

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

#### Oct 11, 2021 - 08:00 PM EDT

PDB ID	:	2GGV
Title	:	Crystal structure of the West Nile virus NS2B-NS3 protease, His51Ala mutant
Authors	:	Aleshin, A.E.; Shiryaev, S.A.; Strongin, A.Y.; Liddington, R.C.
Deposited on		
Resolution	:	1.80  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 following versions of software and data (see references (1)) were used in the production of this report:

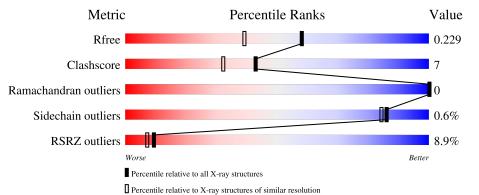
MolProbity Xtriage (Phenix) EDS	:	
		20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 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 1.80 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793(1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 of chain					
1	А	56	<u>9%</u> 59%	20%	21%			
2	В	185	8%		9% 9%			



#### $2 \mathrm{GGV}$

## 2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1738 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 non-structural protein 2B.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	44	Total 365	C 218	N 63	O 82	${ m S} { m 2}$	0	2	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	48	MET	-	cloning artifact	UNP Q203W3
А	94	GLY	-	SEE REMARK 999	UNP Q203W3
А	95	GLY	-	SEE REMARK 999	UNP Q203W3
А	96	GLY	-	SEE REMARK 999	UNP Q203W3
A	97	GLY	-	SEE REMARK 999	UNP Q203W3
A	98	SER	-	SEE REMARK 999	UNP Q203W3
А	99	GLY	-	SEE REMARK 999	UNP Q203W3
А	100	GLY	-	SEE REMARK 999	UNP Q203W3
А	101	GLY	-	SEE REMARK 999	UNP Q203W3
А	102	ARG	-	SEE REMARK 999	UNP Q203W3
А	103	ARG	-	SEE REMARK 999	UNP Q203W3

• Molecule 2 is a protein called non-structural protein 3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	169	Total 1283	C 810	N 220	0 246	S 7	0	1	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	51	ALA	HIS	engineered mutation	UNP Q203W3
В	84	GLN	LYS	conflict	UNP Q203W3
В	104	ARG	LYS	conflict	UNP Q203W3
В	179	LYS	-	cloning artifact	UNP Q203W3
В	180	GLY	-	cloning artifact	UNP Q203W3

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Chain	Residue	Modelled	Actual	Comment	Reference
В	181	HIS	-	expression tag	UNP Q203W3
В	182	HIS	-	expression tag	UNP Q203W3
В	183	HIS	-	expression tag	UNP Q203W3
В	184	HIS	-	expression tag	UNP Q203W3
В	185	HIS	-	expression tag	UNP Q203W3
В	186	HIS	-	expression tag	UNP Q203W3

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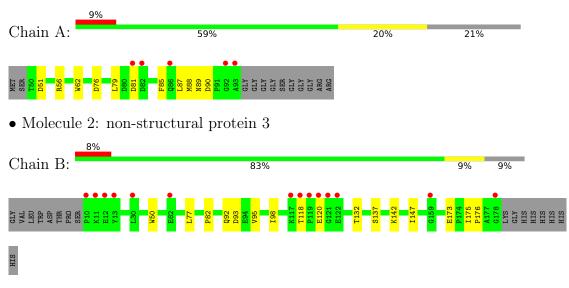
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	19	Total O 19 19	0	0
3	В	71	Total         O           71         71	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: non-structural protein 2B



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64	Depositor
Cell constants	56.74Å $56.74$ Å $103.72$ Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	49.15 - 1.80	Depositor
Resolution (A)	15.85 - 1.80	EDS
% Data completeness	98.4 (49.15-1.80)	Depositor
(in resolution range)	$98.6\ (15.85\text{-}1.80)$	EDS
R <sub>merge</sub>	0.06	Depositor
$R_{sym}$	0.06	Depositor
$< I/\sigma(I) > 1$	$2.18 (at 1.80 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.191 , $0.228$	Depositor
n, n <sub>free</sub>	0.191 , $0.229$	DCC
$R_{free}$ test set	906 reflections $(5.24\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	32.0	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.43, $58.1$	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
Estimated twinning fraction	0.073 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1738	wwPDB-VP
Average B, all atoms $(Å^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.91% 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)

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		lengths	Bond angles		
	Ullalli	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.57	0/370	0.71	0/501	
2	В	0.62	0/1313	0.69	0/1780	
All	All	0.61	0/1683	0.69	0/2281	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts (i)

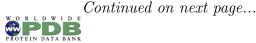
In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	365	0	321	11	0
2	В	1283	0	1259	12	0
3	А	19	0	0	0	0
3	В	71	0	0	2	0
All	All	1738	0	1580	22	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 7.

