



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2016 – 07:06 AM EDT

PDB ID : 5DA1  
Title : A Dimerization-Dependent Mechanism Drives PRRSV NSP11 Functions As a Beta Interferon Antagonist and Endoribonuclease  
Authors : Shi, Y.; Peng, G.  
Deposited on : 2015-08-19  
Resolution : 2.75 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

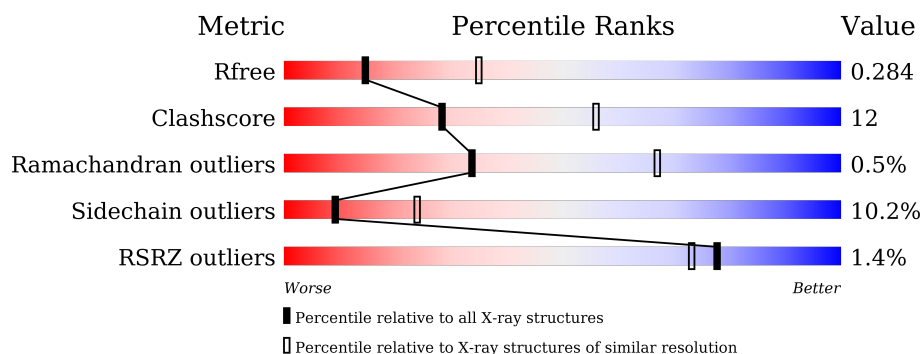
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	229	 69% 24% . .
1	B	229	 68% 19% . 10%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3400 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 endoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1750	1130	297	315	8			
1	B	205	Total	C	N	O	S	0	0	0
			1633	1058	277	290	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	224	HIS	-	expression tag	UNP E3V2B6
A	225	HIS	-	expression tag	UNP E3V2B6
A	226	HIS	-	expression tag	UNP E3V2B6
A	227	HIS	-	expression tag	UNP E3V2B6
A	228	HIS	-	expression tag	UNP E3V2B6
A	229	HIS	-	expression tag	UNP E3V2B6
B	224	HIS	-	expression tag	UNP E3V2B6
B	225	HIS	-	expression tag	UNP E3V2B6
B	226	HIS	-	expression tag	UNP E3V2B6
B	227	HIS	-	expression tag	UNP E3V2B6
B	228	HIS	-	expression tag	UNP E3V2B6
B	229	HIS	-	expression tag	UNP E3V2B6

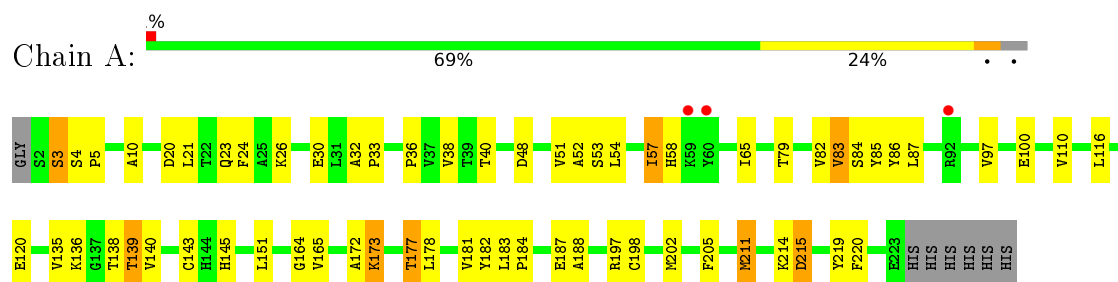
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	10	Total	O	0	0
			10	10		
2	B	7	Total	O	0	0
			7	7		

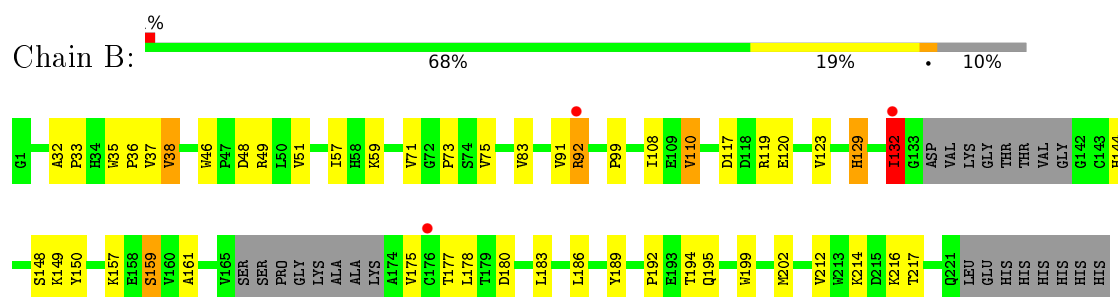
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: endoribonuclease



