

# Full wwPDB NMR Structure Validation Report (i)

### Mar 1, 2022 – 10:41 AM EST

PDB ID	:	2GM0
Title	:	Linear dimer of stemloop SL1 from HIV-1
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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:

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	:	2.27
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

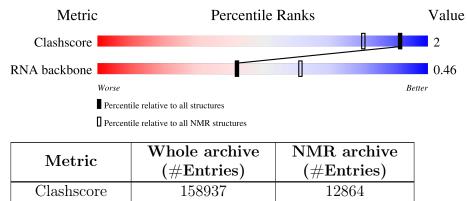
RNA backbone

# 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.



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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%

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Mol	Chain	Length	Quality of chain						
1	А	35	80%	14%	6%				
1	В	35	80%	14%	6%				



# 2 Ensemble composition and analysis (i)

This entry contains 10 models. This entry does not contain polypeptide chains, therefore identification of well-defined residues and clustering analysis are not possible. All residues are included in the validation scores.



# 3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2272 atoms, of which 766 are hydrogens and 0 are deuteriums.

• Molecule 1 is a RNA chain called RNA (35-MER).

Mol	Chain	Residues		Atoms					Trace
1	Δ	35	Total					Р	0
		55	1136	336	383	143	240	34	
1	В	35	Total	С	Н	Ν	0	Р	0
	D	- 55	1136	336	383	143	240	34	0



# 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.

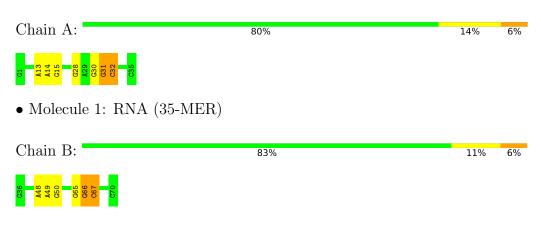
• Molecule 1: RNA (35-MER)

Chain A:	80%	14%	6%
<b>G1</b> A13 A14 A14 A29 G31 G32 C35 C35 C35			
• Molecule 1: RNA (35-MER)			
Chain B:	80%	14%	6%
<b>G</b> <b>G</b> <b>G</b> <b>G</b> <b>G</b> <b>G</b> <b>G</b> <b>G</b>			

## 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





## 4.2.2 Score per residue for model 2

Chain A	A: 83%	11%	6%
<b>G1</b> 615 615	0 03 0 03 0 03 0 03 0 0 0 0 0 0 0 0 0 0		
• Mole	cule 1: RNA (35-MER)		
Chain l	3: 80%	14%	6%
<b>G36</b> 449 G50			
4.2.3	Score per residue for model 3		
• Moleo	cule 1: RNA (35-MER)		
Chain A	A: 74%	17%	9%
<b>G1</b> A13 A14 G15	A27 62.8 63.1 63.1 63.1 63.2 8 63.1		
• Moleo	cule 1: RNA (35-MER)		
Chain l	3: 74%	17%	9%
636 A48 A49 G50	A62 663 666 666 70 70		
4.2.4	Score per residue for model 4		
• Moleo	cule 1: RNA (35-MER)		
Chain A	A: 80%	9%	11%
G1 A13 A14 G15	830 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0		
• Mole	cule 1: RNA (35-MER)		
Chain l	3: 77%	11%	11%
<b>G36</b> A48 A49 G50	C 10 C 10 C 10 C 10 C 10 C 10 C 10 C 10		