All (22) 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:56:ARG:HH11	1:A:88:MET:HE3	1.27	0.98	



A + 1	A + 0	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:A:56:ARG:NH1	1:A:88:MET:CE	2.36	0.88
1:A:56:ARG:HH11	1:A:88:MET:CE	1.90	0.85
1:A:56:ARG:HG2	1:A:88:MET:CE	2.14	0.77
1:A:76:ASP:H	1:A:89:ASN:HD21	1.38	0.71
1:A:56:ARG:NH1	1:A:88:MET:HE1	2.07	0.68
2:B:176:PRO:HD2	3:B:195:HOH:O	2.06	0.55
2:B:82:PRO:HG3	2:B:173:GLU:HB2	1.89	0.55
1:A:87:LEU:HD23	1:A:90:ASP:HB2	1.89	0.54
1:A:76:ASP:H	1:A:89:ASN:ND2	2.07	0.50
1:A:62:TRP:CD2	2:B:142:LYS:HA	2.48	0.49
1:A:81[B]:ASP:N	1:A:81[B]:ASP:OD1	2.47	0.46
2:B:82:PRO:CG	2:B:173:GLU:HB2	2.46	0.46
2:B:95:VAL:HG11	2:B:147:ILE:HD11	1.98	0.45
1:A:79:LEU:HD23	1:A:85:PHE:HA	1.99	0.45
2:B:132:THR:HG22	3:B:187:HOH:O	2.19	0.42
2:B:92:GLN:HG3	2:B:93:ASP:N	2.34	0.42
2:B:118:THR:HG22	2:B:120:GLU:H	1.85	0.42
2:B:175:ILE:HA	2:B:176:PRO:HD3	1.96	0.42
2:B:98:ILE:O	2:B:137:SER:HB3	2.20	0.41
2:B:95:VAL:HG11	2:B:147:ILE:CD1	2.51	0.40
2:B:50:TRP:CE3	2:B:77:LEU:HD13	2.56	0.40

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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	Perce	ntiles
1	А	44/56~(79%)	42 (96%)	2(4%)	0	100	100
2	В	168/185~(91%)	164 (98%)	4(2%)	0	100	100
All	All	212/241 (88%)	206 (97%)	6 (3%)	0	100	100



There are no Ramachandran outliers to report.

#### 5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	40/43~(93%)	39~(98%)	1 (2%)	47 34
2	В	135/148~(91%)	135 (100%)	0	100 100
All	All	175/191~(92%)	174 (99%)	1 (1%)	86 84

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	51	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	89	ASN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

## 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 monosaccharides 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 (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	< <b>RSRZ</b> >	#RSI	RZ>	$\cdot 2$	$OWAB(Å^2)$	Q < 0.9
1	А	44/56~(78%)	0.54	5 (11%)	5	3	26, 37, 50, 57	0
2	В	169/185~(91%)	0.41	14 (8%)	11	8	22, 33, 59, 74	0
All	All	213/241 (88%)	0.43	19 (8%)	9	7	22, 33, 57, 74	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	120	GLU	6.2
2	В	10	PRO	6.0
2	В	121	GLY	5.8
2	В	118	THR	5.7
2	В	119	PRO	5.4
2	В	117	LYS	5.3
1	А	93	ALA	3.9
2	В	30	LEU	3.9
2	В	122	GLU	3.7
2	В	11	LYS	3.7
1	А	81[A]	ASP	3.6
1	А	82	ASP	3.3
2	В	178	GLY	3.0
1	А	92	GLY	2.8
2	В	12	GLU	2.8
1	А	86	GLN	2.8
2	В	62	GLU	2.4
2	В	159	GLY	2.1
2	В	13	TYR	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 monosaccharides 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.