- Molecule 1: endoribonuclease



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.32Å 77.32Å 204.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.75 42.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-2.75) 100.0 (42.66-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.211 , 0.282 0.223 , 0.284	Depositor DCC
$R_{free}$ test set	854 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 20.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 16916 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	3400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.78	1/1801 (0.1%)	0.80	0/2455
1	B	0.79	0/1681	0.80	2/2290 (0.1%)
All	All	0.78	1/3482 (0.0%)	0.80	2/4745 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	CYS	CB-SG	-6.01	1.72	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASP	CB-CG-OD1	6.46	124.12	118.30
1	B	38	VAL	CB-CA-C	-5.74	100.50	111.40

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	1750	0	1744	56	0
1	B	1633	0	1620	24	0
2	A	10	0	0	0	0
2	B	7	0	0	0	0
All	All	3400	0	3364	78	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 12.

All (78) 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:140:VAL:HB	1:A:173:LYS:CE	1.76	1.16
1:A:140:VAL:CB	1:A:173:LYS:HE3	1.82	1.09
1:A:140:VAL:HB	1:A:173:LYS:HE3	0.97	0.96
1:B:159:SER:O	1:B:175:VAL:HG12	1.77	0.84
1:B:129:HIS:HB3	1:B:217:THR:HG22	1.59	0.82
1:A:172:ALA:N	1:A:173:LYS:NZ	2.36	0.74
1:A:135:VAL:HG12	1:A:140:VAL:HG22	1.70	0.74
1:A:172:ALA:C	1:A:173:LYS:NZ	2.41	0.73
1:A:172:ALA:C	1:A:173:LYS:HZ3	1.91	0.72
1:A:140:VAL:H	1:A:173:LYS:CE	2.03	0.71
1:A:172:ALA:N	1:A:173:LYS:HZ3	1.90	0.70
1:A:172:ALA:CA	1:A:173:LYS:NZ	2.56	0.69
1:A:173:LYS:N	1:A:173:LYS:HE2	2.08	0.69
1:A:172:ALA:O	1:A:173:LYS:HD3	1.96	0.64
1:A:140:VAL:H	1:A:173:LYS:NZ	2.00	0.60
1:B:110:VAL:O	1:B:110:VAL:HG13	2.01	0.60
1:A:172:ALA:C	1:A:173:LYS:CE	2.70	0.60
1:A:202:MET:HE3	1:A:205:PHE:HA	1.83	0.59
1:B:91:VAL:HG12	1:B:92:ARG:HG2	1.84	0.59
1:B:32:ALA:N	1:B:33:PRO:HD2	2.18	0.58
1:A:85:TYR:CE1	1:A:87:LEU:HD13	2.39	0.58
1:A:79:THR:OG1	1:A:82:VAL:HB	2.04	0.58
1:B:129:HIS:HB2	1:B:216:LYS:O	2.05	0.56
1:A:3:SER:HB2	1:A:54:LEU:HD21	1.87	0.56
1:A:140:VAL:CA	1:A:173:LYS:HE3	2.36	0.56
1:B:119:ARG:O	1:B:123:VAL:HG23	2.06	0.56
1:A:140:VAL:H	1:A:173:LYS:HZ2	1.52	0.55
1:A:172:ALA:CA	1:A:173:LYS:HZ1	2.19	0.55
1:A:172:ALA:CA	1:A:173:LYS:HZ3	2.17	0.54
1:A:57:ILE:O	1:A:58:HIS:HB2	2.08	0.52
1:B:36:PRO:HA	1:B:48:ASP:O	2.09	0.52
1:A:173:LYS:CE	1:A:173:LYS:N	2.73	0.52
1:A:85:TYR:HE1	1:A:87:LEU:HD13	1.76	0.51
1:A:140:VAL:N	1:A:173:LYS:HZ2	2.09	0.50
1:B:49:ARG:HG3	1:B:51:VAL:HG23	1.92	0.50
1:A:164:GLY:HA3	1:B:71:VAL:O	2.11	0.50
1:A:177:THR:HG21	1:A:220:PHE:O	2.12	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ALA:HB3	1:A:24:PHE:CE1	2.48	0.49
1:B:161:ALA:O	1:B:177:THR:HA	2.12	0.49
1:A:65:ILE:HA	1:A:83:VAL:HA	1.93	0.49
1:B:108:ILE:HG13	1:B:180:ASP:HB3	1.95	0.49
1:A:57:ILE:O	1:A:58:HIS:CB	2.61	0.48
1:A:140:VAL:HB	1:A:173:LYS:NZ	2.25	0.47
1:B:120:GLU:HG3	1:B:183:LEU:HB2	1.96	0.47
1:A:21:LEU:HD21	1:A:40:THR:HG23	1.96	0.47
1:A:5:PRO:HG3	1:A:87:LEU:HD11	1.96	0.47
1:B:192:PRO:HD2	1:B:214:LYS:HG3	1.95	0.47
1:A:145:HIS:CD2	1:A:183:LEU:HD21	2.50	0.47
1:A:20:ASP:OD1	1:A:20:ASP:N	2.47	0.46
1:B:194:THR:O	1:B:214:LYS:HE2	2.15	0.46
1:B:99:PRO:HB2	1:B:202:MET:HE2	1.96	0.45
1:A:181:VAL:HG12	1:A:182:TYR:N	2.29	0.45
1:A:211:MET:HG2	1:A:219:TYR:CE1	2.51	0.45
1:A:139:THR:HG22	1:A:173:LYS:HD2	1.99	0.45
1:B:159:SER:C	1:B:175:VAL:HG12	2.37	0.45
1:B:144:HIS:O	1:B:178:LEU:HA	2.18	0.44
1:A:32:ALA:N	1:A:33:PRO:CD	2.81	0.44
1:A:52:ALA:HA	1:A:86:TYR:O	2.18	0.44
1:B:35:TRP:CG	1:B:36:PRO:HD2	2.53	0.44
1:A:164:GLY:N	1:B:73:PRO:HD2	2.34	0.43
1:A:140:VAL:H	1:A:173:LYS:CD	2.32	0.43
1:A:120:GLU:HG3	1:A:183:LEU:HB2	2.01	0.43
1:B:189:TYR:HD1	1:B:199:TRP:CD2	2.36	0.43
1:A:214:LYS:HA	1:A:215:ASP:HA	1.73	0.42
1:B:132:ILE:HG21	1:B:150:TYR:HD2	1.84	0.42
1:A:183:LEU:N	1:A:184:PRO:CD	2.84	0.41
1:B:32:ALA:HB3	1:B:46:TRP:NE1	2.36	0.41
1:A:51:VAL:O	1:A:87:LEU:HA	2.21	0.41
1:A:23:GLN:HG2	1:A:24:PHE:CD2	2.56	0.41
1:A:140:VAL:CB	1:A:173:LYS:CE	2.66	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.84	0.40
1:A:30:GLU:HG2	1:A:30:GLU:H	1.70	0.40
1:A:110:VAL:O	1:A:110:VAL:HG13	2.22	0.40
1:A:172:ALA:N	1:A:173:LYS:HZ1	2.17	0.40
1:A:36:PRO:HA	1:A:48:ASP:O	2.21	0.40
1:B:189:TYR:O	1:B:212:VAL:HG21	2.22	0.40
1:A:172:ALA:H	1:A:173:LYS:HZ3	1.66	0.40
1:A:116:LEU:HA	1:A:116:LEU:HD23	1.81	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	220/229 (96%)	205 (93%)	14 (6%)	1 (0%)	34	67
1	B	199/229 (87%)	182 (92%)	16 (8%)	1 (0%)	34	67
All	All	419/458 (92%)	387 (92%)	30 (7%)	2 (0%)	34	67

