



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:12 am GMT

PDB ID : 5GXJ
Title : Zika Virus NS2B-NS3 protease
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Deposited on : 2016-09-18
Resolution : 2.60 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 ⓘ symbol.

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

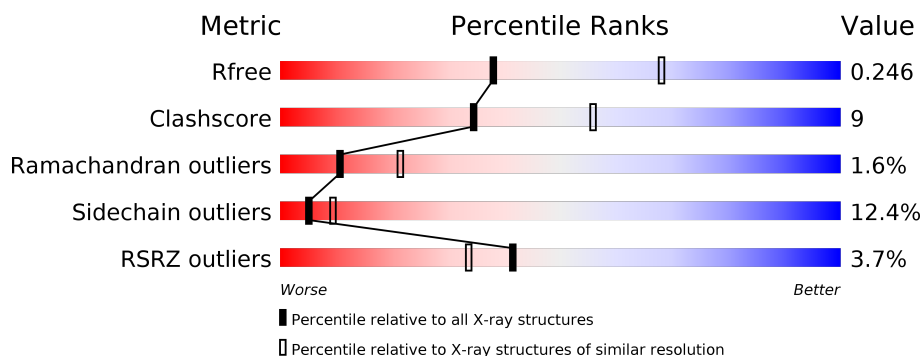
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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 ≥ 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	224	
1	B	224	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2459 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 FLAVIVIRUS_NS2B,LINKER,Peptidase S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1223	771	214	232	6			
1	B	162	Total	C	N	O	S	0	0	0
			1236	779	216	235	6			

i

- Molecule 1: FLAVIVIRUS NS2B,LINKER,Peptidase S7



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	55.21Å 55.21Å 250.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.04 – 2.60 46.03 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.04-2.60) 99.9 (46.03-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.224 , 0.273 0.227 , 0.246	Depositor DCC
R_{free} test set	636 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2459	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.02	0/1249	1.13	6/1694 (0.4%)
1	B	0.87	0/1262	1.02	2/1712 (0.1%)
All	All	0.95	0/2511	1.08	8/3406 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1071	ASP	CB-CG-OD2	9.14	126.53	118.30
1	A	1072	VAL	CG1-CB-CG2	-6.25	100.91	110.90
1	B	1029	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	1145	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	A	1129	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	1145	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	1022	VAL	CB-CA-C	-5.41	101.11	111.40
1	A	1145	ARG	NE-CZ-NH2	5.41	123.00	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	1223	0	1201	17	0
1	B	1236	0	1215	29	0
All	All	2459	0	2416	44	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 9.

