



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:49 am GMT

PDB ID : 3KMQ  
Title : G62S mutant of foot-and-mouth disease virus RNA-polymerase in complex with a template- primer RNA, tetragonal structure  
Authors : Ferrer-Orta, C.; Verdaguer, N.; Perez-Luque, R.  
Deposited on : 2009-11-11  
Resolution : 2.11 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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

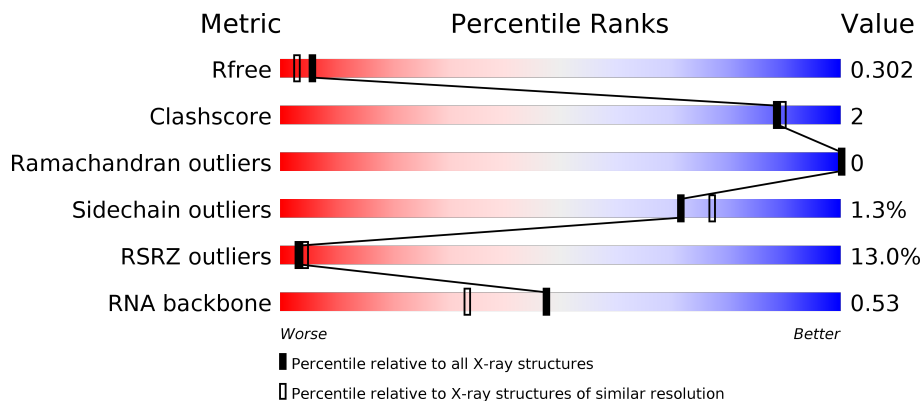
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	5449 (2.14-2.10)
Clashscore	122126	5972 (2.14-2.10)
Ramachandran outliers	120053	5914 (2.14-2.10)
Sidechain outliers	120020	5915 (2.14-2.10)
RSRZ outliers	108989	5321 (2.14-2.10)
RNA backbone	2636	1008 (2.64-1.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . 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 of chain
1	A	476	 12% 94% 5%
2	B	5	 40% 100% 40% 20%
3	C	5	 60% 80% 20%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4065 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 3D polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3758	2388	650	699	21			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	SER	GLY	ENGINEERED MUTATION	UNP Q9QCE3
A	471	ALA	-	EXPRESSION TAG	UNP Q9QCE3
A	472	ALA	-	EXPRESSION TAG	UNP Q9QCE3
A	473	LEU	-	EXPRESSION TAG	UNP Q9QCE3
A	474	GLU	-	EXPRESSION TAG	UNP Q9QCE3
A	475	HIS	-	EXPRESSION TAG	UNP Q9QCE3
A	476	HIS	-	EXPRESSION TAG	UNP Q9QCE3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	P	0	0	0
			109	48	21	35	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	P	0	0	0
			103	47	19	33	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		

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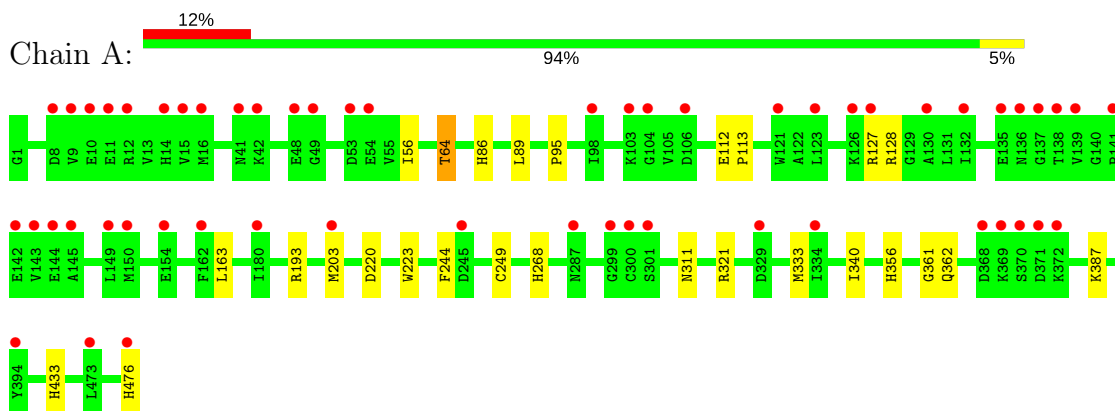
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		

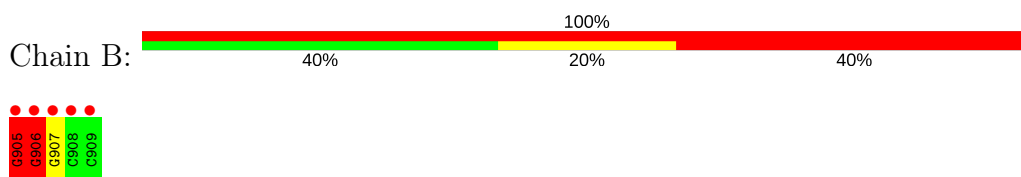
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

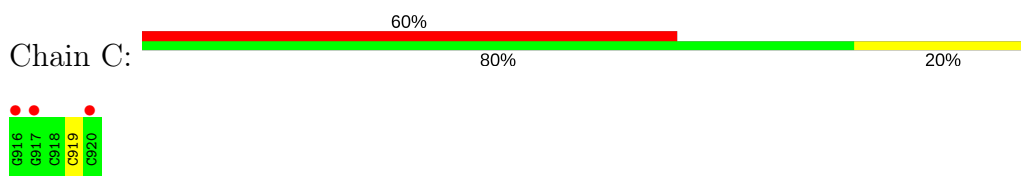
- Molecule 1: 3D polymerase



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.66Å 93.66Å 121.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.11 74.09 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.11) 98.8 (74.09-2.11)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.267 0.272 , 0.302	Depositor DCC
$R_{free}$ test set	1584 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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](#)

