

wwPDB NMR Structure Validation Summary Report (i)

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PDB ID : 1MH6

Title : Solution Structure of the Transposon Tn5-encoding Bleomycin-binding Pro-

tein, BLMT

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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 was not calculated.

There are no overall percentile quality scores available for this entry.

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	125	100%
1	В	125	100%



2 Ensemble composition and analysis (i)

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.



3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 3838 atoms, of which 1886 are hydrogens and 0 are deuteriums.

• Molecule 1 is a protein called BLEOMYCIN RESISTANCE PROTEIN.

Mol	Chain	Residues		Atoms							
1	٨	125	Total	С	Н	N	О	S	0		
$\begin{array}{c c} 1 & A \end{array}$	А	120	1919	623	943	165	182	6			
1	D	125	Total	С	Н	N	О	S	0		
	120	1919	623	943	165	182	6				



4 Residue-property plots (i)

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: BLEOMYCIN RESISTANCE PROTEIN

Chain	A:												1	009	%																	
T202 D203 Q204 A205	N208 L209	S211 R212	D213 F214	D215 S216	T217	A219	F220 Y221	E222 R223	1.224	F226	G227 1228	V229	R231	A233	G234 W235	M236	1237 L238	Q239	G241	D242	M244	L245 F246	F247	F248	A249 H250	P251	G252 1.253	D254	P255	A257	S258 W259	F260 S261
C262 C263 L264 R265	D267 D268 L269	A270 E271 F272	Y273 R274	Q275 C276	K277	V279	G280 I281	Q282 E283	T284	S286 S286	G287 V288	P289	1291	A293	P294 F205	1296	Q297 E298	W299	G301	T302	A304	A305 1306	V307	D308	P309	G311	T312	L314	R315	1317	Q318 N319	E320 L321
L322 A323 G324 I325																																
• Mole	ecule	1:]	BL	ΕC	lΜ	[Υ(CI	N	RI	ES.	IS	ТА	N	CF	ΞΙ	PR	Ο'	ΤF	EIN	J												
Chain	В:												1	00°	%																	
T2 D3 Q4 A5	P7 N8 L9	S11 R12	D13 F14	D15	T17	A19	F20 Y21	E22 R23	L24	F26	G27 T28	V29	R31	A33	G34 U35	M36	137 L38	Q39	G41	D42	M44	L45 F46	F47	F48	H50	P51	G52 1.53	D54	P55	A57	S58 W59	F60 S61
C62 C63 L64 R65	D68 D68 L69	A/O E71 F72	Y73 R74	Q75 C76	K77	077 0779	181	Q82 E83	T84	288 288	G87 V88	P89	191	A93	P94	1.96	197 E98	W99	G101	T102	A104	A105	V107	D108	P109	G111	T112	L114	R115	1117	Q118 N119	E120 L121
L122 A123 G124 I125 S126	O N																															



5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 1 were deposited, based on the following criterion: ?.

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

Software name	Classification	Version				
Discover	refinement	2000				

No chemical shift data was provided.



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	0	0	0	0
1	В	0	0	0	0
All	All	0	0	0	-

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	Percentiles		
1	A	0	-	-	-	-		
1	В	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	0	-	-	-
1	В	0	-	-	-
All	All	0	-	-	-

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

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)

No chemical shift data were provided

