

Full wwPDB NMR Structure Validation Report (i)

Apr 20, 2024 – 09:13 AM EDT

PDB ID : 1MTG

Title: NMR Structure of HO2-Co(III)bleomycin A(2) bound to d(GAGCTC)(2) Authors: Zhao, C.; Xia, C.; Mao, Q.; Forsterling, H.; DeRose, E.; Antholine, W.E.;

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Deposited on : 2002-09-20

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

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

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)

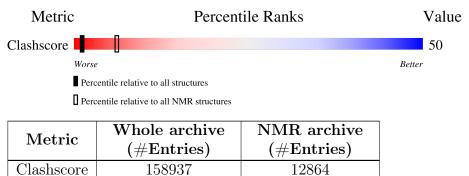
Validation Pipeline (wwPDB-VP) : 2.36.2

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	A	6	50%	50%		
1	В	6	33%	67%		



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 are 4 unique types of molecules in this entry. The entry contains 561 atoms, of which 222 are hydrogens and 0 are deuteriums.

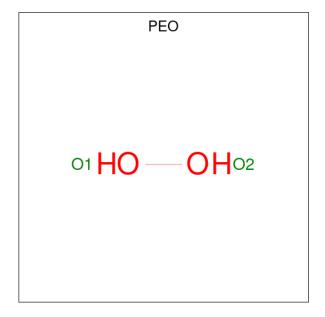
• Molecule 1 is a DNA chain called 5'-D(*GP*AP*GP*CP*TP*C)-3'.

Mol	Chain	Residues	Atoms						Trace
1	۸	6	Total	С	Н	N	О	Р	0
1	A	0	189	58	69	23	34	5	U
1	D	6	Total	С	Н	N	О	Р	0
	1 B	0	189	58	69	23	34	5	U

• Molecule 2 is COBALT (III) ION (three-letter code: 3CO) (formula: Co).

Mol	Chain	Residues	Atoms
9	Λ	1	Total Co
	А	1	1 1

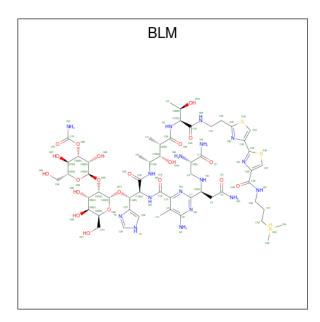
• Molecule 3 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



Mo	Chain	Residues	Ato	oms	
9	Λ	1	Total	Η	О
)	A	1	3	1	2

• Molecule 4 is BLEOMYCIN A2 (three-letter code: BLM) (formula: C₅₅H₈₅N₁₇O₂₁S₃).





Mol	Chain	Residues	Atoms					
1	D	1	Total	С	Н	N	О	S
4	Б	1	179	55	83	17	21	3



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: 5'-D(*GP*AP*GP*CP*TP*C)-3'

Chain A: 50% 50%

• Molecule 1: 5'-D(*GP*AP*GP*CP*TP*C)-3'

Chain B: 33% 67%





Refinement protocol and experimental data overview (i) 5



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

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
X-PLOR	refinement	3.1

No chemical shift data was provided.



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: 3CO, PEO, BLM

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		Boı	$\operatorname{ad} \operatorname{lengths}$	Bond angles		
IVIOI	Chain	RMSZ	#Z>5	RMSZ	#Z>5	
1	A	1.19	1/134 (0.7%)	2.24	10/205 (4.9%)	
1	В	1.16	1/134 (0.7%)	2.29	8/205 (3.9%)	
All	All	1.18	2/268 (0.7%)	2.27	18/410 (4.4%)	

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
1	В	11	DT	C5-C7	5.41	1.53	1.50
1	A	5	DT	C5-C7	5.03	1.53	1.50

