W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2023 – 10:35 PM JST

PDB ID	:	5YF8
Title	:	Crystals structure of Classical swine fever virus NS5B (residues 1-672, Y471A-E472A mutant)
Authors	:	Liu, W.; Gong, P.
Deposited on	:	2017-09-20
Resolution	:	3.40 Å(reported)

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

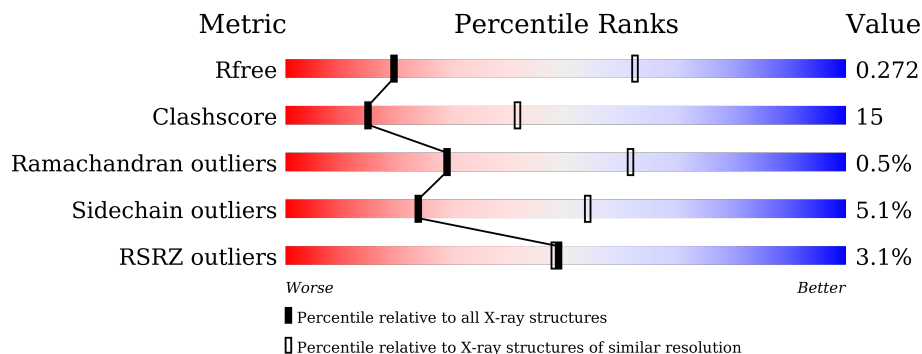|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.40 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		15
Ramachandran outliers		0.5%
Sidechain outliers		5.1%
RSRZ outliers		3.1%

Worse — Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	A	683	3% — 61% — 32% — • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	701	-	-	-	X
2	ACT	A	702	-	-	-	X

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WORLDWIDE PDB
PROTEIN DATA BANK

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	705	-	-	-	X
2	ACT	A	707	-	-	-	X

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4876 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 RdRp catalytic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	645	Total 4839	C 3081	N 825	O 909	S 24	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q5U8X5
A	471	ALA	TYR	engineered mutation	UNP Q5U8X5
A	472	ALA	GLU	engineered mutation	UNP Q5U8X5
A	673	GLY	-	expression tag	UNP Q5U8X5
A	674	SER	-	expression tag	UNP Q5U8X5
A	675	SER	-	expression tag	UNP Q5U8X5
A	676	SER	-	expression tag	UNP Q5U8X5
A	677	HIS	-	expression tag	UNP Q5U8X5
A	678	HIS	-	expression tag	UNP Q5U8X5
A	679	HIS	-	expression tag	UNP Q5U8X5
A	680	HIS	-	expression tag	UNP Q5U8X5
A	681	HIS	-	expression tag	UNP Q5U8X5
A	682	HIS	-	expression tag	UNP Q5U8X5

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

ACT

OXT

O⁻

C

CH3

O

O

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	9	Total 9	O 9	0	0

3 Residue-property plots ⓘ

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: RdRp catalytic
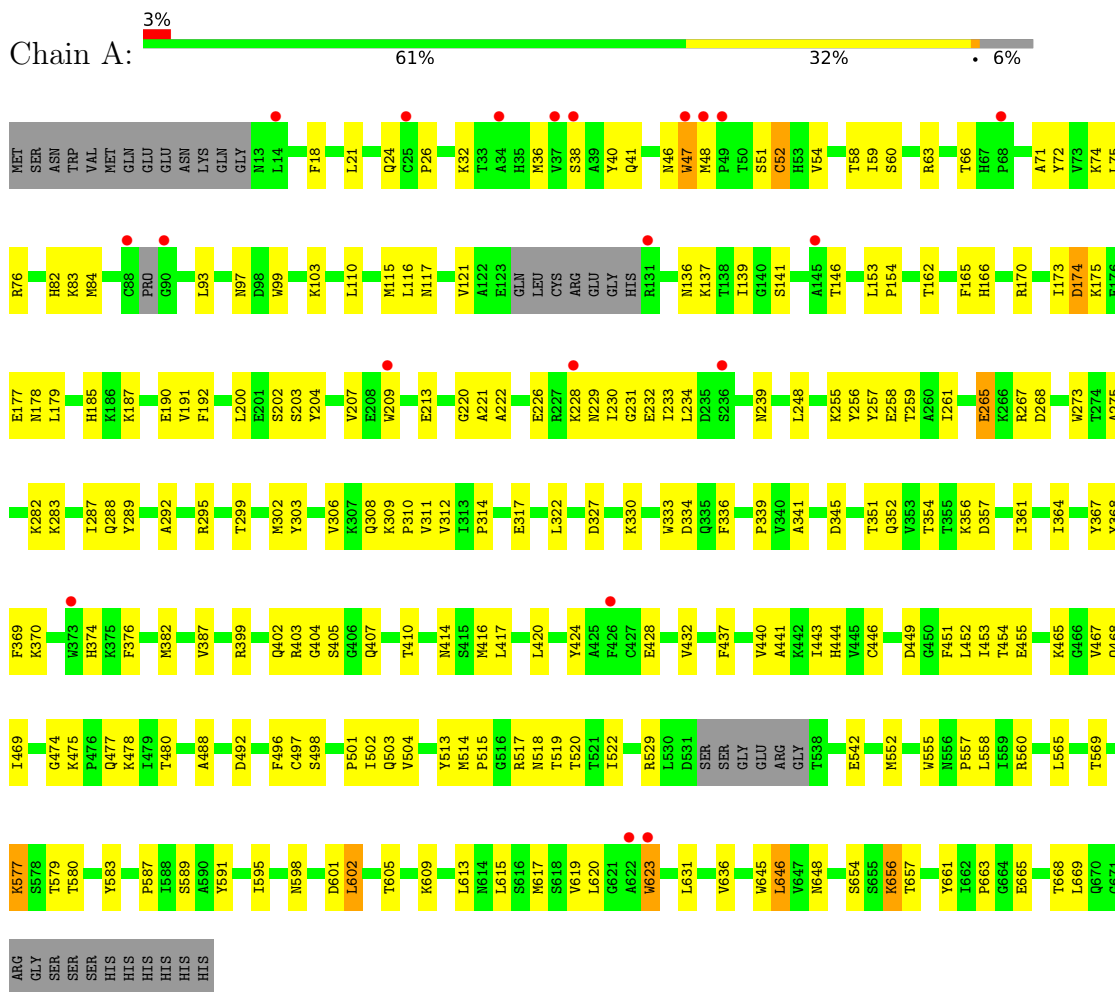
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	115.78Å 115.78Å 393.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.91 – 3.40	Depositor
	49.91 – 3.40	EDS
% Data completeness	98.1 (49.91-3.40)	Depositor
(in resolution range)	98.7 (49.91-3.40)	EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.24 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.230 , 0.271	Depositor
	0.230 , 0.272	DCC
R_{free} test set	956 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	67.4	Xtriage
Anisotropy	1.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.0	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4876	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ACT