All (44) 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:1028:ARG:HH12	1:A:1059:ARG:HH12	1.15	0.91
1:B:1124:GLY:O	1:B:1154:VAL:HG22	1.81	0.79
1:B:1024:ARG:NH2	1:B:1104:GLU:O	2.16	0.77
1:A:1024:ARG:NH2	1:A:1104:GLU:O	2.19	0.76
1:B:1123:ILE:HD13	1:B:1153:GLY:HA3	1.68	0.73
1:B:1107:ARG:HD2	1:B:1107:ARG:N	2.03	0.73
1:A:1028:ARG:HH12	1:A:1059:ARG:NH1	1.86	0.73
1:B:62:GLU:H	1:B:1096:GLN:HE22	1.43	0.67
1:A:1028:ARG:NH1	1:A:1059:ARG:HH12	1.92	0.63
1:B:1152:ASN:OD1	1:B:1153:GLY:N	2.33	0.61
1:B:61:TRP:CE3	1:B:1142:LYS:HA	2.36	0.61
1:B:1104:GLU:OE2	1:B:1107:ARG:NH2	2.33	0.60
1:A:62:GLU:H	1:A:1096:GLN:HE22	1.50	0.60
1:A:1028:ARG:NH1	1:A:1059:ARG:NH1	2.50	0.59
1:B:1123:ILE:HD13	1:B:1153:GLY:CA	2.33	0.58
1:A:1030:LEU:HD11	1:B:1118:THR:HG23	1.85	0.57
1:B:1071:ASP:CG	1:B:1074:GLN:HG3	2.25	0.57
1:B:1049:MET:HE1	1:B:1152:ASN:HB2	1.88	0.56
1:B:1035:GLN:HB3	1:B:1102:PRO:HB3	1.88	0.56
1:B:1097:LEU:HD22	1:B:1099:ALA:HB2	1.89	0.55
1:B:61:TRP:CH2	1:B:1142:LYS:HG3	2.42	0.55
1:B:1071:ASP:OD2	1:B:1074:GLN:HG3	2.06	0.55
1:B:1105:ARG:O	1:B:1107:ARG:NE	2.27	0.53
1:B:1122:ASP:OD2	1:B:1122:ASP:N	2.42	0.52
1:B:1049:MET:CE	1:B:1152:ASN:HB2	2.40	0.51
1:B:1124:GLY:C	1:B:1154:VAL:HG22	2.30	0.51
1:A:1097:LEU:HD12	1:A:1126:VAL:HG11	1.93	0.50
1:A:1122:ASP:N	1:A:1122:ASP:OD2	2.45	0.50
1:A:1031:LEU:H	1:A:1031:LEU:HD12	1.77	0.48
1:A:1097:LEU:HD22	1:A:1099:ALA:HB2	1.96	0.48
1:B:1097:LEU:HD12	1:B:1126:VAL:HG11	1.96	0.48
1:B:1033:SER:O	1:B:1034:THR:HG23	2.13	0.48
1:A:1130:TYR:O	1:B:1034:THR:HG21	2.17	0.45
1:B:1107:ARG:N	1:B:1107:ARG:CD	2.73	0.44
1:A:1035:GLN:HB3	1:A:1102:PRO:HB3	1.97	0.44
1:B:1154:VAL:HG23	1:B:1154:VAL:O	2.18	0.44
1:B:1064:ARG:O	1:B:1065:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:LEU:HB3	1:A:1138:PRO:HG2	2.00	0.43
1:A:61:TRP:CD1	1:A:62:GLU:N	2.87	0.43
1:B:1043:GLU:HB2	1:B:1084:LYS:HD2	2.01	0.43
1:A:1093:SER:OG	1:A:1142:LYS:NZ	2.49	0.41
1:B:1104:GLU:HB3	1:B:1107:ARG:HH21	1.86	0.41
1:B:61:TRP:CD1	1:B:62:GLU:N	2.89	0.41
1:A:1093:SER:CB	1:A:1142:LYS:HZ1	2.34	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	156/224 (70%)	147 (94%)	6 (4%)	3 (2%)	9	17
1	B	158/224 (70%)	147 (93%)	9 (6%)	2 (1%)	13	27
All	All	314/448 (70%)	294 (94%)	15 (5%)	5 (2%)	11	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1031	LEU
1	B	1030	LEU
1	B	1121	GLY
1	A	1121	GLY
1	A	1144	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	128/173 (74%)	111 (87%)	17 (13%)	4	7
1	B	130/173 (75%)	115 (88%)	15 (12%)	6	11
All	All	258/346 (75%)	226 (88%)	32 (12%)	5	9

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	68	THR
1	A	1018	THR
1	A	1019	THR
1	A	1022	VAL
1	A	1031	LEU
1	A	1059	ARG
1	A	1064	ARG
1	A	1073	LYS
1	A	1107	ARG
1	A	1111	THR
1	A	1118	THR
1	A	1120	ASP
1	A	1122	ASP
1	A	1137	SER
1	A	1142	LYS
1	A	1157	LYS
1	B	54	GLU
1	B	63	LYS
1	B	68	THR
1	B	1018	THR
1	B	1019	THR
1	B	1022	VAL
1	B	1059	ARG
1	B	1064	ARG
1	B	1107	ARG
1	B	1111	THR
1	B	1118	THR
1	B	1120	ASP
1	B	1122	ASP
1	B	1142	LYS
1	B	1157	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1096	GLN
1	B	1096	GLN

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, 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	160/224 (71%)	0.00	1 (0%) 89 88	62, 89, 139, 155	0
1	B	162/224 (72%)	0.29	11 (6%) 17 12	74, 106, 181, 207	0
All	All	322/448 (71%)	0.15	12 (3%) 41 33	62, 98, 149, 207	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	GLU	7.0
1	B	1158	ASN	4.4
1	B	1157	LYS	4.4
1	B	1117	LYS	3.2
1	B	67	VAL	3.1
1	A	1158	ASN	3.0
1	B	1128	LEU	3.0
1	B	1129	ASP	2.6
1	B	1073	LYS	2.5
1	B	68	THR	2.4
1	B	1156	ILE	2.4
1	B	1121	GLY	2.3

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.