



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2017 – 08:20 PM EDT

PDB ID : 4M9F
Title : Dengue virus NS2B-NS3 protease A125C variant at pH 8.5
Authors : Yildiz, M.; Ghosh, S.; Bell, J.A.; Sherman, W.; Hardy, J.A.
Deposited on : unknown
Resolution : 2.70 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

<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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

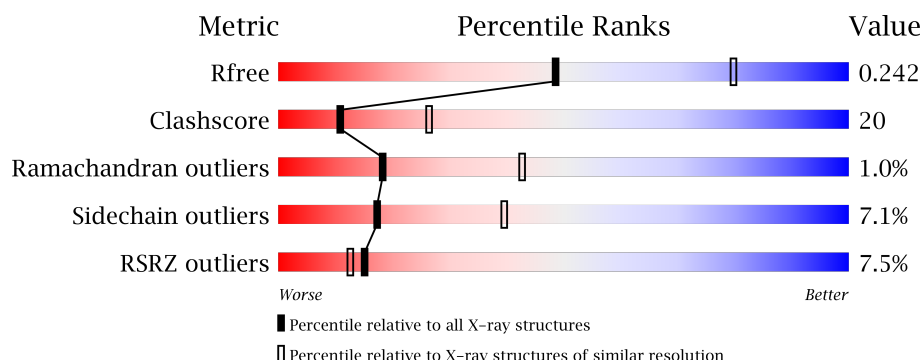
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.70 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}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	247	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1626 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 NS2B-NS3 protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	14	0
			1590	1011	274	300	5			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	GLY	-	EXPRESSION TAG	UNP Q91H74
A	44	SER	-	EXPRESSION TAG	UNP Q91H74
A	45	HIS	-	EXPRESSION TAG	UNP Q91H74
A	46	MET	-	EXPRESSION TAG	UNP Q91H74
A	47	LEU	-	EXPRESSION TAG	UNP Q91H74
A	48	GLU	-	EXPRESSION TAG	UNP Q91H74
A	96	GLY	-	LINKER	UNP Q91H74
A	993	GLY	-	LINKER	UNP Q91H74
A	994	GLY	-	LINKER	UNP Q91H74
A	995	GLY	-	LINKER	UNP Q91H74
A	996	SER	-	LINKER	UNP Q91H74
A	997	GLY	-	LINKER	UNP Q91H74
A	998	GLY	-	LINKER	UNP Q91H74
A	999	GLY	-	LINKER	UNP Q91H74
A	1000	GLY	-	LINKER	UNP Q91H74
A	1125	CYS	ALA	ENGINEERED MUTATION	UNP Q91H74
A	1167	ASN	GLN	CONFLICT	UNP Q91H74

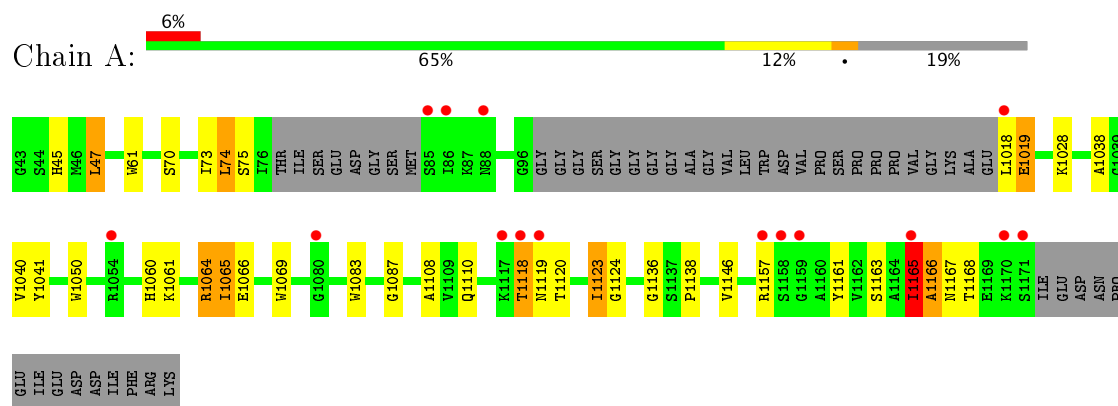
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	36	Total	O	0	0
			36	36		

