



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:47 PM GMT

PDB ID : 3KMS
Title : G62S mutant of foot-and-mouth disease virus RNA-polymerase in complex with a template- primer RNA trigonal structure
Authors : Ferrer-Orta, C.; Verdaguer, N.; Perez-Luque, R.
Deposited on : 2009-11-11
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

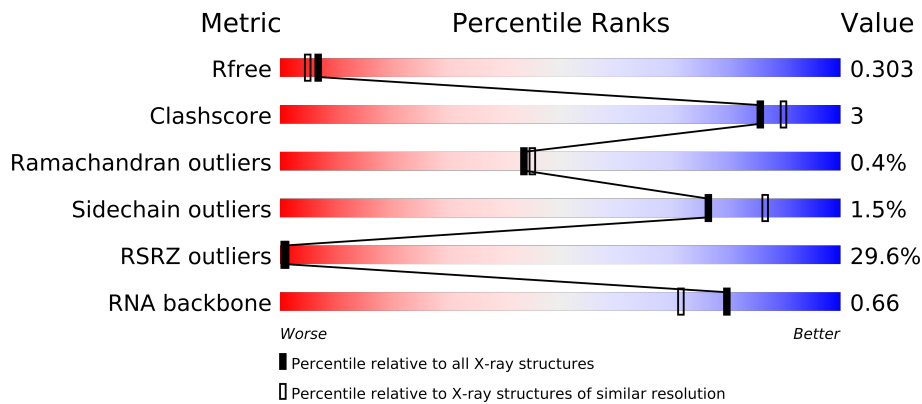
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)
RNA backbone	1838	1120 (3.00-1.40)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	476	
2	B	7	
3	C	5	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4051 atoms, of which 0 are hydrogen and 0 are deuterium.

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
			3731	2374	643	693	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(*AP*UP*GP*GP*GP*CP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	62	0	0
			148	67	28	47	6			

- 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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

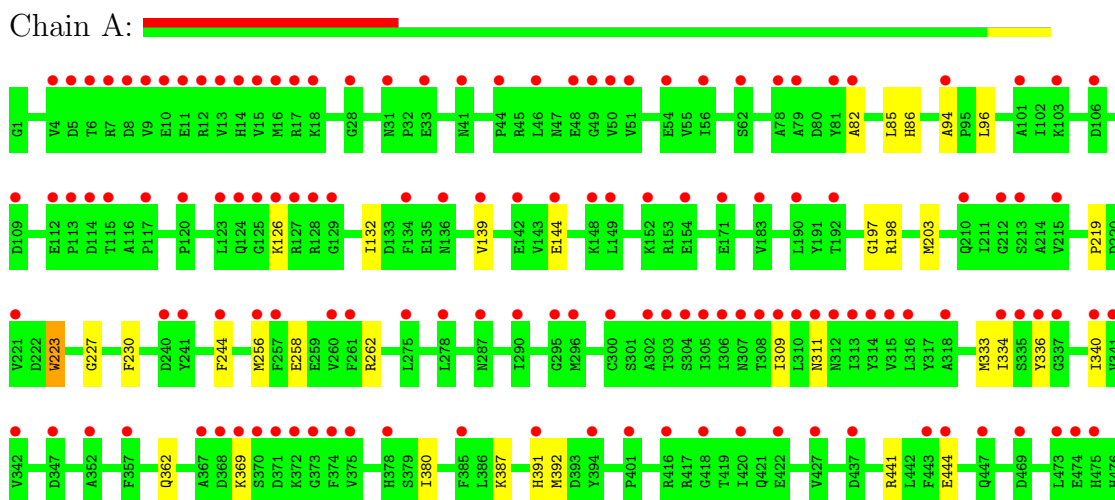
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	59	Total 59	O 59	0	0
5	B	5	Total 5	O 5	0	0
5	C	4	Total 4	O 4	0	0