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	3	DG	N7-C8-N9	9.61	117.91	113.10
1	В	9	DG	N7-C8-N9	9.27	117.74	113.10
1	A	1	DG	N7-C8-N9	9.13	117.67	113.10
1	В	7	DG	N7-C8-N9	9.12	117.66	113.10
1	A	2	DA	N7-C8-N9	7.72	117.66	113.80
1	В	8	DA	N7-C8-N9	7.60	117.60	113.80
1	В	7	DG	C8-N9-C4	-7.07	103.57	106.40
1	В	9	DG	C8-N9-C4	-6.53	103.79	106.40
1	A	3	DG	C8-N9-C4	-6.43	103.83	106.40
1	A	1	DG	C8-N9-C4	-6.40	103.84	106.40
1	A	2	DA	C8-N9-C4	-5.91	103.44	105.80
1	В	11	DT	C6-C5-C7	-5.77	119.44	122.90
1	A	5	DT	C6-C5-C7	-5.60	119.54	122.90
1	A	3	DG	C5-N7-C8	-5.44	101.58	104.30
1	В	8	DA	C8-N9-C4	-5.42	103.63	105.80
1	A	3	DG	O4'-C1'-N9	5.25	111.68	108.00
1	A	1	DG	C5-N7-C8	-5.25	101.67	104.30
1	В	9	DG	C5-N7-C8	-5.24	101.68	104.30



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	120	69	69	5
1	В	120	69	69	13
3	A	2	1	0	1
4	В	96	83	84	18
All	All	339	222	222	28

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 50.

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

Atom-1	Atom-2	$\operatorname{Clash}(ext{\AA})$	$\operatorname{Distance}(\text{\AA})$
1:A:5:DT:H2"	1:A:6:DC:C6	0.62	2.29
1:A:3:DG:H2"	1:A:4:DC:C6	0.60	2.30
1:B:10:DC:H2"	1:B:11:DT:C6	0.60	2.30
1:A:5:DT:C2	4:B:21:BLM:S43	0.59	2.95
4:B:21:BLM:O12	4:B:21:BLM:HAA	0.58	1.97
4:B:21:BLM:NC	4:B:21:BLM:O40	0.58	2.37
1:B:8:DA:C4	4:B:21:BLM:S46	0.57	2.98
4:B:21:BLM:C7	4:B:21:BLM:O4	0.53	2.56
1:A:2:DA:H2"	1:A:3:DG:C8	0.50	2.42
4:B:21:BLM:H3E	4:B:21:BLM:C4	0.50	2.37
1:B:11:DT:H2"	1:B:12:DC:C6	0.48	2.44
4:B:21:BLM:C4	4:B:21:BLM:C3	0.48	2.91
4:B:21:BLM:O36	4:B:21:BLM:OH3	0.47	2.28
1:B:9:DG:C6	4:B:21:BLM:S46	0.47	3.07
4:B:21:BLM:OH1	4:B:21:BLM:H59	0.47	2.10
4:B:21:BLM:OH1	4:B:21:BLM:C59	0.46	2.62
1:A:2:DA:C2'	1:A:3:DG:C8	0.45	2.99
1:B:7:DG:H2"	1:B:8:DA:C8	0.44	2.47
1:B:8:DA:C4	4:B:21:BLM:C47	0.44	2.99
1:B:11:DT:C2'	1:B:12:DC:C6	0.44	3.01
1:B:7:DG:C5	1:B:8:DA:C6	0.42	3.07

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Atom-1	Atom-2	$\operatorname{Clash}(ext{\AA})$	$\operatorname{Distance}(\text{\AA})$
1:B:9:DG:C5	4:B:21:BLM:S46	0.41	3.13
1:B:7:DG:C2'	1:B:8:DA:C8	0.41	3.03
1:B:8:DA:N3	4:B:21:BLM:S46	0.41	2.94
4:B:21:BLM:H38	4:B:21:BLM:H29	0.41	1.91
1:B:11:DT:C1'	4:B:21:BLM:HD1	0.41	2.29
3:A:23:PEO:O1	4:B:21:BLM:NK	0.40	2.52
1:B:9:DG:C6	4:B:21:BLM:C47	0.40	3.03

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

There are no protein molecules in this entry.

6.3.2 Protein sidechains (i)

There are no protein molecules in this entry.

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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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.

Mal	Trunc	Chain	Dag	Timle	Во	nd lengt	ths
Mol	туре	Chain	nes	Lilik	Counts	RMSZ	#Z>2
4	BLM	В	21	2	88,101,101	4.22	17 (19%)
3	PEO	A	23	2	1,1,1	0.26	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.

