

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 19, 2024 – 12:48 AM EST

PDB ID	:	4GV9
Title	:	Lassa nucleoprotein C-terminal domain in complex with triphosphated dsRNA
		soaking for 5 min
Authors	:	Jiang, X.; Huang, Q.; Wang, W.; Dong, H.; Ly, H.; Liang, Y.; Dong, C.
Deposited on	:	2012-08-30
Resolution	:	2.46  Å(reported)

This is a Full wwPDB X-ray 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/XrayValidationReportHelp 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:

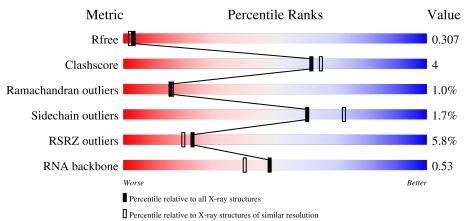
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.46 Å.

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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)
RNA backbone	3102	1001 (2.80-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality	v of chain	
1	Е	4	50%	25%	25%
2	F	5	60%		40%
3	А	213	<u>6%</u> 86%		6% 7%



#### 4GV9

# 2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 1778 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a RNA chain called RNA (5'-R(\*(GTP)P\*GP\*GP\*C)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	F	4	Total	С	Ν	0	Р	0	0	0
	Ľ	4	98	39	18	35	6	0	0	0

• Molecule 2 is a RNA chain called RNA (5'-R(P\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	F	5	Total 103	С 46	N 17	O 35	Р 5	0	0	0

• Molecule 3 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	А	198	Total 1564	C 990	N 265	O 296	S 13	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	ALA	-	expression tag	UNP P13699
A	358	MET	-	expression tag	UNP P13699
А	359	ASP	-	expression tag	UNP P13699
А	360	HIS	-	expression tag	UNP P13699
А	361	VAL	-	expression tag	UNP P13699
А	362	GLU	-	expression tag	UNP P13699
А	363	PHE	-	expression tag	UNP P13699

• Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Е	3	Total Mn 3 3	0	0



• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Zn 1 1	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total O 1 1	0	0
6	А	8	Total O 8 8	0	0



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# 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: RNA (5'-R(\*(GTP)P\*GP\*GP\*C)-3')

Chain E:	50%	25%	25%
00 01 01 01 01 01 01 01 01 01 01 01 01 0			
• Molecule 2: R	ANA (5'-R(P*CP*GP*CP))	*CP*C)-3')	
Chain F:	60%		40%
8 <mark>8</mark> 8			
• Molecule 3: N	lucleoprotein		
Chain A:	86%		6% 7%
ALA MET ASP ASP ASP VAL CALU F363 F363 L380 L380	1001 <b>E395</b> 1411 1411 1414 1414 1428 1428 1428 1445 1445	0451 0462 0462 0463 0463 0463 0463 0463 0460 0460 0460	LYS ARG GLY K522 E523 E523 E523 E523 E523 F1R F1R F1R F1R F1865 R1565 R1565 R1565 R1565



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	44.78Å 44.78Å 221.74Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	43.89 - 2.46	Depositor
Resolution (A)	43.89 - 2.47	EDS
% Data completeness	99.8 (43.89-2.46)	Depositor
(in resolution range)	99.7 (43.89-2.47)	EDS
R <sub>merge</sub>	0.06	Depositor
R <sub>sym</sub>	0.06	Depositor
$< I/\sigma(I) > 1$	$23.63 (at 2.45 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
D D.	0.259 , $0.305$	Depositor
$R, R_{free}$	0.259 , $0.307$	DCC
$R_{free}$ test set	423 reflections $(4.76%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	58.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 50.2	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.41, \langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	1778	wwPDB-VP
Average B, all atoms $(Å^2)$	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MN, GTP

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 root-mean-square of all Z scores of the bond lengths (or angles).

Mol	ol Chain Bond lengths		Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	Е	0.23	0/73	1.43	2/112~(1.8%)
2	F	0.24	0/113	0.69	0/173
3	А	0.27	0/1593	0.47	0/2153
All	All	0.27	0/1779	0.57	2/2438~(0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Е	9	G	P-O3'-C3'	12.75	135.00	119.70
1	Е	9	G	OP1-P-O3'	5.41	117.09	105.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Е	98	0	45	7	0
2	F	103	0	56	0	0
3	А	1564	0	1559	5	0
4	Е	3	0	0	0	0
5	А	1	0	0	0	0
6	А	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1	0	0	0	0
All	All	1778	0	1660	12	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 4.

