



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:09 PM UTC

PDB ID : 3NMA / pdb\_00003nma  
Title : Mutant P169S of Foot-and-mouth disease Virus RNA dependent RNA-polymerase  
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Deposited on : 2010-06-22  
Resolution : 2.60 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](mailto: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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49



## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3853 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 protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	476	3704	2354	643	687	20	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	SER	PRO	engineered mutation	UNP Q0QEE0
A	471	ALA	-	expression tag	UNP Q0QEE0
A	472	ALA	-	expression tag	UNP Q0QEE0
A	473	LEU	-	expression tag	UNP Q0QEE0
A	474	ALA	-	expression tag	UNP Q0QEE0
A	475	HIS	-	expression tag	UNP Q0QEE0
A	476	HIS	-	expression tag	UNP Q0QEE0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	3	63	29	13	19	2	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	2	40	18	6	14	2	0	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		

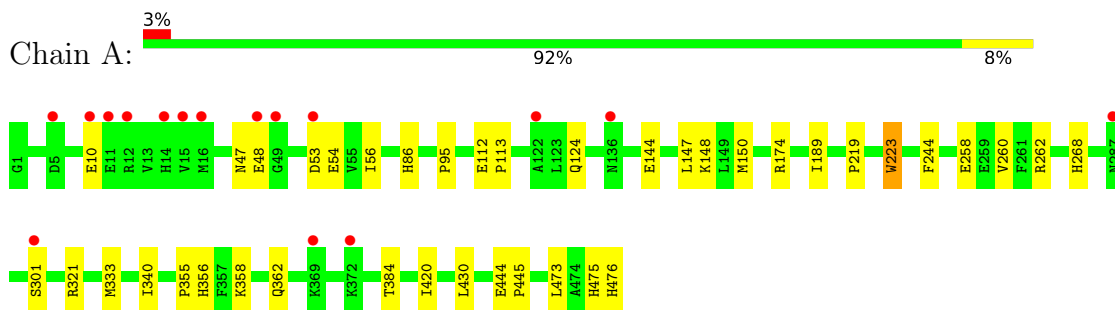
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	44	Total O 44 44	0	0
5	B	1	Total O 1 1	0	0

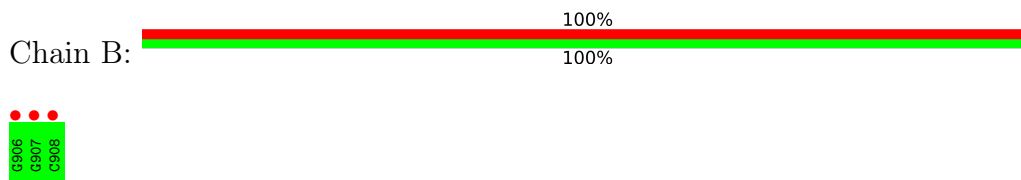
### 3 Residue-property plots [i](#)

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.

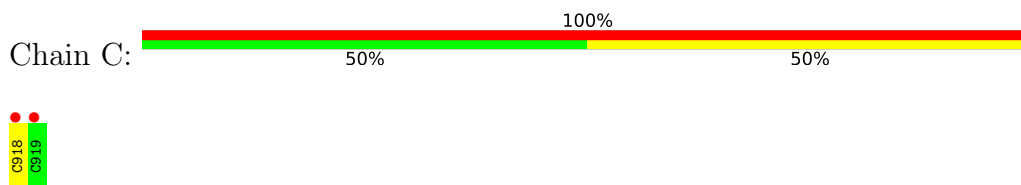
- Molecule 1: Genome polyprotein



- Molecule 2: 5'-R(\*GP\*GP\*C)-3'



- Molecule 3: 5'-R(P\*CP\*C)-3'



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.83Å 93.83Å 121.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.42 – 2.60 19.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.42-2.60) 98.8 (19.42-2.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 2.59Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.221 , 0.260 0.255 , 0.294	Depositor DCC
$R_{free}$ test set	868 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.6	Xtrriage
Anisotropy	0.119	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 28.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3853	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<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.