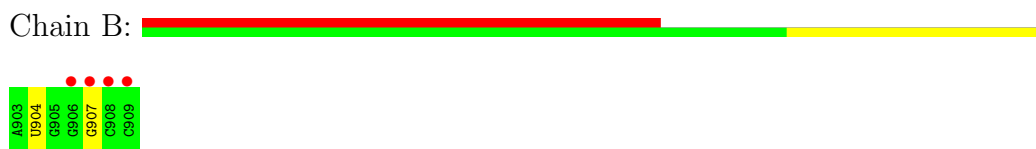
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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(*AP*UP*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 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.95Å 93.95Å 100.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.40 – 2.20 29.39 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.40-2.20) 99.0 (29.39-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.266 0.285 , 0.303	Depositor DCC
R_{free} test set	1318 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.7	EDS
Estimated twinning fraction	0.033 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 26076 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4051	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.33	0/3822	0.46	0/5180
2	B	0.59	0/165	1.00	0/256
3	C	0.60	0/114	0.97	0/176
All	All	0.35	0/4101	0.52	0/5612

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3731	0	3631	21	0
2	B	148	0	78	0	0
3	C	103	0	57	1	0
4	A	1	0	0	0	0
5	A	59	0	0	3	0
5	B	5	0	0	0	0
5	C	4	0	0	0	0
All	All	4051	0	3766	21	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:ALA:O	5:A:599:HOH:O	1.59	1.16
1:A:256:MET:HE2	1:A:309:ILE:HG21	1.49	0.94
1:A:230:PHE:HB2	1:A:380:ILE:HD12	1.49	0.92
1:A:387:LYS:HD3	3:C:919:C:H5"	1.77	0.67
1:A:94:ALA:O	1:A:198:ARG:HD2	2.03	0.58
1:A:227:GLY:HA2	1:A:380:ILE:HD13	1.86	0.57
1:A:256:MET:CE	1:A:309:ILE:HG21	2.30	0.56
1:A:441:ARG:O	1:A:444:GLU:HG2	2.08	0.53
1:A:256:MET:HE2	1:A:309:ILE:CG2	2.31	0.53
1:A:244:PHE:HA	1:A:362:GLN:HE22	1.73	0.53
1:A:85:LEU:HD11	1:A:203:MET:SD	2.52	0.49
1:A:132:ILE:HG12	1:A:139:VAL:HG12	1.96	0.47
1:A:86:HIS:HD2	5:A:525:HOH:O	1.98	0.47
1:A:230:PHE:CB	1:A:380:ILE:HD12	2.35	0.47
1:A:82:ALA:C	5:A:599:HOH:O	2.33	0.44
1:A:333:MET:CE	1:A:340:ILE:HD13	2.48	0.44
1:A:333:MET:HE1	1:A:340:ILE:HD13	1.99	0.43
1:A:96:LEU:HD22	1:A:197:GLY:HA3	2.00	0.42
1:A:258:GLU:O	1:A:262:ARG:HG2	2.19	0.42
1:A:219:PRO:O	1:A:223:TRP:HB2	2.19	0.42
1:A:139:VAL:HG23	1:A:144:GLU:HG3	2.03	0.41

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%)	461 (97%)	11 (2%)	2 (0%)	43 45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	369	LYS

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	393/400 (98%)	387 (98%)	6 (2%)	76 86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	TRP
1	A	311	ASN
1	A	334	ILE
1	A	336	TYR
1	A	391	HIS
1	A	392	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	160	GLN
1	A	280	ASN
1	A	311	ASN
1	A	322	HIS
1	A	356	HIS
1	A	362	GLN
1	A	447	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	6/7 (85%)	2 (33%)	0
3	C	4/5 (80%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	10/12 (83%)	2 (20%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	904	U
2	B	907	G

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	476/476 (100%)	1.47	135 (28%) 1 1	40, 49, 59, 63	0
2	B	4/7 (57%)	7.34	4 (100%) 0 0	81, 82, 82, 82	4 (100%)
3	C	5/5 (100%)	6.83	5 (100%) 0 0	74, 74, 75, 76	5 (100%)
All	All	485/488 (99%)	1.58	144 (29%) 1 1	40, 49, 60, 82	9 (1%)