## 4.2.5 Score per residue for model 5

Chain A:	83%	149	% •
61 A13 A14 G15 G30 G31 G31			
• Molecule	1: RNA (35-MER)		
Chain B:	89%		11%
<mark>636</mark> 49 665 665 666 C67	2 <mark>0</mark> 10 10 10 10 10 10 10 10 10 10 10 10 10		
4.2.6 Sc	ore per residue for model 6		
• Molecule	1: RNA (35-MER)		
Chain A:	74%	20%	6%
G1 G5 A13 A14 G15	A21 630 631 631 631 631 631 631 631		
• Molecule	1: RNA (35-MER)		
Chain B:	74%	17%	9%
<b>G36</b> G40 A48 A49 G50	A56 464 665 666 666 70 70 70		
4.2.7 Sc	ore per residue for model 7		
• Molecule	1: RNA (35-MER)		
Chain A:	80%	11%	9%
G1 614 615 A21 A27	82 33 39 82 33 49 82 33 49 82 33 49 82 33 49 82 33 49 82 33 49 82 34 82 34 82 83 82 34 82 83 82 83 83 83 83 83 83 83 83 83 83 83 83 83		
• Molecule	1: RNA (35-MER)		
Chain B:	80%	9%	11%





## 4.2.8 Score per residue for model 8

Chain A:	77%	23%	6
G1 G12 A13 A14 G15	<b>6 8 2 3</b> <b>6 9 3</b> 10 <b>6 9</b> <b>7 1</b> <b>7 11111111111111</b>		
• Molecu	le 1: RNA (35-MER)		
Chain B:	80%	9%	11%
<b>G36</b> A48 A49 G50 G50	0 665 667 667 667 667 667 667 667 667 667		
4.2.9	Score per residue for model 9		
• Molecu	le 1: RNA (35-MER)		
Chain A:	86%		14%
G1 A14 A29 G30 C31	8		
• Molecu	le 1: RNA (35-MER)		
Chain B:	86%		14%
<b>G36</b> A49 A64 G65 G65	2 <mark>2</mark> 2 - 2 2 - 2 2 - 2 2 - 2 2 - 2 2 - 2 2 - 2 2		
4.2.10	Score per residue for model 10		
• Molecu	le 1: RNA (35-MER)		
Chain A:	80%	179	<b>%</b> ••
G1 A13 A14 G15 G15	8 9 3 3 1 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9 9		
• Molecu	le 1: RNA (35-MER)		
Chain B:	83%	119	6%
<mark>636</mark> 49 650 A56	A 64 665 C 70 C 70		



# 5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: Restrained Metropolis Monte Carlo and restrained minimization in helical parameter's space.

Of the 20 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
DYANA	refinement	1.5
miniCarlo	refinement	

No chemical shift data was provided.



# 6 Model quality (i)

## 6.1 Standard geometry (i)

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	Bond angles		
		RMSZ	$\#Z{>}5$	RMSZ	#Z>5	
1	А	$0.73 {\pm} 0.00$	$0{\pm}0/843~(~0.0{\pm}~0.0\%)$	$1.13 \pm 0.01$	$0{\pm}0/1315~(~0.0{\pm}~0.0\%)$	
1	В	$0.73 {\pm} 0.00$	$0{\pm}0/843~(~0.0{\pm}~0.0\%)$	$1.12 \pm 0.01$	$0{\pm}0/1315~(~0.0{\pm}~0.0\%)$	
All	All	0.73	0/16860 ( $0.0%$ )	1.12	9/26300 ( $0.0%$ )	

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mal	Mol Chain		Res Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
10101	Unam	nes	Type	Atoms			Ideal()	Worst	Total
1	А	21	A	C3'-C2'-C1'	6.85	106.98	101.50	10	3
1	В	56	A	C3'-C2'-C1'	5.70	106.06	101.50	10	3
1	А	15	G	C3'-C2'-C1'	5.69	106.06	101.50	4	1
1	А	28	G	C3'-C2'-C1'	5.39	105.81	101.50	1	1
1	В	50	G	C3'-C2'-C1'	5.02	105.52	101.50	4	1

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	А	753	383	383	$2\pm1$
1	В	753	383	383	2±2
All	All	15060	7660	7660	34