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 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: NS2B-NS3 protease



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	59.63Å 62.16Å 115.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 21.52 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.70) 98.6 (21.52-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.38 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.227 , 0.244 0.224 , 0.242	Depositor DCC
R_{free} test set	300 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.059 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1626	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.89% 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	0.75	4/1658 (0.2%)	0.81	1/2234 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1083	TRP	CD2-CE2	5.50	1.48	1.41
1	A	1069	TRP	CD2-CE2	5.40	1.47	1.41
1	A	61	TRP	CD2-CE2	5.26	1.47	1.41
1	A	1050	TRP	CD2-CE2	5.11	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1165	ILE	CG1-CB-CG2	-5.48	99.34	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1118	THR	Peptide
1	A	1166	ALA	Peptide

5.2 Too-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 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	1590	0	1614	65	0
2	A	36	0	0	19	0
All	All	1626	0	1614	65	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 20.

All (65) 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:1018[A]:LEU:HB2	1:A:1041[A]:TYR:CE2	1.81	1.15
1:A:1118:THR:HB	1:A:1119:ASN:HB3	1.19	1.15
1:A:1018[B]:LEU:HD22	2:A:1233:HOH:O	1.54	1.04
1:A:1018[B]:LEU:CD2	2:A:1233:HOH:O	2.04	1.02
1:A:1018[A]:LEU:O	1:A:1041[A]:TYR:CZ	2.16	0.99
1:A:1166:ALA:CB	2:A:1228:HOH:O	2.11	0.98
1:A:1166:ALA:C	1:A:1168:THR:H	1.66	0.97
1:A:1018[A]:LEU:CB	1:A:1041[A]:TYR:CE2	2.46	0.97
1:A:74:LEU:HB2	2:A:1231:HOH:O	1.63	0.96
1:A:1118:THR:CB	1:A:1119:ASN:HB3	1.97	0.93
1:A:1166:ALA:HB1	2:A:1228:HOH:O	1.67	0.92
1:A:1166:ALA:H	1:A:1168:THR:HG22	1.35	0.89
1:A:47:LEU:CD1	2:A:1229:HOH:O	2.21	0.89
1:A:1157[B]:ARG:HG2	2:A:1230:HOH:O	1.71	0.89
1:A:1166:ALA:N	1:A:1168:THR:HG22	1.93	0.82
1:A:1028:LYS:HD3	2:A:1225:HOH:O	1.81	0.79
1:A:1157[B]:ARG:HD2	1:A:1157[B]:ARG:H	1.47	0.78
1:A:1018[A]:LEU:HB2	1:A:1041[A]:TYR:HE2	1.49	0.76
1:A:1018[A]:LEU:HG	1:A:1060:HIS:ND1	1.99	0.76
1:A:1018[A]:LEU:O	1:A:1041[A]:TYR:OH	2.08	0.72
1:A:1040:VAL:HG21	1:A:1138:PRO:HB3	1.70	0.72
1:A:1166:ALA:HB2	2:A:1218:HOH:O	1.88	0.72
1:A:1166:ALA:CB	2:A:1218:HOH:O	2.40	0.70
1:A:1166:ALA:C	1:A:1168:THR:N	2.38	0.69
1:A:47:LEU:HD11	2:A:1229:HOH:O	1.90	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1018[A]:LEU:HB3	1:A:1041[A]:TYR:CE2	2.30	0.65
1:A:74:LEU:CB	2:A:1231:HOH:O	2.32	0.65
1:A:1018[A]:LEU:HB3	1:A:1041[A]:TYR:CD2	2.34	0.63