Mal	Tuno	Chain	Dec Link		Res Link		Во	nd angle	es
IVIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	#Z>2		
4	BLM	В	21	2	108,143,143	2.73	17 (15%)		
3	PEO	A	23	2	-	-	-		

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
4	BLM	В	21	2	-	2,86,142,142	0,6,6,6

All bond outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	$Ideal(\AA)$
4	В	21	BLM	C47-S46	26.38	1.37	1.70
4	В	21	BLM	C44-S43	21.45	1.36	1.70
4	В	21	BLM	C43-S43	11.89	1.37	1.73
4	В	21	BLM	C10-C12	7.37	1.39	1.50
4	В	21	BLM	C48-C49	5.37	1.37	1.50
4	В	21	BLM	O64-C64	4.68	1.53	1.41
4	В	21	BLM	O62-C63	4.54	1.53	1.41
4	В	21	BLM	O62-C60	4.13	1.54	1.44
4	В	21	BLM	O64-C65	3.87	1.53	1.44
4	В	21	BLM	C8-NE	3.83	1.40	1.35
4	В	21	BLM	C6-NC	3.45	1.53	1.47
4	В	21	BLM	C42-C43	2.34	1.50	1.49

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Mol	Chain	Res	Type	Atoms	${f Z}$	Observed(A)	$\operatorname{Ideal}(ext{\AA})$
4	В	21	BLM	C7-NE	2.29	1.38	1.34
4	В	21	BLM	O70-C70	2.26	1.25	1.21
4	В	21	BLM	C13-NH	2.17	1.50	1.45
4	В	21	BLM	C3-NC	2.03	1.52	1.47
4	В	21	BLM	O68-C70	2.01	1.40	1.35

All angle outliers are listed below. They are sorted according to the Z-score.

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	В	21	BLM	C45-C44-S43	16.71	107.87	112.53
4	В	21	BLM	C47-S46-C46	13.68	107.62	91.12
4	В	21	BLM	C54-S53-C55	6.25	109.70	101.49
4	В	21	BLM	O68-C70-NQ	6.09	120.05	110.58
4	В	21	BLM	O68-C70-O70	5.41	118.22	123.69
4	В	21	BLM	NE-C7-NG	5.40	118.21	126.00
4	В	21	BLM	C68-O68-C70	5.17	109.74	117.12
4	В	21	BLM	C54-S53-C52	4.60	109.79	101.63
4	В	21	BLM	C55-S53-C52	4.59	109.76	101.63
4	В	21	BLM	C12-C10-NG	4.04	112.23	115.99
4	В	21	BLM	C9-C10-NG	3.88	119.17	123.31
4	В	21	BLM	C48-C47-S46	3.31	107.73	111.79
4	В	21	BLM	C64-O56-C57	2.82	110.99	117.96
4	В	21	BLM	C9-C10-C12	2.80	128.60	123.14
4	В	21	BLM	C48-C49-NP	2.71	119.38	115.59
4	В	21	BLM	C63-OH1-C14	2.55	110.84	114.99
4	В	21	BLM	O70-C70-NQ	2.29	121.73	125.51

There are no chirality outliers.

All torsion outliers are listed below.

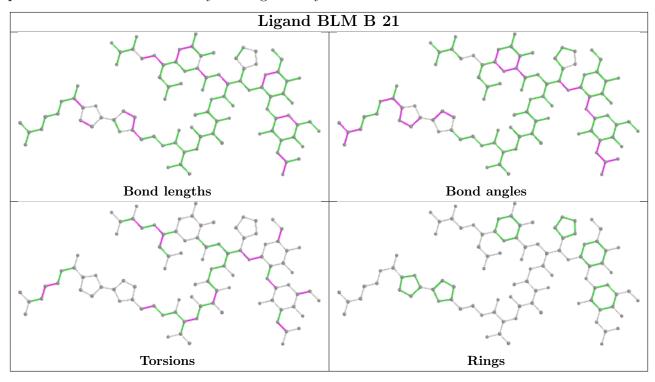
Mol	Chain	Res	Type	Atoms
4	В	21	BLM	NQ-C70-O68-C68
4	В	21	BLM	O70-C70-O68-C68

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring



in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