All (12) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:566:ARG:HB3	3:A:567:VAL:HB	1.67	0.77
1:E:8:GTP:HO2'	1:E:9:G:H8	1.36	0.70
3:A:381:ASP:H	3:A:404:GLN:HE22	1.44	0.66
3:A:462:GLN:HE22	3:A:486:LEU:H	1.46	0.63
1:E:8:GTP:H2'	1:E:9:G:C8	2.37	0.58
1:E:8:GTP:O2'	1:E:9:G:H8	1.89	0.55
1:E:8:GTP:C2'	1:E:9:G:H8	2.25	0.49
3:A:414:PHE:CZ	3:A:508:MET:HG3	2.49	0.47
1:E:8:GTP:C2'	1:E:9:G:C8	2.98	0.47
1:E:8:GTP:O2'	1:E:9:G:C8	2.67	0.46
1:E:8:GTP:H2'	1:E:9:G:H8	1.81	0.45
3:A:380:LEU:HD11	3:A:411:ILE:HD11	2.01	0.42

There are no symmetry-related clashes.

## 5.3 Torsion angles (i)

#### 5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution.

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
3	А	192/213~(90%)	188 (98%)	2(1%)	2(1%)	15 16

All (2) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
3	А	463	GLY
3	А	567	VAL

#### 5.3.2 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 X-ray entries followed by that with respect to entries of similar resolution.

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
3	А	175/187~(94%)	172 (98%)	3~(2%)	60 73

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	А	420	LEU
3	А	445	LEU
3	А	451	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	А	379	GLN
3	А	404	GLN
3	А	462	GLN
3	А	474	GLN
3	А	496	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	Ε	3/4~(75%)	0	1 (33%)
2	F	5/5~(100%)	1 (20%)	1 (20%)
All	All	8/9~(88%)	1 (12%)	2(25%)

All (1) RNA backbone outliers are listed below:



Mol	Chain	Res	Type
2	F	2	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	Е	8	GTP
2	F	1	С

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or 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 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Type	Гуре Chain	Res	Res Link	Bond lengths			Bond angles		
MOI	туре				Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
1	GTP	Е	8	2,1	26,34,34	0.93	1 (3%)	32,54,54	1.41	5 (15%)

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	GTP	Е	8	2,1	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Е	8	GTP	C6-N1	-2.20	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	8	GTP	C3'-C2'-C1'	3.18	105.77	100.98
1	Е	8	GTP	PB-O3B-PG	-3.08	122.27	132.83

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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	Е	8	GTP	PA-O3A-PB	-2.85	123.05	132.83
1	Е	8	GTP	C8-N7-C5	2.36	107.48	102.99
1	Ε	8	GTP	C5-C6-N1	2.27	117.97	113.95

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There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	Е	8	GTP	O4'-C4'-C5'-O5'
1	Е	8	GTP	C3'-C4'-C5'-O5'
1	Е	8	GTP	PB-O3A-PA-O5'
1	Е	8	GTP	PA-O3A-PB-O1B
1	Е	8	GTP	PA-O3A-PB-O2B
1	Е	8	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	Ε	8	GTP	7	0

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.



## 5.7 Other polymers (i)

There are no such residues in this entry.

## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

## 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	Ε	3/4~(75%)	-0.01	0 100 10	0	74, 74, 76, 84	0
2	F	5/5~(100%)	0.42	0 100 10	0	113, 122, 151, 183	0
3	А	198/213~(92%)	0.38	12 (6%) 21	18	41, 64, 92, 135	0
All	All	206/222~(92%)	0.38	12 (5%) 23	20	41, 64, 96, 183	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	А	567	VAL	3.6
3	А	428	LYS	3.3
3	А	367	TYR	3.2
3	А	514	VAL	2.9
3	А	395	GLU	2.8
3	А	566	ARG	2.8
3	А	429	TYR	2.7
3	А	522	LYS	2.7
3	А	565	PRO	2.6
3	А	439	PHE	2.5
3	А	523	GLU	2.3
3	А	420	LEU	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q < 0.9
1	GTP	Ε	8	32/32	0.44	0.29	$99,\!111,\!150,\!159$	0



### 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
4	MN	Е	101	1/1	0.95	0.19	$55,\!55,\!55,\!55$	0
4	MN	Е	103	1/1	0.95	0.06	78,78,78,78	0
4	MN	Е	102	1/1	0.96	0.14	81,81,81,81	0
5	ZN	А	601	1/1	1.00	0.12	57,57,57,57	0

#### 6.5 Other polymers (i)

There are no such residues in this entry.