## 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: MG

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	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.42	0/3794	0.75	1/5146 (0.0%)
2	B	0.45	0/70	0.70	0/108
3	C	0.58	0/43	0.88	0/64
All	All	0.42	0/3907	0.75	1/5318 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	GLU	N-CA-C	-5.52	107.80	114.75

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	A	3704	0	3580	20	0
2	B	63	0	35	0	0
3	C	40	0	23	1	0
4	A	1	0	0	0	0
5	A	44	0	0	0	0
5	B	1	0	0	0	0
All	All	3853	0	3638	20	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 3.

All (20) 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)
1:A:189:ILE:HG23	1:A:301:SER:HB3	1.75	0.67
1:A:95:PRO:HG3	1:A:268:HIS:HB2	1.83	0.61
1:A:333:MET:HE3	1:A:340:ILE:HD13	1.85	0.58
1:A:333:MET:HE3	1:A:340:ILE:CD1	2.38	0.54
1:A:244:PHE:HA	1:A:362:GLN:HE22	1.73	0.53
1:A:321:ARG:HH11	1:A:356:HIS:CD2	2.28	0.51
1:A:53:ASP:HA	1:A:56:ILE:HG12	1.92	0.51
1:A:321:ARG:HH11	1:A:356:HIS:HD2	1.57	0.51
1:A:355:PRO:HA	1:A:358:LYS:HB2	1.95	0.47
1:A:258:GLU:O	1:A:262:ARG:HG2	2.15	0.47
1:A:147:LEU:HA	1:A:150:MET:HE3	1.97	0.46
1:A:473:LEU:C	1:A:475:HIS:H	2.25	0.45
1:A:112:GLU:HA	1:A:113:PRO:HD3	1.84	0.44
1:A:430:LEU:HD11	3:C:918:C:H4'	1.99	0.43
1:A:420:ILE:HD12	1:A:420:ILE:H	1.84	0.43
1:A:219:PRO:O	1:A:223:TRP:HB2	2.19	0.43
1:A:444:GLU:HB3	1:A:445:PRO:HD3	2.02	0.42
1:A:47:ASN:OD1	1:A:174:ARG:HG2	2.20	0.41
1:A:86:HIS:HE1	1:A:260:VAL:O	2.04	0.41
1:A:144:GLU:O	1:A:148:LYS:HG2	2.22	0.40

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
1	A	474/476 (100%)	458 (97%)	15 (3%)	1 (0%)	43 66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU

### 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
1	A	385/398 (97%)	380 (99%)	5 (1%)	61 82

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	124	GLN
1	A	223	TRP
1	A	384	THR
1	A	476	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	60	HIS
1	A	86	HIS
1	A	93	ASN
1	A	124	GLN
1	A	210	GLN
1	A	232	GLN
1	A	280	ASN
1	A	311	ASN
1	A	356	HIS
1	A	362	GLN
1	A	378	HIS
1	A	389	HIS
1	A	464	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	2/3 (66%)	0	0
3	C	1/2 (50%)	0	0
All	All	3/5 (60%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

### 6.1 Protein, DNA and RNA chains

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<sup>th</sup> 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	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	476/476 (100%)	0.40	16 (3%) 48 42	45, 52, 63, 67	0
2	B	3/3 (100%)	4.13	3 (100%) 0 0	84, 84, 84, 84	3 (100%)
3	C	2/2 (100%)	3.08	2 (100%) 0 0	75, 75, 75, 76	2 (100%)
All	All	481/481 (100%)	0.43	21 (4%) 39 33	45, 52, 63, 84	5 (1%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	906	G	5.5
1	A	10	GLU	4.2
2	B	908	C	3.9
1	A	16	MET	3.8
1	A	136	ASN	3.5
3	C	918	C	3.1
1	A	14	HIS	3.0
3	C	919	C	3.0
1	A	49	GLY	3.0
2	B	907	G	3.0
1	A	15	VAL	3.0
1	A	372	LYS	2.9
1	A	287	ASN	2.9
1	A	12	ARG	2.6
1	A	301	SER	2.5
1	A	122	ALA	2.4
1	A	48	GLU	2.3
1	A	369	LYS	2.3
1	A	5	ASP	2.3
1	A	53	ASP	2.2
1	A	11	GLU	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MG	A	1055	1/1	0.75	0.21	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.