



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 10:41 PM EDT

PDB ID : 5HIY  
Title : Crystal structure of PEDV NSP9 Mutant-C59A  
Authors : Deng, F.; Peng, G.  
Deposited on : 2016-01-12  
Resolution : 3.00 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>.

---

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	:	2.37.1
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)	:	2.37.1

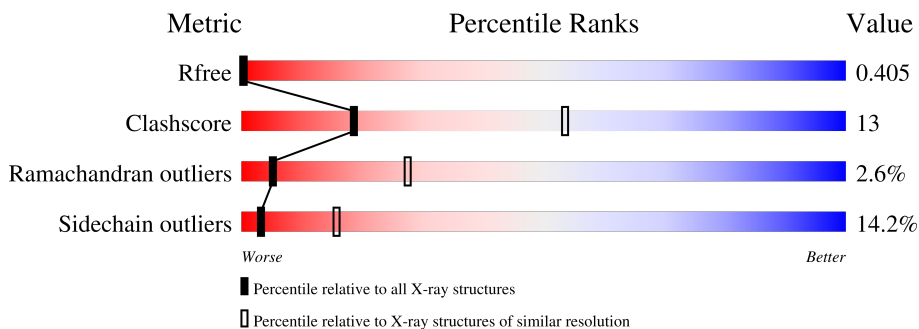
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	114	<div> <div>58%</div> <div>25%</div> <div>•</div> <div>17%</div> </div>
1	B	114	<div> <div>52%</div> <div>25%</div> <div>8%</div> <div>16%</div> </div>
1	C	114	<div> <div>49%</div> <div>29%</div> <div>•</div> <div>18%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2249 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 Non-structural protein 9.

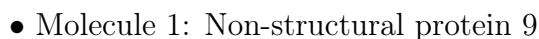
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			749	480	133	135	1			
1	B	96	Total	C	N	O	S	0	0	0
			765	491	137	136	1			
1	C	93	Total	C	N	O	S	0	0	0
			735	472	131	131	1			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ALA	CYS	engineered mutation	UNP P0C6Y4
A	109	HIS	-	expression tag	UNP P0C6Y4
A	110	HIS	-	expression tag	UNP P0C6Y4
A	111	HIS	-	expression tag	UNP P0C6Y4
A	112	HIS	-	expression tag	UNP P0C6Y4
A	113	HIS	-	expression tag	UNP P0C6Y4
A	114	HIS	-	expression tag	UNP P0C6Y4
B	59	ALA	CYS	engineered mutation	UNP P0C6Y4
B	109	HIS	-	expression tag	UNP P0C6Y4
B	110	HIS	-	expression tag	UNP P0C6Y4
B	111	HIS	-	expression tag	UNP P0C6Y4
B	112	HIS	-	expression tag	UNP P0C6Y4
B	113	HIS	-	expression tag	UNP P0C6Y4
B	114	HIS	-	expression tag	UNP P0C6Y4
C	59	ALA	CYS	engineered mutation	UNP P0C6Y4
C	109	HIS	-	expression tag	UNP P0C6Y4
C	110	HIS	-	expression tag	UNP P0C6Y4
C	111	HIS	-	expression tag	UNP P0C6Y4
C	112	HIS	-	expression tag	UNP P0C6Y4
C	113	HIS	-	expression tag	UNP P0C6Y4
C	114	HIS	-	expression tag	UNP P0C6Y4



- Molecule 1: Non-structural protein 9



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	58.73Å 58.73Å 193.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 38.15 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.00-3.00) 98.5 (38.15-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.99 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.249 , 0.354 0.314 , 0.405	Depositor DCC
$R_{free}$ test set	335 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	111.5	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 76.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	2249	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.39% 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

### 5.1 Standard geometry

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	0.46	0/762	0.59	0/1024
1	B	0.49	0/779	0.64	0/1044
1	C	0.58	0/748	0.65	0/1005
All	All	0.51	0/2289	0.63	0/3073

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	749	0	764	18	0
1	B	765	0	777	24	0
1	C	735	0	753	19	0
All	All	2249	0	2294	60	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 13.

The worst 5 of 60 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:73:ASP:HA	1:A:78:ALA:HA	1.49	0.94

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:HH11	1:C:49:ARG:HG2	1.40	0.86
1:C:46:PRO:HA	1:C:84:TYR:OH	1.77	0.83
1:C:89:LEU:O	1:C:94:ARG:NH1	2.18	0.77
1:B:17:GLU:HB3	1:B:52:LYS:HE2	1.68	0.74

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	91/114 (80%)	76 (84%)	13 (14%)	2 (2%)	6	31
1	B	90/114 (79%)	77 (86%)	11 (12%)	2 (2%)	6	31
1	C	89/114 (78%)	75 (84%)	11 (12%)	3 (3%)	3	20
All	All	270/342 (79%)	228 (84%)	35 (13%)	7 (3%)	5	27

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	91	THR
1	C	19	ASP
1	A	66	PRO
1	B	8	LYS
1	C	46	PRO

### 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	77/94 (82%)	71 (92%)	6 (8%)	12	42
1	B	79/94 (84%)	63 (80%)	16 (20%)	1	6
1	C	76/94 (81%)	65 (86%)	11 (14%)	3	15
All	All	232/282 (82%)	199 (86%)	33 (14%)	3	16

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	43	SER
1	C	49	ARG
1	C	68	ARG
1	B	47	ASP
1	B	44	ASP

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

Mol	Chain	Res	Type
1	B	30	ASN

### 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 ⓘ

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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.