



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 6JPW  
Title : Crystal structure of Zika NS2B-NS3 protease with compound 1C  
Authors : Quek, J.P.  
Deposited on : 2019-03-28  
Resolution : 1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 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) : 2.36

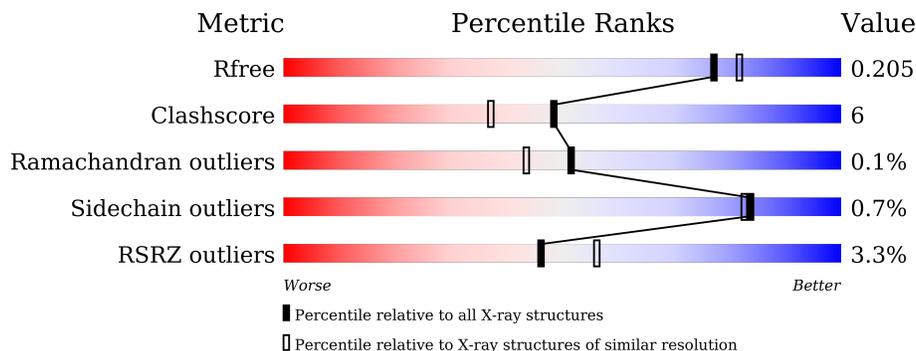
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	53	 4% 66% 6% 28%
1	C	53	 68% 28%
1	E	53	 2% 62% 9% 28%
1	G	53	 66% 6% 28%
2	B	178	 3% 75% 12% 13%
2	D	178	 3% 78% 11% 11%

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Mol	Chain	Length	Quality of chain
2	F	178	 <p>2% 78% 9% 13%</p>
2	H	178	 <p>3% 78% 9% 13%</p>
3	J	6	 <p>17% 33% 67%</p>
3	K	6	 <p>17% 33% 67%</p>
3	L	6	 <p>17% 50% 33% 17%</p>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6371 atoms, of which 171 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 Serine protease subunit NS2B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	38	284	176	46	61	1	0	0	0
1	C	38	284	176	46	61	1	0	0	0
1	E	38	284	176	46	61	1	0	0	0
1	G	38	284	176	46	61	1	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	MET	-	initiating methionine	UNP Q32ZE1
A	45	THR	-	expression tag	UNP Q32ZE1
C	44	MET	-	initiating methionine	UNP Q32ZE1
C	45	THR	-	expression tag	UNP Q32ZE1
E	44	MET	-	initiating methionine	UNP Q32ZE1
E	45	THR	-	expression tag	UNP Q32ZE1
G	44	MET	-	initiating methionine	UNP Q32ZE1
G	45	THR	-	expression tag	UNP Q32ZE1

- Molecule 2 is a protein called NS3 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	154	1134	721	195	213	5	0	2	0
2	D	159	1188	755	207	221	5	0	2	0
2	F	154	1131	718	195	213	5	0	2	0
2	H	154	1131	718	195	213	5	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP A0A142IX72
D	0	GLY	-	expression tag	UNP A0A142IX72
F	0	GLY	-	expression tag	UNP A0A142IX72
H	0	GLY	-	expression tag	UNP A0A142IX72

- Molecule 3 is a protein called SER-C0F-GLY-LYS-ARG-LYS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	J	6	Total 116	C 35	H 57	N 14	O 9	S 1	0	0	0
3	K	6	Total 116	C 35	H 57	N 14	O 9	S 1	0	0	0
3	L	6	Total 116	C 35	H 57	N 14	O 9	S 1	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	65	Total 65	O 65	0	0
4	C	21	Total 21	O 21	0	0
4	D	64	Total 64	O 64	0	0
4	E	11	Total 11	O 11	0	0
4	F	54	Total 54	O 54	0	0
4	G	15	Total 15	O 15	0	0
4	H	44	Total 44	O 44	0	0
4	J	3	Total 3	O 3	0	0
4	K	2	Total 2	O 2	0	0
4	L	6	Total 6	O 6	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: Serine protease subunit NS2B



- Molecule 1: Serine protease subunit NS2B



- Molecule 1: Serine protease subunit NS2B



- Molecule 1: Serine protease subunit NS2B



- Molecule 2: NS3 protease





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.11Å 60.47Å 215.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.26 – 1.95 46.26 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.4 (46.26-1.95) 99.4 (46.26-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.95Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.169 , 0.205 0.169 , 0.205	Depositor DCC
$R_{free}$ test set	1997 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.384	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.63% 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: C0F

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	0.35	0/288	0.58	0/392
1	C	0.34	0/288	0.59	0/392
1	E	0.31	0/288	0.52	0/392
1	G	0.30	0/288	0.59	0/392
2	B	0.40	0/1164	0.61	0/1585
2	D	0.42	0/1218	0.59	0/1653
2	F	0.36	0/1161	0.56	0/1581
2	H	0.35	0/1161	0.55	0/1581
3	J	2.88	3/38 (7.9%)	1.78	0/43
3	K	2.82	3/38 (7.9%)	1.57	0/43
3	L	2.93	3/38 (7.9%)	1.89	2/43 (4.7%)
All	All	0.54	9/5970 (0.2%)	0.61	2/8097 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	5	ARG	NE-CZ	9.98	1.46	1.33
3	J	5	ARG	CZ-NH1	9.97	1.46	1.33
3	K	5	ARG	CZ-NH1	9.62	1.45	1.33
3	L	5	ARG	CZ-NH1	9.19	1.45	1.33
3	K	5	ARG	NE-CZ	9.07	1.44	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	5	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	L	5	ARG	NE-CZ-NH1	6.04	123.32	120.30

