSZ	#Z>2
1	PHL	А	16	1	11, 13, 13	$0.46 {\pm} 0.06$	0±0 (0±0%)
1	HYP	А	13	1	$5,\!10,\!12$	$1.24{\pm}0.05$	0±0 (0±0%)
1	HYP	А	10	1	5,10,12	1.22 ± 0.08	0±0 (0±0%)
1	AIB	А	9	1	2,7,9	$0.65 {\pm} 0.04$	0±0 (0±0%)
1	DIV	А	4	1	$3,\!8,\!10$	$1.30 {\pm} 0.06$	0±0 (0±0%)
1	AIB	А	14	1	2,7,9	$0.73 {\pm} 0.04$	0±0 (0±0%)
1	AIB	А	12	1	2,7,9	$0.70 {\pm} 0.05$	0±0 (0±0%)
1	AIB	А	7	1	$2,\!7,\!9$	$0.73 {\pm} 0.04$	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.



1DDD

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	AIB	А	9	1	-	$0\pm 0,2,3,6$	-
1	AIB	А	12	1	-	$0\pm 0,2,3,6$	-
1	HYP	А	10	1	-	$0\pm0,0,11,13$	$0\pm 0,1,1,1$
1	DIV	А	4	1	-	$0\pm 0,3,6,9$	-
1	PHL	А	16	1	-	$0\pm 0,\!6,\!6,\!6$	$0\pm 0,1,1,1$
1	HYP	А	13	1	-	$0\pm0,0,11,13$	$0\pm 0,1,1,1$
1	AIB	А	7	1	-	$0\pm 0,2,3,6$	-
1	AIB	А	14	1	-	$0\pm 0,2,3,6$	-

There are no bond-length outliers.

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 (i)

There are no chain breaks in this entry.



7 Chemical shift validation (i)

No chemical shift data were provided