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	916	G	12.7
2	B	909	C	11.0
2	B	907	G	10.1
1	A	10	GLU	6.6
3	C	920	C	6.6
1	A	370	SER	6.4
3	C	917	G	6.3
1	A	114	ASP	5.7
1	A	394	TYR	5.6
3	C	919	C	5.6
1	A	8	ASP	5.6
1	A	7	ARG	5.2
1	A	51	VAL	5.1
1	A	12	ARG	5.0
2	B	906	G	4.9
1	A	113	PRO	4.9
1	A	9	VAL	4.6
1	A	469	ASP	4.6
1	A	371	ASP	4.6
1	A	5	ASP	4.6
1	A	306	ILE	4.5
1	A	473	LEU	4.5
1	A	6	THR	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	369	LYS	4.4
1	A	309	ILE	4.1
1	A	17	ARG	4.1
1	A	149	LEU	4.1
1	A	15	VAL	3.9
1	A	313	ILE	3.9
1	A	310	LEU	3.9
1	A	372	LYS	3.8
1	A	305	ILE	3.8
1	A	125	GLY	3.8
1	A	303	THR	3.7
1	A	308	THR	3.7
1	A	287	ASN	3.6
1	A	475	HIS	3.6
1	A	49	GLY	3.6
1	A	373	GLY	3.5
1	A	28	GLY	3.5
1	A	447	GLN	3.5
1	A	378	HIS	3.4
2	B	908	C	3.4
1	A	109	ASP	3.4
1	A	302	ALA	3.4
1	A	18	LYS	3.4
1	A	129	GLY	3.3
1	A	340	ILE	3.3
1	A	46	LEU	3.2
1	A	128	ARG	3.2
1	A	134	PHE	3.2
1	A	81	TYR	3.2
1	A	48	GLU	3.2
1	A	16	MET	3.1
1	A	101	ALA	3.1
1	A	367	ALA	3.1
1	A	154	GLU	3.1
1	A	336	TYR	3.1
1	A	123	LEU	3.1
1	A	352	ALA	3.1
1	A	314	TYR	3.1
3	C	918	C	3.0
1	A	31	ASN	3.0
1	A	375	VAL	2.9
1	A	275	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	14	HIS	2.9
1	A	244	PHE	2.9
1	A	152	LYS	2.9
1	A	139	VAL	2.8
1	A	106	ASP	2.8
1	A	148	LYS	2.8
1	A	437	ASP	2.8
1	A	257	PHE	2.8
1	A	278	LEU	2.8
1	A	368	ASP	2.8
1	A	335	SER	2.7
1	A	307	ASN	2.7
1	A	385	PHE	2.7
1	A	126	LYS	2.7
1	A	82	ALA	2.7
1	A	416	ARG	2.7
1	A	347	ASP	2.6
1	A	171	GLU	2.6
1	A	11	GLU	2.6
1	A	115	THR	2.6
1	A	261	PHE	2.6
1	A	474	GLU	2.6
1	A	337	GLY	2.5
1	A	144	GLU	2.5
1	A	422	GLU	2.5
1	A	210	GLN	2.5
1	A	312	ASN	2.5
1	A	117	PRO	2.5
1	A	215	VAL	2.5
1	A	342	VAL	2.5
1	A	290	ILE	2.5
1	A	13	VAL	2.5
1	A	341	VAL	2.5
1	A	221	VAL	2.5
1	A	315	VAL	2.5
1	A	418	GLY	2.4
1	A	136	ASN	2.4
1	A	357	PHE	2.4
1	A	401	PRO	2.4
1	A	4	VAL	2.3
1	A	296	MET	2.3
1	A	212	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	112	GLU	2.3
1	A	311	ASN	2.3
1	A	54	GLU	2.3
1	A	190	LEU	2.3
1	A	213	SER	2.3
1	A	316	LEU	2.3
1	A	44	PRO	2.3
1	A	94	ALA	2.3
1	A	120	PRO	2.3
1	A	334	ILE	2.2
1	A	295	GLY	2.2
1	A	50	VAL	2.2
1	A	391	HIS	2.2
1	A	78	ALA	2.2
1	A	256	MET	2.2
1	A	142	GLU	2.2
1	A	124	GLN	2.2
1	A	192	THR	2.2
1	A	300	CYS	2.2
1	A	62	SER	2.2
1	A	241	TYR	2.2
1	A	103	LYS	2.2
1	A	183	VAL	2.2
1	A	33	GLU	2.1
1	A	318	ALA	2.1
1	A	304	SER	2.1
1	A	56	ILE	2.1
1	A	420	ILE	2.1
1	A	41	ASN	2.1
1	A	260	VAL	2.1
1	A	79	ALA	2.1
1	A	443	PHE	2.1
1	A	427	VAL	2.1
1	A	444	GLU	2.1
1	A	374	PHE	2.1
1	A	127	ARG	2.0
1	A	240	ASP	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MG	A	950	1/1	0.32	1.77	67,67,67,67	0

6.5 Other polymers

There are no such residues in this entry.