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including



A + ama 1	Atom 2	$C \ln a \ln \left( \frac{3}{2} \right)$	$\mathbf{D}^{\mathbf{i}}_{\mathbf{i}}$	Models	
Atom-1	Atom-2	$\operatorname{Clash}(\operatorname{\AA})$	$\operatorname{Distance}(\operatorname{\AA})$	Worst	Total
1:B:48:A:O2'	1:B:49:A:C8	0.53	2.62	6	1
1:B:64:A:O2'	1:B:65:G:C8	0.49	2.63	7	1
1:B:49:A:HO2'	1:B:50:G:P	0.49	2.31	4	1
1:B:66:G:O2'	1:B:67:C:C6	0.48	2.66	2	6
1:B:64:A:O2'	1:B:65:G:C2'	0.47	2.62	6	1
1:A:31:G:O2'	1:A:32:C:C6	0.47	2.67	2	4
1:A:29:A:O2'	1:A:30:G:C2'	0.47	2.62	6	1
1:A:14:A:N3	1:A:15:G:C8	0.46	2.83	5	1
1:A:31:G:C3'	1:A:32:C:H5"	0.45	2.39	7	1
1:A:30:G:O2'	1:A:31:G:C8	0.44	2.70	7	1
1:B:66:G:C3'	1:B:67:C:H5"	0.43	2.43	7	1
1:B:49:A:O2'	1:B:50:G:P	0.42	2.77	4	1
1:A:13:A:H2'	1:A:14:A:C8	0.42	2.50	5	2
1:A:14:A:O2'	1:A:15:G:P	0.42	2.78	4	1
1:B:48:A:H2'	1:B:49:A:C8	0.42	2.50	4	1
1:B:48:A:C2'	1:B:49:A:O4'	0.41	2.68	3	2
1:B:66:G:O2'	1:B:67:C:C5	0.41	2.73	4	1
1:A:14:A:HO2'	1:A:15:G:P	0.41	2.37	4	1
1:A:31:G:O2'	1:A:32:C:C5	0.41	2.73	2	2
1:B:65:G:O2'	1:B:66:G:C8	0.41	2.74	7	1
1:A:13:A:C2'	1:A:14:A:O4'	0.41	2.69	10	2
1:B:57:C:O2	1:B:57:C:H2'	0.40	2.16	4	1

hydrogen atoms). The all-atom clashscore for this structure is 1.

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

### 6.3 Torsion angles (i)

#### Protein backbone (i) 6.3.1

There are no protein molecules in this entry.

#### Protein sidechains (i) 6.3.2

There are no protein molecules in this entry.

#### RNA (i) 6.3.3

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	А	34/35~(97%)	$6{\pm}1~(18{\pm}4\%)$	$2\pm1~(5\pm3\%)$	$0.46 {\pm} 0.03$

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	Chain	Analysed	Backbone Outliers	Pucker Outliers	Suiteness
1	В	34/35~(97%)	$6\pm1 (18\pm4\%)$	$1\pm1~(4\pm2\%)$	$0.45 {\pm} 0.04$
All	All	680/700~(97%)	120 (18%)	30 (4%)	0.46

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The overall RNA backbone suiteness is 0.46.

All unique RNA backbone outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	А	14	А	10
1	А	31	G	10
1	А	32	С	10
1	В	49	А	10
1	В	66	G	10
1	В	67	С	10
1	А	30	G	9
1	В	65	G	9
1	А	15	G	7
1	В	50	G	7
1	В	64	А	6
1	А	29	А	5
1	А	13	А	3
1	В	63	G	3
1	В	48	А	2
1	А	27	А	2
1	А	28	G	2
1	В	62	А	1
1	А	5	G	1
1	А	21	А	1
1	В	40	G	1
1	В	56	А	1

All unique RNA pucker outliers are listed below:

Mol	Chain	Res	Type	Models (Total)
1	А	31	G	9
1	В	66	G	9
1	А	14	А	4
1	В	49	А	3
1	А	12	G	1
1	А	29	А	1
1	А	30	G	1
1	В	64	А	1
1	В	65	G	1



## 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