1:A:1124:GLY:H	1:A:1168:THR:CG2	2.12	0.62
1:A:1018[A]:LEU:O	1:A:1041[A]:TYR:CE1	2.53	0.61
1:A:1064:ARG:HG2	1:A:1064:ARG:HH11	1.65	0.61
1:A:1064:ARG:HG2	1:A:1064:ARG:NH1	2.15	0.61
1:A:1118:THR:HB	1:A:1119:ASN:CB	2.13	0.61
1:A:1118:THR:CA	1:A:1119:ASN:HB3	2.30	0.60
1:A:1118:THR:HG23	1:A:1123:ILE:HD12	1.83	0.60
1:A:1064:ARG:HD2	2:A:1213:HOH:O	2.02	0.58
1:A:1165:ILE:O	1:A:1166:ALA:HB3	2.05	0.56
1:A:1124:GLY:H	1:A:1168:THR:HG23	1.70	0.55
1:A:45:HIS:HD2	2:A:1219:HOH:O	1.89	0.54
1:A:1018[B]:LEU:O	1:A:1019:GLU:HB3	2.07	0.54
1:A:1064:ARG:CD	2:A:1213:HOH:O	2.55	0.54
1:A:1038:ALA:O	1:A:1136:GLY:HA3	2.07	0.54
1:A:47:LEU:HD13	2:A:1229:HOH:O	1.98	0.54
1:A:1166:ALA:HA	2:A:1228:HOH:O	2.08	0.53
1:A:1040:VAL:CG2	1:A:1138:PRO:HB3	2.40	0.52
1:A:1166:ALA:H	1:A:1168:THR:CG2	2.17	0.49
1:A:1064:ARG:CG	1:A:1064:ARG:HH11	2.26	0.49
1:A:45:HIS:CD2	2:A:1219:HOH:O	2.64	0.48
1:A:1166:ALA:CA	2:A:1228:HOH:O	2.54	0.48
1:A:1087:GLY:HA3	1:A:1146:VAL:C	2.34	0.47
1:A:1018[A]:LEU:N	1:A:1018[A]:LEU:HD12	2.30	0.47
1:A:1166:ALA:O	1:A:1168:THR:N	2.40	0.46
1:A:1018[A]:LEU:HD21	1:A:1065:ILE:HD11	1.98	0.45
1:A:1124:GLY:O	1:A:1165:ILE:HG12	2.17	0.45
1:A:1019:GLU:HA	1:A:1041[A]:TYR:CE1	2.52	0.45
1:A:73:ILE:HD11	1:A:1108:ALA:HB2	1.99	0.45
1:A:1157[B]:ARG:H	1:A:1157[B]:ARG:CD	2.25	0.44
1:A:1018[B]:LEU:HD23	1:A:1018[B]:LEU:N	2.33	0.43
1:A:1018[A]:LEU:HB2	1:A:1041[A]:TYR:CZ	2.43	0.43
1:A:1060:HIS:NE2	1:A:1061:LYS:HE2	2.33	0.43
1:A:1118:THR:CG2	1:A:1123:ILE:HD12	2.47	0.43
1:A:70:SER:HA	1:A:1108:ALA:O	2.19	0.43
1:A:1165:ILE:O	1:A:1166:ALA:CB	2.68	0.42
1:A:1123:ILE:H	1:A:1123:ILE:HD13	1.86	0.41
1:A:1064:ARG:NH2	1:A:1066:GLU:OE2	2.54	0.41

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	208/247 (84%)	200 (96%)	6 (3%)	2 (1%)	18	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1167	ASN
1	A	1019	GLU

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	170/195 (87%)	158 (93%)	12 (7%)	17	39

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	74	LEU
1	A	75[A]	SER
1	A	75[B]	SER
1	A	1064	ARG
1	A	1065	ILE
1	A	1110	GLN
1	A	1120	THR
1	A	1123	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1161	TYR
1	A	1163	SER
1	A	1165	ILE

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	45	HIS
1	A	64	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	200/247 (80%)	0.24	15 (7%) 15 12	14, 27, 53, 72	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1157[A]	ARG	4.0
1	A	1018[A]	LEU	3.8
1	A	1171	SER	3.7
1	A	86	ILE	3.4
1	A	1119	ASN	3.3
1	A	1080[A]	GLY	2.9
1	A	1117	LYS	2.6
1	A	85	SER	2.6
1	A	1054[A]	ARG	2.6
1	A	1170	LYS	2.3
1	A	1159	GLY	2.3
1	A	1165	ILE	2.3
1	A	1118	THR	2.2
1	A	88	ASN	2.1
1	A	1158	SER	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 [i](#)

There are no such residues in this entry.