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	0.49	0/4947	0.66	0/6732

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 ⓘ

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	4839	0	4511	144	0
2	A	28	0	21	2	0
3	A	9	0	0	0	0
All	All	4876	0	4532	144	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 15.

The worst 5 of 144 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:357:ASP:OD2	1:A:475:LYS:NZ	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:ASP:HA	1:A:501:PRO:HG2	1.59	0.83
1:A:258:GLU:OE2	1:A:399:ARG:NH2	2.15	0.80
1:A:228:LYS:HB3	1:A:232:GLU:HB2	1.64	0.79
1:A:579:THR:HG22	1:A:580:THR:H	1.48	0.78

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	637/683 (93%)	560 (88%)	74 (12%)	3 (0%)	29	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	83	LYS
1	A	497	CYS

5.3.2 Protein sidechains ⓘ

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	475/596 (80%)	451 (95%)	24 (5%)	24	54

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	382	MET
1	A	577	LYS
1	A	468	GLN
1	A	589	SER
1	A	76	ARG

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

Mol	Chain	Res	Type
1	A	193	ASN
1	A	477	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	ACT	A	706	-	3,3,3	0.92	0	3,3,3	1.55	1 (33%)
2	ACT	A	707	-	3,3,3	1.41	0	3,3,3	1.68	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	ACT	A	705	-	3,3,3	1.14	0	3,3,3	1.43	0
2	ACT	A	702	-	3,3,3	1.16	0	3,3,3	1.53	1 (33%)
2	ACT	A	704	-	3,3,3	1.28	0	3,3,3	1.12	0
2	ACT	A	703	-	3,3,3	0.98	0	3,3,3	1.99	1 (33%)
2	ACT	A	701	-	3,3,3	1.04	0	3,3,3	0.89	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	703	ACT	OXT-C-O	-2.85	111.56	122.05
2	A	707	ACT	OXT-C-O	-2.25	113.78	122.05
2	A	706	ACT	OXT-C-CH3	2.17	124.14	115.18
2	A	702	ACT	OXT-C-CH3	2.13	123.98	115.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	706	ACT	1	0
2	A	703	ACT	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	645/683 (94%)	0.30	20 (3%)	49	48	49, 68, 107, 123	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	37	VAL	4.6
1	A	48	MET	3.9
1	A	88	CYS	3.3
1	A	49	PRO	3.2
1	A	228	LYS	3.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACT	A	707	4/4	0.58	0.59	55,72,74,78	0
2	ACT	A	705	4/4	0.59	0.72	69,76,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	ACT	A	701	4/4	0.66	0.55	68,75,75,81	0
2	ACT	A	702	4/4	0.69	0.49	58,70,70,74	0
2	ACT	A	704	4/4	0.84	0.29	81,87,89,89	0
2	ACT	A	706	4/4	0.88	0.26	51,54,59,65	0
2	ACT	A	703	4/4	0.88	0.34	48,52,54,57	0

6.5 Other polymers ⓘ

There are no such residues in this entry.