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	284	0	254	2	0
1	C	284	0	254	2	0
1	E	284	0	254	7	0
1	G	284	0	254	7	0
2	B	1134	0	1114	17	0
2	D	1188	0	1193	17	0
2	F	1131	0	1105	13	0
2	H	1131	0	1105	12	0
3	J	59	57	49	2	0
3	K	59	57	49	1	0
3	L	59	57	49	2	0
4	A	18	0	0	0	0
4	B	65	0	0	7	0
4	C	21	0	0	0	0
4	D	64	0	0	3	0
4	E	11	0	0	3	0
4	F	54	0	0	2	0
4	G	15	0	0	1	0
4	H	44	0	0	1	0
4	J	3	0	0	0	0
4	K	2	0	0	0	0
4	L	6	0	0	1	0
All	All	6200	171	5680	69	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 6.

The worst 5 of 69 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)
2:B:143:CYS:SG	4:B:264:HOH:O	2.19	0.99
3:L:6:LYS:OXT	4:L:101:HOH:O	1.84	0.93
2:B:160:SER:OG	4:B:201:HOH:O	1.90	0.89
2:D:27:THR:HG22	2:D:34:THR:H	1.40	0.85
2:F:64:ARG:NH1	4:F:202:HOH:O	2.11	0.84

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	36/53 (68%)	36 (100%)	0	0	100	100
1	C	36/53 (68%)	35 (97%)	1 (3%)	0	100	100
1	E	36/53 (68%)	35 (97%)	1 (3%)	0	100	100
1	G	36/53 (68%)	35 (97%)	1 (3%)	0	100	100
2	B	154/178 (86%)	150 (97%)	4 (3%)	0	100	100
2	D	159/178 (89%)	157 (99%)	2 (1%)	0	100	100
2	F	154/178 (86%)	149 (97%)	5 (3%)	0	100	100
2	H	154/178 (86%)	151 (98%)	2 (1%)	1 (1%)	25	14
3	J	3/6 (50%)	3 (100%)	0	0	100	100
3	K	3/6 (50%)	3 (100%)	0	0	100	100
3	L	3/6 (50%)	3 (100%)	0	0	100	100
All	All	774/942 (82%)	757 (98%)	16 (2%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	61	GLY

### 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	29/45 (64%)	29 (100%)	0	100	100
1	C	29/45 (64%)	29 (100%)	0	100	100
1	E	29/45 (64%)	29 (100%)	0	100	100
1	G	29/45 (64%)	29 (100%)	0	100	100
2	B	115/140 (82%)	115 (100%)	0	100	100
2	D	123/140 (88%)	123 (100%)	0	100	100
2	F	114/140 (81%)	113 (99%)	1 (1%)	78	77
2	H	114/140 (81%)	113 (99%)	1 (1%)	78	77
3	J	4/4 (100%)	4 (100%)	0	100	100
3	K	4/4 (100%)	3 (75%)	1 (25%)	0	0
3	L	4/4 (100%)	3 (75%)	1 (25%)	0	0
All	All	594/752 (79%)	590 (99%)	4 (1%)	84	82

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	140	LEU
2	H	19	THR
3	K	4	LYS
3	L	1	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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<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	38/53 (71%)	0.17	2 (5%) 26 35	23, 35, 55, 65	0
1	C	38/53 (71%)	0.17	0 100 100	24, 36, 53, 63	0
1	E	38/53 (71%)	0.40	1 (2%) 56 65	33, 50, 72, 76	0
1	G	38/53 (71%)	0.20	0 100 100	31, 41, 57, 71	0
2	B	154/178 (86%)	0.12	5 (3%) 47 57	16, 26, 59, 73	0
2	D	159/178 (89%)	0.24	5 (3%) 49 58	16, 27, 63, 89	0
2	F	154/178 (86%)	0.22	4 (2%) 56 65	21, 37, 62, 82	0
2	H	154/178 (86%)	0.14	6 (3%) 39 49	21, 33, 69, 93	0
3	J	5/6 (83%)	1.82	1 (20%) 1 1	31, 34, 44, 101	0
3	K	5/6 (83%)	1.83	1 (20%) 1 1	41, 45, 55, 98	0
3	L	5/6 (83%)	2.21	1 (20%) 1 1	37, 38, 43, 104	0
All	All	788/942 (83%)	0.22	26 (3%) 46 56	16, 33, 65, 104	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1	SER	8.1
3	L	1	SER	7.6
2	D	12	GLU	7.6
3	K	1	SER	7.5
2	F	170	ARG	6.5

### 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.