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	0.33	0/3849	0.44	0/5212
2	B	0.57	0/121	1.37	4/187 (2.1%)
3	C	0.62	0/114	1.02	0/176
All	All	0.35	0/4084	0.53	4/5575 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	906	G	O4'-C1'-N9	5.93	112.95	108.20
2	B	905	G	C3'-C2'-C1'	5.70	106.06	101.50
2	B	906	G	C4'-C3'-C2'	-5.62	96.98	102.60
2	B	906	G	C1'-O4'-C4'	-5.47	105.53	109.90

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	3758	0	3674	15	0
2	B	109	0	56	3	0
3	C	103	0	57	1	0
4	A	93	0	0	1	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4065	0	3787	16	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 2.

All (16) 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:193:ARG:NH1	2:B:906:G:OP2	2.33	0.60
1:A:95:PRO:HG3	1:A:268:HIS:HB2	1.85	0.59
1:A:387:LYS:HD3	3:C:919:C:H5''	1.89	0.53
1:A:220:ASP:OD1	1:A:433:HIS:HE1	1.93	0.51
1:A:244:PHE:HA	1:A:362:GLN:HE22	1.73	0.51
1:A:86:HIS:HD2	4:A:491:HOH:O	1.94	0.51
1:A:89:LEU:HD11	1:A:203:MET:HG3	1.94	0.49
1:A:321:ARG:HH11	1:A:356:HIS:HD2	1.62	0.46
1:A:112:GLU:HA	1:A:113:PRO:HD3	1.83	0.45
1:A:128:ARG:HH12	2:B:905:G:P	2.40	0.45
1:A:333:MET:HE1	1:A:340:ILE:HD13	2.01	0.42
1:A:64:THR:HG21	1:A:361:GLY:HA3	2.02	0.41
1:A:64:THR:HG23	1:A:249:CYS:HB3	2.02	0.41
1:A:56:ILE:HD11	1:A:163:LEU:HD21	2.03	0.41
1:A:333:MET:CE	1:A:340:ILE:HD13	2.51	0.40
2:B:906:G:H2'	2:B:907:G:C8	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	466 (98%)	8 (2%)	0	100	100



There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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	399/400 (100%)	394 (99%)	5 (1%)	71 77

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

Mol	Chain	Res	Type
1	A	64	THR
1	A	127	ARG
1	A	223	TRP
1	A	311	ASN
1	A	476	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	86	HIS
1	A	124	GLN
1	A	160	GLN
1	A	280	ASN
1	A	311	ASN
1	A	356	HIS
1	A	362	GLN
1	A	433	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	5/5 (100%)	1 (20%)	2 (40%)
3	C	4/5 (80%)	0	0
All	All	9/10 (90%)	1 (11%)	2 (22%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	906	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	905	G
2	B	906	G

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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%)	0.87	55 (11%) 4 6	36, 46, 59, 62	0
2	B	5/5 (100%)	4.96	5 (100%) 0 0	92, 93, 94, 94	5 (100%)
3	C	5/5 (100%)	2.64	3 (60%) 0 0	71, 72, 73, 73	5 (100%)
All	All	486/486 (100%)	0.93	63 (12%) 3 4	36, 46, 60, 94	10 (2%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	473	LEU	7.0
1	A	16	MET	6.9
1	A	136	ASN	6.3
1	A	15	VAL	6.3
1	A	301	SER	6.2
2	B	906	G	6.1
2	B	905	G	6.0
1	A	48	GLU	5.6
1	A	372	LYS	5.4
1	A	14	HIS	5.2
1	A	369	LYS	4.7
2	B	908	C	4.6
1	A	12	ARG	4.5
2	B	907	G	4.5
1	A	370	SER	4.4
3	C	916	G	4.4
1	A	10	GLU	4.3
1	A	476	HIS	4.1
1	A	149	LEU	3.7
1	A	139	VAL	3.5
2	B	909	C	3.5
1	A	11	GLU	3.3
1	A	53	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	127	ARG	3.2
1	A	9	VAL	3.2
1	A	126	LYS	3.1
1	A	287	ASN	3.1
1	A	130	ALA	3.0
3	C	920	C	3.0
1	A	144	GLU	3.0
1	A	132	ILE	3.0
1	A	137	GLY	2.9
1	A	138	THR	2.9
1	A	106	ASP	2.8
1	A	121	TRP	2.7
1	A	371	ASP	2.7
1	A	49	GLY	2.7
1	A	123	LEU	2.6
1	A	8	ASP	2.6
1	A	103	LYS	2.6
1	A	299	GLY	2.6
1	A	54	GLU	2.6
1	A	145	ALA	2.5
1	A	142	GLU	2.5
1	A	104	GLY	2.5
3	C	917	G	2.4
1	A	300	CYS	2.4
1	A	143	VAL	2.4
1	A	150	MET	2.3
1	A	180	ILE	2.3
1	A	245	ASP	2.2
1	A	203	MET	2.2
1	A	42	LYS	2.2
1	A	394	TYR	2.1
1	A	98	ILE	2.1
1	A	334	ILE	2.0
1	A	368	ASP	2.0
1	A	162	PHE	2.0
1	A	41	ASN	2.0
1	A	329	ASP	2.0
1	A	141	PRO	2.0
1	A	135	GLU	2.0
1	A	154	GLU	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.