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	ALA
1	B	132	ILE

### 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	192/198 (97%)	170 (88%)	22 (12%)	7	19
1	B	179/198 (90%)	163 (91%)	16 (9%)	12	31
All	All	371/396 (94%)	333 (90%)	38 (10%)	9	24

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	4	SER
1	A	26	LYS
1	A	38	VAL
1	A	53	SER
1	A	57	ILE
1	A	83	VAL
1	A	84	SER
1	A	97	VAL
1	A	100	GLU
1	A	136	LYS
1	A	138	THR
1	A	139	THR
1	A	143	CYS
1	A	165	VAL
1	A	173	LYS
1	A	177	THR
1	A	178	LEU
1	A	187	GLU
1	A	197	ARG
1	A	211	MET
1	A	215	ASP
1	B	37	VAL
1	B	38	VAL
1	B	57	ILE
1	B	59	LYS
1	B	75	VAL
1	B	83	VAL
1	B	92	ARG
1	B	110	VAL
1	B	129	HIS
1	B	132	ILE
1	B	148	SER
1	B	149	LYS
1	B	157	LYS
1	B	159	SER
1	B	186	LEU
1	B	195	GLN

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

Mol	Chain	Res	Type
1	B	34	HIS

### 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 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 [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<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	222/229 (96%)	0.18	3 (1%) 78 73	36, 54, 76, 85	0
1	B	205/229 (89%)	0.08	3 (1%) 76 72	37, 57, 76, 83	0
All	All	427/458 (93%)	0.13	6 (1%) 78 73	36, 55, 76, 85	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	ARG	3.0
1	B	92	ARG	2.3
1	B	176	CYS	2.3
1	A	60	TYR	2.2
1	B	132	ILE	2.1
1	A	59	LYS	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

There are no such residues in this entry.